wwPDB EM Validation Summary Report (i)

Mar 25, 2026 – 08:32 PM UTC

PDB ID	:	6JHN / pdb_00006jhn
EMDB ID	:	EMD-9826
Title	:	Structure of RyR2 (F/C/Ca2+ dataset)
Authors	:	Chi, X.M.; Gong, D.S.; Ren, K.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Zhou, Q.; Yan, N.
Deposited on	:	2019-02-18
Resolution	:	4.50 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 (i) 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 (1)) were used in the production of this report:

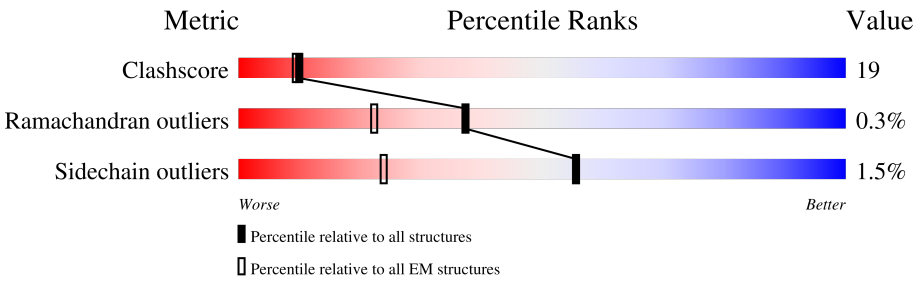
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

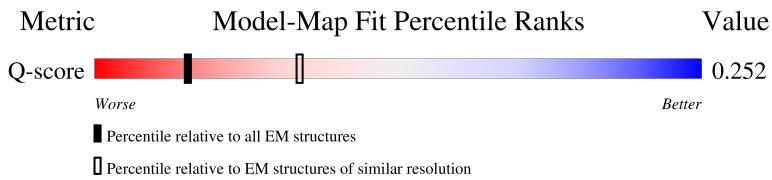
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	4968	8% 42% 27% • 30%
1	C	4968	8% 42% 27% • 30%
1	E	4968	8% 42% 27% • 30%
1	G	4968	8% 42% 27% • 30%

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Mol	Chain	Length	Quality of chain
2	B	108	46% 52%
2	D	108	48% 50%
2	F	108	48% 50%
2	H	108	48% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFF	A	6002	-	X	-	-
5	CFF	C	6002	-	X	-	-
5	CFF	E	6002	-	X	-	-
5	CFF	G	6002	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 109488 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3476	26537	16896	4538	4946	157	0	0
1	C	3476	26537	16896	4538	4946	157	0	0
1	E	3476	26537	16896	4538	4946	157	0	0
1	G	3476	26537	16896	4538	4946	157	0	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	107	819	516	144	155	4	0	0
2	D	107	819	516	144	155	4	0	0
2	F	107	819	516	144	155	4	0	0
2	H	107	819	516	144	155	4	0	0

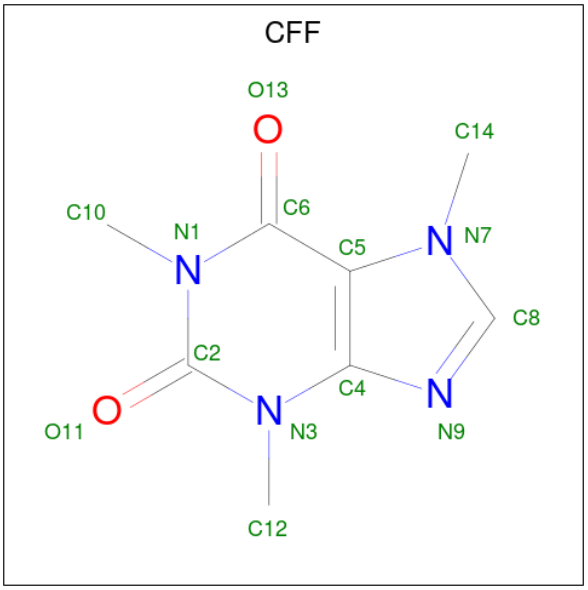
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0
3	C	1	1	1	0
3	E	1	1	1	0
3	G	1	1	1	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	1	1	0
4	C	1	1	1	0
4	E	1	1	1	0
4	G	1	1	1	0

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



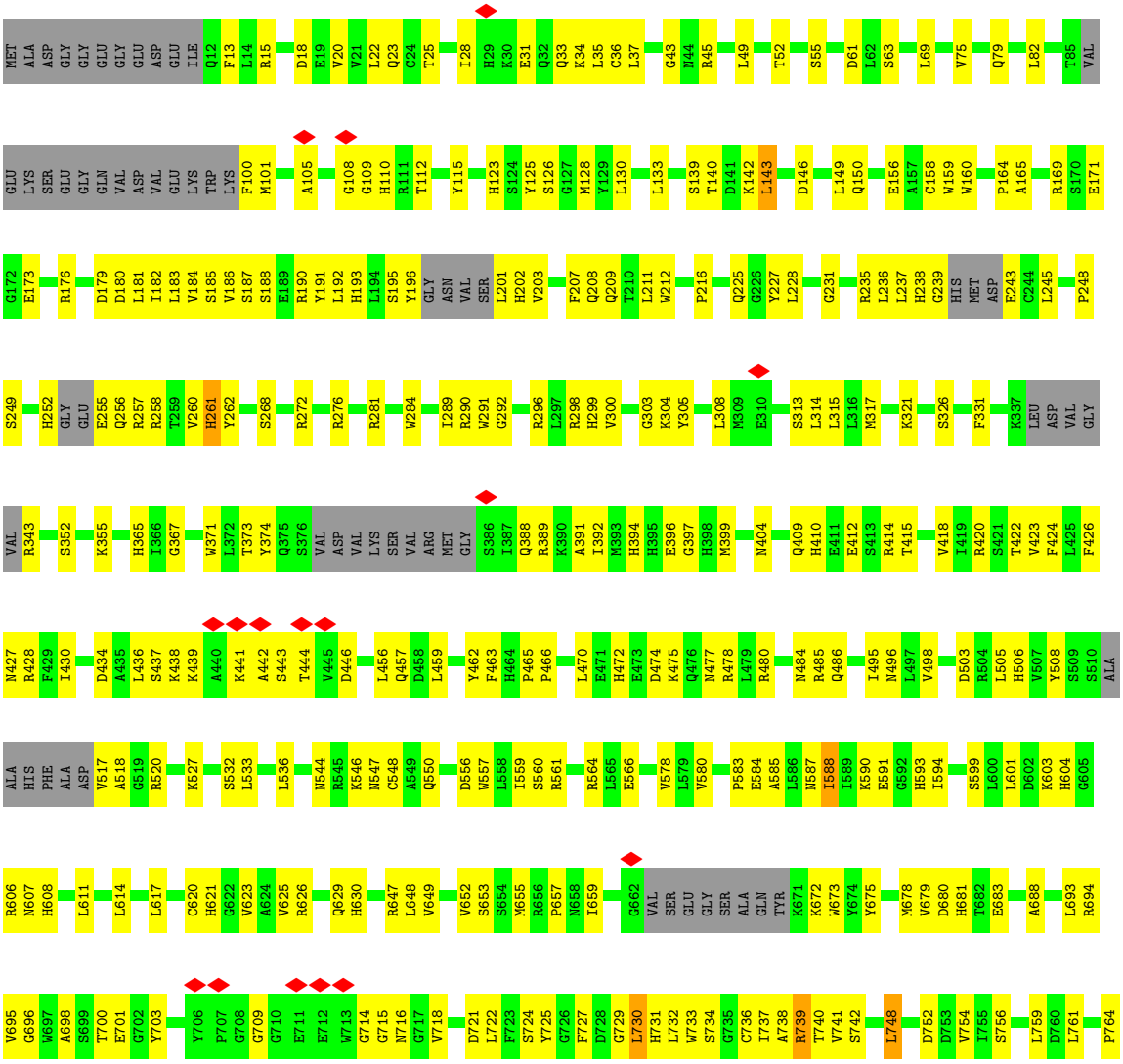
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	4	2	0
5	C	1	14	8	4	2	0
5	E	1	14	8	4	2	0
5	G	1	14	8	4	2	0

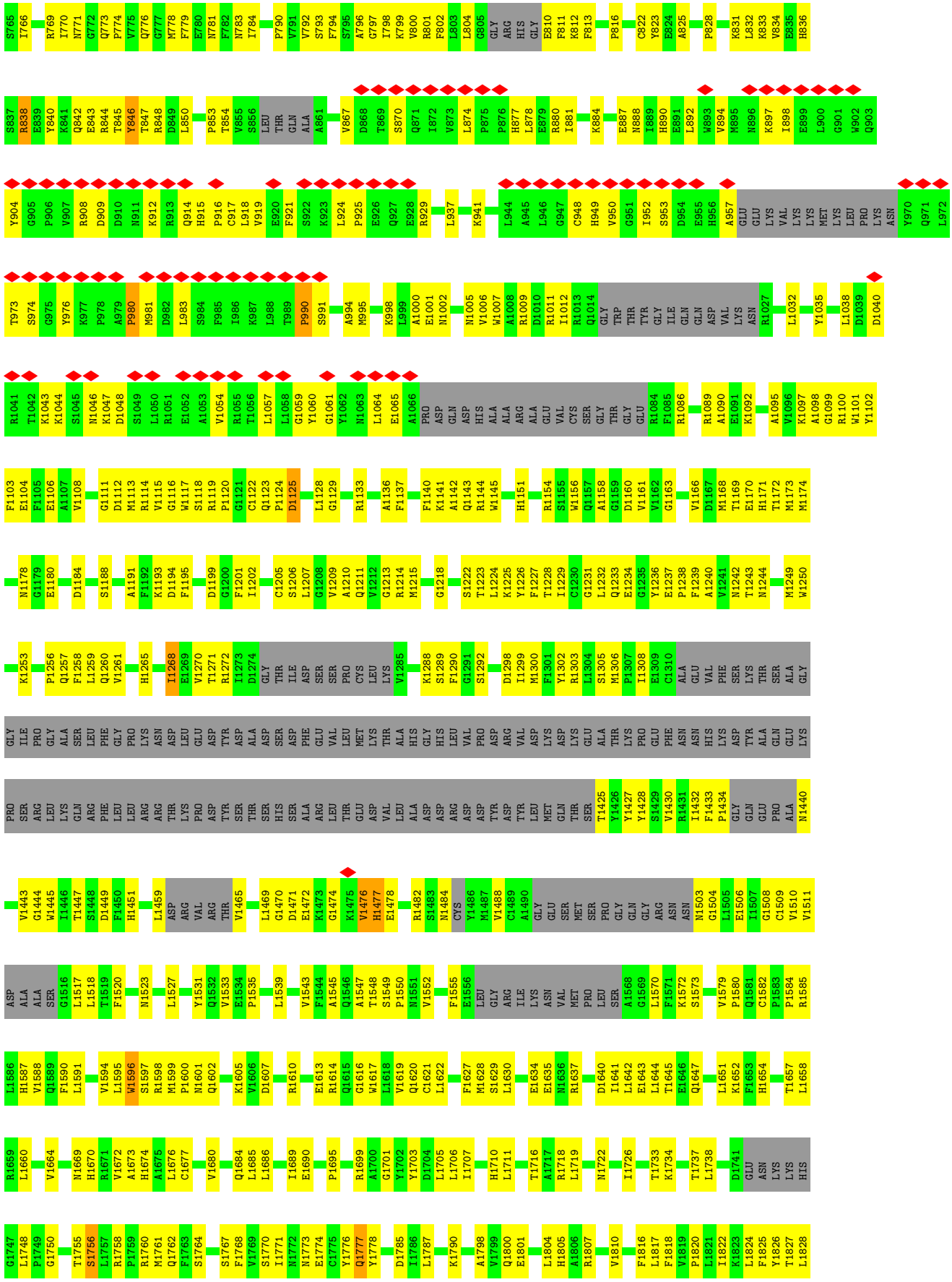
3 Residue-property plots (i)

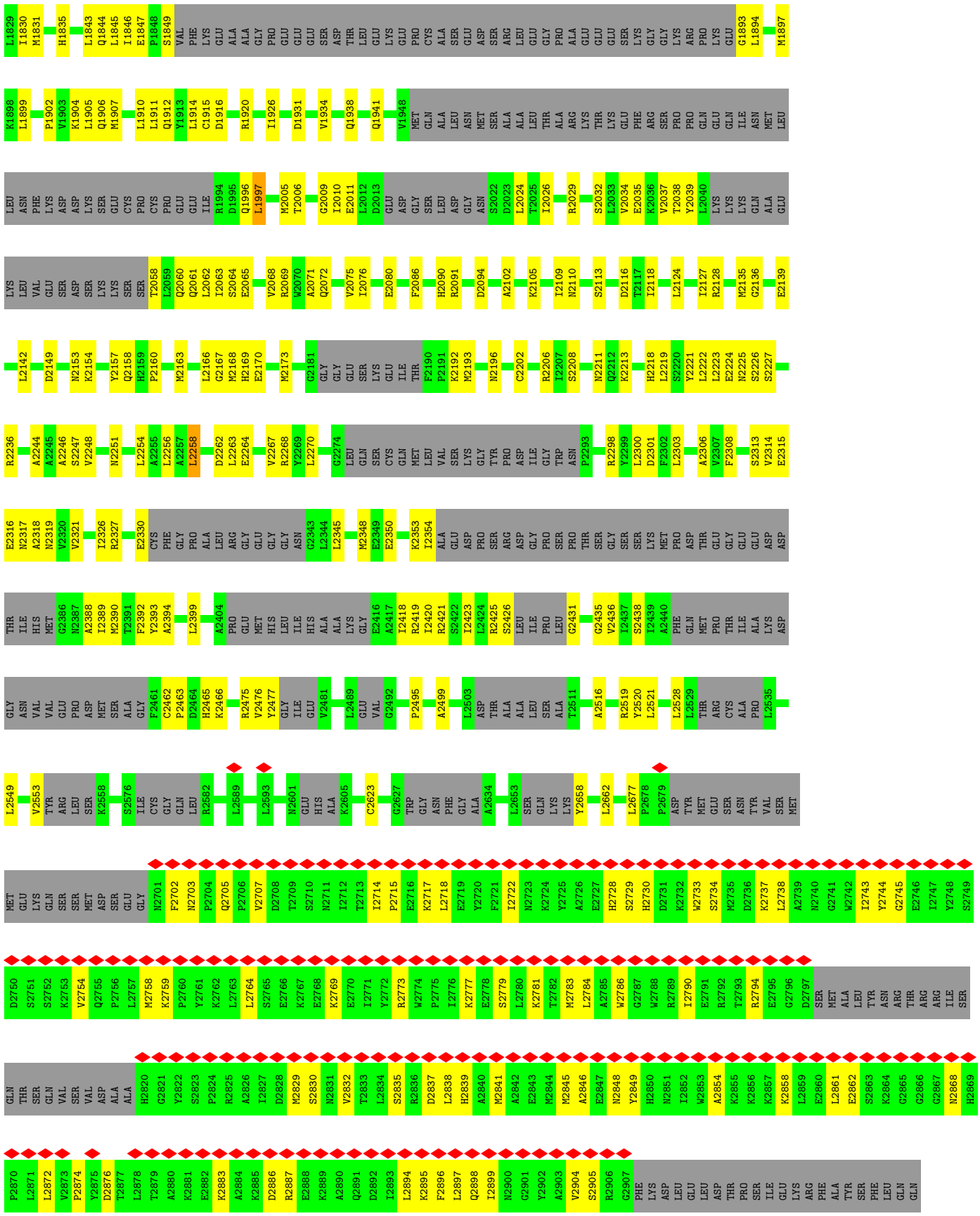
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

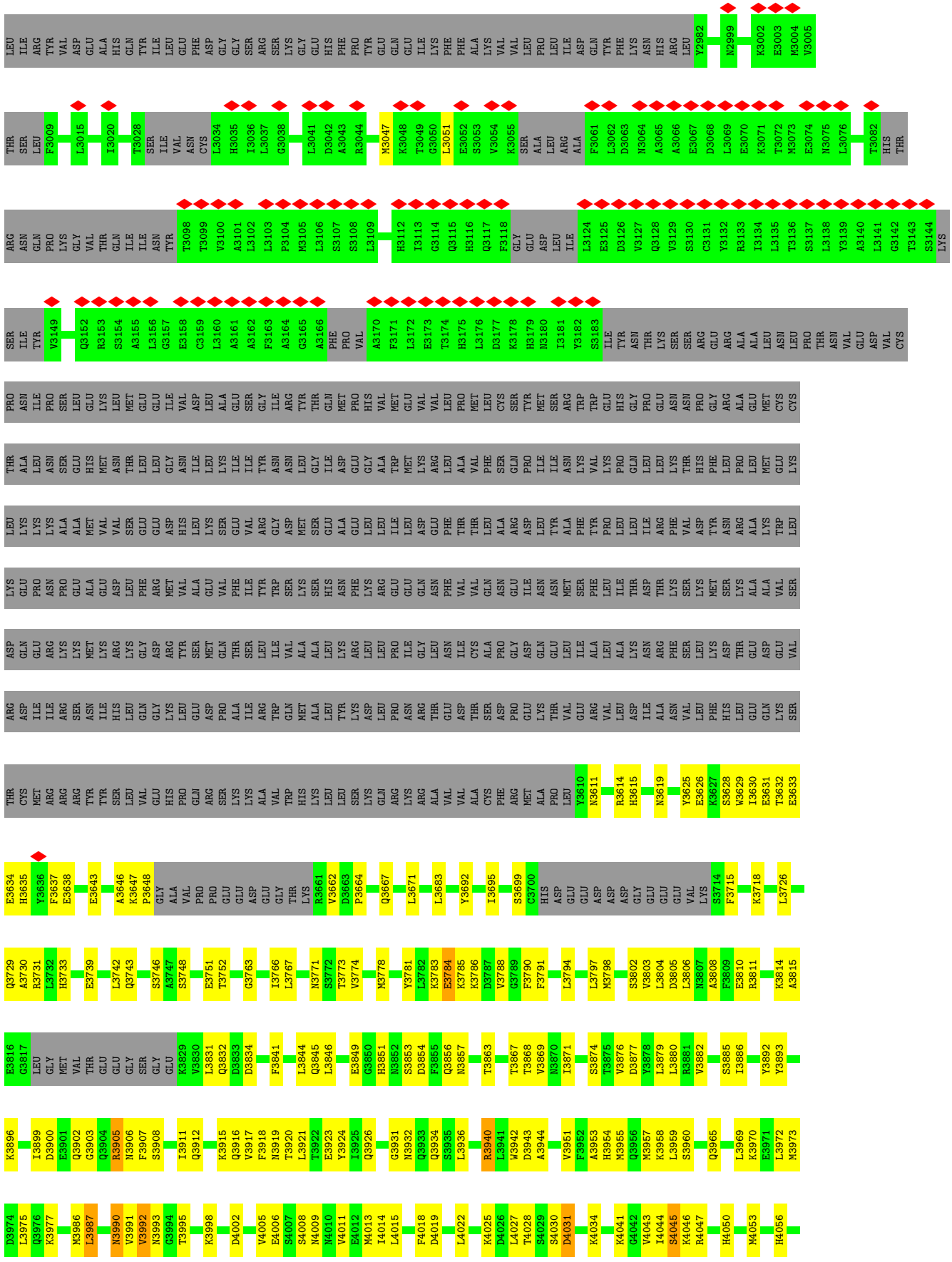
- Molecule 1: RyR2

Chain A:




S765 I766 R769 I770 N771 G772 Q773 P774 V775 Q776 G777 M778 F779 E780 N781 F782 N783 I784 P790 V791 V792 S793 F794 S795 A796 G797 I798 K799 V800 R801 F802 L803 L804 G805 GLY ARG HIS GLY E810 F811 K812 F813 P816 C822 Y823 E824 A825 P828 K831 L832 K833 V834 E835 H836
S837 R838 E839 Y840 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 L850 P853 T854 V855 S856 LEU THR GLN ALA A861 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 K884 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903
Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 L937 K941 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972
T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 A994 M995 K998 L999 A1000 E1001 N1002 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 L1032 Y1035 L1038 D1039 D1040
R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 R1089 A1090 E1091 K1092 A1095 V1096 K1097 A1098 G1099 R1100 W1101 Y1102
F1103 E1104 F1105 E1106 A1107 V1108 G1111 D1112 M1113 R1114 V1115 G1116 W1117 S1118 R1119 P1120 G1121 C1122 Q1123 P1124 D1125 L1128 G1129 R1133 A1136 F1137 F1140 K1141 A1142 Q1143 R1144 W1145 H1151 R1154 S1155 W1156 Q1157 A1158 G1159 D1160 V1161 V1162 G1163 V1166 D1167 M1168 T1169 E1170 H1171 T1172 M1173 M1174
N1178 G1179 E1180 D1184 S1188 A1191 F1192 K1193 D1194 F1195 D1199 G1200 F1201 I1202 C1205 S1206 L1207 G1208 V1209 A1210 Q1211 V1212 G1213 R1214 M1215 G1218 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235 Y1236 E1237 P1238 F1239 A1240 V1241 N1242 T1243 N1244 M1249 W1250
K1253 P1256 Q1257 F1258 L1259 Q1260 V1261 H1265 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 K1288 S1289 F1290 G1291 S1292 D1298 I1299 M1300 F1301 Y1302 R1303 L1304 S1305 M1306 P1307 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY
GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS
PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP ASP TYR LEU MET GLN THR SER T1425 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440
V1443 G1444 W1445 I1446 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 L1469 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO LEU SER A1568 G1569 L1570 F1571 K1572 S1573 N1503 G1504 L1505 E1506 I1507 G1508 C1509 V1510 V1511
ASP ALA ALA SER G1516 L1517 L1518 T1519 F1520 N1523 L1527 Y1531 Q1532 V1533 E1534 P1535 L1539 V1543 F1544 A1545 Q1546 A1547 T1548 S1549 P1550 N1551 V1552 F1555 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 F1571 K1572 S1573 V1579 P1580 Q1581 C1582 P1583 P1584 R1585
L1586 H1587 V1588 Q1589 F1590 L1591 V1594 L1595 W1596 S1597 R1598 M1599 P1600 N1601 Q1602 K1605 V1606 D1607 R1610 E1613 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 F1627 M1628 S1629 L1630 E1634 E1635 M1636 R1637 D1640 I1641 L1642 E1643 L1644 T1645 E1646 Q1647 L1651 K1652 F1653 H1654 T1657 L1658
R1659 L1660 V1664 N1669 H1670 R1671 V1672 A1673 H1674 A1675 L1676 C1677 V1680 Q1684 L1685 L1686 I1689 E1690 P1695 R1699 A1700 G1701 Y1702 Y1703 D1704 L1705 L1706 I1707 H1710 L1711 T1716 A1717 R1718 L1719 N1722 V1726 T1733 K1734 T1737 L1738 D1741 GLU ASN LYS LYS HIS
G1747 L1748 P1749 G1750 T1755 S1756 L1757 R1758 P1759 R1760 M1761 Q1762 F1763 S1764 S1767 F1768 V1769 S1770 I1771 N1772 N1773 E1774 C1775 Y1776 Q1777 Y1778 D1785 I1786 L1787 K1790 A1798 V1799 Q1800 E1801 L1804 H1805 A1806 R1807 V1810 F1816 L1817 F1818 V1819 P1820 L1821 I1822 K1823 L1824 F1825 Y1826 T1827 L1828


L1829 I1830 M1831 H1835 L1843 Q1844 L1845 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS GLU G1893 L1894 M1897
K1898 L1899 P1902 V1903 K1904 L1905 Q1906 M1907 L1910 L1911 Q1912 Y1913 L1914 C1915 D1916 R1920 I1926 D1931 V1934 Q1938 Q1941 V1948 MET GLN ALA LEU ASN MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU
LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE R1994 D1995 Q1996 L1997 M2005 T2006 G2009 I2010 E2011 L2012 D2013 GLU ASP GLY SER LEU ASP GLY ASN S2022 D2023 L2024 T2025 I2026 R2029 S2032 L2033 V2034 E2035 K2036 V2037 T2038 Y2039 L2040 LYS LYS LYS GLN ALA GLU
LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 L2059 Q2060 Q2061 L2062 I2063 S2064 E2065 V2068 R2069 W2070 A2071 Q2072 V2075 I2076 E2080 F2086 H2090 R2091 D2094 A2102 K2105 I2109 N2110 S2113 D2116 T2117 I2118 L2124 I2127 R2128 M2135 G2136 E2139
L2142 D2149 N2153 K2154 Y2157 Q2158 H2159 P2160 M2163 L2166 G2167 M2168 H2169 E2170 M2173 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191 K2192 M2193 N2196 C2202 R2206 I2207 S2208 N2211 Q2212 K2213 H2218 L2219 S2220 Y2221 L2222 L2223 E2224 N2225 S2226 S2227
R2236 A2244 A2245 A2246 S2247 V2248 N2251 L2254 A2255 L2256 A2257 L2258 D2262 L2263 E2264 V2267 R2268 Y2269 L2270 G2274 LEU GLN SER CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 R2298 Y2299 L2300 D2301 F2302 L2303 A2306 V2307 F2308 S2313 V2314 E2315
E2316 N2317 A2318 N2319 V2320 V2321 I2326 R2327 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 L2344 L2345 M2348 E2349 E2350 K2353 I2354 ALA GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS MET PRO ASP THR GLU GLY GLU GLU ASP ASP
THR ILE HIS MET G2386 N2387 A2388 I2389 M2390 T2391 F2392 Y2393 A2394 L2399 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 A2417 I2418 R2419 I2420 R2421 S2422 I2423 L2424 R2425 S2426 LEU ILE PRO LEU G2431 G2435 V2436 I2437 S2438 I2439 A2440 PHE GLN MET PRO THR ILE ALA LYS ASP
GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 C2462 P2463 D2464 H2465 K2466 R2475 V2476 Y2477 GLY ILE GLU V2481 L2489 GLU VAL G2492 P2495 A2499 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2516 R2519 Y2520 L2521 L2528 L2529 THR ARG CYS ALA PRO L2535
L2549 V2553 TYR ARG LEU SER K2558 S2576 ILE CYS GLY GLN LEU R2582 L2589 L2593 N2601 GLU HIS ALA K2605 C2623 G2627 TRP GLY ASN PHE GLY ALA A2634 L2653 SER GLN LYS LYS Y2658 L2662 L2677 P2678 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET
MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728 S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749
D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788 R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER
GLN THR SER GLN VAL SER VAL ASP ALA ALA H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869
P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN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THR SER LEU F3009 L3015 I3020 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 G3038 L3041 D3042 A3043 R3044 M3047 K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER ALA LEU ARG ARG ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070 K3071 T3072 M3073 E3074 N3075 L3076 T3082 HIS THR
ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135 T3136 S3137 L3138 Y3139 A3140 L3141 G3142 T3143 S3144 LYS
SER ILE TYR V3149 Q3152 R3153 S3154 A3155 L3156 G3157 E3158 C3159 L3160 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS
PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS
THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU GLU LYS
LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU
LYS GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL VAL ILE ASN GLU ILE ASN ASN MET SER PHE LEU LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER
ASP GLN GLU ARG LYS LYS MET VAL ARG LYS ARG ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU LYS ASN LEU ALA LEU LEU ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL
ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP SER PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA PHE LYS HIS LYS LEU GLU PHE GLY PHE ARG LYS LEU PHE
THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU Y3610 N3611 R3614 H3615 N3619 Y3625 E3626 K3627 S3628 W3629 I3630 E3631 T3632 E3633
E3634 H3635 Y3636 F3637 E3638 E3643 A3646 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 P3664 Q3667 L3671 L3683 Y3692 I3695 S3699 C3700 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU VAL LYS S3714 F3715 K3718 L3726
Q3729 A3730 R3731 L3732 H3733 E3739 L3742 Q3743 S3746 A3747 S3748 E3751 T3752 G3763 I3766 L3767 N3771 S3772 T3773 V3774 M3778 Y3781 L3782 K3783 E3784 K3785 K3786 D3787 V3788 G3789 F3790 F3791 L3794 L3797 M3798 S3802 V3803 L3804 D3805 L3806 N3807 A3808 F3809 E3810 R3811 K3814 A3815
E3816 G3817 LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU K3829 V3830 L3831 Q3832 D3833 D3834 F3841 L3844 Q3845 L3846 E3849 G3850 H3851 N3852 S3853 D3854 F3855 Q3856 N3857 T3863 T3867 T3868 V3869 N3870 I3871 S3874 T3875 V3876 D3877 Y3878 L3879 L3880 R3881 V3882 S3885 I3886 Y3892 Y3893
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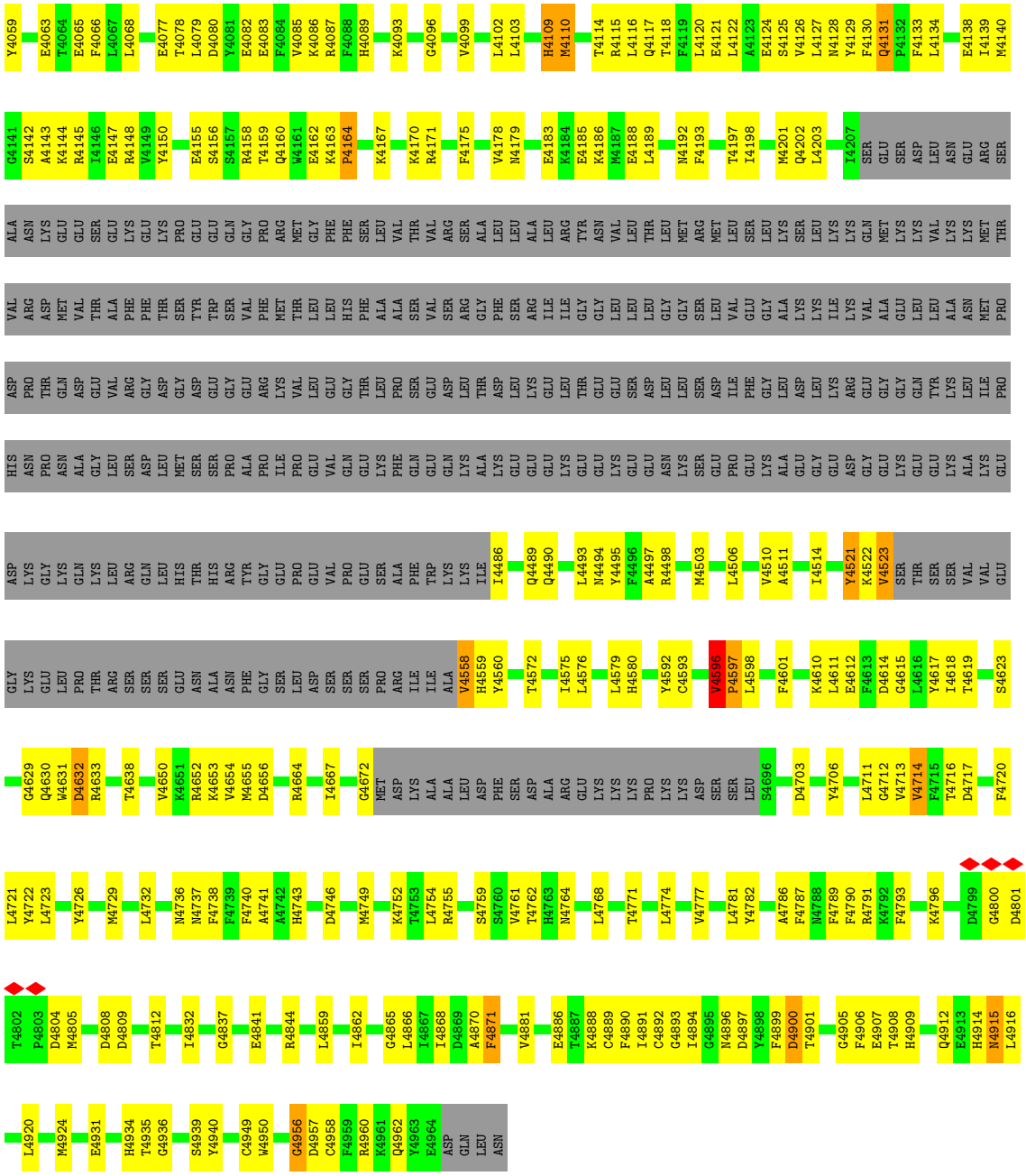
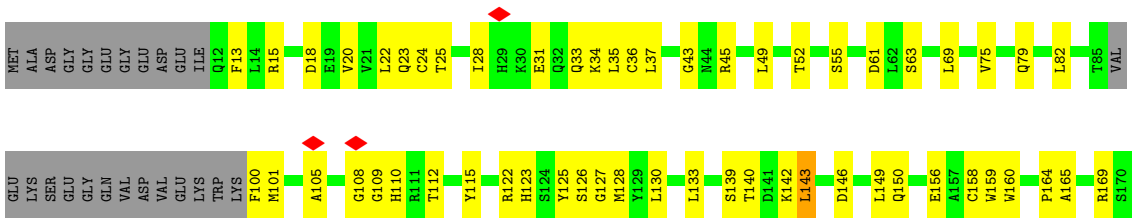
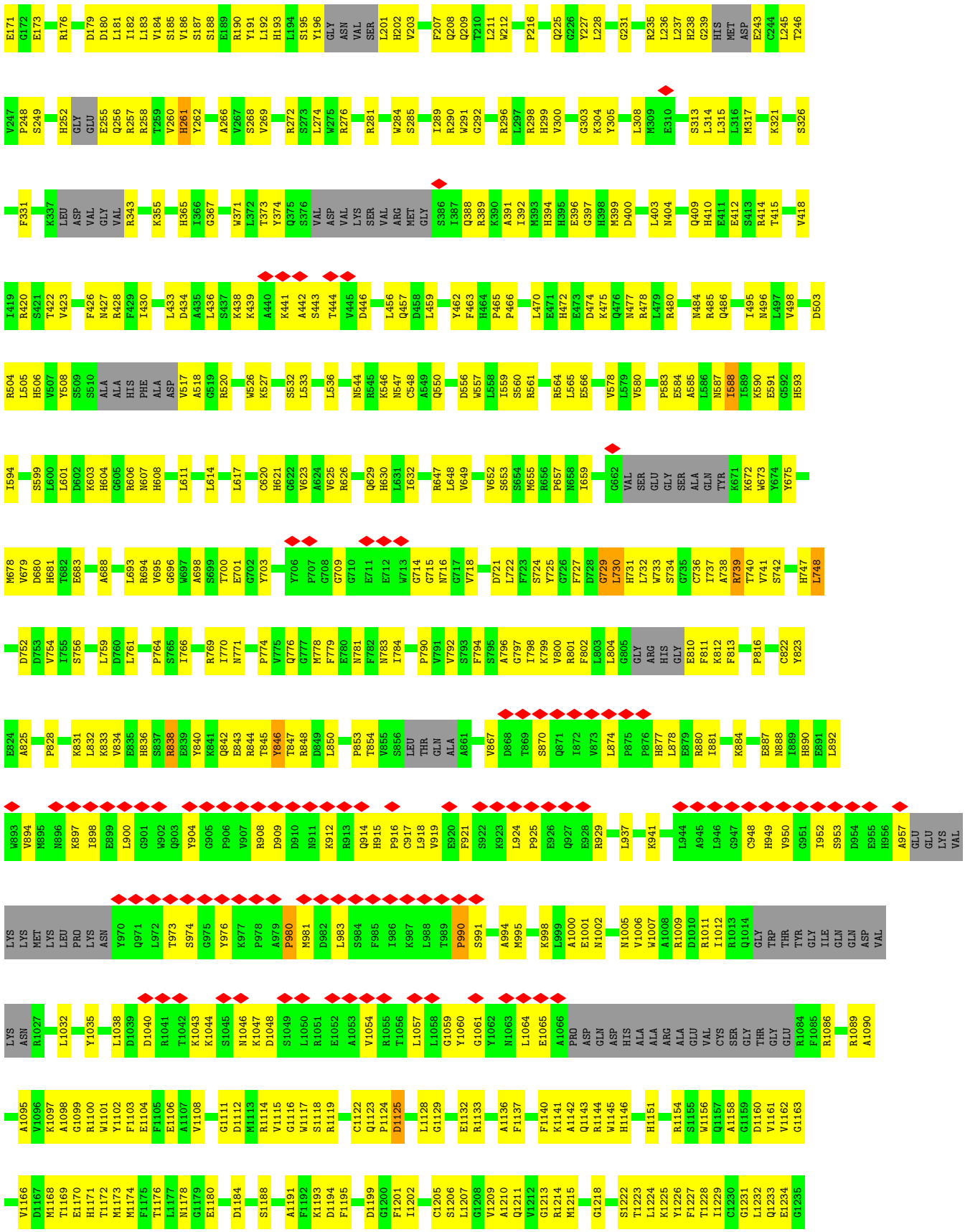
D3974 L3975 Q3976 K3977 M3986 L3987 N3990 V3991 V3992 N3993 G3994 T3995 K3998 D4002 V4005 E4006 S4007 S4008 N4009 N4010 V4011 E4012 M4013 I4014 L4015 F4018 D4019 L4022 K4025 D4026 L4027 T4028 S4029 S4030 D4031 K4034 K4041 G4042 V4043 I4044 S4045 K4046 R4047 H4050 M4053 H4056



- Molecule 1: RyR2

Chain C:

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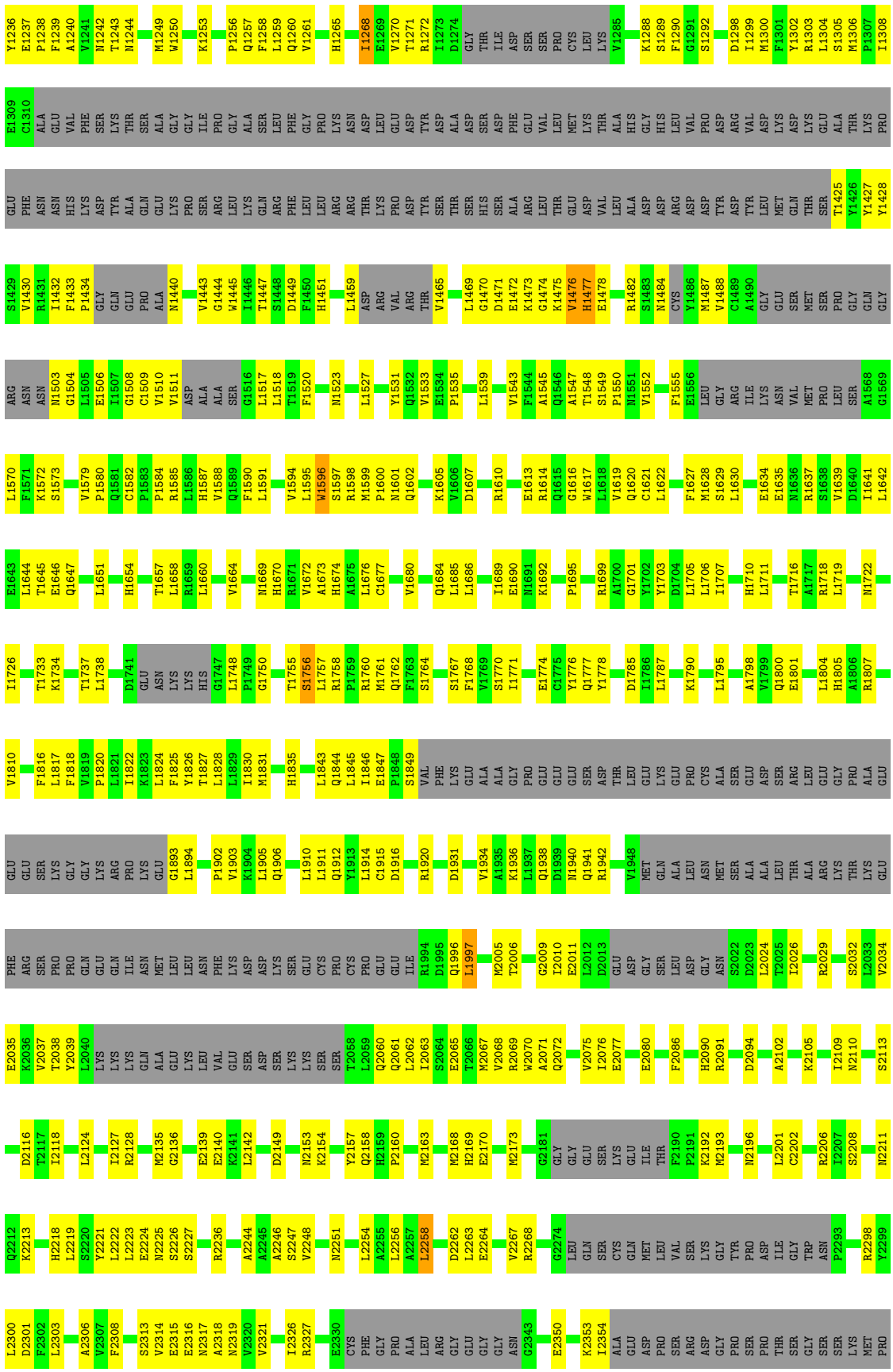
V247 P248 S249 H252 GLY GLU E255 Q256 R257 R258 T259 V260 H261 Y262 A266 V267 S268 V269 R272 S273 L274 W275 R276 R281 W284 S285 I289 R290 W291 G292 R296 L297 R298 H299 V300 G303 K304 Y305 L308 M309 E310 S313 L314 L315 L316 M317 K321 S326
F331 K337 LEU ASP VAL GLY VAL R343 K355 H365 I366 G367 W371 L372 T373 Y374 Q375 S376 VAL ASP VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 K390 A391 I392 M393 H394 H395 E396 G397 H398 M399 D400 L403 N404 Q409 H410 E411 E412 S413 R414 T415 V418
I419 R420 S421 T422 V423 F426 N427 R428 F429 I430 L433 D434 A435 L436 S437 K438 K439 A440 K441 A442 S443 T444 V445 D446 L456 Q457 D458 L459 Y462 F463 H464 P465 P466 L470 E471 H472 E473 D474 K475 Q476 N477 R478 L479 R480 N484 R485 Q486 I495 N496 L497 V498 D503
R504 L505 H506 V507 Y508 S509 S510 ALA ALA HIS PHE ALA ASP V517 A518 G519 R520 W526 K527 S532 L533 L536 N544 R545 K546 N547 C548 A549 Q550 D556 W557 L558 I559 S560 R561 R564 L565 E566 V578 L579 V580 P583 E584 A585 L586 N587 I588 I589 K590 E591 G592 H593
I594 S599 L600 L601 D602 K603 H604 G605 R606 N607 H608 L611 L614 L617 C620 H621 G622 V623 A624 V625 R626 Q629 H630 L631 I632 R647 L648 V649 V652 S653 S654 M655 R656 P657 N658 I659 G662 VAL SER GLU GLY SER ALA GLN TYR K671 K672 W673 Y674 Y675
M678 V679 D680 H681 T682 E683 A688 L693 R694 V695 G696 W697 A698 S699 T700 E701 G702 Y703 Y706 P707 G708 G709 G710 E711 E712 W713 G714 G715 N716 G717 V718 D721 L722 F723 S724 Y725 G726 F727 D728 G729 L730 H731 L732 W733 S734 G735 C736 I737 A738 R739 T740 V741 S742 H747 L748
D752 D753 V754 I755 S756 L759 D760 L761 P764 S765 I766 R769 I770 N771 P774 V775 Q776 G777 M778 F779 E780 N781 F782 N783 I784 P790 V791 V792 S793 F794 S795 A796 G797 I798 K799 V800 R801 F802 L803 L804 G805 GLY ARG HIS GLY E810 F811 K812 F813 P816 C822 Y823
E824 A825 P828 K831 L832 K833 V834 E835 H836 S837 R838 E839 Y840 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 L850 P853 T854 V855 S856 LEU THR GLN ALA A861 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 K884 E887 N888 I889 H890 E891 L892
W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 L937 K941 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 GLU GLU LYS VAL
LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 A994 M995 K998 L999 A1000 E1001 N1002 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL
LYS ASN R1027 L1032 Y1035 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 R1089 A1090
A1095 Y1096 K1097 A1098 G1099 R1100 W1101 Y1102 F1103 E1104 F1105 E1106 A1107 V1108 G1111 D1112 M1113 R1114 V1115 G1116 W1117 S1118 R1119 C1122 Q1123 P1124 D1125 L1128 G1129 E1132 R1133 A1136 F1137 F1140 K1141 A1142 Q1143 R1144 W1145 H1146 H1151 R1154 S1155 W1156 Q1157 A1158 G1159 D1160 V1161 V1162 G1163
V1166 D1167 M1168 T1169 E1170 H1171 T1172 M1173 M1174 F1175 T1176 L1177 N1178 G1179 E1180 D1184 S1188 A1191 F1192 K1193 D1194 F1195 D1199 G1200 F1201 I1202 C1205 S1206 L1207 G1208 V1209 A1210 Q1211 V1212 G1213 R1214 M1215 G1218 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235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Q2212 K2213 H2218 L2219 S2220 Y2221 L2222 L2223 E2224 N2225 S2226 S2227 R2236 A2244 A2245 A2246 S2247 V2248 N2251 L2254 A2255 L2256 A2257 L2258 D2262 L2263 E2264 V2267 R2268 G2274 LEU GLN SER CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 R2298 Y2299
D2116 T2117 I2118 L2124 I2127 R2128 M2135 G2136 E2139 E2140 R2141 L2142 D2149 N2153 K2154 Y2157 Q2158 H2159 P2160 M2163 M2168 H2169 E2170 M2173 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191 K2192 M2193 N2196 L2201 C2202 R2206 I2207 S2208 N2211
E2035 K2036 V2037 T2038 Y2039 L2040 LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 L2059 Q2060 Q2061 L2062 I2063 S2064 E2065 T2066 M2067 V2068 R2069 W2070 A2071 Q2072 V2075 I2076 E2077 E2080 F2086 H2090 R2091 D2094 A2102 K2105 I2109 N2110 S2113
PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU GLU GLU ILE R1994 D1995 Q1996 L1997 M2005 T2006 G2009 I2010 E2011 L2012 D2013 GLU ASP GLY SER LEU ASP GLY ASN S2022 D2023 L2024 T2025 I2026 R2029 S2032 L2033 V2034
GLU GLU SER LYS GLY GLY LYS LYS ARG PRO LYS GLU G1893 L1894 P1902 V1903 K1904 L1905 Q1906 L1910 L1911 Q1912 Y1913 L1914 C1915 D1916 R1920 D1931 V1934 A1935 K1936 L1937 Q1938 D1939 N1940 Q1941 R1942 V1948 MET GLN ALA LEU ASN MET SER ALA ALA THR ARG LEU LYS THR LYS GLU
V1810 F1816 L1817 F1818 V1819 P1820 L1821 I1822 R1823 L1824 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 H1835 L1843 Q1844 L1845 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU
I1726 T1733 K1734 T1737 L1738 D1741 GLU ASN LYS LYS HIS G1747 L1748 P1749 G1750 T1755 S1756 L1757 R1758 P1759 R1760 M1761 Q1762 F1763 S1764 S1767 F1768 V1769 S1770 I1771 E1774 C1775 Y1776 Q1777 Y1778 D1785 I1786 L1787 K1790 L1795 A1798 V1799 Q1800 E1801 L1804 H1805 A1806 R1807
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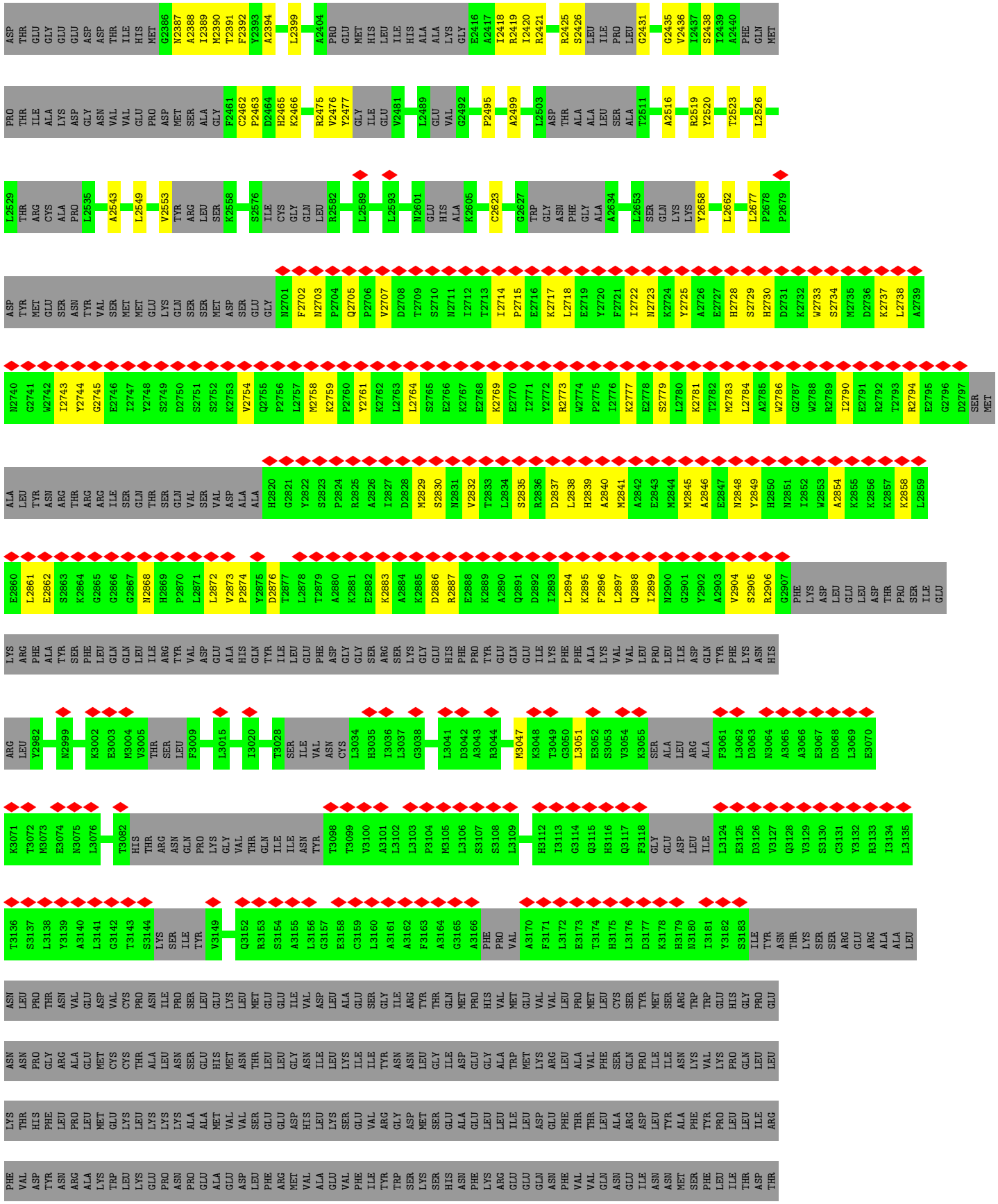
L1570 F1571 K1572 S1573 V1579 P1580 Q1581 C1582 P1583 P1584 R1585 L1586 H1587 V1588 Q1589 F1590 L1591 V1594 L1595 W1596 S1597 R1598 M1599 P1600 N1601 Q1602 K1605 V1606 D1607 R1610 E1613 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 F1627 M1628 S1629 L1630 E1634 E1635 N1636 R1637 S1638 V1639 D1640 I1641 L1642
ARG ASN ASN N1503 G1504 E1505 E1506 I1507 G1508 C1509 V1510 V1511 ASP ALA ALA SER G1516 L1517 L1518 T1519 F1520 N1523 L1527 Y1531 Q1532 V1533 E1534 P1535 L1539 V1543 F1544 A1545 Q1546 A1547 T1548 S1549 P1550 M1551 V1552 F1555 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569
S1429 V1430 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 I1446 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 L1469 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY
GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU GLY LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS ASN HIS SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP HIS GLY HIS LEU VAL PRO ASP ARG ASP TYR ASP TYR LEU MET GLN THR SER T1425 Y1426 Y1427 Y1428
E1309 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY ILE PRO GLY GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO
Y1236 E1237 P1238 F1239 A1240 V1241 N1242 T1243 N1244 M1249 W1250 K1253 P1256 Q1257 F1258 L1259 Q1260 V1261 H1265 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER SER PRO CYS LEU LYS V1285 K1288 S1289 F1290 G1291 S1292 D1298 I1299 M1300 F1301 Y1302 R1303 L1304 S1305 M1306 P1307 I1308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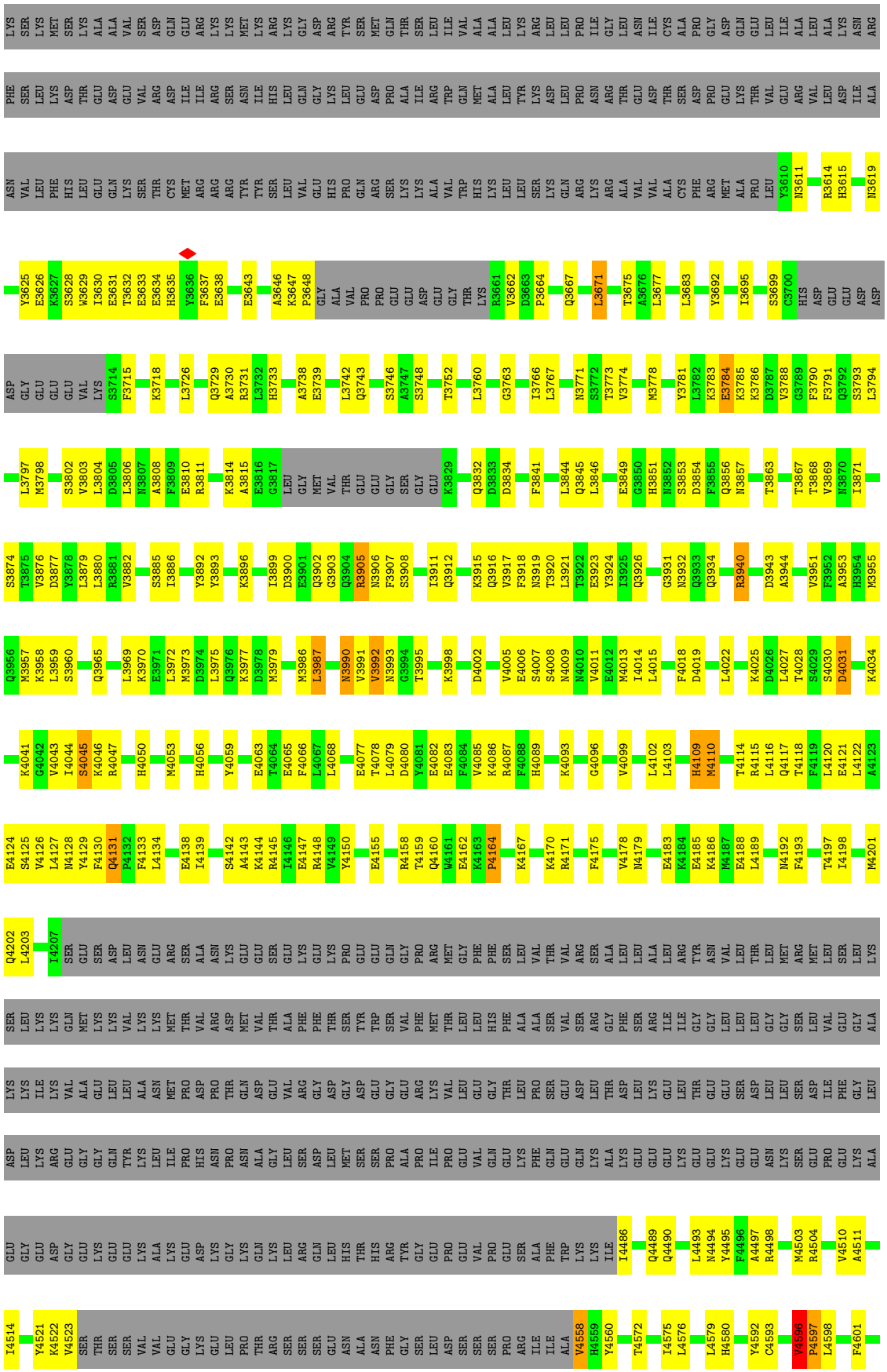
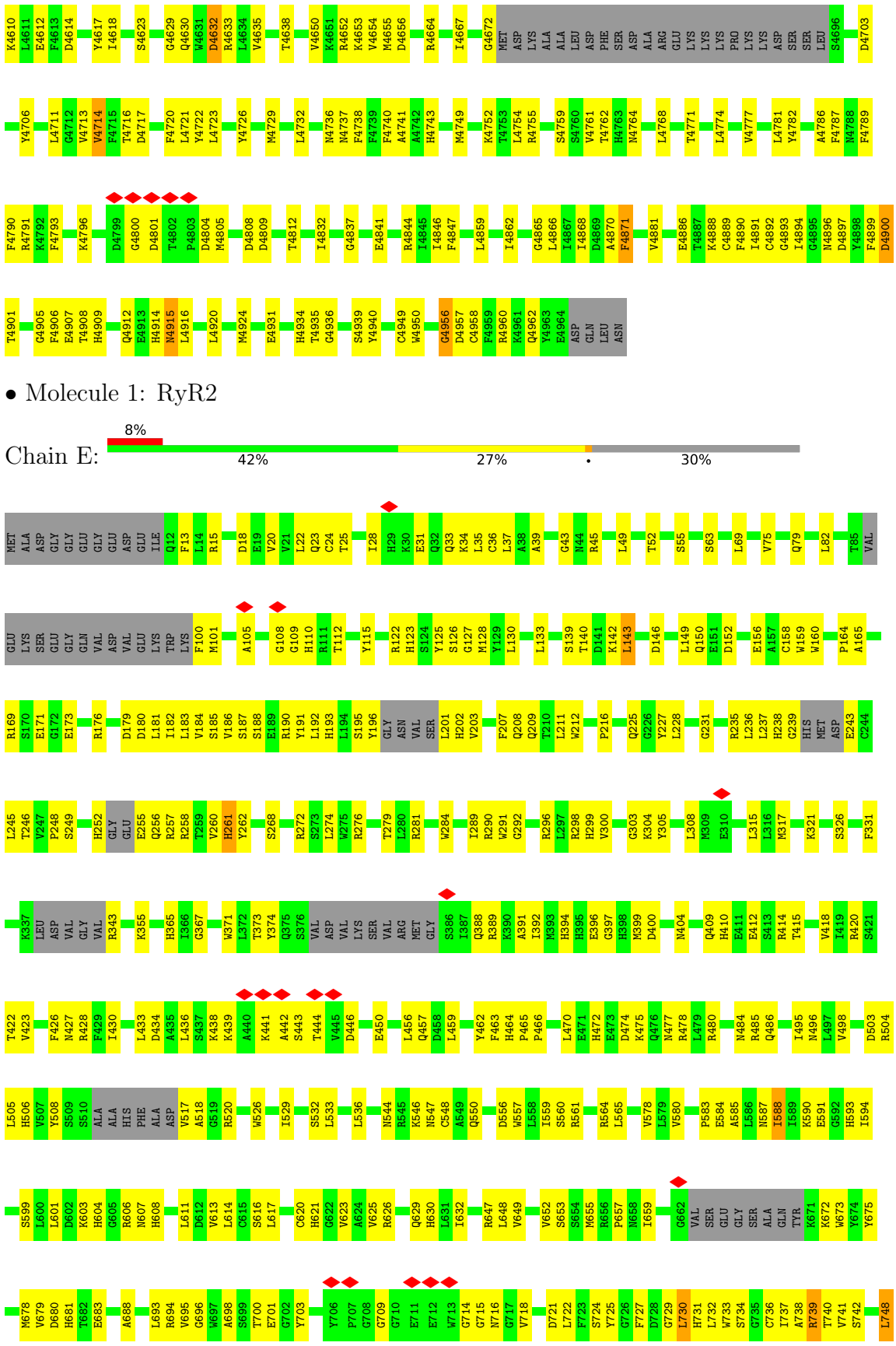
PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 C2462 P2463 D2464 H2465 K2466 R2475 V2476 Y2477 GLY ILE GLU V2481 L2489 GLU VAL G2492 P2495 A2499 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2516 R2519 Y2520 T2523 L2526
L2529 THR ARG CYS ALA PRO L2535 A2543 L2549 V2553 TYR ARG LEU SER K2558 S2576 ILE CYS GLY GLN LEU R2582 L2589 L2593 N2601 GLU HIS ALA K2605 C2623 G2627 TRP GLY ASN PHE GLY ALA A2634 L2653 SER GLN LYS LYS Y2658 L2662 L2677 P2678 P2679
ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728 S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739
N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788 R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET
ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859
E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU
LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS
ARG LEU Y2982 N2999 K3002 E3003 M3004 V3005 THR SER LEU F3009 L3015 I3020 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 G3038 L3041 D3042 A3043 R3044 M3047 K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070
K3071 T3072 M3073 E3074 N3075 L3076 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135
T3136 S3137 L3138 Y3139 A3140 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 Q3152 R3153 S3154 A3155 L3156 G3157 E3158 C3159 L3160 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 I3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU
ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU
ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE ILE LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU
LYS THR HIS PHE LEU PRO LEU MET GLU LYS LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLY ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG
PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR





- Molecule 1: RyR2

Chain E:

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C822 Y823 E824 A825 P828 K831 L832 K833 V834 E835 H836 S837 R838 E839 Y840 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 L850 P853 T854 V855 S856 LEU THR GLN ALA A861 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 K884 E887 N888 I889 H890
E891 L892 W893 V894 H895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 I918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 L937 K941 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 GLU GLU
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ASP VAL LYS ASN R1027 L1032 Y1035 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086
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THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ARG TYR LEU MET GLN THR SER T1425
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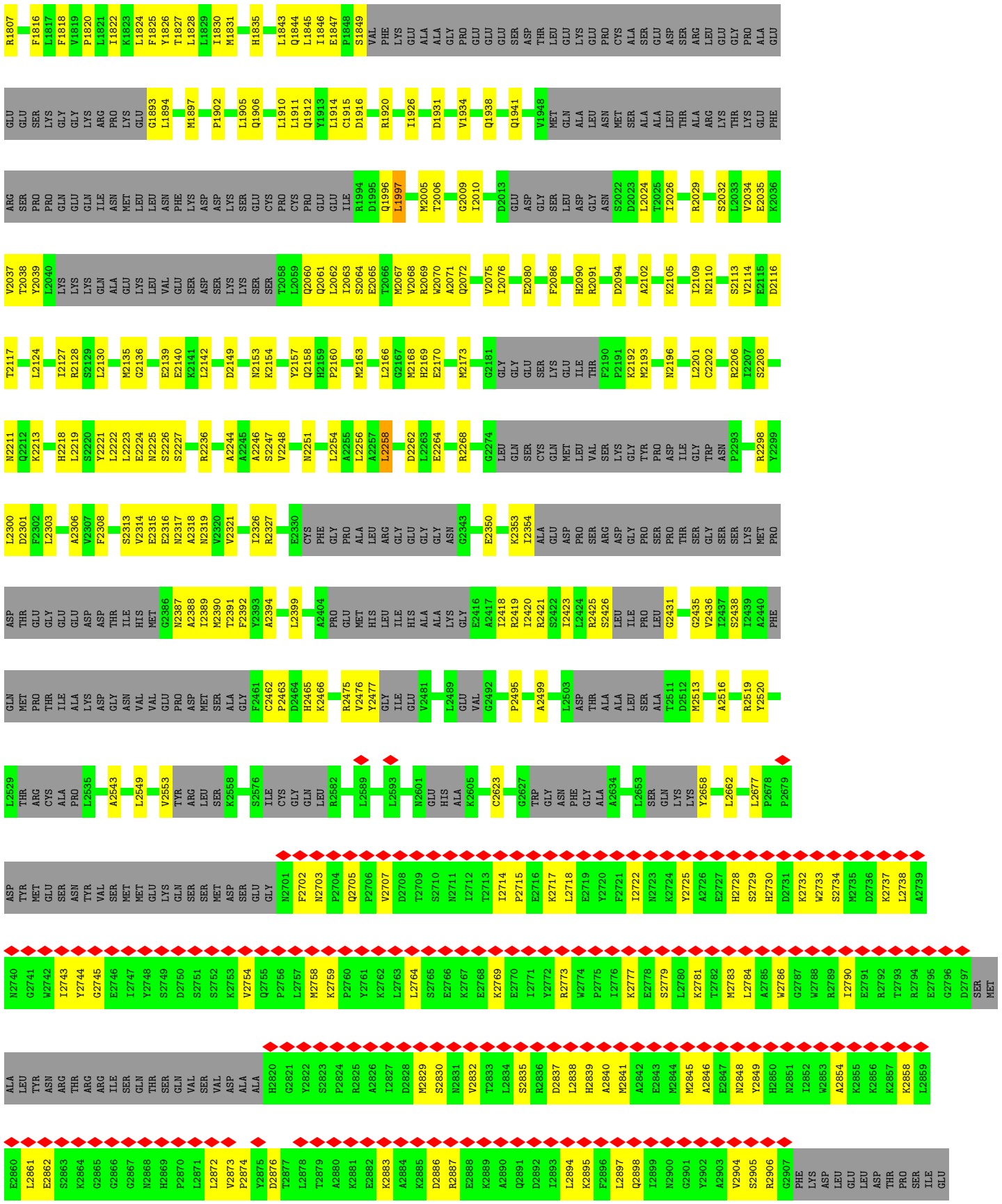
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V2037 T2038 Y2039 L2040 LYS LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP ASP SER LYS LYS SER SER T2058 L2059 Q2060 Q2061 L2062 I2063 S2064 E2065 T2066 M2067 V2068 R2069 W2070 A2071 Q2072 V2075 I2076 E2080 F2086 H2090 R2091 D2094 A2102 K2105 I2109 N2110 S2113 V2114 E2115 D2116
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ASP THR GLU GLY GLU GLU ASP ASP THR ILE ILE HIS MET G2386 N2387 A2388 I2389 M2390 T2391 F2392 Y2393 A2394 L2399 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 A2417 I2418 R2419 I2420 R2421 S2422 I2423 L2424 R2425 S2426 LEU ILE PRO LEU G2431 G2435 Y2436 I2437 S2438 I2439 A2440 PHE
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ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859
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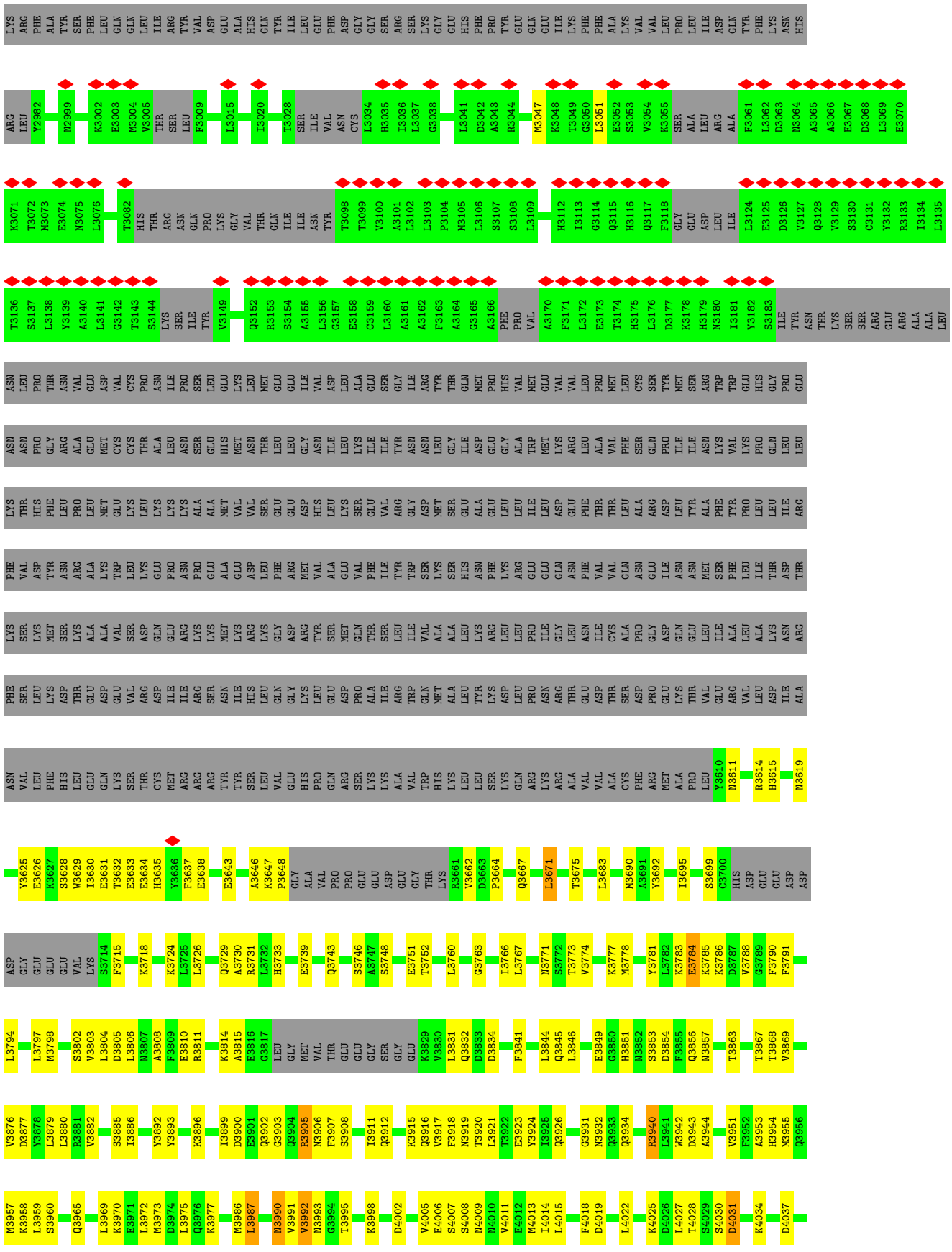
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ARG LEU Y2982 N2999 K3002 E3003 M3004 V3005 THR SER LEU F3009 L3015 I3020 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 G3038 L3041 D3042 A3043 R3044 M3047 K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070
K3071 T3072 M3073 E3074 M3075 L3076 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135
T3136 S3137 L3138 Y3139 A3140 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 Q3152 R3153 S3154 A3155 L3156 G3157 E3158 C3159 L3160 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU
ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU
ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU
LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG
PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR
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ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL PRO LEU Y3610 N3611 R3614 H3615 N3619
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ASP GLY GLU GLU GLU VAL LYS S3714 F3715 K3718 K3724 L3725 L3726 Q3729 A3730 R3731 L3732 H3733 E3739 Q3743 S3746 A3747 S3748 E3751 T3752 L3760 G3763 I3766 L3767 N3771 S3772 T3773 V3774 K3777 M3778 Y3781 L3782 K3783 E3784 K3785 K3786 D3787 V3788 G3789 F3790 F3791
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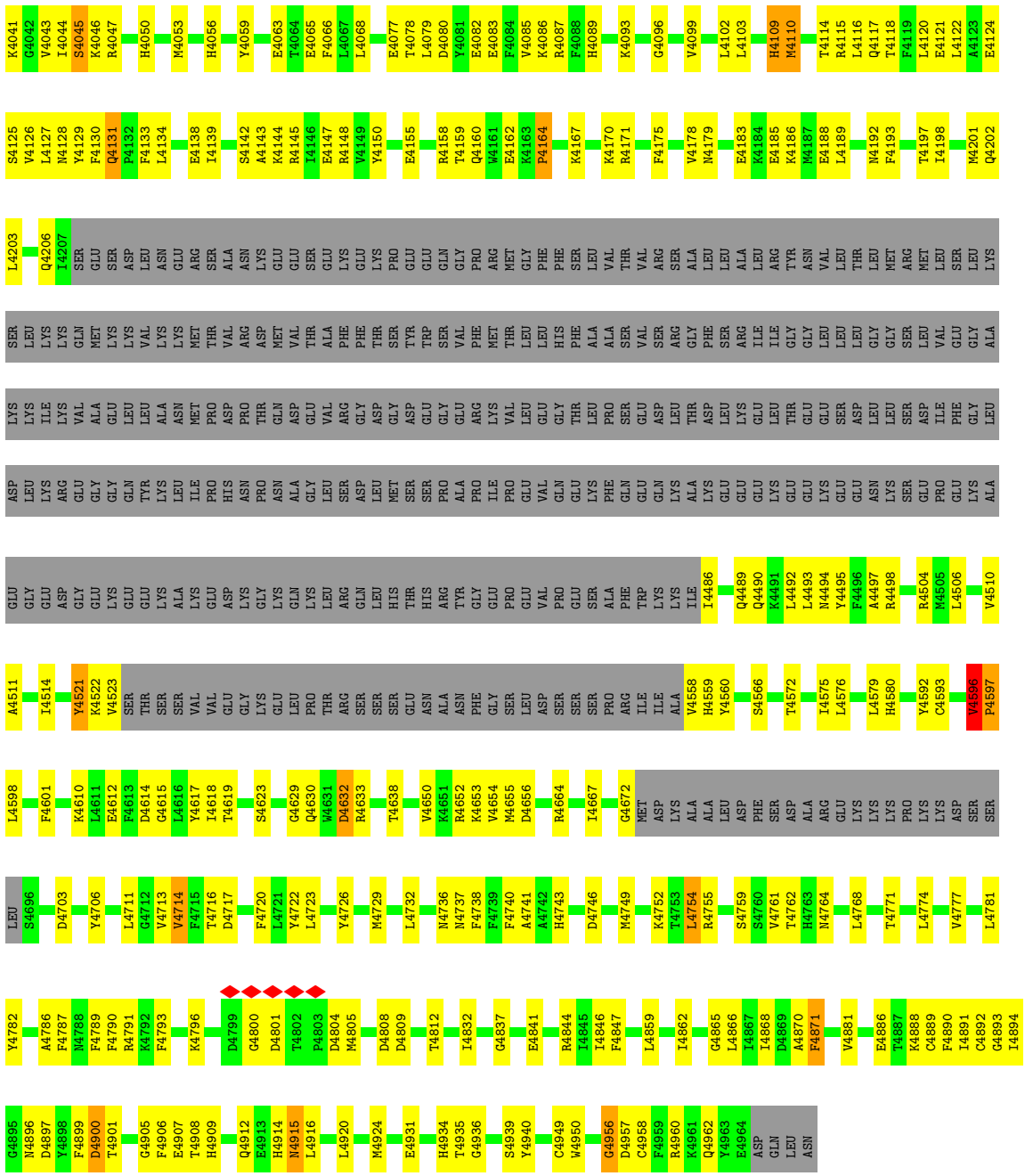

- Molecule 1: RyR2

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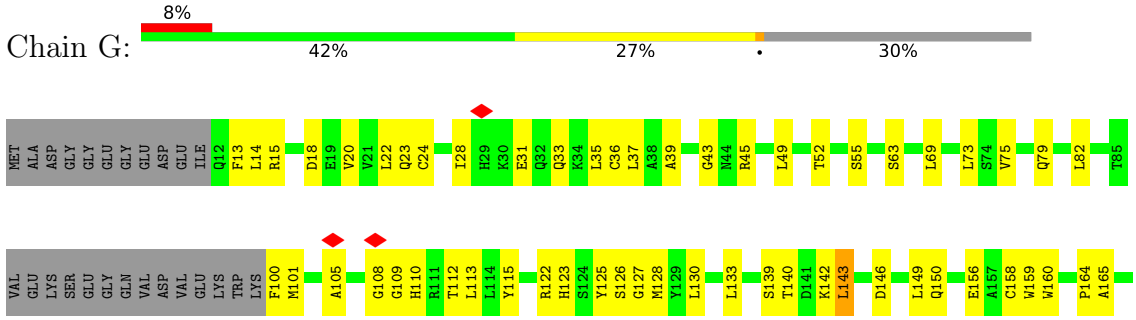

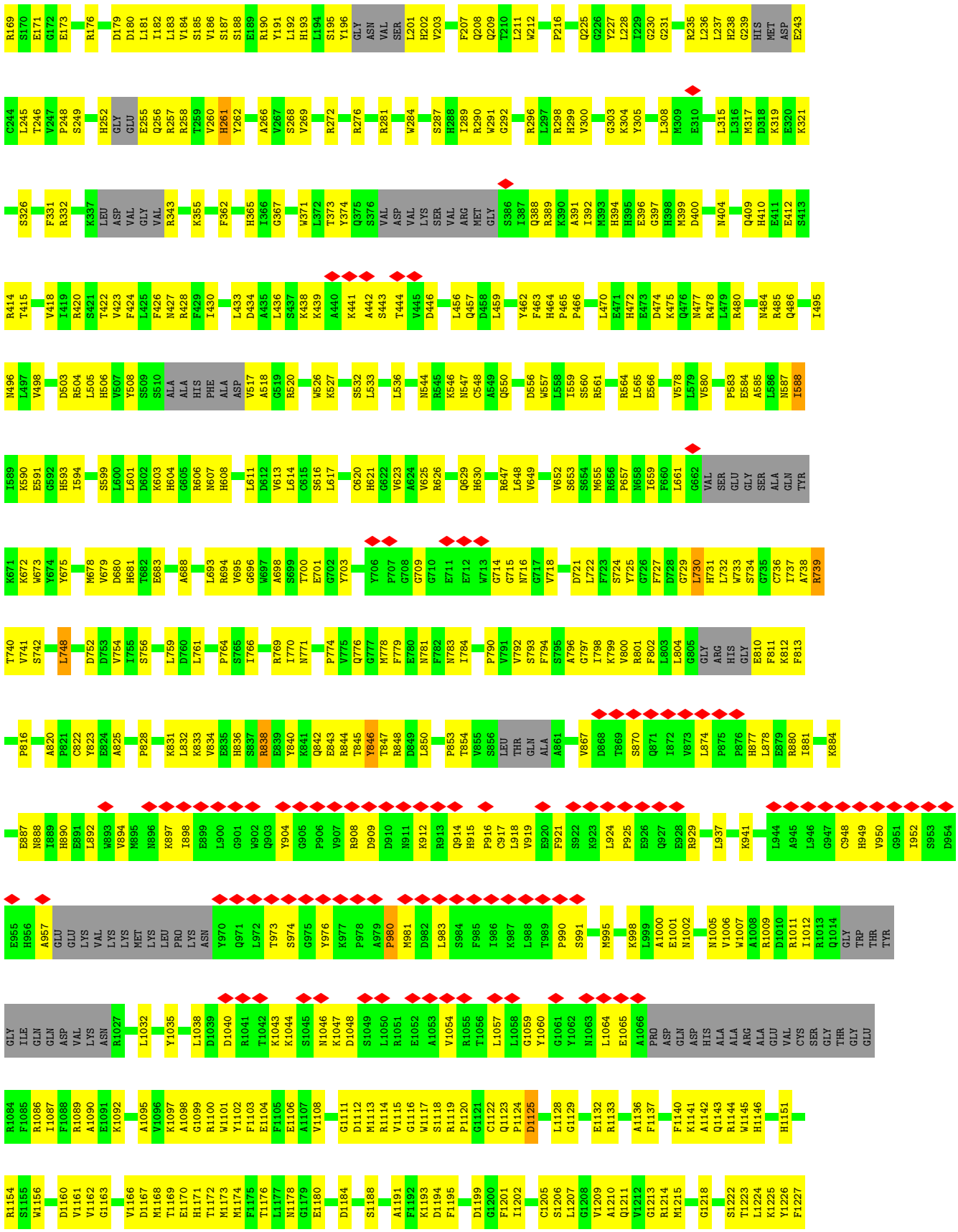
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R1084 F1085 R1086 I1087 F1088 R1089 A1090 E1091 K1092 A1095 Y1096 K1097 A1098 G1099 R1100 W1101 Y1102 F1103 E1104 F1105 E1106 A1107 V1108 G1111 D1112 M1113 R1114 V1115 G1116 W1117 S1118 R1119 P1120 G1121 C1122 Q1123 P1124 D1125 L1128 G1129 E1132 R1133 A1136 F1137 F1140 K1141 A1142 Q1143 R1144 W1145 H1146 H1151
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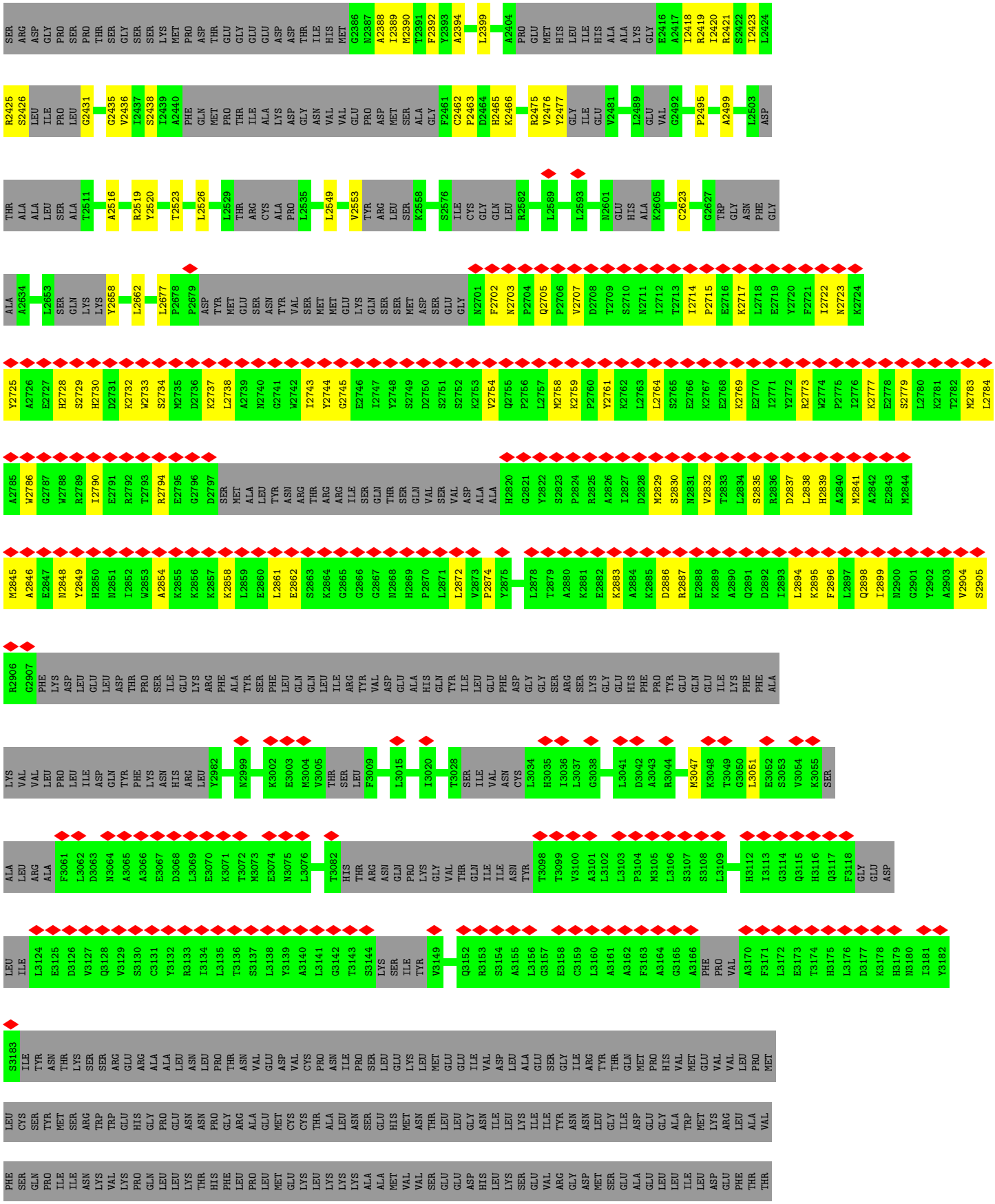
VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 R2298 Y2299 L2300 D2301 F2302 L2303 A2306 V2307 F2308 S2313 V2314 E2315 E2316 N2317 A2318 N2319 V2320 V2321 I2326 R2327 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 E2350 K2353 I2354 ALA GLU ASP PRO
K2192 M2193 N2196 L2201 C2202 R2206 I2207 S2208 N2211 Q2212 K2213 H2218 L2219 S2220 Y2221 L2222 L2223 E2224 N2225 S2226 S2227 R2236 A2244 A2245 A2246 S2247 V2248 N2251 L2254 A2255 L2256 A2257 L2258 D2262 L2263 E2264 V2267 R2268 Y2269 L2270 G2274 LEU GLN SER CYS GLN MET LEU
R2091 D2094 A2102 K2105 I2109 N2110 S2113 D2116 L2124 I2127 R2128 S2129 L2130 M2135 G2136 E2139 L2142 D2149 N2153 K2154 Y2157 Q2158 H2159 P2160 M2163 L2166 G2167 M2168 H2169 E2170 M2173 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191
S2022 D2023 L2024 T2025 I2026 R2029 S2032 L2033 V2034 E2035 K2036 V2037 T2038 Y2039 L2040 LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS SER GLU CYS PRO CYS PRO GLU GLU ILE R1994 D1995 Q1996 L1997 M2005 T2006 G2009 I2010 D2013 GLU ASP GLY SER LEU ASP GLY ASN
MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU GLU GLU ILE R1920 I1926 D1931 V1934 A1935 K1936 L1937 Q1938 D1939 N1940 Q1941 R1942 V1948 MET GLN ALA LEU ASN
SER ARG LEU GLU GLY PRO ALA GLU GLU SER LYS GLY GLY LYS GLU GLN G1893 L1894 M1897 P1902 L1905 Q1906 L1909 L1910 L1911 Q1912 Y1913 L1914 C1915 D1916 A1798 V1799 Q1800 E1801 L1804 H1805 A1806 R1807 F1816 L1817 F1818 V1819 P1820 L1821 I1822 K1823 L1824 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 H1835 L1843 Q1844 L1845 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP
H1710 L1711 T1716 A1717 R1718 L1719 N1722 I1726 T1733 K1734 T1737 L1738 D1741 GLU ASN LYS LYS HIS G1747 L1748 P1749 G1750 L1753 S1754 T1755 S1756 L1757 R1758 P1759 R1760 M1761 Q1762 F1763 S1764 S1767 F1768 V1769 S1770 I1771 N1772 N1773 E1774 Q1777 Y1778 D1785 I1786 L1787 L1795
S1629 L1630 E1634 E1635 N1636 R1637 D1640 I1641 L1642 E1643 L1644 T1645 E1646 Q1647 L1651 K1652 F1653 H1654 T1657 L1658 R1659 L1660 V1664 N1669 H1670 R1671 V1672 A1673 H1674 A1675 L1676 C1677 V1680 Q1684 L1685 L1686 I1689 P1695 R1699 A1700 G1701 Y1702 Y1703 D1704 L1705 L1706 I1707 D1708 I1709
ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 F1571 K1572 S1573 K1576 V1579 P1580 Q1581 C1582 P1583 P1584 R1585 L1586 H1587 V1588 Q1589 F1590 L1591 V1594 L1595 W1596 S1597 R1598 M1599 P1600 N1601 Q1602 K1605 V1606 D1607 R1610 E1613 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 F1627 M1628
SER MET SER PRO GLY GLN GLY ARG ASN ASN N1503 G1504 L1505 E1506 I1507 G1508 C1509 V1510 V1511 ASP ALA ALA SER G1516 L1517 L1518 T1519 F1520 T1521 A1522 N1523 G1524 K1525 D1526 L1527 Y1531 Q1532 V1533 E1534 P1535 L1539 V1543 F1544 A1545 Q1546 A1547 T1548 S1549 P1550 N1551 V1552 F1555 E1556 LEU GLY ARG
MET GLN THR SER T1425 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 L1469 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU
LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU
F1301 Y1302 R1303 L1304 S1305 M1306 P1307 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP
T1228 I1229 C1230 G1231 L1232 Q1233 E1234 G1235 Y1236 E1237 P1238 F1239 A1240 V1241 N1242 T1243 N1244 M1249 W1250 K1253 P1256 Q1257 F1258 L1259 Q1260 V1261 H1265 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 K1288 S1289 F1290 G1291 S1292 D1298 I1299 M1300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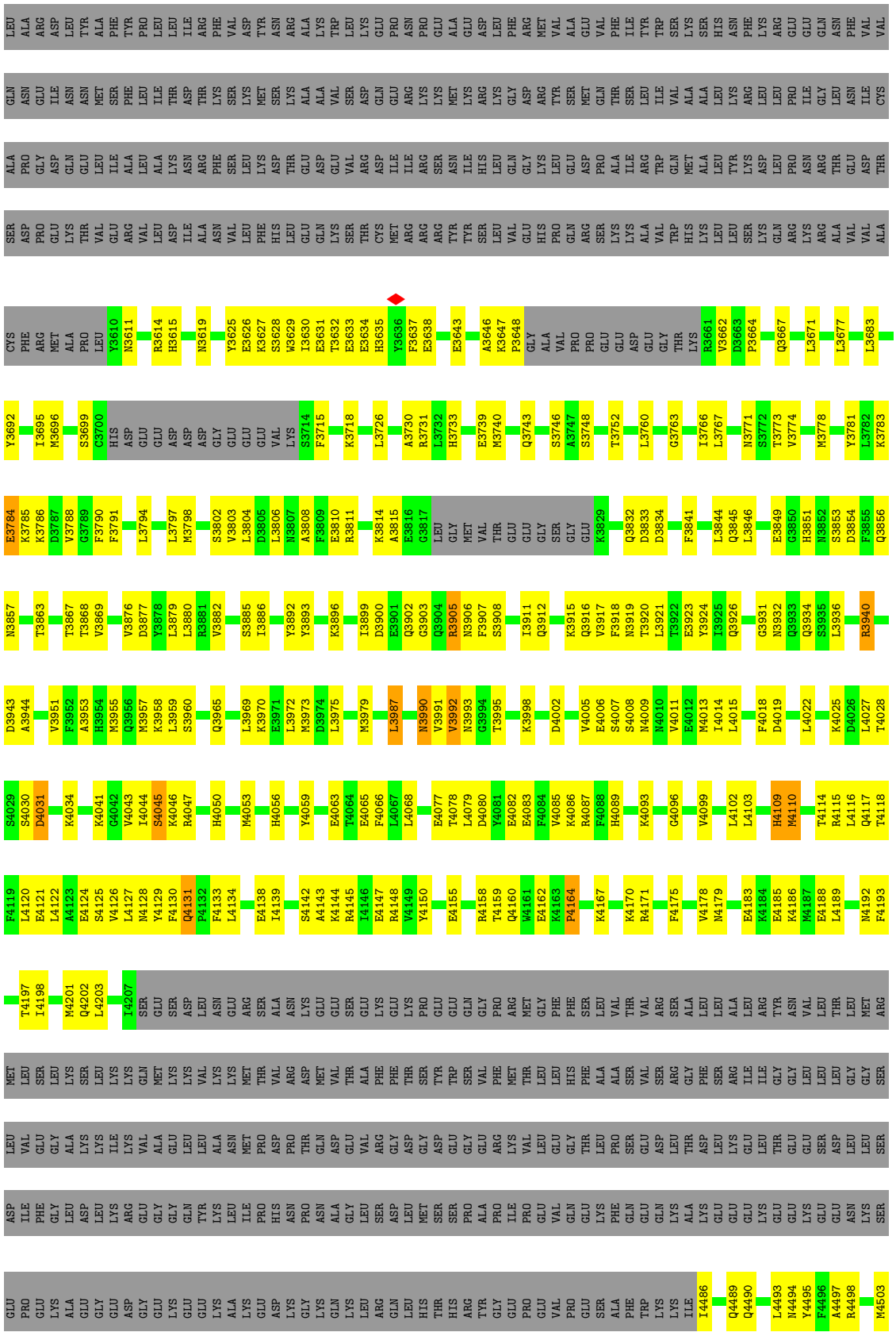
R2425 S2426 LEU ILE PRO LEU G2431 G2435 V2436 I2437 S2438 I2439 A2440 PHE GLN MET MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 C2462 P2463 D2464 H2465 K2466 R2475 V2476 Y2477 GLY ILE GLU V2481 L2489 GLU VAL G2492 P2495 A2499 L2503 ASP
THR ALA ALA LEU SER ALA T2511 A2516 R2519 Y2520 T2523 L2526 L2529 THR ARG CYS ALA PRO L2535 L2549 V2553 TYR ARG LEU SER K2558 S2576 ILE CYS GLY GLN LEU R2582 L2589 L2593 N2601 GLU HIS ALA K2605 C2623 G2627 TRP GLY ASN PHE GLY
ALA A2634 L2653 SER GLN LYS LYS Y2658 L2662 L2677 P2678 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724
Y2725 A2726 E2727 H2728 S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784
A2785 W2786 G2787 W2788 R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844
M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905
R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA
LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 N2999 K3002 E3003 M3004 V3005 THR SER LEU F3009 L3015 I3020 T3028 SER ILE ILE VAL ASN CYS L3034 H3035 I3036 L3037 G3038 L3041 D3042 A3043 R3044 M3047 K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER
ALA LEU ARG ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070 K3071 T3072 M3073 E3074 M3075 L3076 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP
LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135 T3136 S3137 L3138 Y3139 A3140 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 Q3152 R3153 S3154 A3155 L3156 G3157 E3158 C3159 L3160 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182
S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET
LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL
PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR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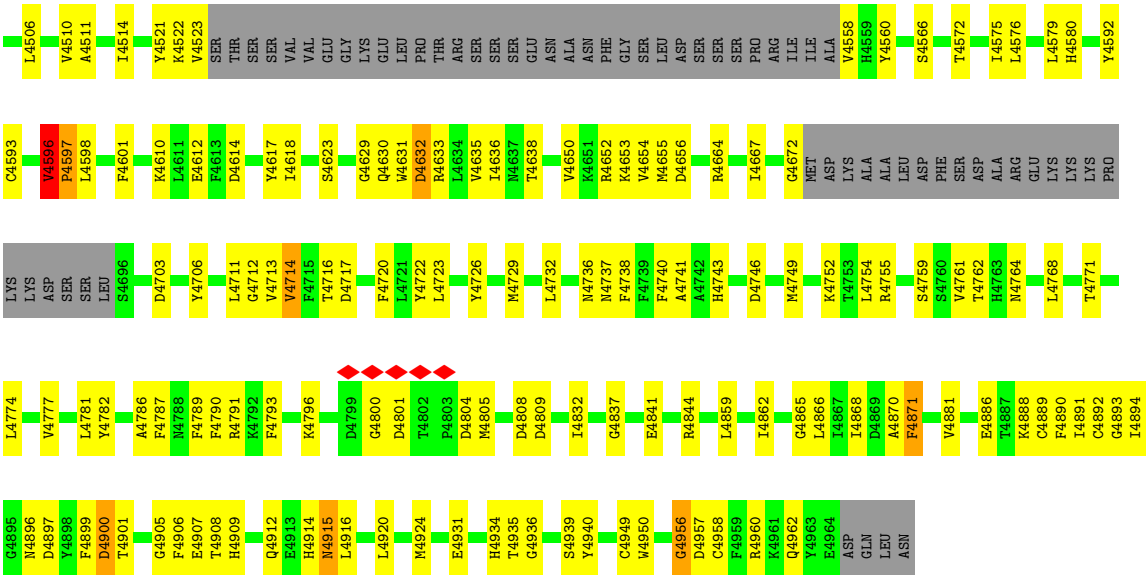
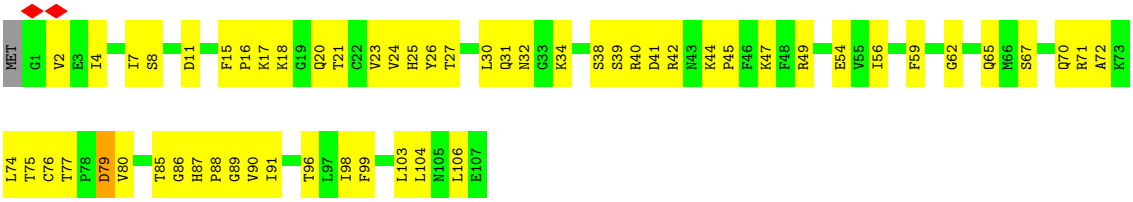
GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS ASP ARG TYR SER VAL GLN GLY ARG LEU LYS ASP LEU PRO ILE GLY LEU ASN ARG THR GLU ASP THR CYS
ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG ARG THR GLU ASP THR
SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA
CYS PHE ARG MET ALA PRO LEU Y3610 N3611 R3614 H3615 N3619 Y3625 E3626 K3627 S3628 W3629 I3630 E3631 T3632 E3633 E3634 H3635 Y3636 F3637 E3638 E3643 A3646 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 P3664 Q3667 L3671 L3677 L3683
Y3692 I3695 M3696 S3699 C3700 HIS ASP GLU GLU GLU ASP ASP GLY GLU GLU GLU VAL LYS S3714 F3715 K3718 L3726 A3730 R3731 L3732 H3733 E3739 M3740 Q3743 S3746 A3747 S3748 T3752 L3760 G3763 I3766 L3767 N3771 S3772 T3773 V3774 M3778 Y3781 L3782 K3783
E3784 K3785 K3786 D3787 V3788 G3789 F3790 F3791 L3794 L3797 M3798 S3802 V3803 L3804 D3805 L3806 N3807 A3808 F3809 E3810 R3811 K3814 A3815 E3816 G3817 LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU K3829 Q3832 D3833 D3834 F3841 L3844 Q3845 L3846 E3849 G3850 H3851 N3852 S3853 D3854 F3855 Q3856
N3857 T3863 T3867 T3868 V3869 V3876 D3877 Y3878 L3879 L3880 R3881 V3882 S3885 I3886 Y3892 Y3893 K3896 I3899 D3900 E3901 Q3902 G3903 Q3904 R3905 N3906 F3907 S3908 I3911 Q3912 K3915 Q3916 V3917 F3918 N3919 T3920 L3921 T3922 E3923 Y3924 I3925 Q3926 G3931 N3932 Q3933 Q3934 S3935 L3936 R3940
D3943 A3944 V3951 F3952 A3953 H3954 M3955 Q3956 M3957 K3958 L3959 S3960 Q3965 L3969 K3970 E3971 L3972 M3973 D3974 L3975 M3979 L3987 N3990 V3991 V3992 N3993 G3994 T3995 K3998 D4002 V4005 Q4006 E4006 S4007 S4008 N4009 N4010 V4011 E4012 M4013 I4014 L4015 F4018 D4019 L4022 K4025 D4026 L4027 T4028
S4029 S4030 D4031 K4034 K4041 G4042 V4043 I4044 S4045 K4046 R4047 H4050 M4053 H4056 Y4059 E4063 T4064 E4065 F4066 L4067 L4068 E4077 T4078 L4079 D4080 Y4081 E4082 E4083 F4084 V4085 K4086 R4087 F4088 H4089 K4093 G4096 V4099 L4102 L4103 H4109 M4110 T4114 R4115 L4116 Q4117 T4118
F4119 L4120 E4121 L4122 A4123 E4124 S4125 V4126 L4127 N4128 Y4129 F4130 Q4131 P4132 F4133 L4134 E4138 I4139 S4142 A4143 K4144 R4145 I4146 E4147 R4148 V4149 Y4150 E4155 R4158 T4159 Q4160 W4161 E4162 K4163 P4164 K4167 K4170 R4171 F4175 V4178 N4179 E4183 K4184 E4185 K4186 M4187 E4188 L4189 N4192 F4193
T4197 I4198 M4201 Q4202 L4203 I4207 SER GLU SER ASP ALA ASN LYS GLU GLU SER GLU LYS GLU LYS PRO GLU GLU GLN GLY PRO ARG MET GLY PHE PHE SER LEU VAL THR VAL ARG SER ALA LEU LEU ALA LEU ARG TYR ASN VAL LEU LEU THR LEU MET ARG
MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS LYS VAL LYS LYS MET THR VAL ARG ASP MET VAL ALA THR ALA PHE PHE THR SER TYR TRP SER VAL PHE MET THR LEU LEU HIS PHE LEU ALA ALA SER VAL SER ARG GLY PHE SER ARG ILE ILE GLY GLY LEU LEU LEU LEU GLY SER
LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LYS ALA ASN MET PRO ASP PRO THR GLN ASP ALA GLU VAL ARG GLY ASP GLY ASP GLY GLU GLU ASP LEU THR ASP LEU LYS GLU LYS LEU LYS GLU GLU LEU THR LYS THR GLU GLU LEU LEU LEU ASP LEU THR GLU GLU SER ASP LEU LEU SER
ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLU GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER SER PRO ALA PRO ILE PRO GLU VAL GLN GLU GLN LYS LYS ALA LYS GLU GLU LYS PHE GLN GLU GLN LYS SER
GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU GLU LYS LYS GLU LYS GLY LYS LYS GLU GLU LYS LYS GLU ASP LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU GLU PRO GLU VAL PRO GLU SER ALA PHE TRP LYS LYS ILE I4486 Q4489 Q4490 L4493 N4494 Y4495 F4496 A4497 R4498 M4503



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:

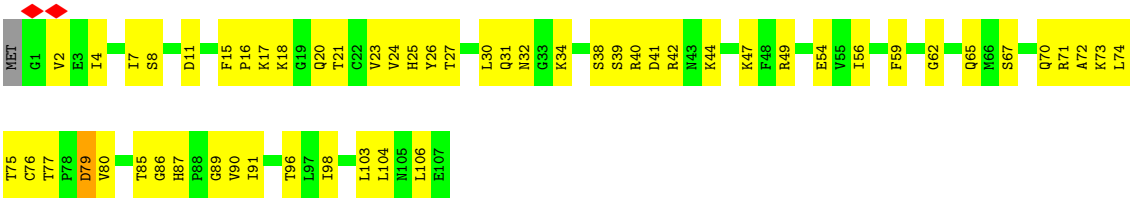


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:

- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

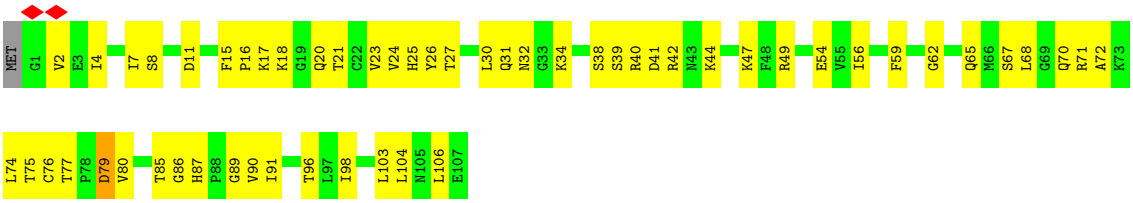
Chain F:



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:

48%
50%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L74 T75 C76 T77 P78 D79 V80 T85 G86 H87 P88 G89 V90 I91 T96 L97 I98 L103 L104 N105 L106 E107

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77339	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CFF, 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	0.50	0/27032	0.71	12/36559 (0.0%)
1	C	0.50	0/27032	0.71	12/36559 (0.0%)
1	E	0.50	0/27032	0.71	12/36559 (0.0%)
1	G	0.50	0/27032	0.71	12/36559 (0.0%)
2	B	0.47	0/835	0.64	1/1123 (0.1%)
2	D	0.47	0/835	0.64	1/1123 (0.1%)
2	F	0.47	0/835	0.64	1/1123 (0.1%)
2	H	0.47	0/835	0.64	1/1123 (0.1%)
All	All	0.50	0/111468	0.71	52/150728 (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
1	A	0	33
1	C	0	33
1	E	0	33
1	G	0	33
All	All	0	132

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2039	TYR	N-CA-C	9.27	123.96	112.47
1	E	2039	TYR	N-CA-C	9.26	123.95	112.47
1	G	2039	TYR	N-CA-C	9.23	123.92	112.47
1	C	2039	TYR	N-CA-C	9.21	123.90	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	139	SER	CA-C-N	7.37	134.96	121.70

There are no chirality outliers.

5 of 132 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Peptide
1	A	142	LYS	Peptide
1	A	588	ILE	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	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	26537	0	25033	1033	0
1	C	26537	0	25033	1044	0
1	E	26537	0	25033	1045	0
1	G	26537	0	25033	1042	0
2	B	819	0	824	44	0
2	D	819	0	824	43	0
2	F	819	0	824	44	0
2	H	819	0	824	43	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	14	0	10	0	0
5	C	14	0	10	0	0
5	E	14	0	10	0	0
5	G	14	0	10	0	0
All	All	109488	0	103468	4127	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 19.

The worst 5 of 4127 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:4522:LYS:O	1:C:4560:TYR:HB3	1.25	1.36
1:G:4522:LYS:O	1:G:4560:TYR:HB3	1.30	1.30
1:C:4808:ASP:CB	1:E:4523:VAL:HG11	1.65	1.25
1:G:4522:LYS:CB	1:G:4560:TYR:HD2	1.50	1.22
1:E:4522:LYS:CB	1:E:4560:TYR:HD2	1.56	1.19

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	3356/4968 (68%)	2877 (86%)	469 (14%)	10 (0%)	36	71
1	C	3356/4968 (68%)	2877 (86%)	469 (14%)	10 (0%)	36	71
1	E	3356/4968 (68%)	2876 (86%)	470 (14%)	10 (0%)	36	71
1	G	3356/4968 (68%)	2879 (86%)	467 (14%)	10 (0%)	36	71
2	B	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
All	All	13844/20304 (68%)	11884 (86%)	1920 (14%)	40 (0%)	37	71

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1477	HIS

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Mol	Chain	Res	Type
1	C	1477	HIS
1	E	1477	HIS
1	G	1477	HIS
1	A	730	LEU

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	2673/4355 (61%)	2632 (98%)	41 (2%)	57	70
1	C	2672/4355 (61%)	2632 (98%)	40 (2%)	57	70
1	E	2672/4355 (61%)	2633 (98%)	39 (2%)	57	70
1	G	2671/4355 (61%)	2632 (98%)	39 (2%)	57	70
2	B	88/89 (99%)	86 (98%)	2 (2%)	44	63
2	D	88/89 (99%)	86 (98%)	2 (2%)	44	63
2	F	88/89 (99%)	86 (98%)	2 (2%)	44	63
2	H	88/89 (99%)	86 (98%)	2 (2%)	44	63
All	All	11040/17776 (62%)	10873 (98%)	167 (2%)	55	70

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4521	TYR
1	G	3905	ARG
1	E	4754	LEU
1	G	625	VAL
1	G	4044	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 217 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	394	HIS

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Mol	Chain	Res	Type
1	E	2740	ASN
1	G	3611	ASN
1	E	547	ASN
1	E	1265	HIS

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CFF	A	6002	-	15,15,15	2.25	8 (53%)	23,23,23	2.83	9 (39%)
5	CFF	E	6002	-	15,15,15	2.25	8 (53%)	23,23,23	2.82	9 (39%)
5	CFF	C	6002	-	15,15,15	2.25	8 (53%)	23,23,23	2.83	9 (39%)
5	CFF	G	6002	-	15,15,15	2.25	8 (53%)	23,23,23	2.83	9 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CFF	A	6002	-	-	-	0/2/2/2
5	CFF	E	6002	-	-	-	0/2/2/2
5	CFF	C	6002	-	-	-	0/2/2/2
5	CFF	G	6002	-	-	-	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	6002	CFF	C6-N1	-4.37	1.31	1.40
5	A	6002	CFF	C6-N1	-4.37	1.31	1.40
5	E	6002	CFF	C6-N1	-4.37	1.31	1.40
5	C	6002	CFF	C6-N1	-4.34	1.31	1.40
5	G	6002	CFF	C4-N3	-3.29	1.32	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	6002	CFF	C14-N7-C8	-7.86	111.57	126.28
5	C	6002	CFF	C14-N7-C8	-7.86	111.57	126.28
5	E	6002	CFF	C14-N7-C8	-7.86	111.57	126.28
5	G	6002	CFF	C14-N7-C8	-7.86	111.57	126.28
5	E	6002	CFF	C14-N7-C5	5.33	140.45	127.77

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.

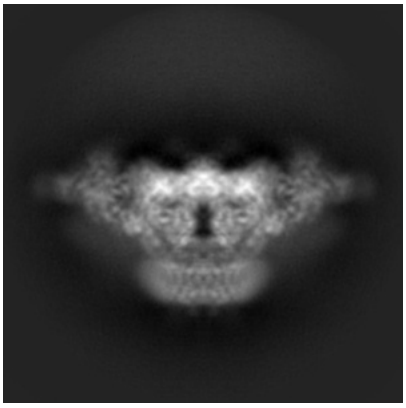
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9826. These allow visual inspection of the internal detail of the map and identification of artifacts.

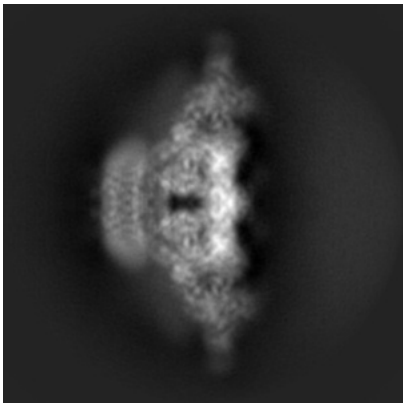
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

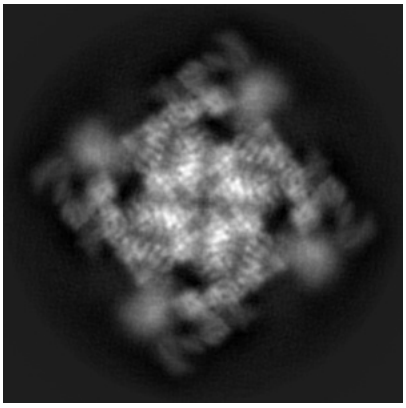
6.1.1 Primary map



X



Y

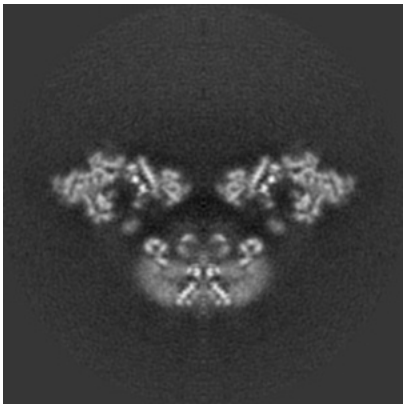


Z

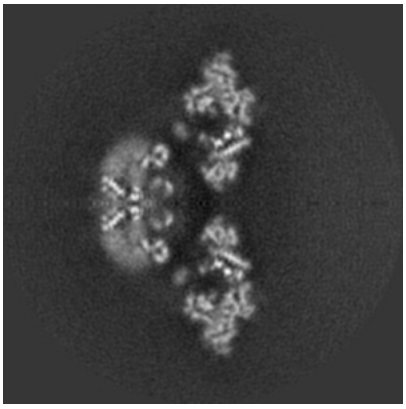
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

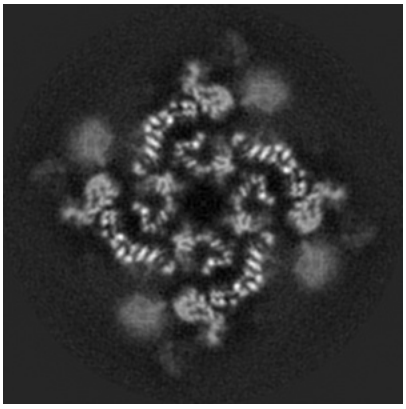
6.2.1 Primary map



X Index: 200



Y Index: 200

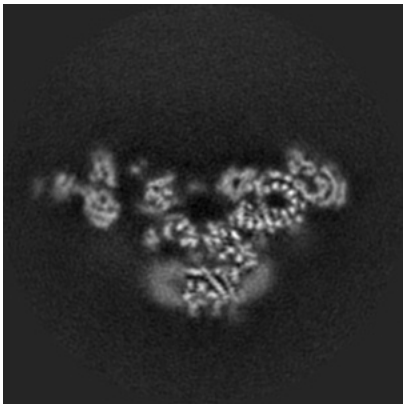


Z Index: 200

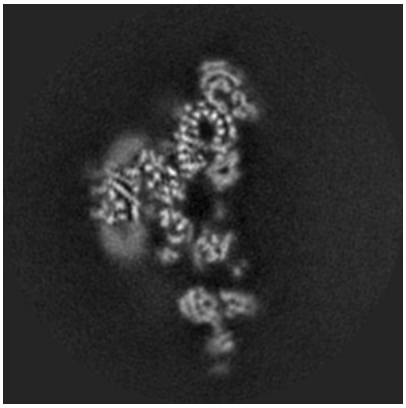
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

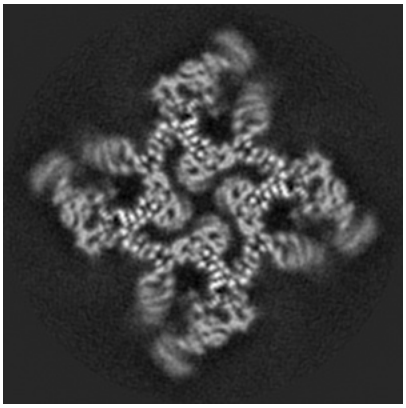
6.3.1 Primary map



X Index: 187



Y Index: 213

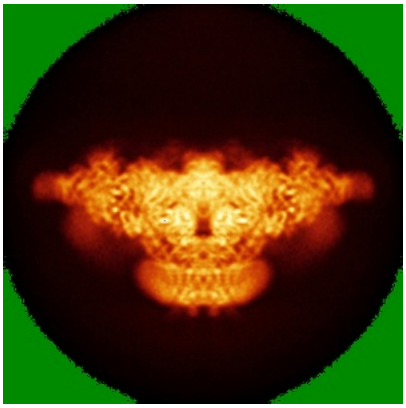


Z Index: 217

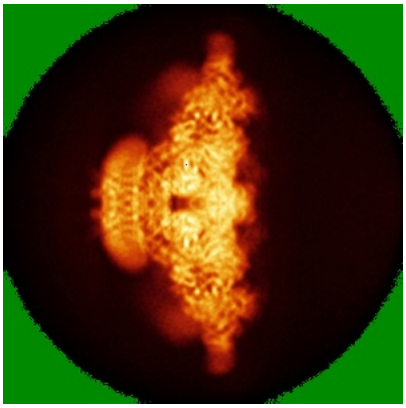
The images above show the largest variance slices of the map in three orthogonal directions.

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

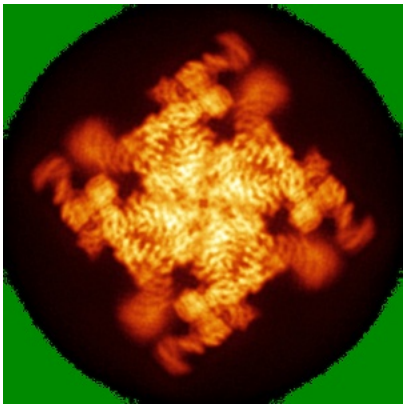
6.4.1 Primary map



X



Y

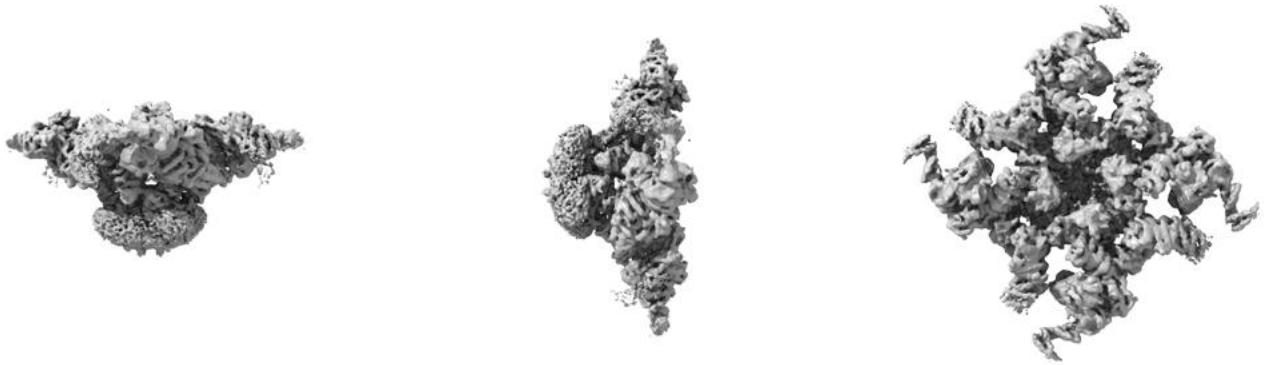


Z

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

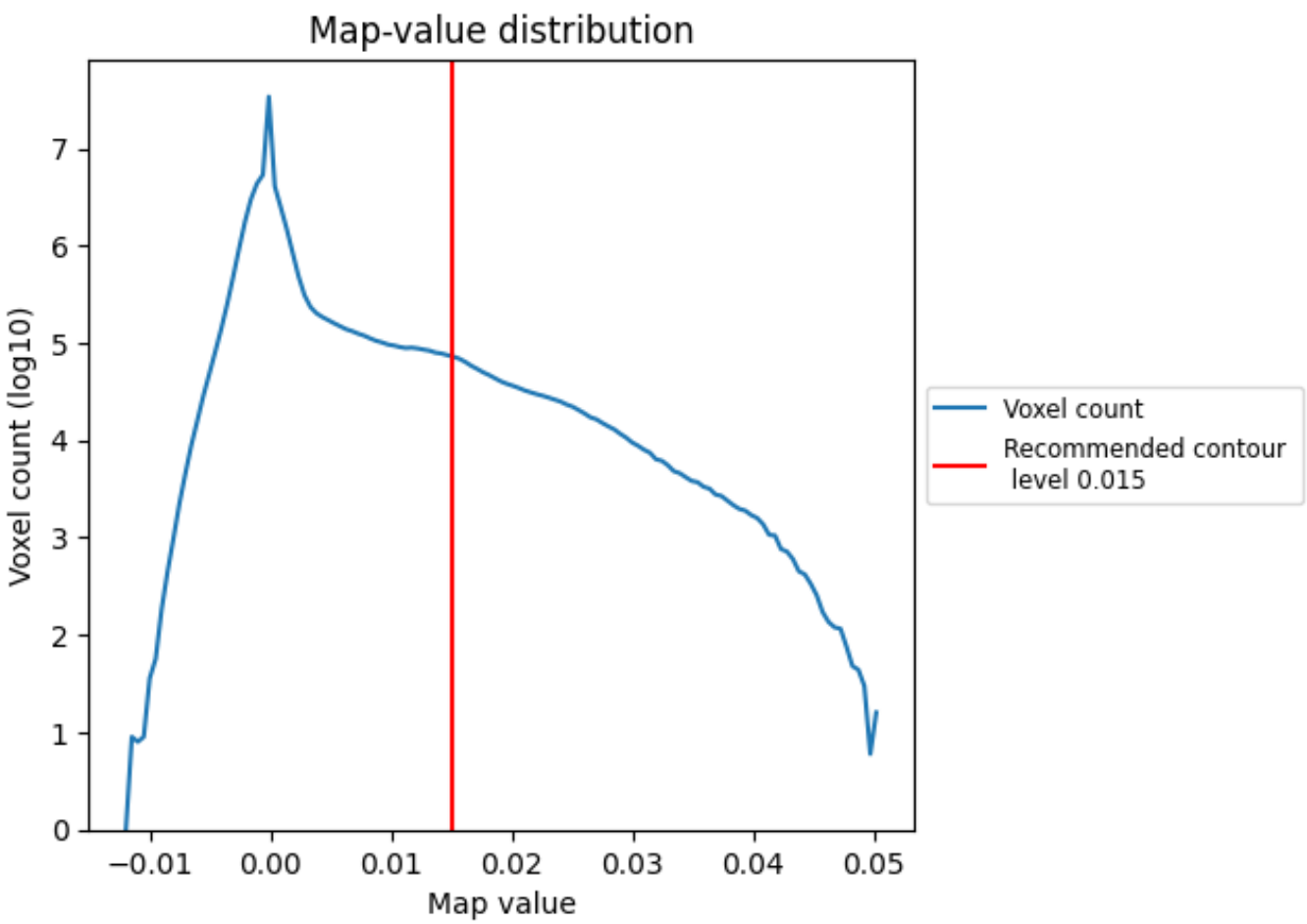
6.6 Mask visualisation (i)

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

7 Map analysis (i)

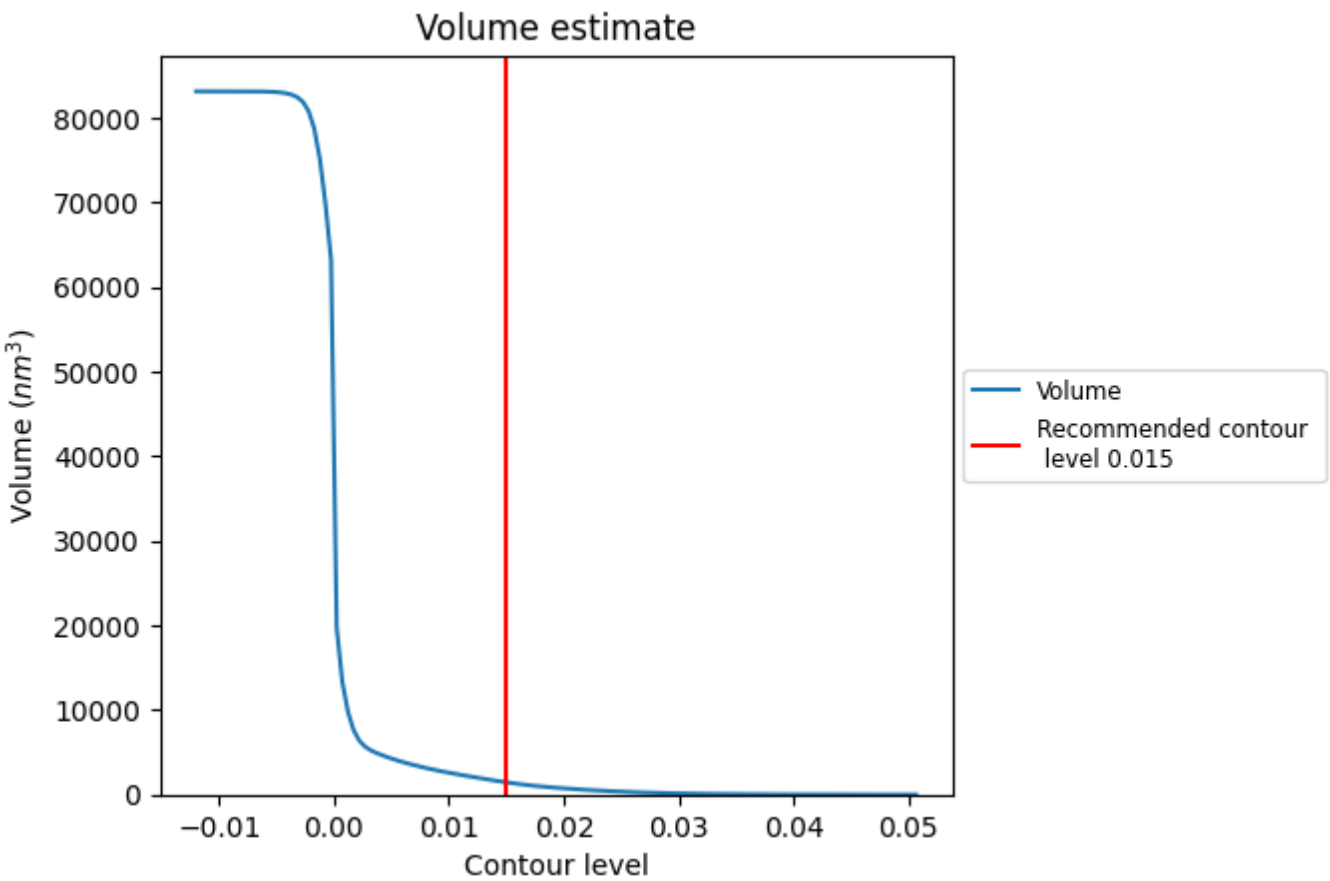
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

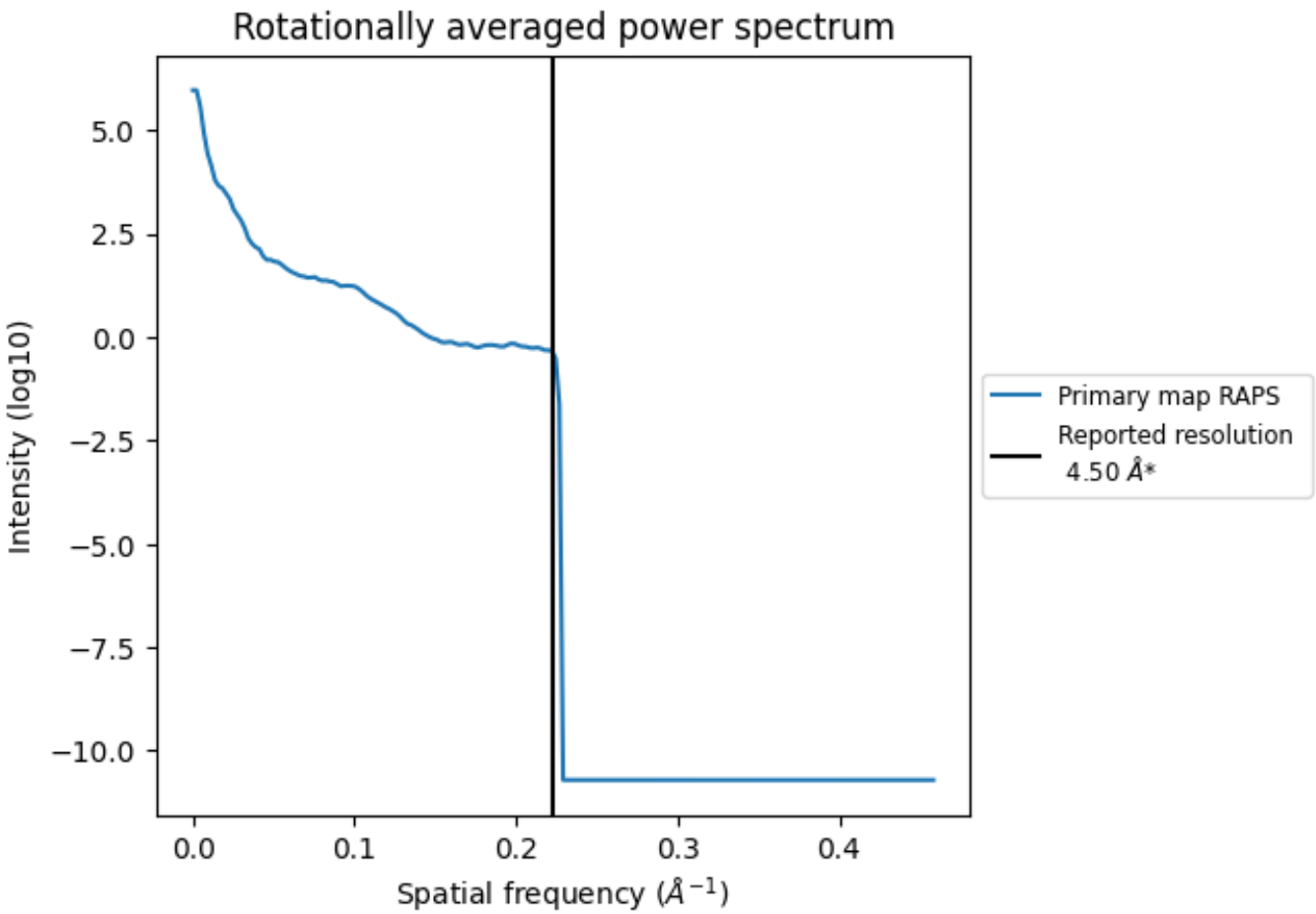
7.2 Volume estimate (i)



The volume at the recommended contour level is 1448 nm^3; this corresponds to an approximate mass of 1308 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)

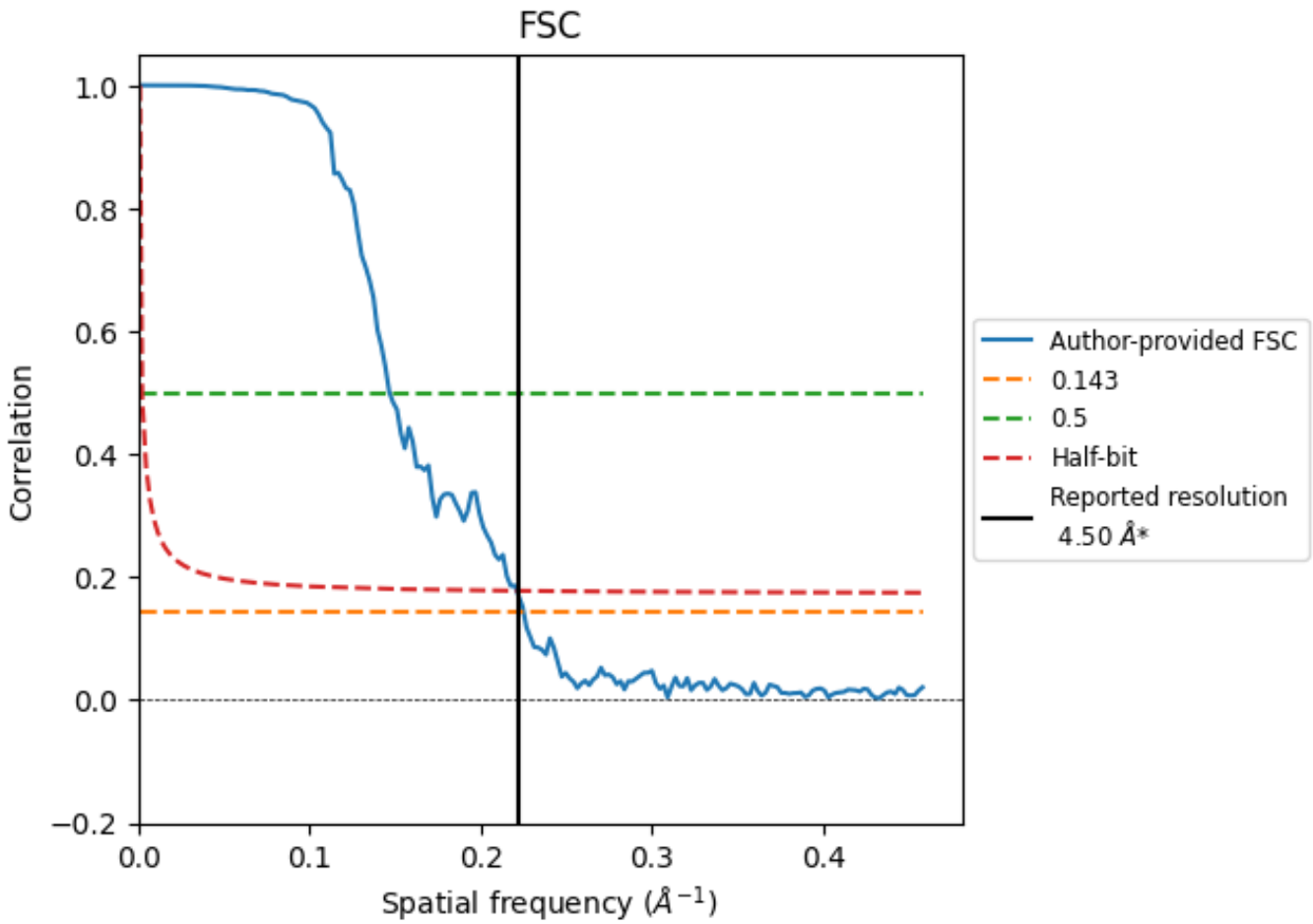


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

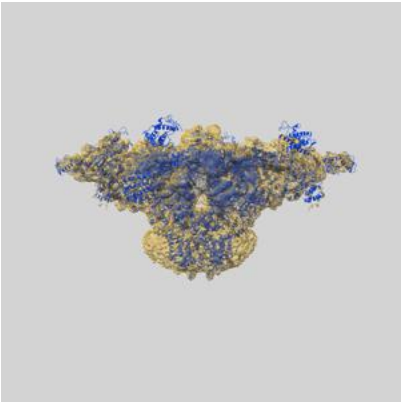
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.44	6.81	4.52
Unmasked-calculated*	-	-	-

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

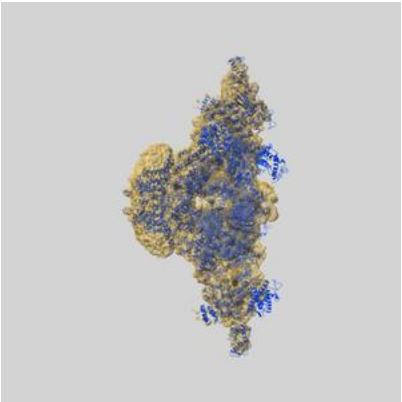
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9826 and PDB model 6JHN. Per-residue inclusion information can be found in section 3 on page 6.

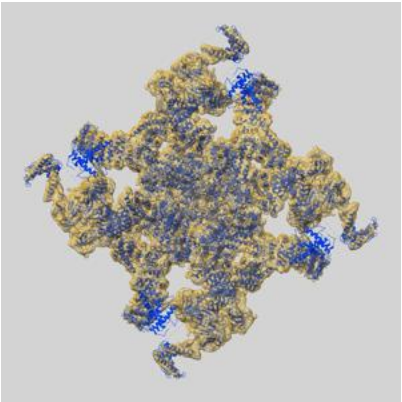
9.1 Map-model overlay (i)



X



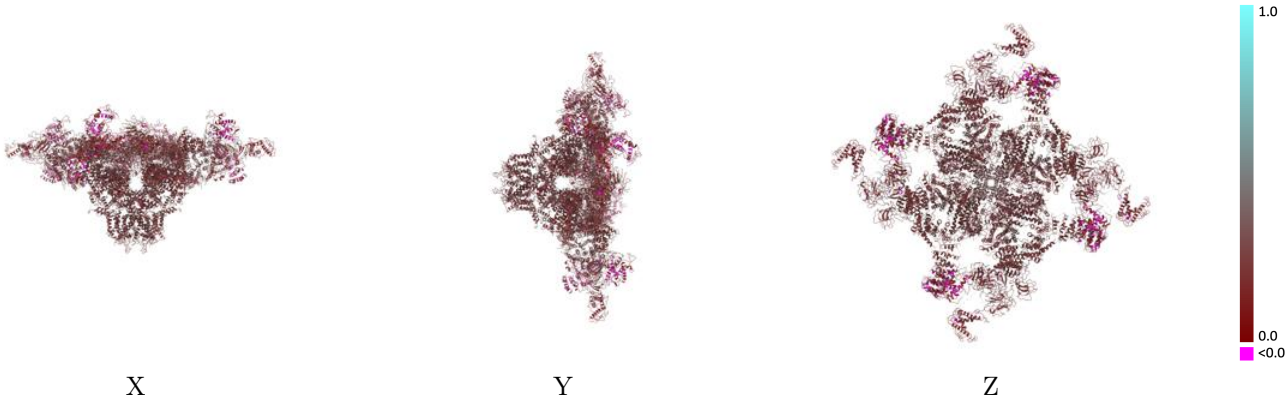
Y



Z

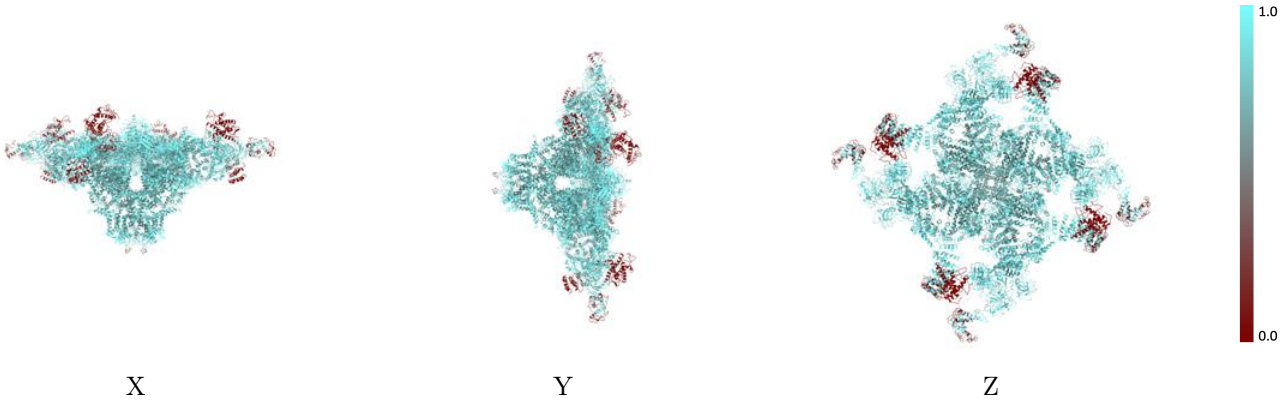
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



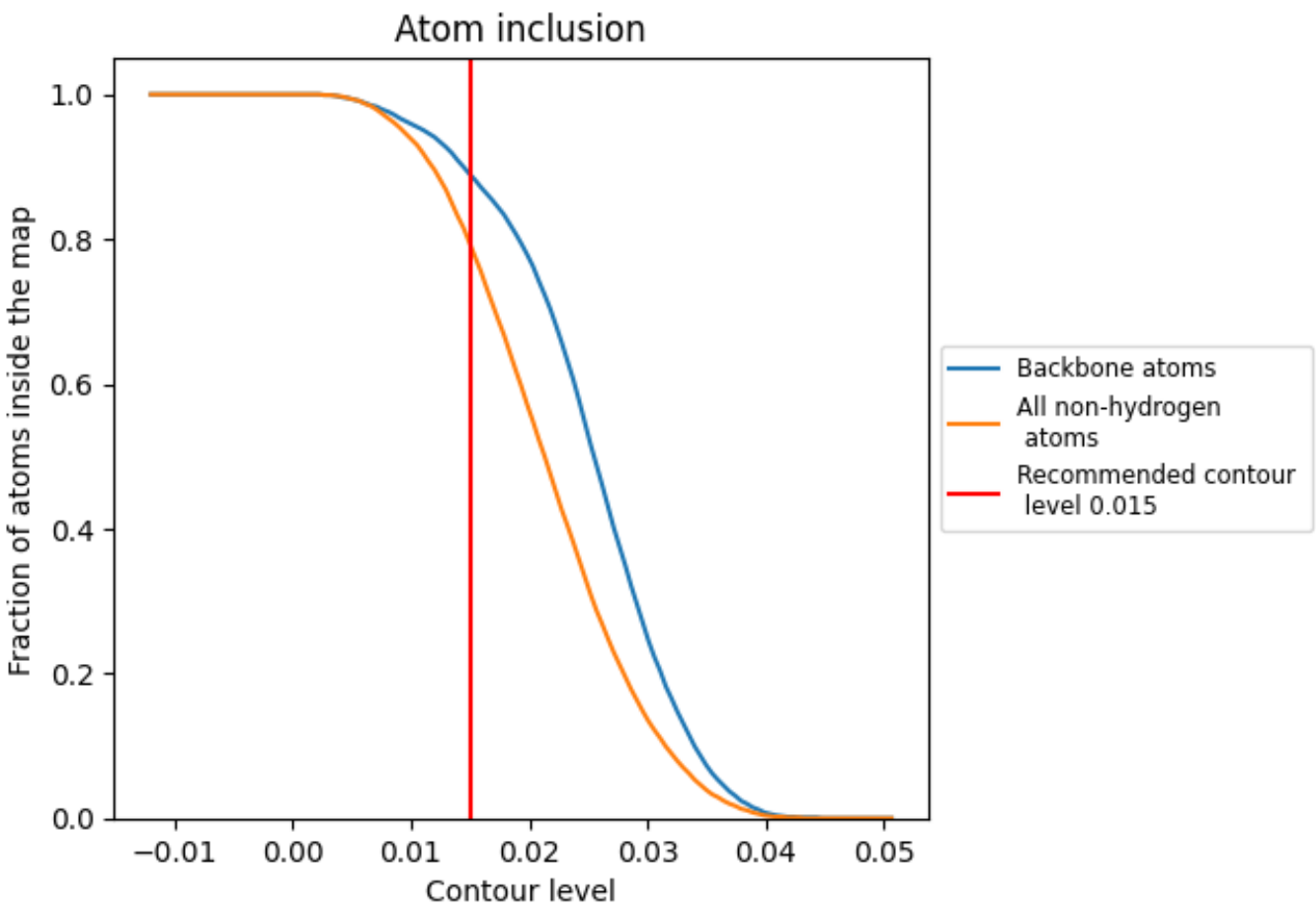
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.2520
A	0.7920	0.2520
B	0.8320	0.2670
C	0.7920	0.2520
D	0.8320	0.2660
E	0.7920	0.2520
F	0.8320	0.2680
G	0.7920	0.2520
H	0.8320	0.2670