wwPDB EM Validation Summary Report

Mar 3, 2025 – 07:30 PM JST

PDB ID	:	8X4B
EMDB ID	:	EMD-38045
Title	:	Cryo-EM structure of Ryanodine receptor 1 (TM helix S0,100 nM Ca2+, open state)
Authors	:	Chen, Q.; Hu, H.
Deposited on	:	2023-11-15
Resolution	:	4.20 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:

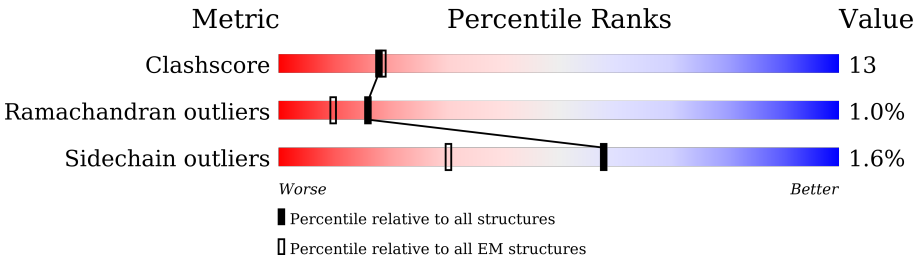
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 4.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5037	10% 66% 16% • 17%
1	B	5037	10% 66% 16% • 17%
1	C	5037	10% 66% 16% • 17%
1	D	5037	10% 66% 16% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 110456 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4173	Total 27613	C 17058	N 5114	O 5292	S 149	0	0
1	B	4173	Total 27613	C 17058	N 5114	O 5292	S 149	0	0
1	C	4173	Total 27613	C 17058	N 5114	O 5292	S 149	0	0
1	D	4173	Total 27613	C 17058	N 5114	O 5292	S 149	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

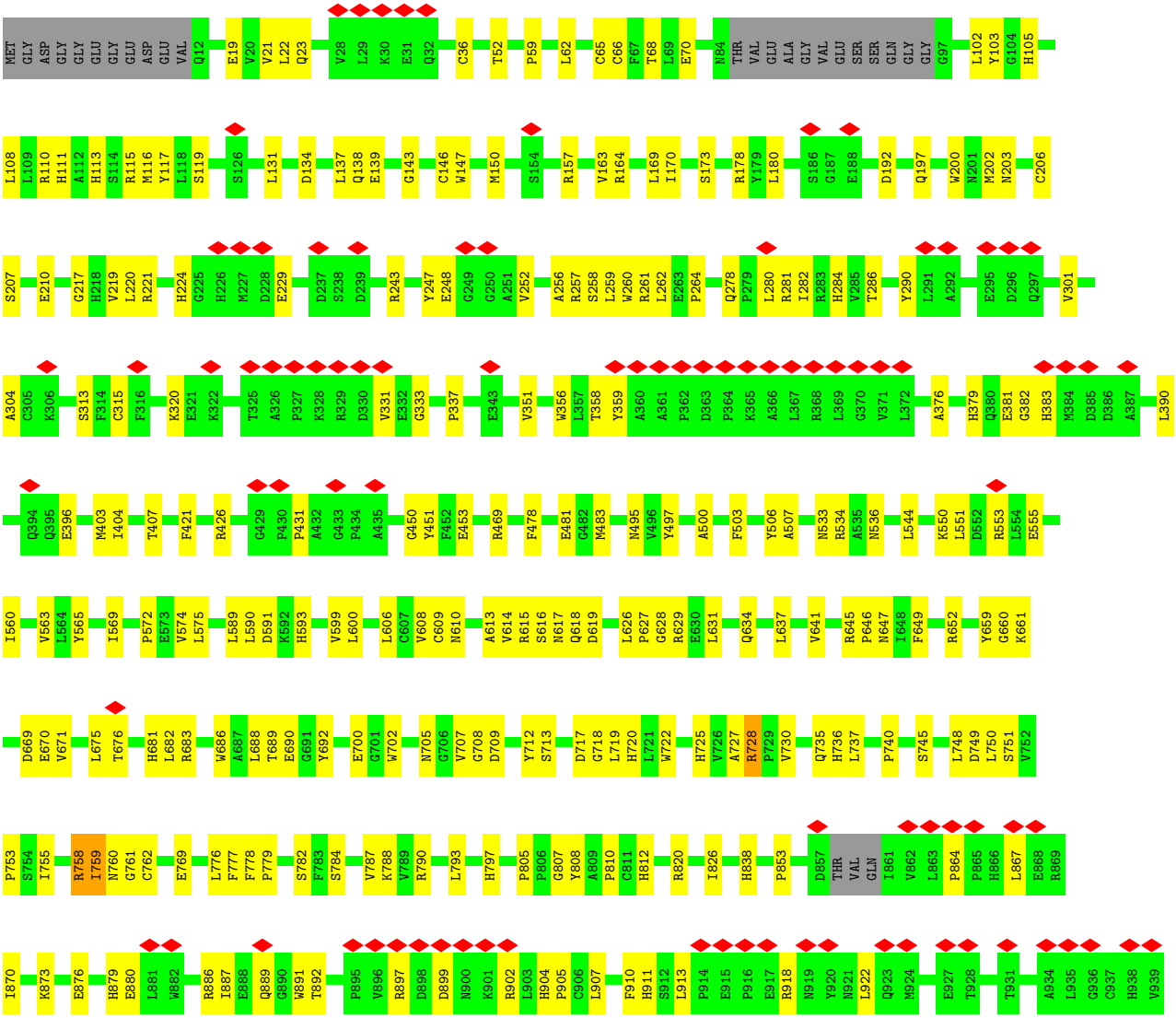
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Ca 1	0
2	B	1	Total 1	Ca 1	0
2	C	1	Total 1	Ca 1	0
2	D	1	Total 1	Ca 1	0

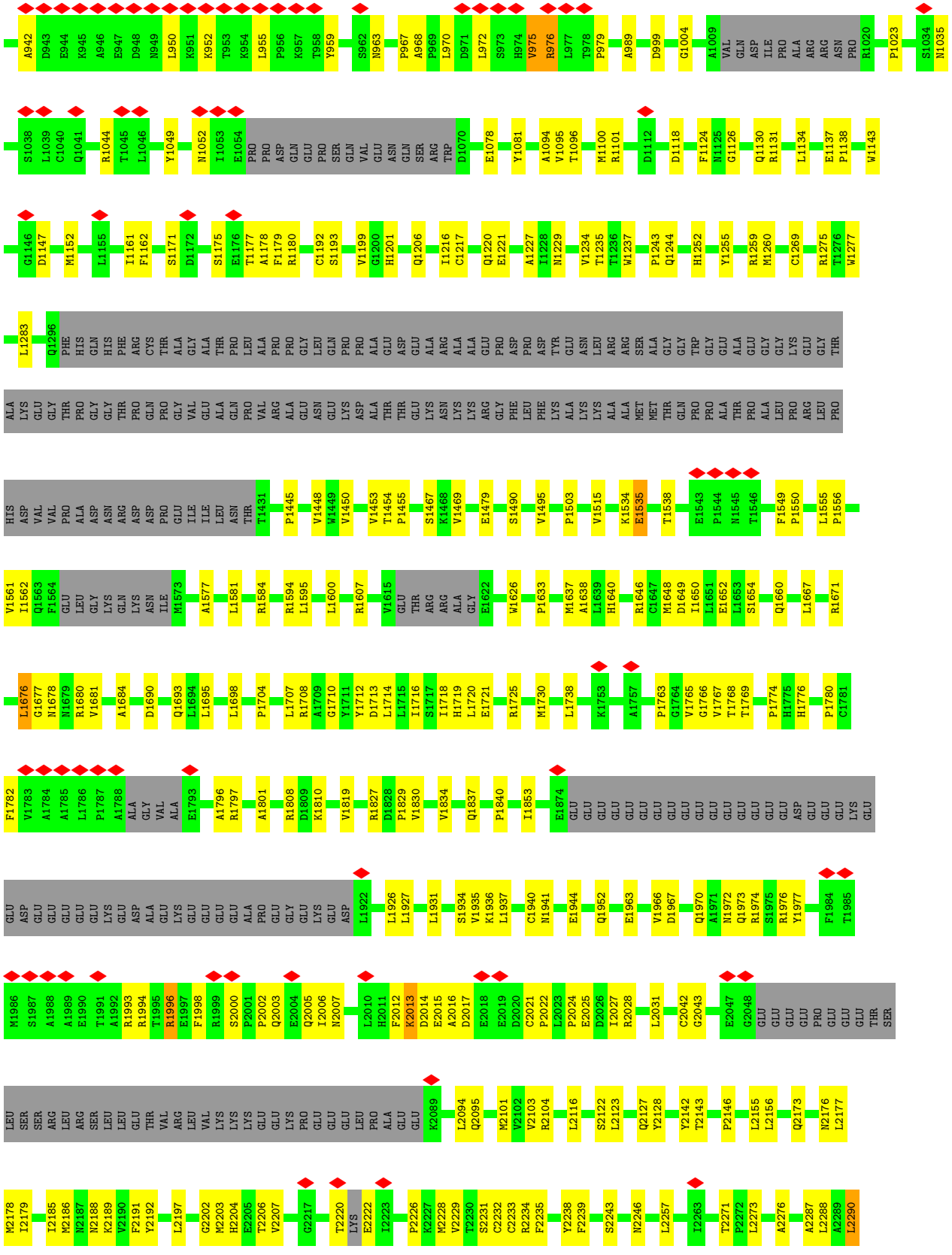
3 Residue-property plots (i)

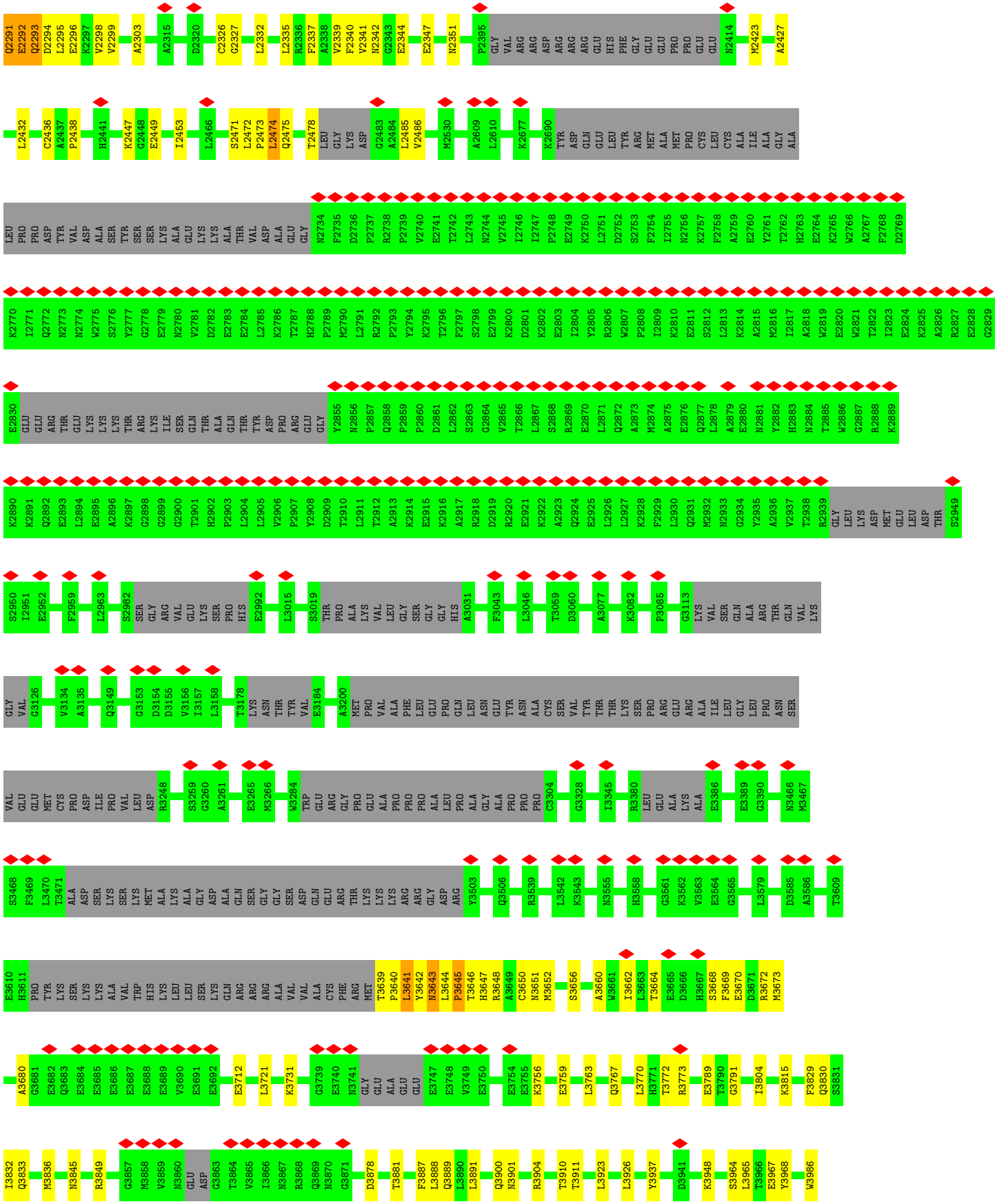
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

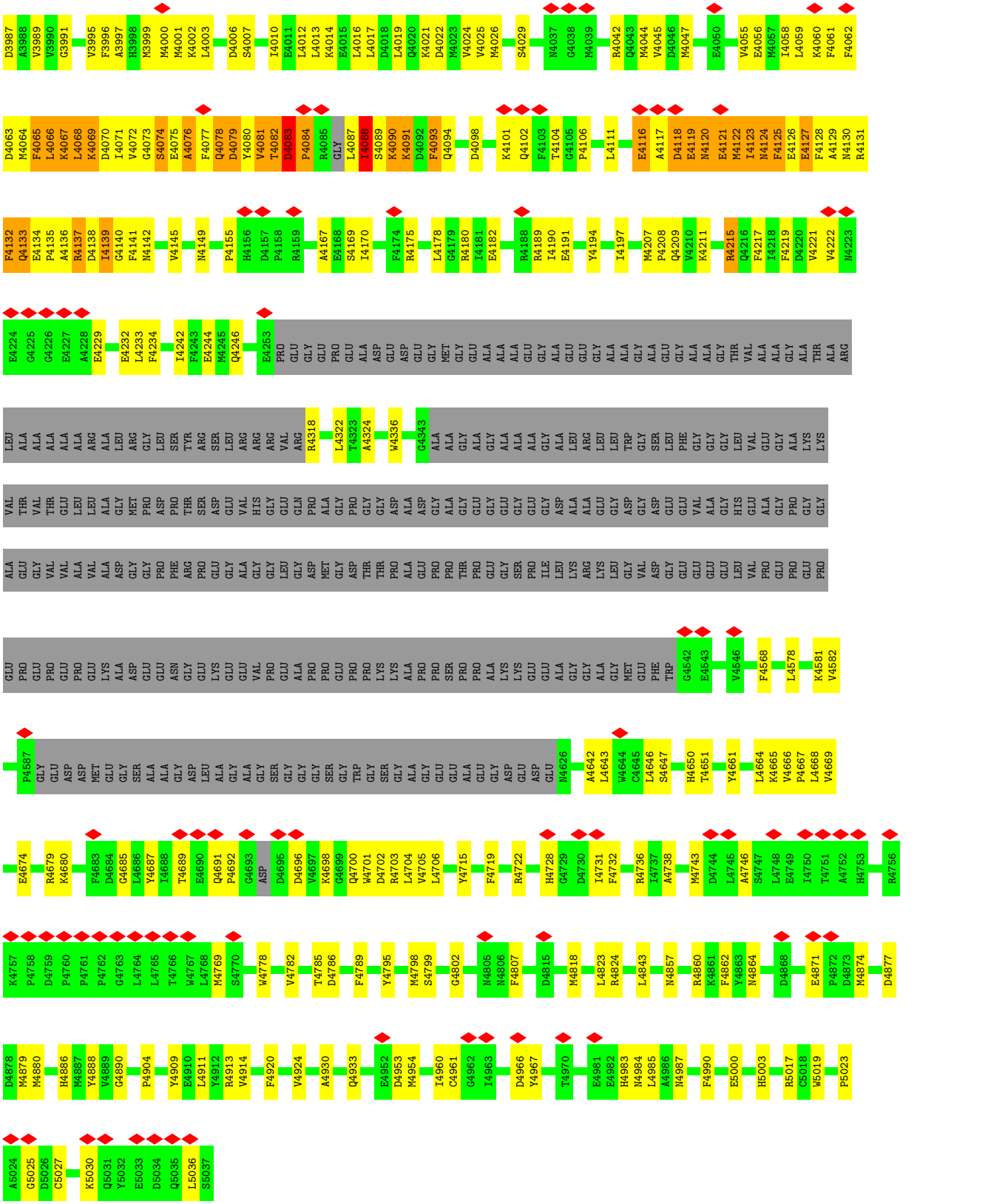
- Molecule 1: Ryanodine receptor 1

Chain A:



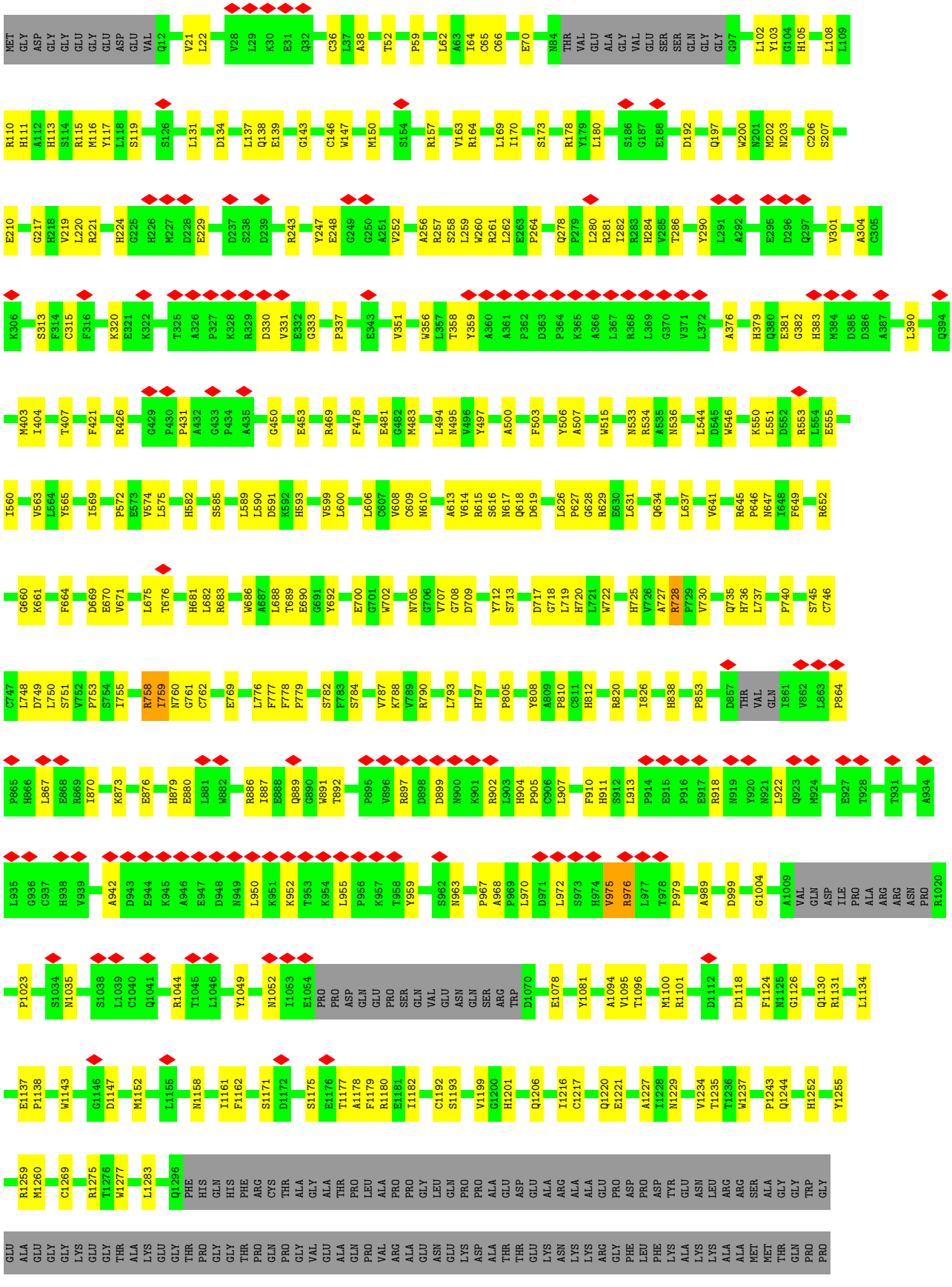

A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 S962 N963 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A989 D999 G1004 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 P1023 S1034 N1035
S1038 L1039 C1040 Q1041 R1044 T1045 L1046 Y1049 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 E1078 Y1081 A1094 V1095 T1096 M1100 R1101 D1112 D1118 F1124 N1125 G1126 Q1130 R1131 L1134 E1137 P1138 W1143
G1146 D1147 M1152 L1155 I1161 F1162 S1171 D1172 S1175 E1176 T1177 A1178 F1179 R1180 C1192 S1193 V1199 G1200 H1201 Q1206 I1216 C1217 Q1220 E1221 A1227 T1228 N1229 V1234 T1235 T1236 W1237 P1243 Q1244 H1252 Y1255 R1259 M1260 C1269 R1275 T1276 W1277
L1283 Q1296 PHE HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR
ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO
HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN THR T1431 P1445 V1448 W1449 V1450 V1453 T1454 P1455 S1467 K1468 V1469 E1479 S1490 V1495 P1503 V1515 K1534 E1535 T1538 E1543 P1544 N1545 T1546 F1549 P1550 L1555 P1556
V1561 I1562 Q1563 F1564 GLU LEU GLY LYS GLN LYS ASN ILE M1573 A1577 L1581 R1584 R1594 L1595 L1600 R1607 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 P1633 M1637 A1638 L1639 H1640 R1646 C1647 M1648 D1649 I1650 L1651 E1652 L1653 S1654 Q1660 L1667 R1671
L1676 G1677 N1678 N1679 R1680 V1681 A1684 D1690 Q1693 L1694 L1695 L1698 P1704 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 L1714 L1715 I1716 S1717 I1718 H1719 L1720 E1721 R1725 M1730 L1738 K1753 A1757 P1763 G1764 V1765 G1766 V1767 T1768 T1769 P1774 H1775 H1776 P1780 C1781
F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1796 R1797 A1801 R1808 D1809 K1810 V1819 R1827 D1828 P1829 V1830 V1834 Q1837 P1840 I1853 E1874 GLU 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 LYS GLU ASP ALA GLU LYS GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 L1927 L1931 S1934 V1935 K1936 L1937 C1940 N1941 E1944 Q1952 E1963 V1966 D1967 Q1970 A1971 N1972 Q1973 R1974 S1975 R1976 Y1977 F1984 T1985
M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 L2031 C2042 G2043 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 L2094 Q2095 M2101 V2102 V2103 R2104 L2116 S2122 L2123 Q2127 Y2128 Y2142 T2143 P2146 L2155 L2156 Q2173 N2176 L2177
W2178 I2179 I2185 M2186 N2187 N2188 K2189 Y2190 F2191 Y2192 L2197 G2202 M2203 H2204 E2205 T2206 V2207 G2217 T2220 LYS E2222 T2223 P2226 K2227 M2228 V2229 T2230 S2231 C2232 C2233 R2234 F2235 Y2238 F2239 S2243 N2246 L2257 I2263 T2271 P2272 L2273 A2276 A2287 L2288 A2289 L2290





• Molecule 1: Ryanodine receptor 1

Chain B: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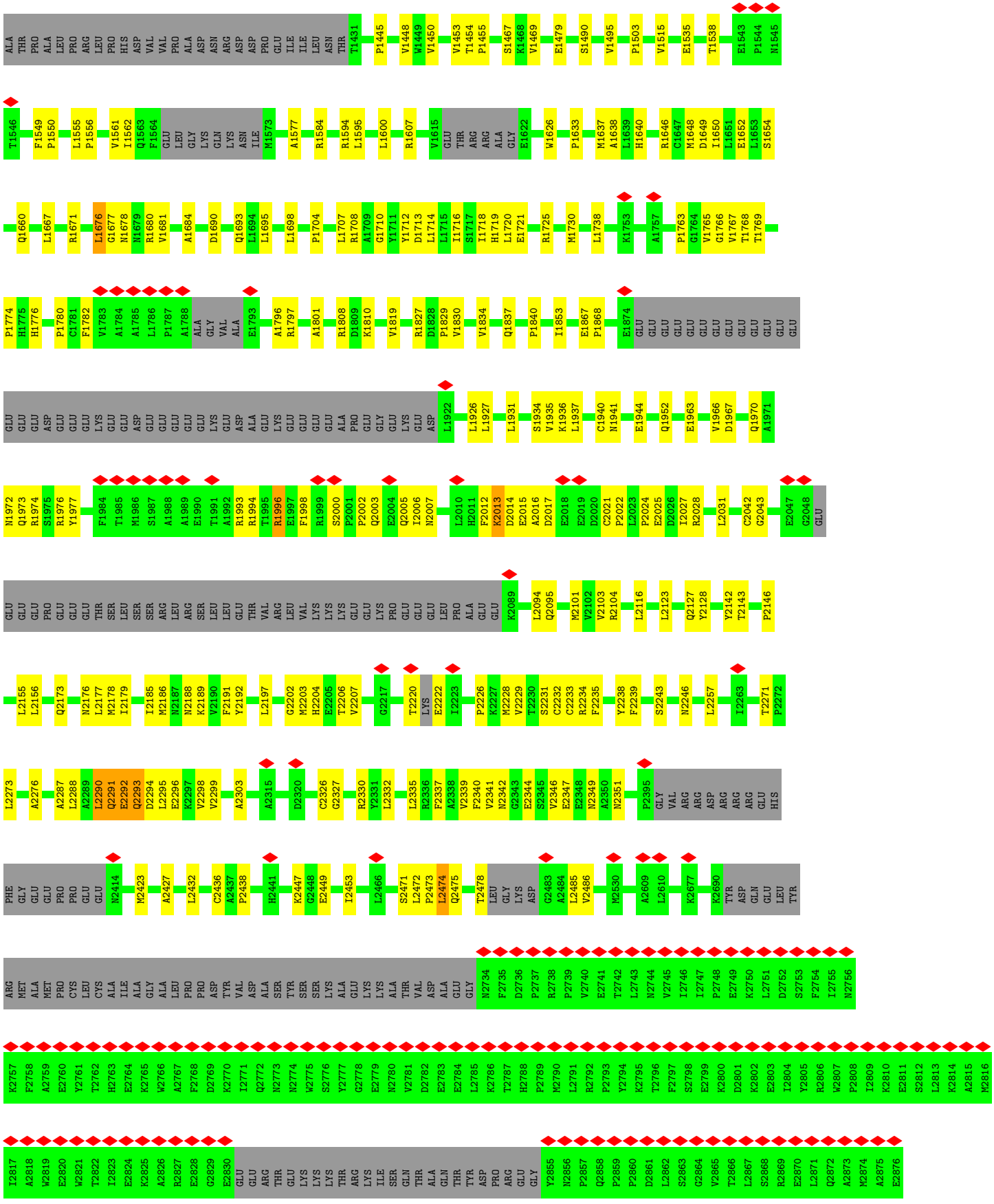
R110 H111 A112 H113 S114 R115 M116 Y117 L118 S119 S126 L131 D134 L137 Q138 E139 G143 C146 W147 M150 S154 R157 V163 R164 L169 I170 S173 R178 Y179 L180 S186 G187 E188 D192 Q197 W200 N201 M202 N203 C206 S207
E210 G217 H218 V219 L220 R221 H224 G225 H226 M227 D228 E229 D237 S238 D239 R243 Y247 E248 G249 G250 A251 V252 A256 R257 S258 L259 W260 R261 L262 E263 P264 Q278 P279 L280 R281 I282 R283 H284 V285 T286 Y290 L291 A292 E295 D296 Q297 V301 A304 G305
K306 S313 F314 C315 F316 K320 E321 K322 T325 A326 P327 K328 R329 D330 V331 E332 G333 P337 E343 V351 W356 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 A376 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L390 Q394
M403 I404 T407 F421 R426 G429 P430 P431 A432 G433 P434 A435 G450 E453 R469 F478 E481 G482 M483 L494 N495 V496 Y497 A500 F503 Y506 A507 W515 N533 R534 A535 N536 L544 D545 W546 K550 L551 D552 R553 L554 E555
I560 V563 L564 Y565 I569 P572 E573 V574 L575 H582 S585 L589 L590 D591 K592 H593 V599 L600 L606 C607 V608 C609 N610 A613 V614 R615 S616 N617 Q618 D619 L626 P627 G628 R629 E630 L631 Q634 L637 V641 R645 P646 N647 I648 F649 R652
G660 K661 F664 D669 E670 V671 L675 T676 H681 L682 R683 W686 A687 L688 T689 E690 G691 Y692 E700 G701 W702 N705 G706 V707 G708 D709 Y712 S713 D717 G718 L719 H720 L721 W722 H725 V726 A727 R728 P729 V730 Q735 H736 L737 P740 S745 C746
C747 L748 D749 L750 S751 V752 P753 S754 T755 R758 I759 N760 G761 C762 E769 L776 F777 F778 P779 S782 F783 S784 V787 K788 W789 R790 L793 H797 P805 Y808 A809 P810 C811 H812 R820 I826 H838 P853 D857 THR VAL GLN I861 V862 L863 P864
P865 H866 L867 E868 R869 I870 K873 E876 H879 E880 L881 W882 R886 I887 E888 Q889 G890 W891 T892 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 N924 E927 T928 T931 A934
L935 G936 C937 H938 V939 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 S962 N963 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A989 D999 G1004 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020
P1023 S1034 N1035 S1038 L1039 C1040 Q1041 R1044 T1045 L1046 Y1049 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 E1078 Y1081 A1094 V1095 T1096 M1100 R1101 D1112 D1118 F1124 N1125 G1126 Q1130 R1131 L1134
E1137 P1138 W1143 G1146 D1147 M1152 L1155 N1158 I1161 F1162 S1171 D1172 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1182 C1192 S1193 V1199 G1200 H1201 Q1206 I1216 C1217 Q1220 E1221 A1227 I1228 N1229 V1234 T1235 T1236 W1237 P1243 Q1244 H1252 Y1255
R1259 M1260 C1269 R1275 T1276 W1277 L1283 Q1296 PHE HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY
GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO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T1546 F1549 P1550 L1555 P1556 V1561 I1562 Q1563 F1564 GLU LEU GLY LYS GLN LYS ASN ILE M1573 A1577 R1584 R1594 L1595 L1600 R1607 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 P1633 M1637 A1638 L1639 H1640 R1646 G1647 M1648 D1649 I1650 L1651 E1652 L1653 S1654
Q1660 L1667 R1671 L1676 G1677 N1678 N1679 R1680 V1681 A1684 D1690 Q1693 L1694 L1695 L1698 P1704 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 L1714 L1715 I1716 S1717 I1718 H1719 L1720 E1721 R1725 M1730 L1738 K1753 A1757 P1763 G1764 V1765 G1766 V1767 T1768 T1769
P1774 H1775 H1776 P1780 C1781 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1796 R1797 A1801 R1808 D1809 K1810 V1819 R1827 D1828 P1829 V1830 V1834 Q1837 P1840 I1853 E1867 P1868 E1874 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 ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1926 L1927 L1931 S1934 V1935 K1936 L1937 C1940 N1941 E1944 Q1952 E1963 V1966 D1967 Q1970 A1971
N1972 Q1973 R1974 S1975 R1976 Y1977 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 L2031 C2042 G2043 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 LEU PRO ALA GLU GLU K2089 L2094 Q2095 M2101 V2102 V2103 R2104 L2116 L2123 Q2127 Y2128 Y2142 T2143 P2146
L2155 L2156 Q2173 N2176 L2177 M2178 I2179 I2185 M2186 N2187 N2188 K2189 V2190 F2191 Y2192 L2197 G2202 M2203 H2204 E2205 T2206 V2207 G2217 T2220 LYS E2222 I2223 P2226 K2227 M2228 V2229 T2230 S2231 C2232 C2233 R2234 F2235 Y2238 F2239 S2243 N2246 L2257 I2263 T2271 P2272
L2273 A2276 A2287 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 E2296 K2297 V2298 V2299 A2303 A2315 D2320 C2326 G2327 R2330 Y2331 L2332 L2335 R2336 F2337 A2338 V2339 F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 N2351 P2395 GLY VAL ARG ASP ARG ARG ARG GLU HIS
PHE GLY GLU GLU PRO PRO GLU GLU N2414 M2423 A2427 L2432 C2436 A2437 P2438 H2441 K2447 G2448 E2449 I2453 L2466 S2471 L2472 P2473 L2474 Q2475 T2478 LEU GLY LYS ASP G2483 A2484 L2485 V2486 M2530 A2609 L2610 K2677 K2690 TYR ASP GLN GLU LEU TYR
ARG MET ALA MET PRO CYS LEU CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756
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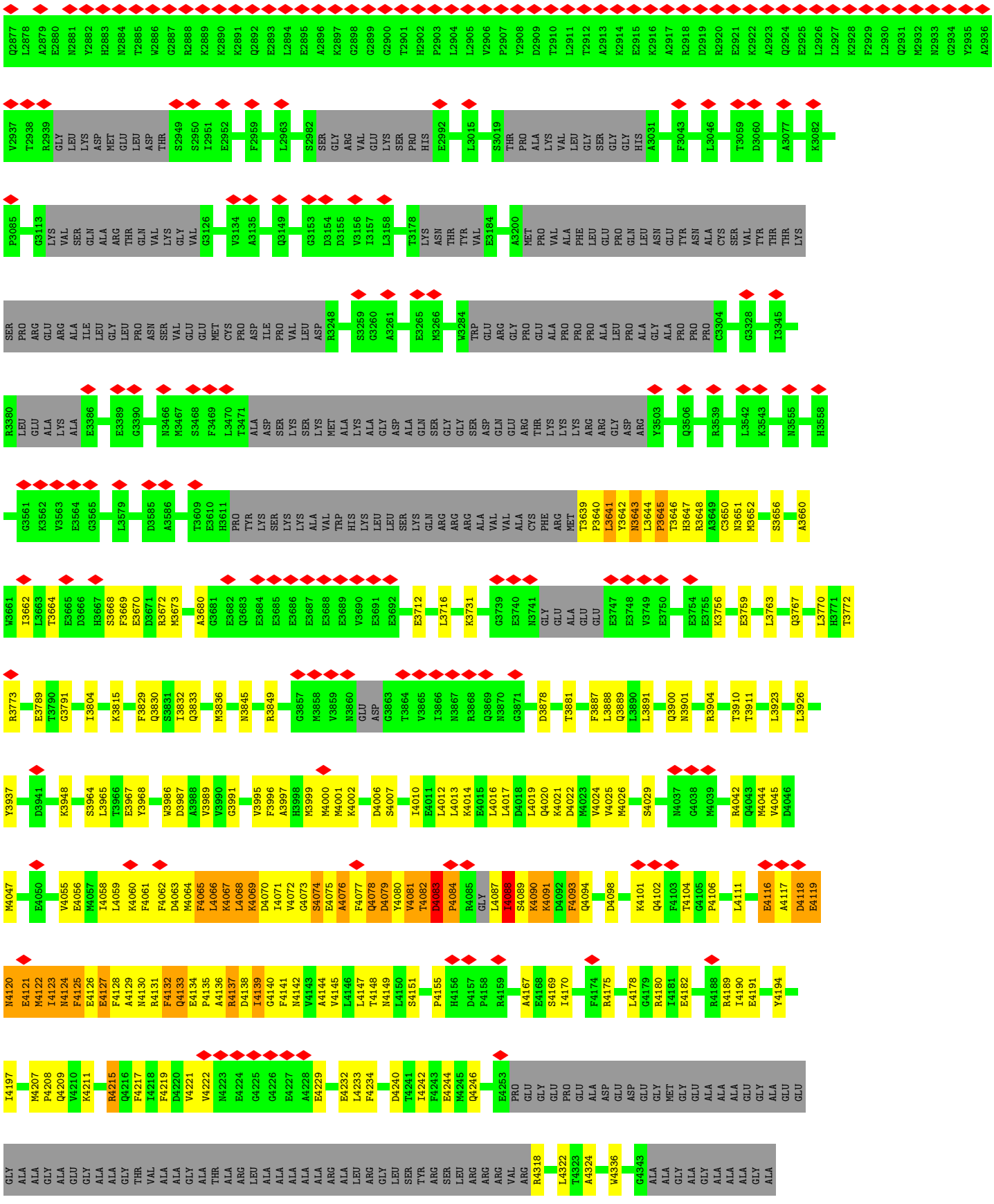
I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 W2874 A2875 E2876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V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR S2949 S2950 I2951 E2952 F2959 L2963 S2982 SER GLY ARG VAL GLU LYS SER PRO HIS E2992 L3015 S3019 THR PRO ALA LYS VAL LEU GLY SER GLY GLY HIS A3031 F3043 L3046 T3059 D3060 A3077 K3082
P3085 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL G3126 V3134 A3135 Q3149 G3153 D3154 D3155 V3156 I3157 L3158 T3178 LYS ASN THR TYR VAL E3184 A3200 MET PRO VAL ALA PHE LEU GLU PRO GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS
SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP R3248 S3259 G3260 A3261 E3265 M3266 W3284 TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO C3304 G3328 I3345
R3380 LEU GLU ALA LYS ALA E3386 E3389 G3390 N3466 M3467 S3468 F3469 L3470 T3471 ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3503 Q3506 R3539 L3542 K3543 N3555 H3558
G3561 K3562 V3563 E3564 G3565 L3579 D3585 A3586 T3609 E3610 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 Y3642 N3643 L3644 P3645 T3646 H3647 R3648 A3649 C3650 N3651 M3652 S3656 A3660
W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 P3669 E3670 D3671 R3672 M3673 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 E3712 L3716 K3731 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 E3754 E3755 K3756 E3759 L3763 Q3767 L3770 H3771 T3772
R3773 E3789 T3790 G3791 I3804 K3815 F3829 Q3830 S3831 I3832 Q3833 M3836 N3845 R3849 G3857 M3858 V3859 N3860 GLU ASP G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 D3878 T3881 F3887 L3888 Q3889 L3890 L3891 Q3900 N3901 R3904 T3910 T3911 L3923 L3926
Y3937 D3941 K3948 S3964 I3965 T3966 E3967 Y3968 W3986 D3987 A3988 Y3989 Y3990 G3991 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002 D4006 S4007 I4010 E4011 L4012 L4013 K4014 E4015 L4016 L4017 D4018 L4019 Q4020 K4021 D4022 M4023 V4024 V4025 M4026 S4029 W4037 G4038 M4039 R4042 Q4043 M4044 V4045 D4046
M4047 E4050 V4055 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 D4070 I4071 V4072 G4073 S4074 A4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 GLY L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 D4098 K4101 Q4102 F4103 T4104 G4105 P4106 L4111 E4116 A4117 D4118 E4119
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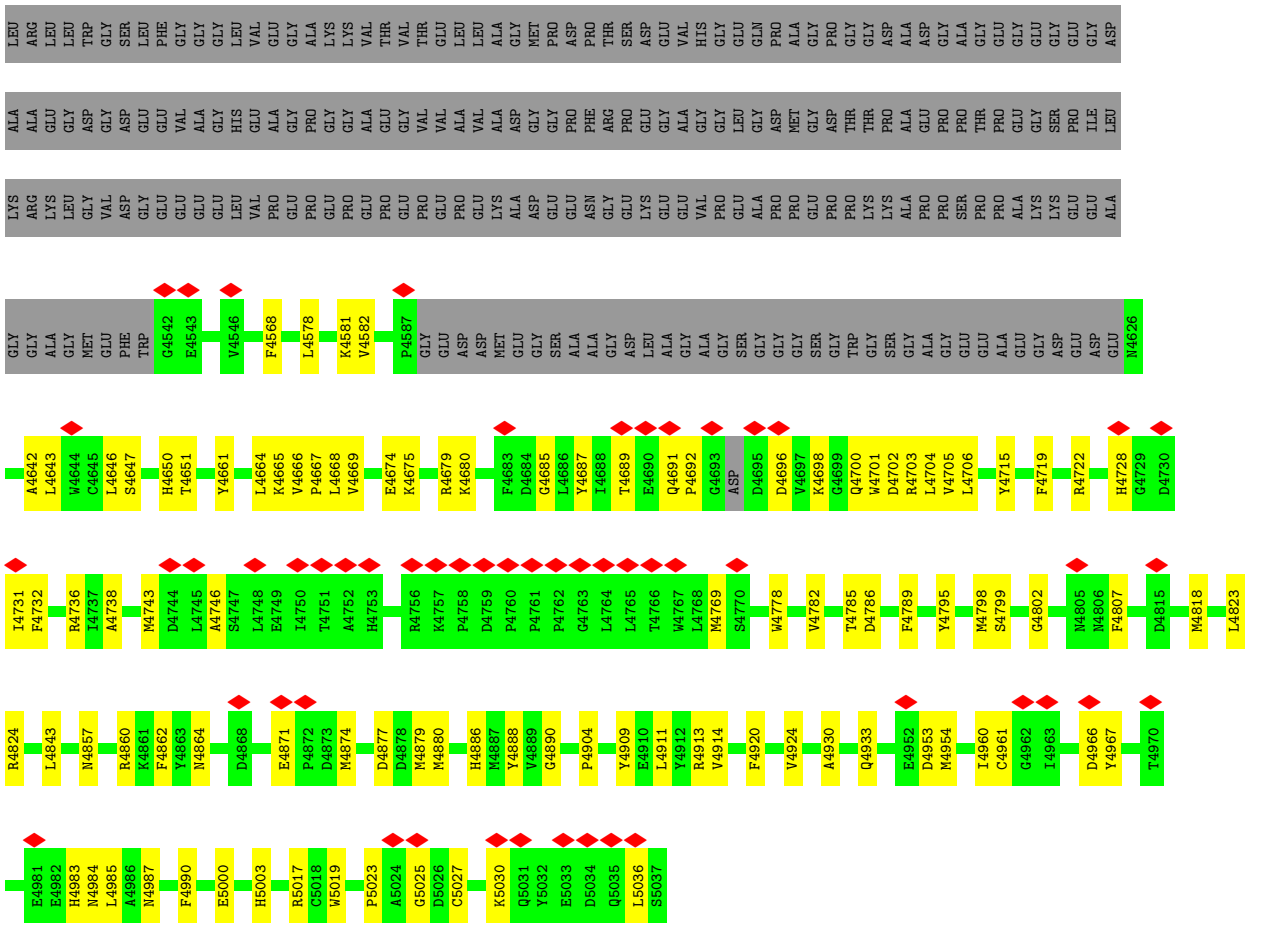
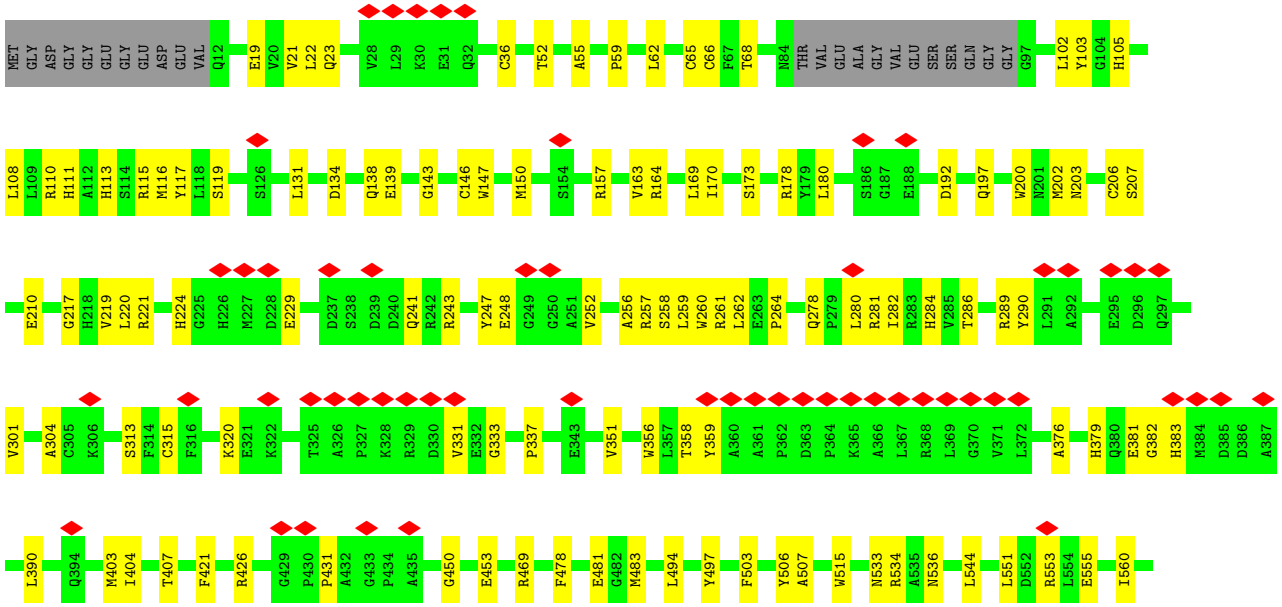
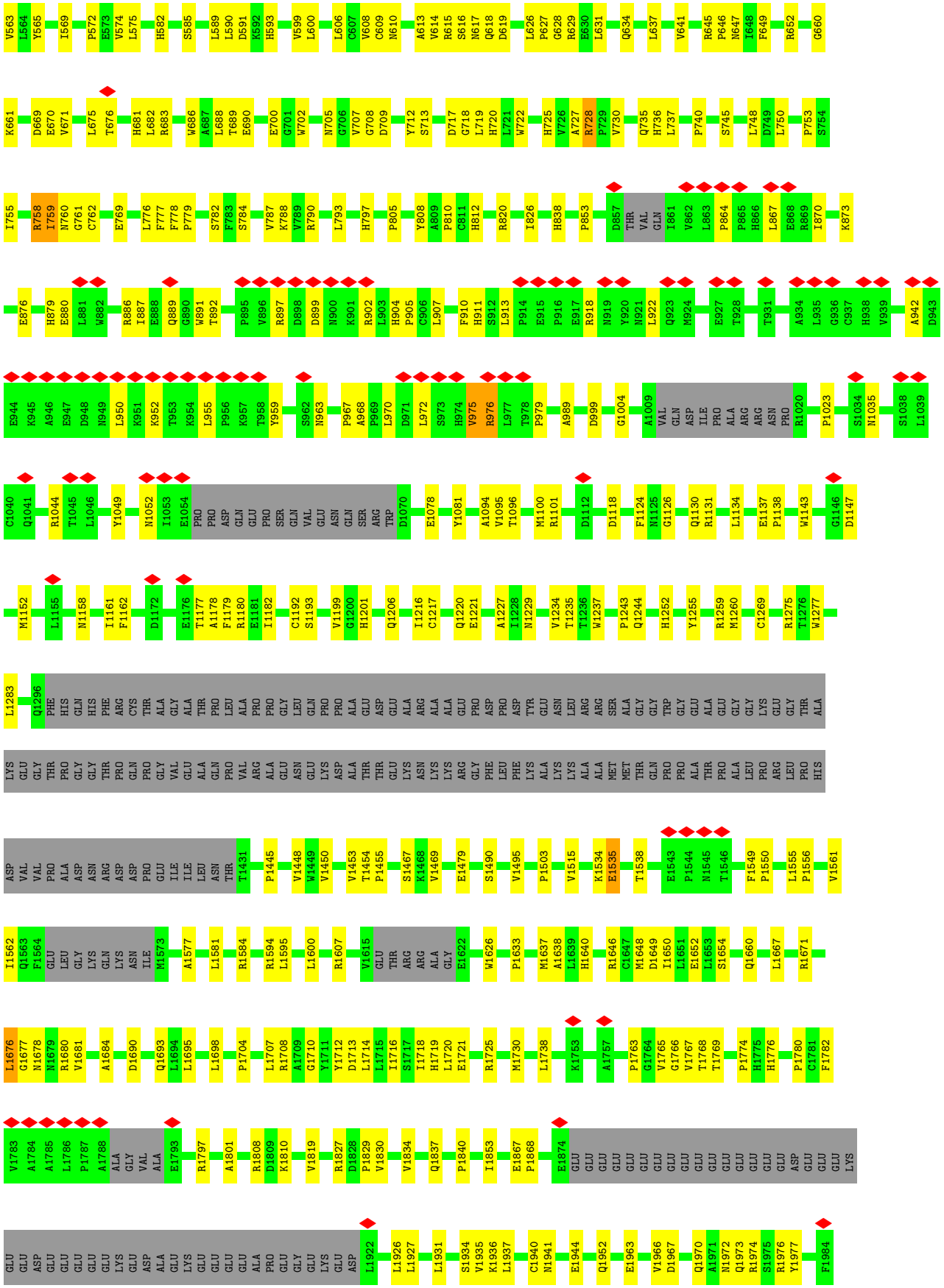
GLY ALA ALA GLY GLU GLY ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG R4318 L4322 T4323 A4324 W4336 G4343 ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA



• Molecule 1: Ryanodine receptor 1

Chain C:

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E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 S962 N963 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A989 D999 G1004 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 P1023 S1034 N1035 S1038 L1039
C1040 Q1041 R1044 T1045 L1046 Y1049 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 E1078 Y1081 A1094 V1095 T1096 M1100 R1101 D1112 D1118 F1124 N1125 G1126 Q1130 R1131 L1134 E1137 P1138 W1143 G1146 D1147
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L1283 Q1296 PHE HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA
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ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO PRO GLU ILE ILE LEU ASN THR T1431 P1445 V1448 W1449 V1450 V1453 T1454 P1455 S1467 K1468 V1469 E1479 S1490 V1495 P1503 V1515 K1534 E1535 T1538 E1543 P1544 N1545 T1546 F1549 P1550 L1555 P1556 V1561
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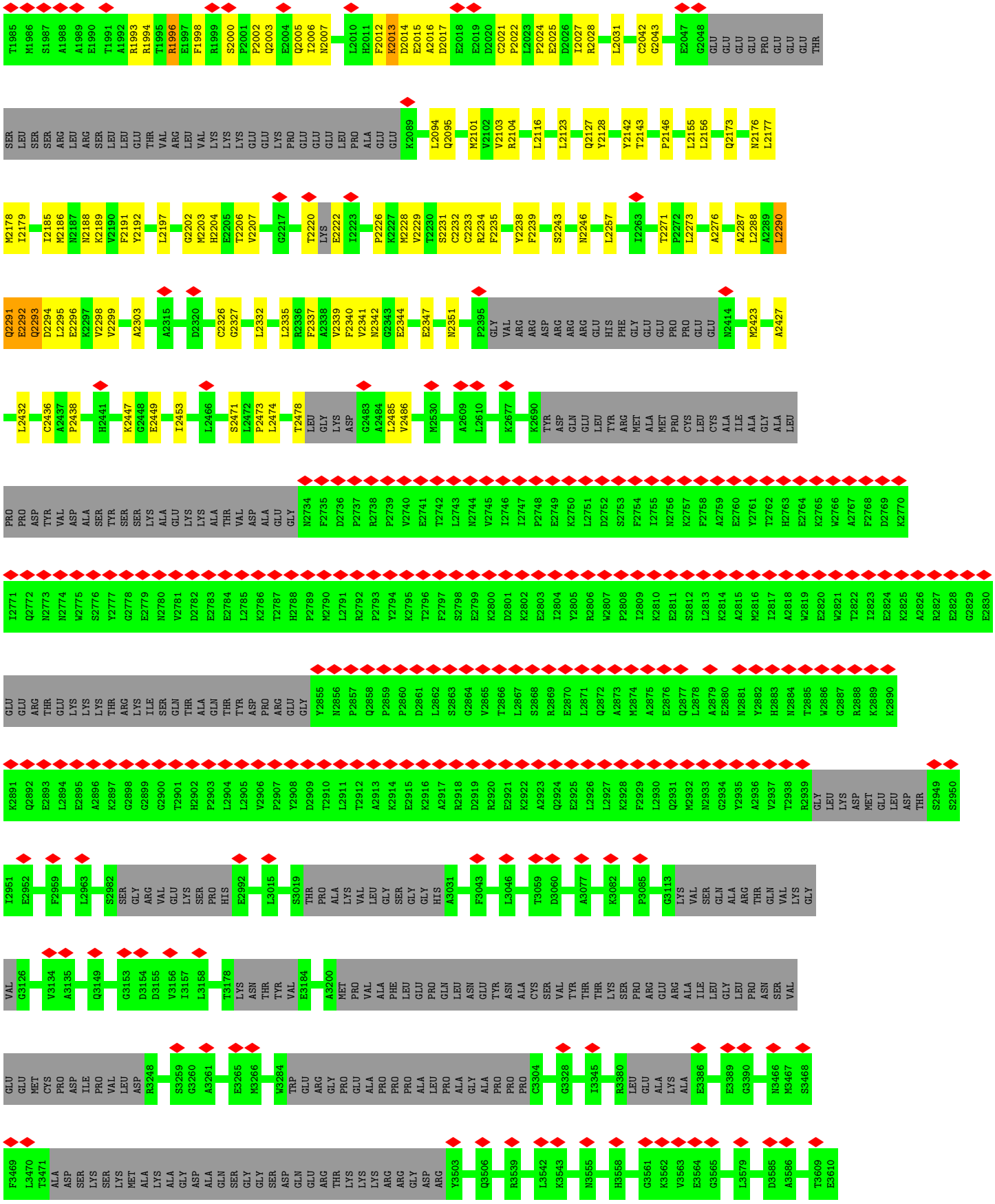
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PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 P2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 P2768 D2769 K2770
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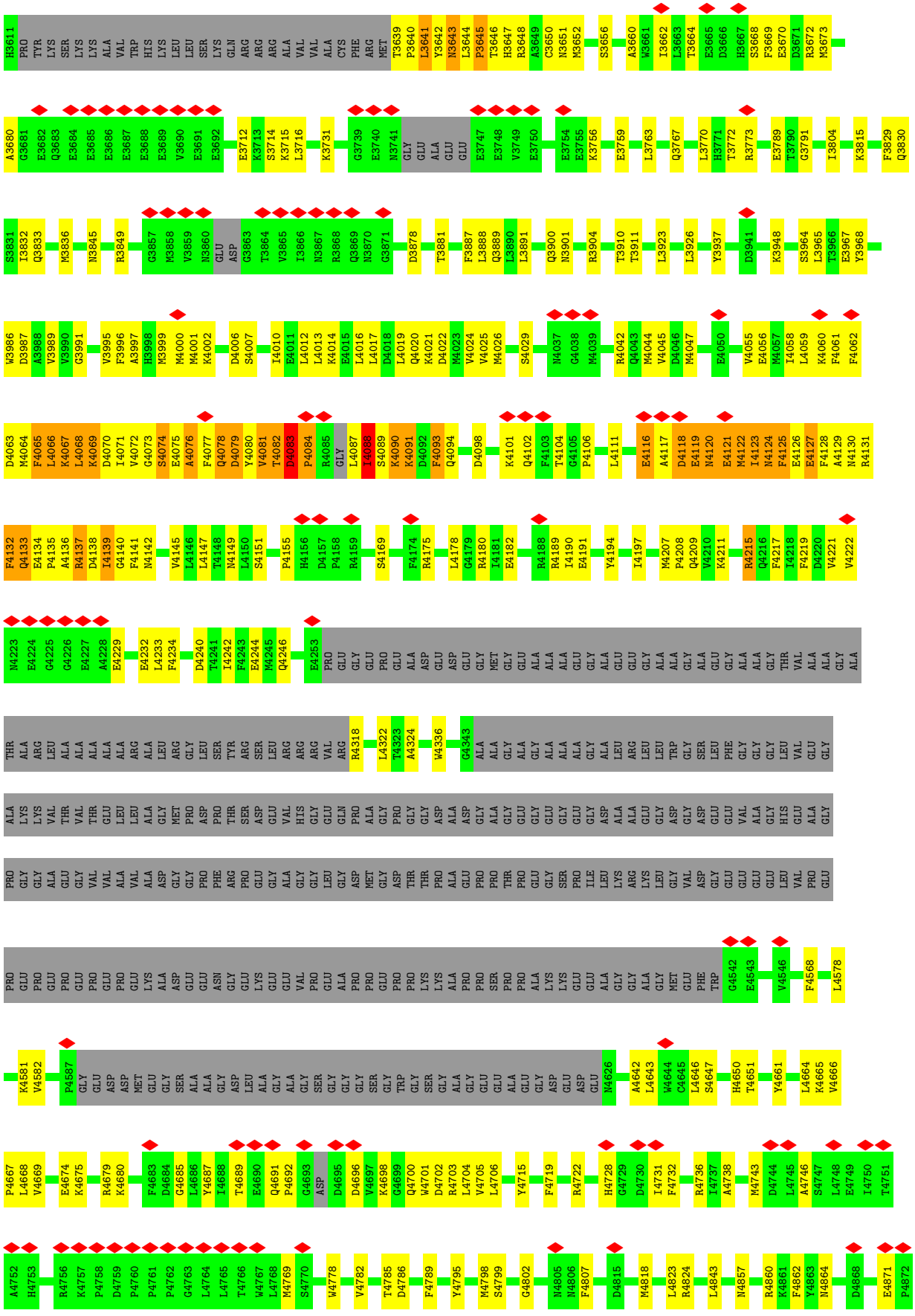
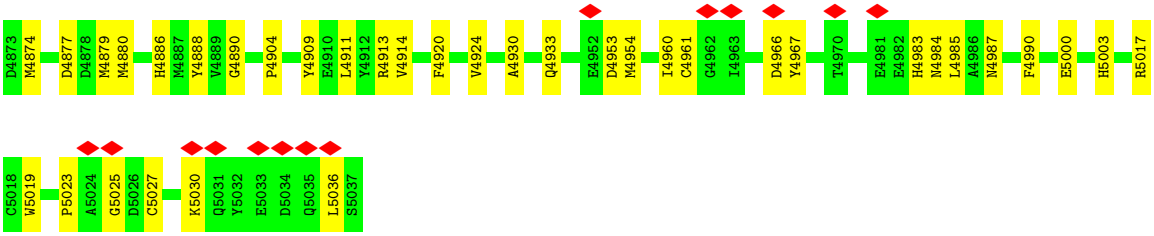
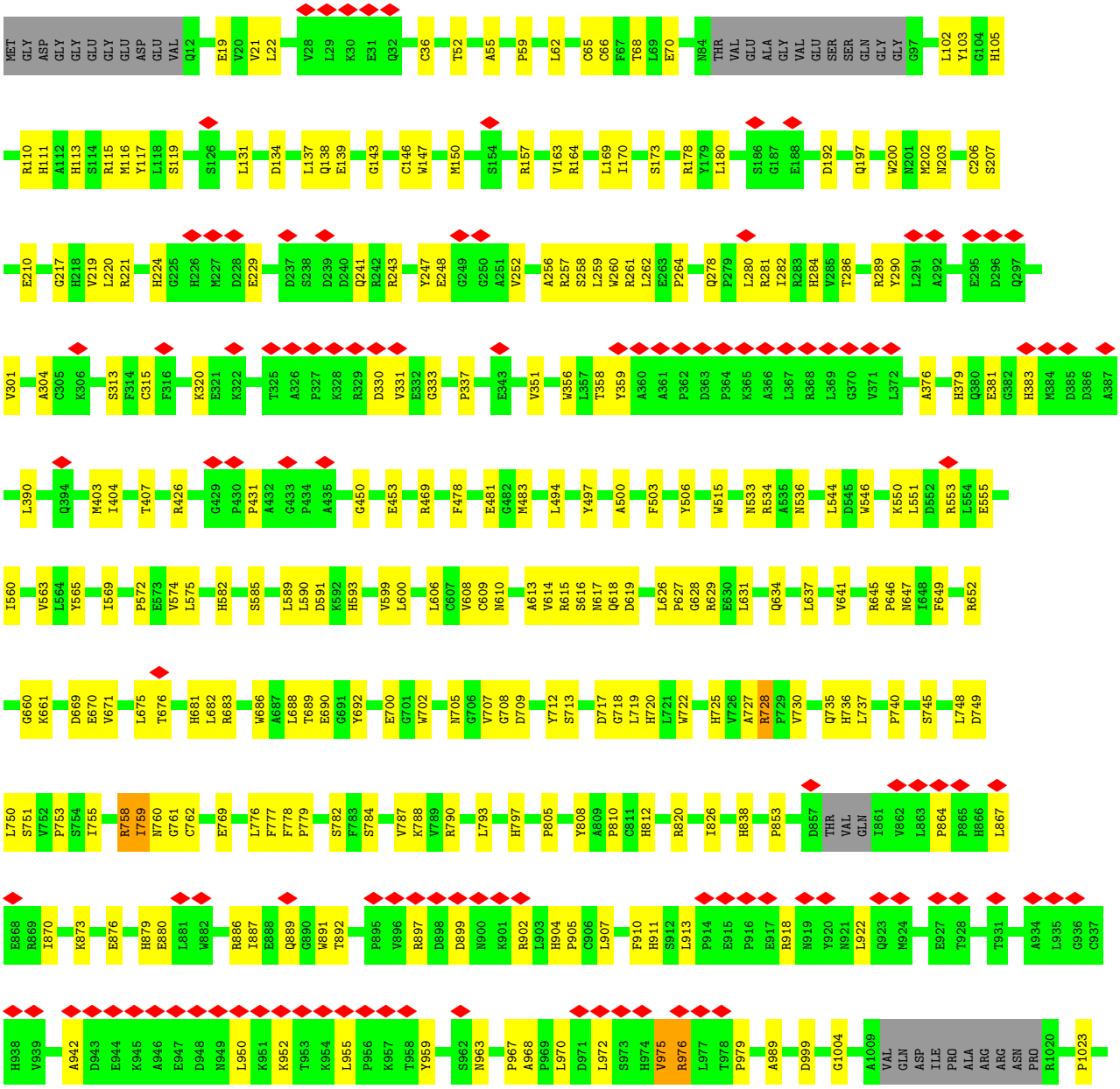
VAL G3126 V3134 A3135 Q3149 G3153 D3154 D3155 V3156 I3157 L3158 T3178 LYS ASN THR TYR VAL E3184 A3200 MET PRO VAL ALA PHE LEU GLU PRO GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL
GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP R3248 S3259 G3260 A3261 E3265 M3266 W3284 TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA ALA LEU PRO PRO ALA GLY ALA PRO PRO PRO C3304 G3328 I3345 B3380 LEU GLU ALA LYS ALA E3386 E3389 G3390 N3466 M3467 S3468
F3469 L3470 T3471 ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG GLY THR LYS LYS LYS ARG ARG GLY ASP ARG Y3503 Q3506 R3539 L3542 K3543 N3555 H3558 G3561 K3562 V3563 E3564 G3565 L3579 D3585 A3586 T3609 E3610

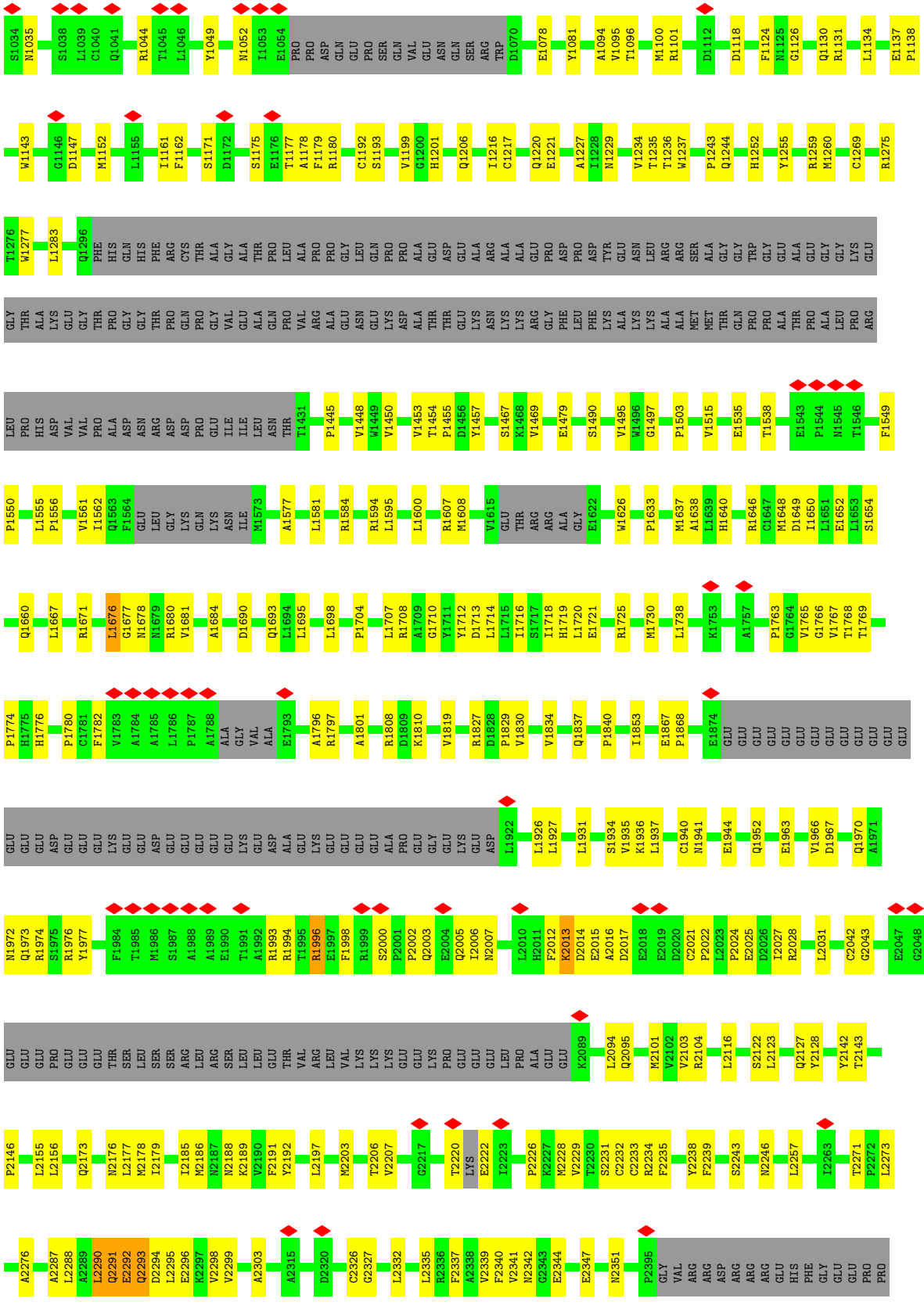


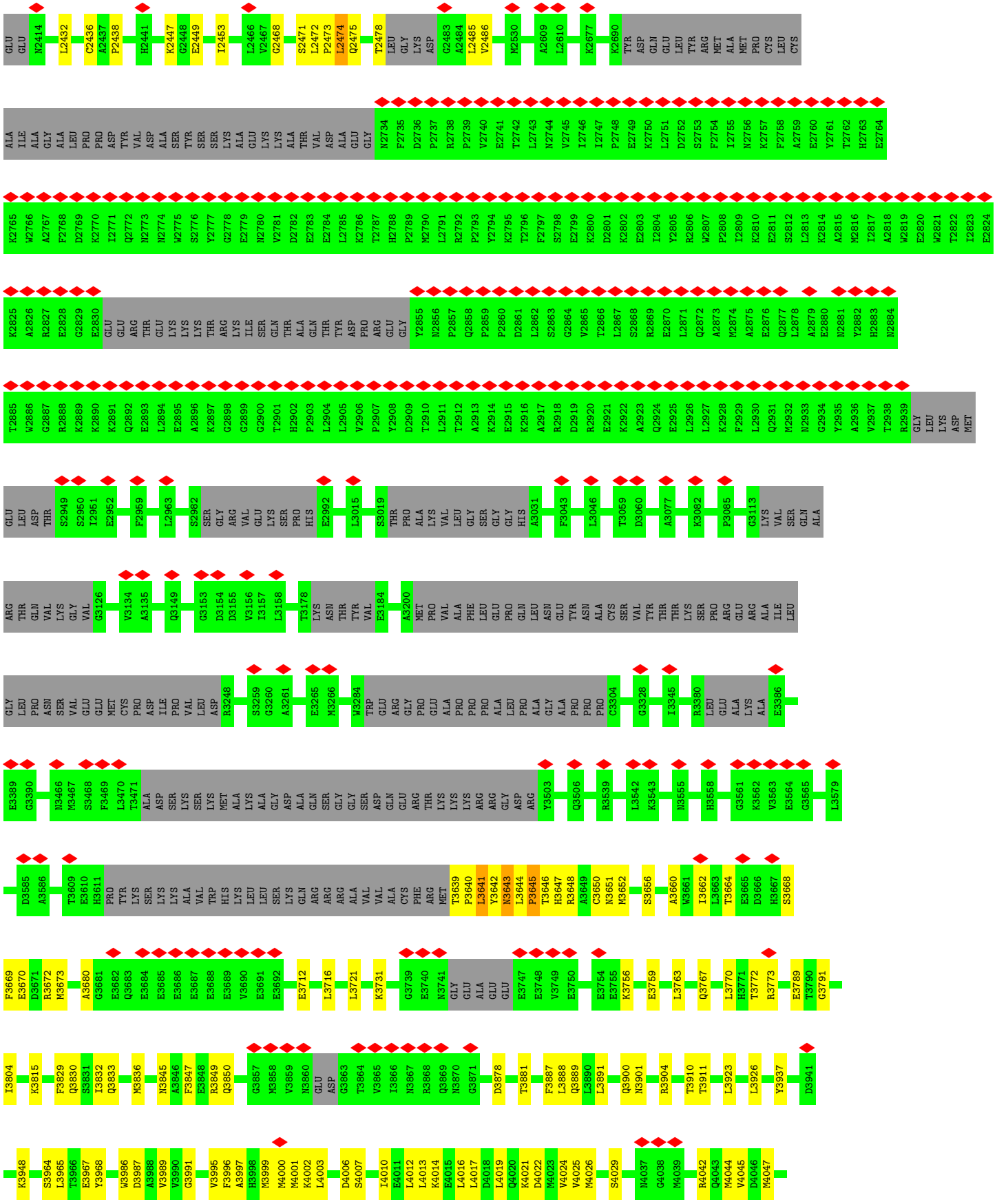


• Molecule 1: Ryanodine receptor 1

Chain D:



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ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764
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GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP R3248 S3259 G3260 A3261 E3265 M3266 W3284 TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO C3304 G3328 T3345 R3380 LEU GLU ALA LYS ALA E3386
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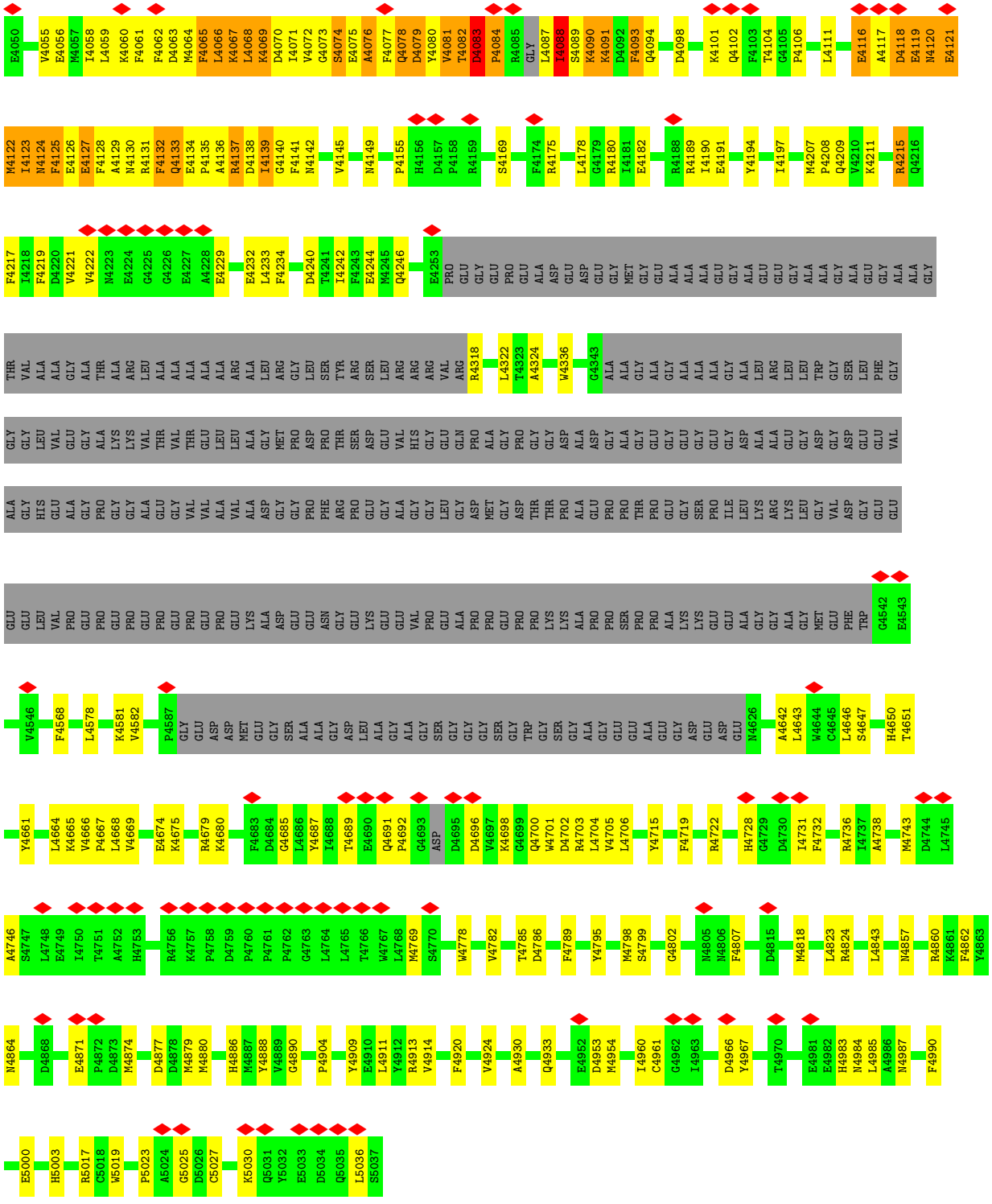


4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52414	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.049	Depositor
Minimum map value	-0.431	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.237	Depositor
Map size (Å)	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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

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	0.27	0/28107	0.46	0/37709
1	B	0.27	0/28107	0.46	0/37709
1	C	0.27	0/28107	0.46	0/37709
1	D	0.27	0/28107	0.46	0/37709
All	All	0.27	0/112428	0.46	0/150836

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	27613	0	23271	696	0
1	B	27613	0	23271	710	0
1	C	27613	0	23271	695	0
1	D	27613	0	23271	696	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	110456	0	93084	2673	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 13.

The worst 5 of 2673 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:1963:GLU:HA	1:C:3650:CYS:SG	1.69	1.32
1:B:1963:GLU:HA	1:B:3650:CYS:SG	1.69	1.31
1:D:1963:GLU:HA	1:D:3650:CYS:SG	1.69	1.30
1:A:1963:GLU:HA	1:A:3650:CYS:SG	1.69	1.29
1:B:4888:TYR:OH	1:C:4904:PRO:HG3	1.29	1.26

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	4107/5037 (82%)	3689 (90%)	378 (9%)	40 (1%)	13	48
1	B	4107/5037 (82%)	3689 (90%)	378 (9%)	40 (1%)	13	48
1	C	4107/5037 (82%)	3689 (90%)	378 (9%)	40 (1%)	13	48
1	D	4107/5037 (82%)	3689 (90%)	378 (9%)	40 (1%)	13	48
All	All	16428/20148 (82%)	14756 (90%)	1512 (9%)	160 (1%)	16	48

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1455	PRO
1	A	1490	SER
1	A	1495	VAL
1	A	1503	PRO
1	A	1549	PHE

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	2310/4276 (54%)	2273 (98%)	37 (2%)	58	73
1	B	2310/4276 (54%)	2273 (98%)	37 (2%)	58	73
1	C	2310/4276 (54%)	2273 (98%)	37 (2%)	58	73
1	D	2310/4276 (54%)	2273 (98%)	37 (2%)	58	73
All	All	9240/17104 (54%)	9092 (98%)	148 (2%)	58	73

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	976	ARG
1	D	4123	ILE
1	D	2291	GLN
1	D	4070	ASP
1	B	2474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4124	ASN
1	D	2005	GLN
1	C	4691	GLN
1	D	720	HIS
1	D	4124	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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)

There are no chain breaks in this entry.

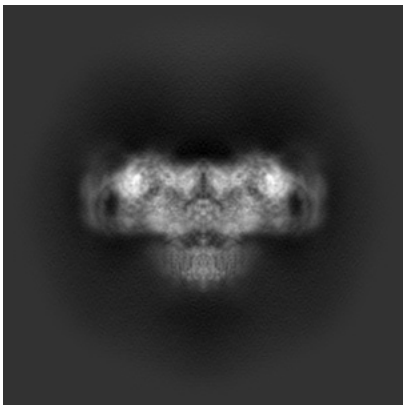
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38045. These allow visual inspection of the internal detail of the map and identification of artifacts.

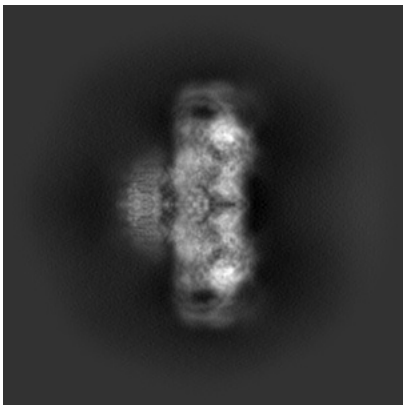
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

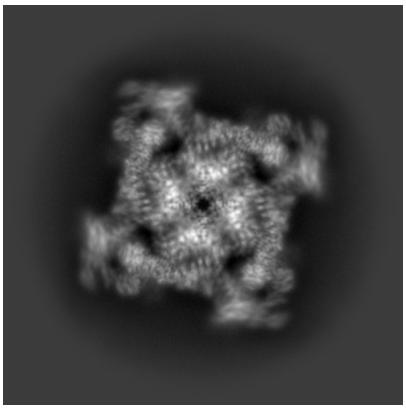
6.1.1 Primary map



X

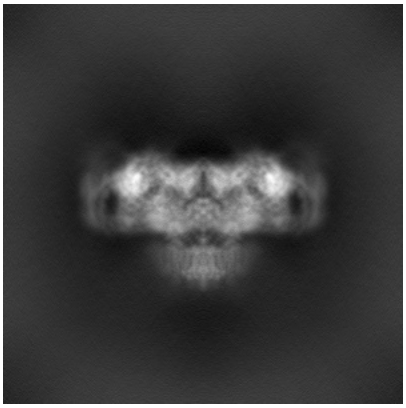


Y

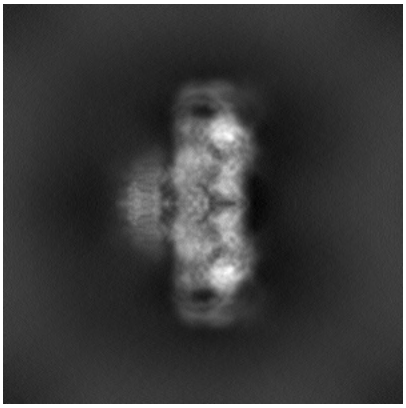


Z

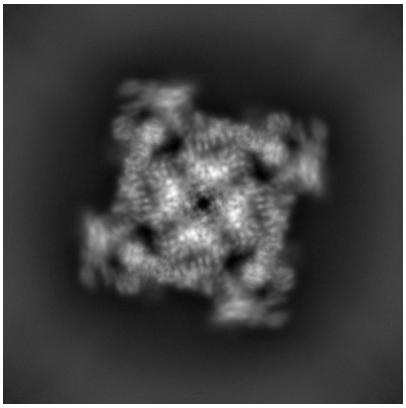
6.1.2 Raw map



X



Y

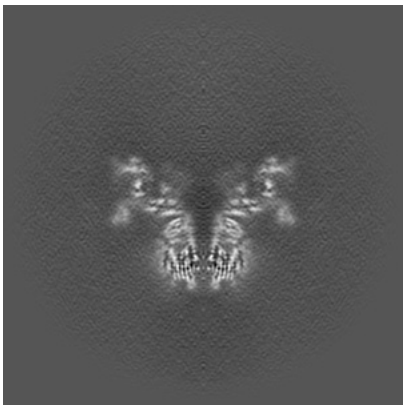


Z

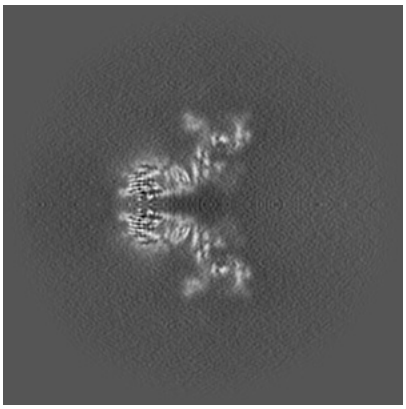
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

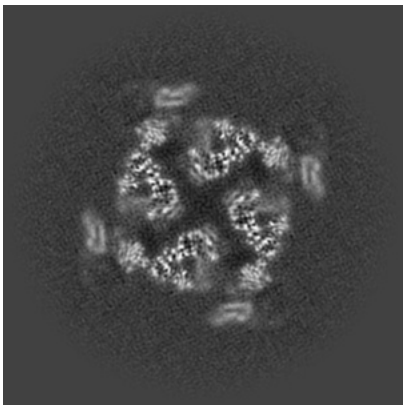
6.2.1 Primary map



X Index: 240

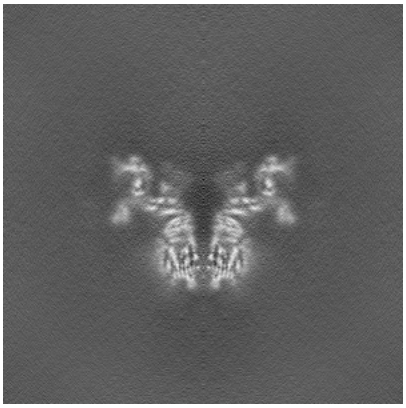


Y Index: 240

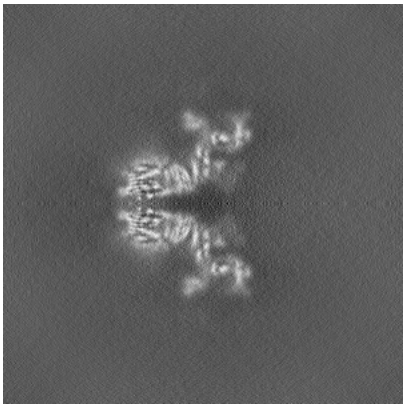


Z Index: 240

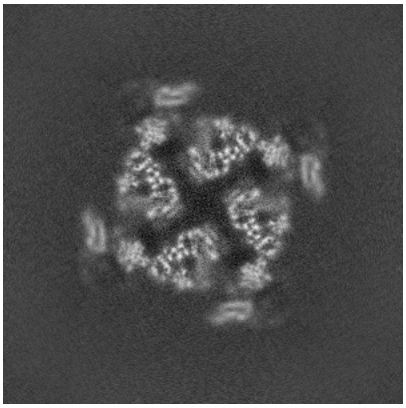
6.2.2 Raw map



X Index: 240



Y Index: 240

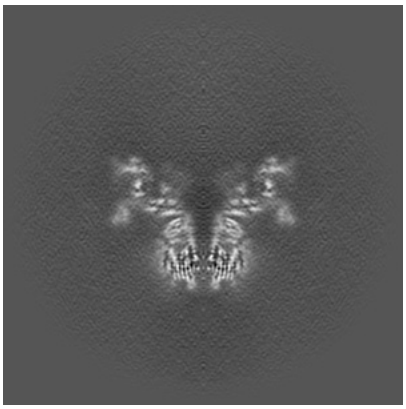


Z Index: 240

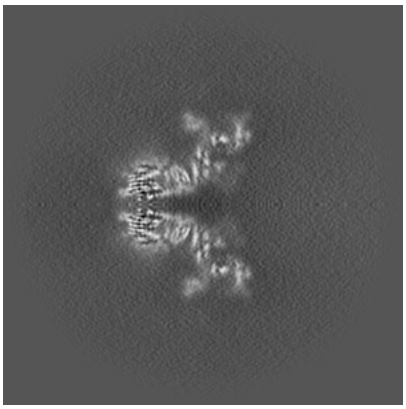
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

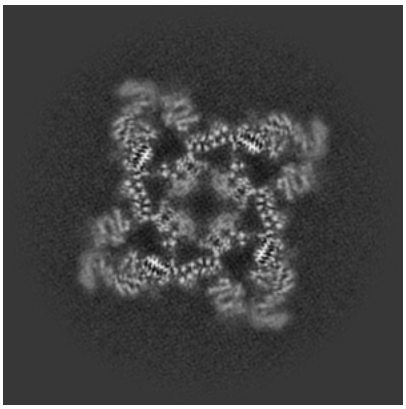
6.3.1 Primary map



X Index: 240

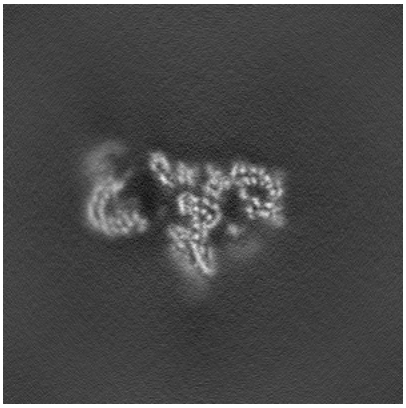


Y Index: 240

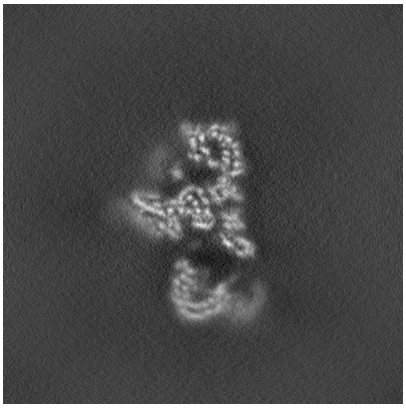


Z Index: 262

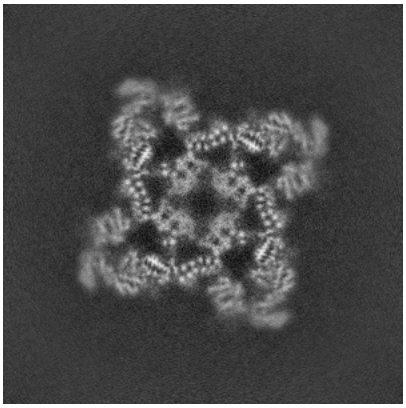
6.3.2 Raw map



X Index: 281



Y Index: 199

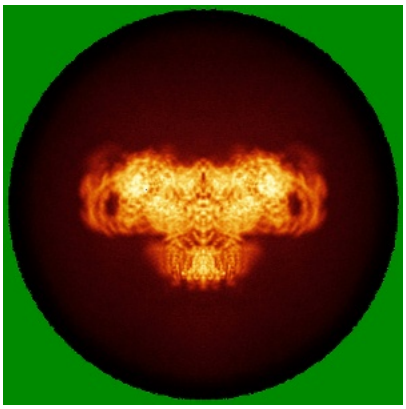


Z Index: 262

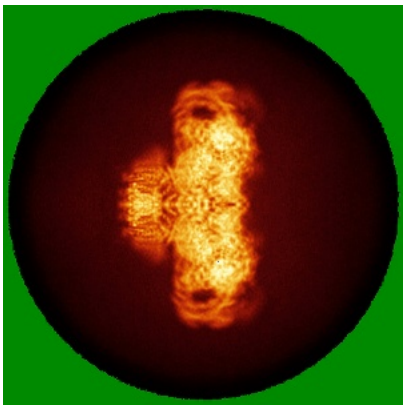
The images above show the largest variance slices of the map in three orthogonal directions.

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

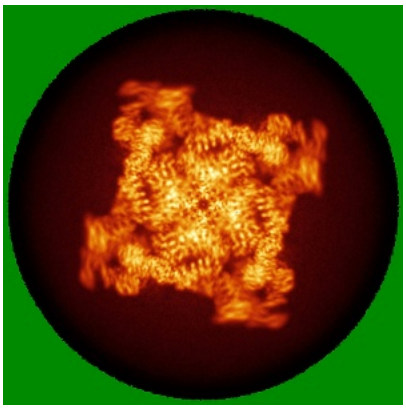
6.4.1 Primary map



X

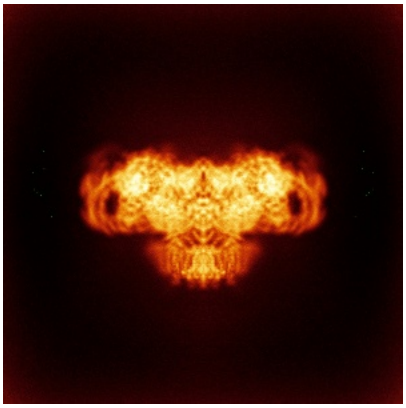


Y

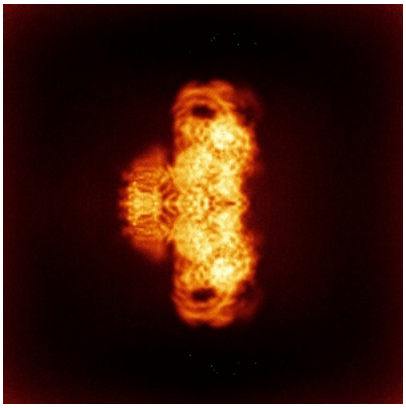


Z

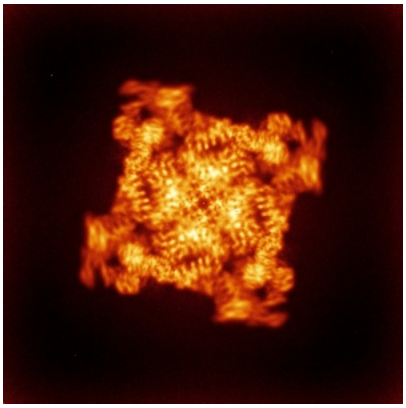
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

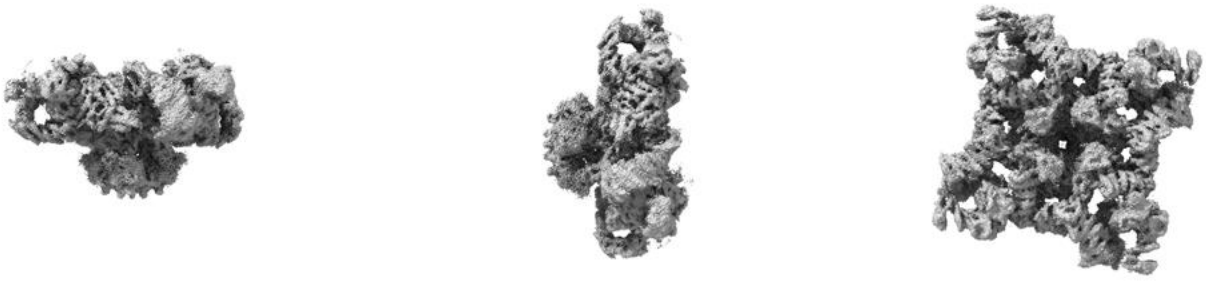
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.237. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

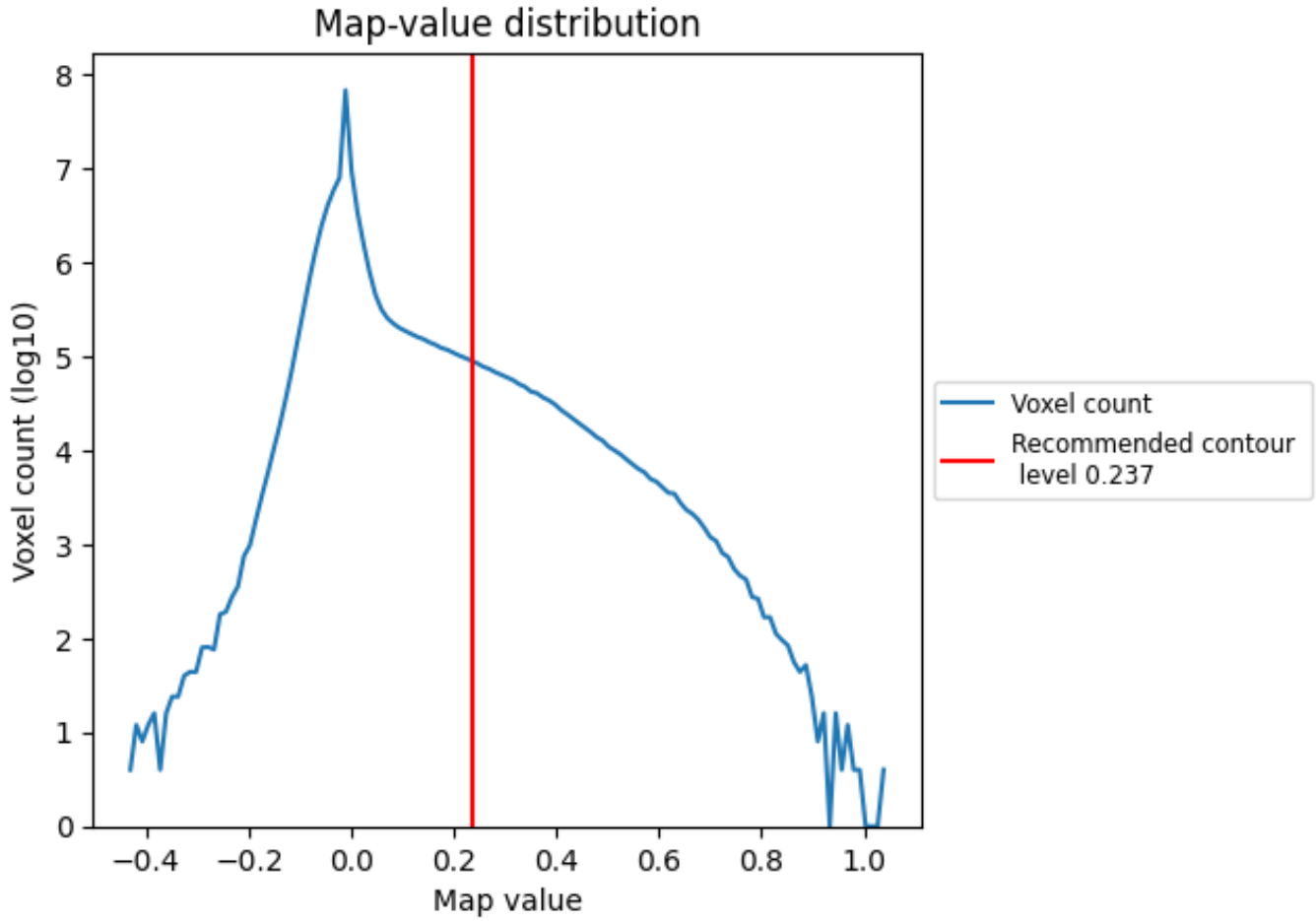
6.6 Mask visualisation (i)

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

7 Map analysis

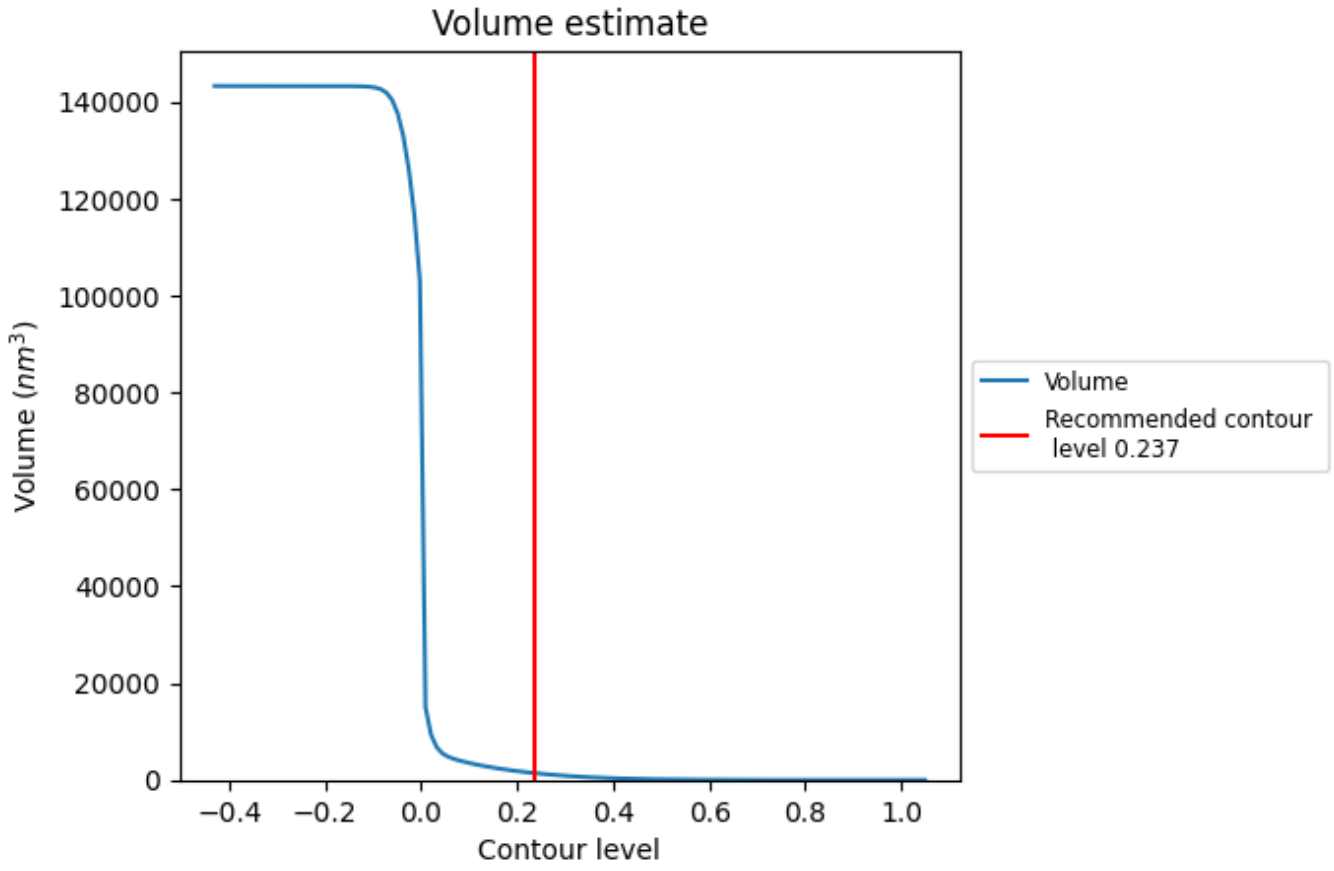
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

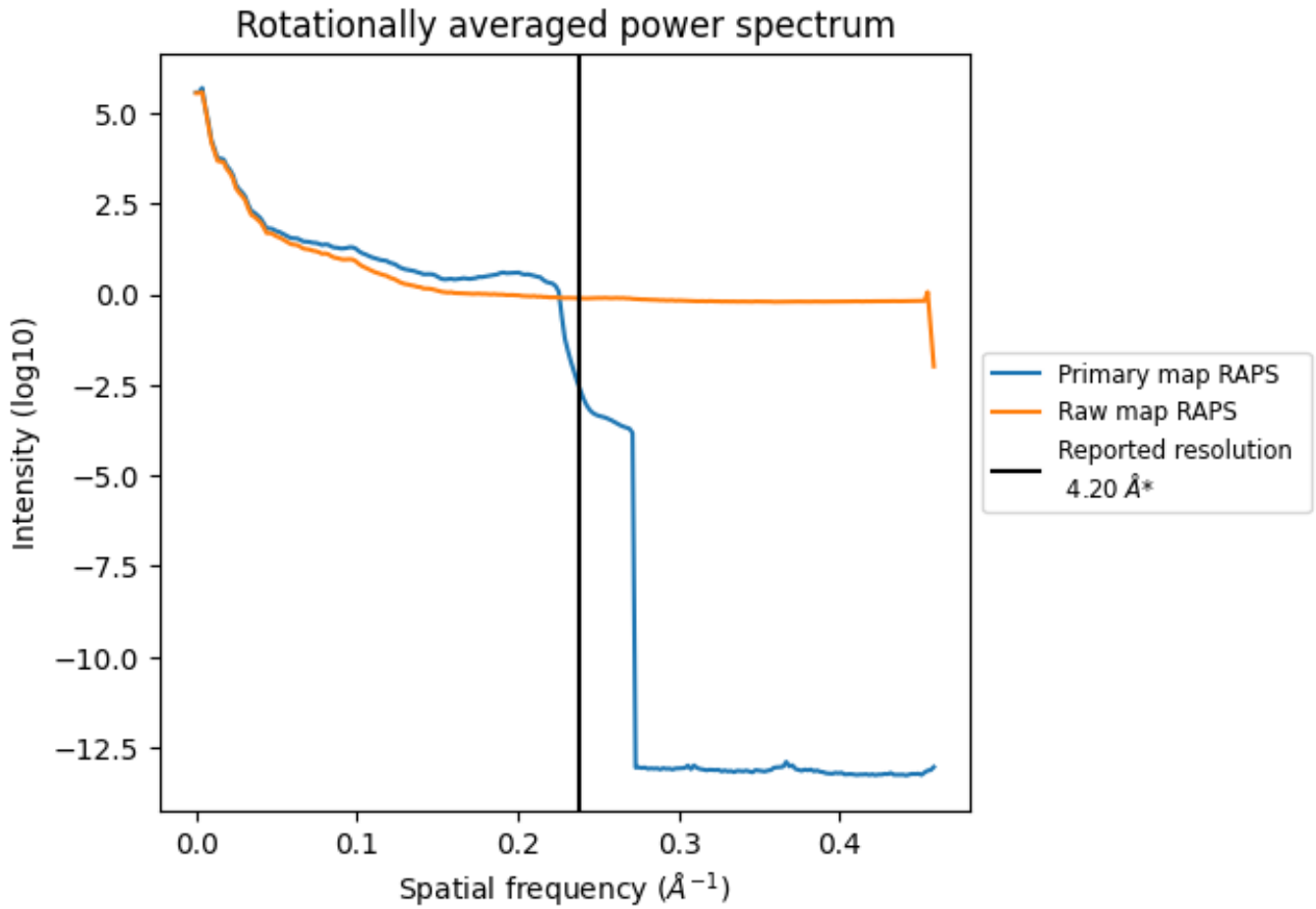
7.2 Volume estimate (i)



The volume at the recommended contour level is 1401 nm^3; this corresponds to an approximate mass of 1265 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)

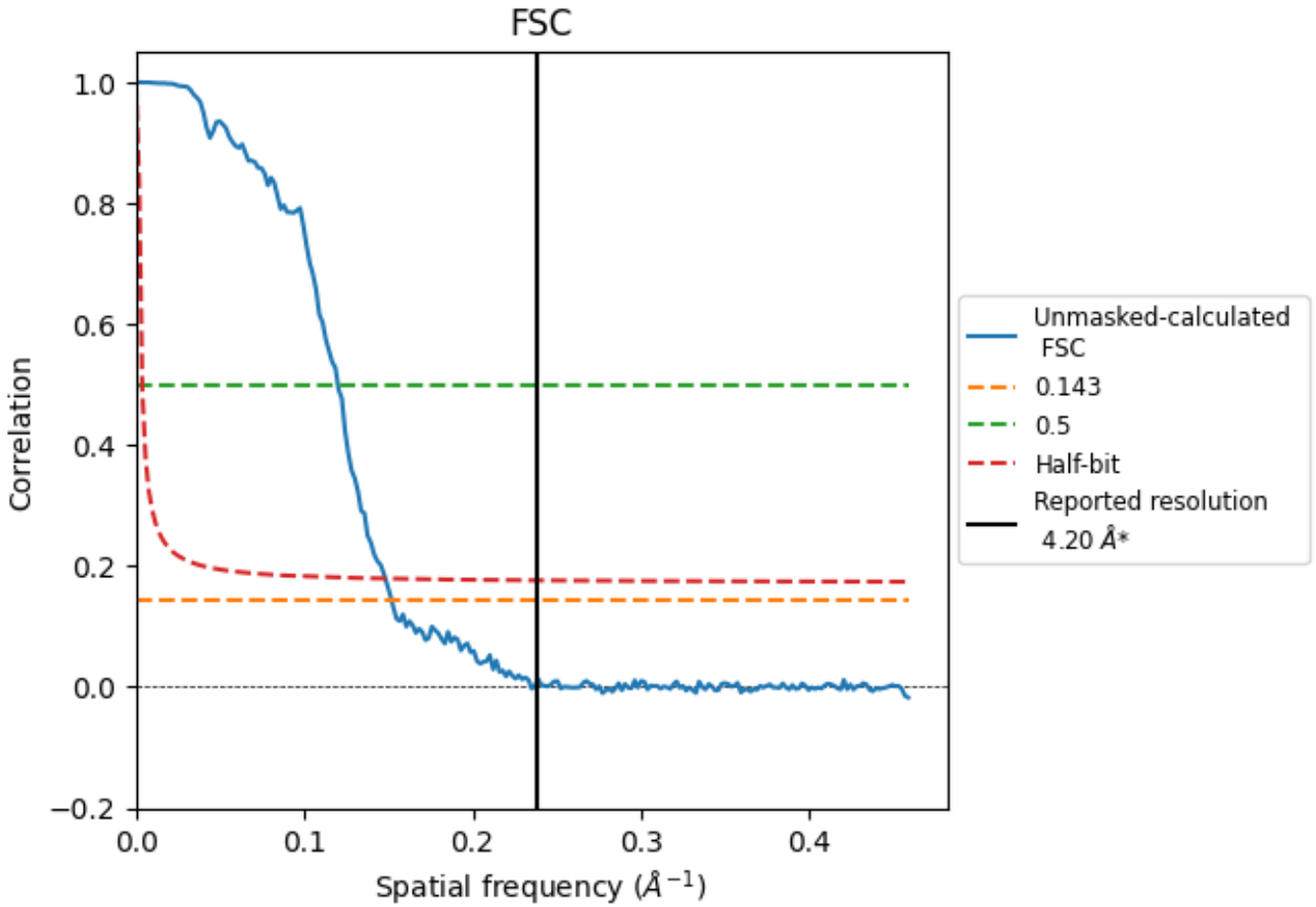


*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

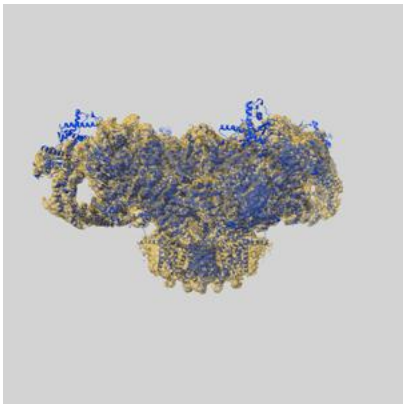
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.58	8.33	6.75

*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 6.58 differs from the reported value 4.2 by more than 10 %

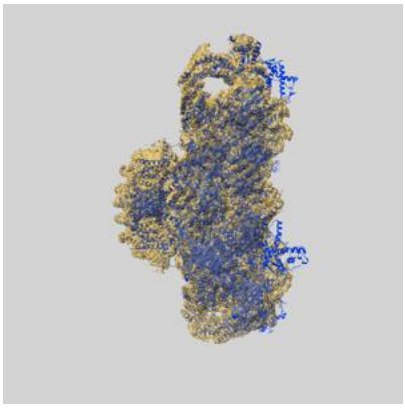
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38045 and PDB model 8X4B. Per-residue inclusion information can be found in section 3 on page 4.

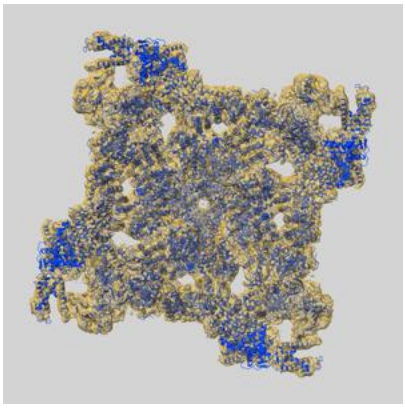
9.1 Map-model overlay



X



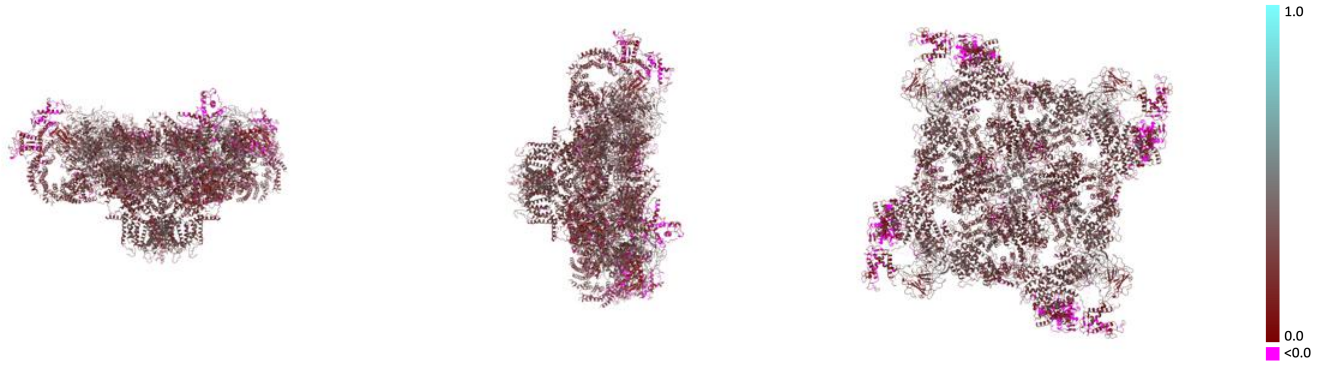
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.237 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.

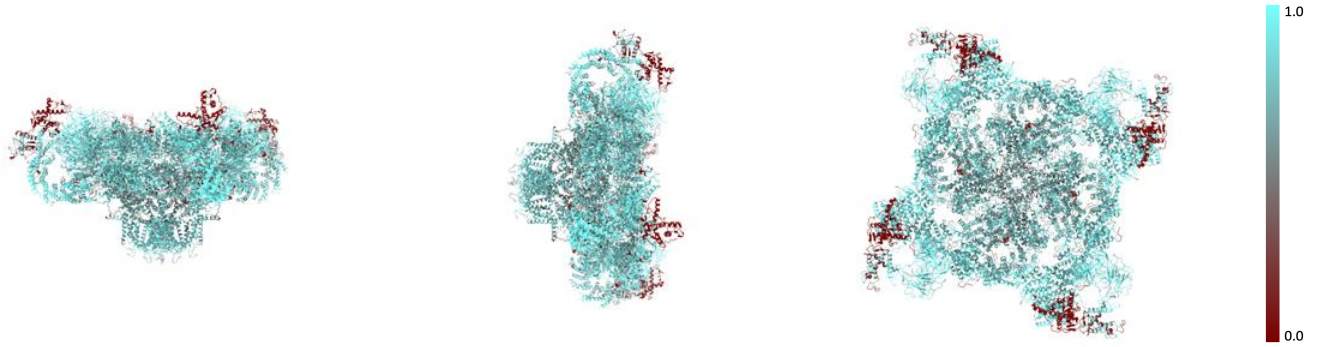
9.2 Q-score mapped to coordinate model (i)



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.

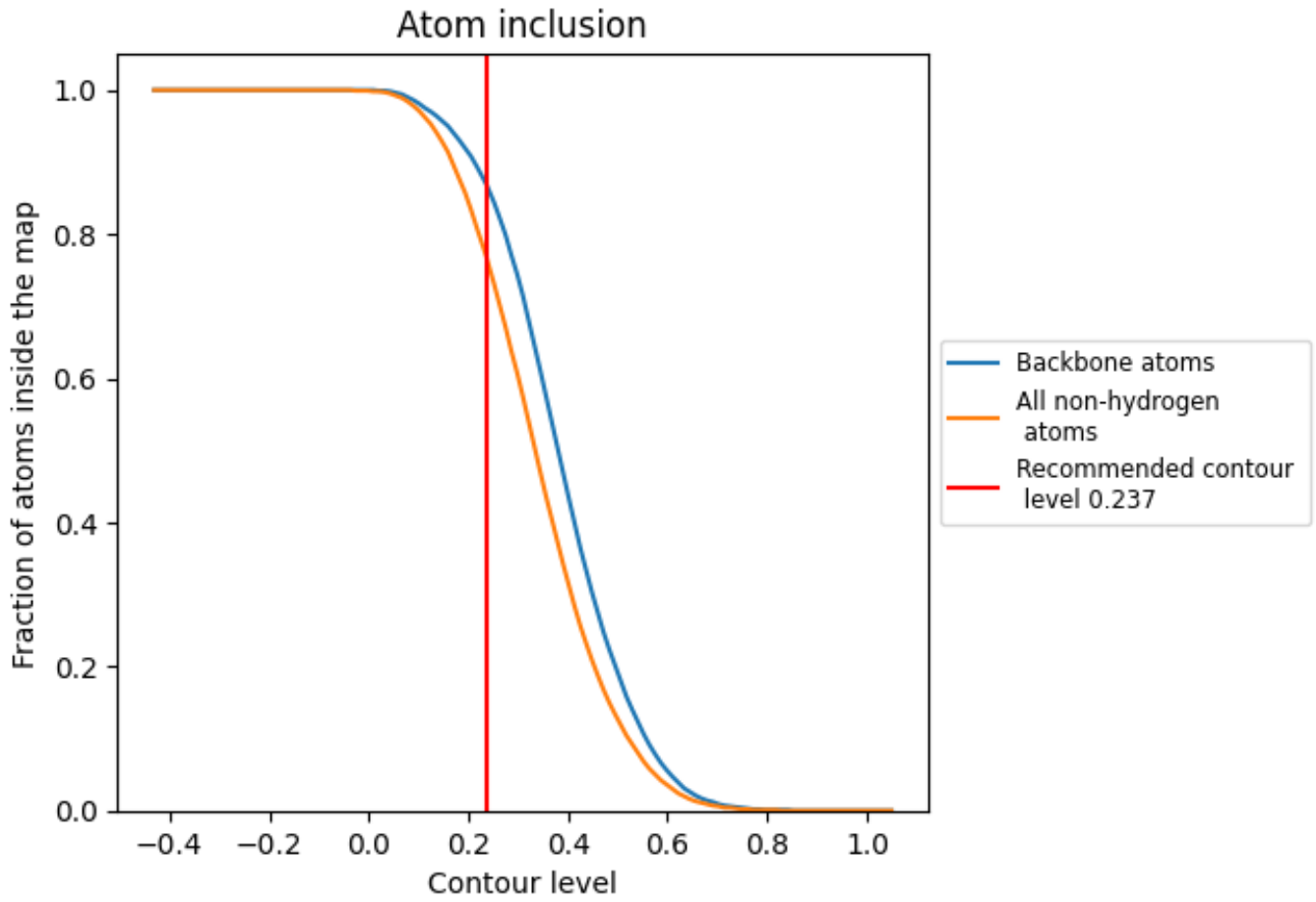
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.237).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 77% 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 (0.237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.2600
A	0.7670	0.2600
B	0.7670	0.2600
C	0.7670	0.2600
D	0.7670	0.2600