wwPDB EM Validation Summary Report (i)

Mar 19, 2024 – 09:35 PM JST

PDB ID	:	6JI0
EMDB ID	:	EMD-9831
Title	:	Structure of RyR2 (F/A/C/Ca2+ dataset)
Authors	:	Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on	:	2019-02-19
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 (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:

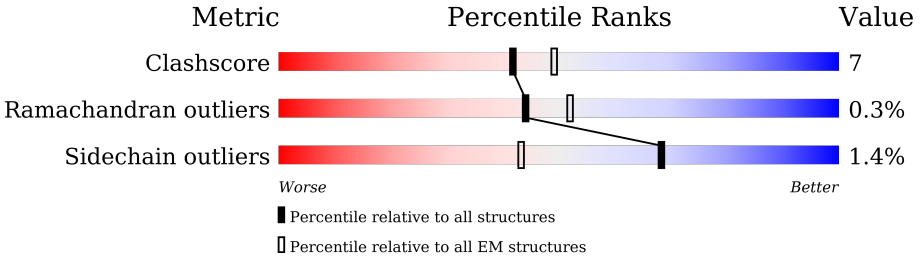
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4968	16% 57% 13% 30%
1	C	4968	16% 57% 12% 30%
1	E	4968	16% 57% 13% 30%
1	G	4968	16% 57% 12% 30%
2	B	108	81% 19%
2	D	108	81% 18%
2	F	108	83% 16%
2	H	108	82% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 109772 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	26577	16924	4546	4949	158	0	0
1	C	3476	26577	16924	4546	4949	158	0	0
1	E	3476	26577	16924	4546	4949	158	0	0
1	G	3476	26577	16924	4546	4949	158	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

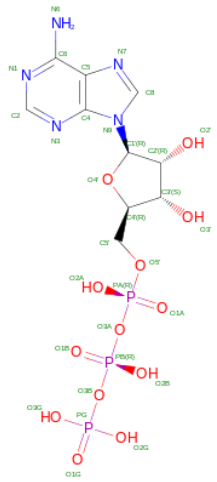
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$).

ATP

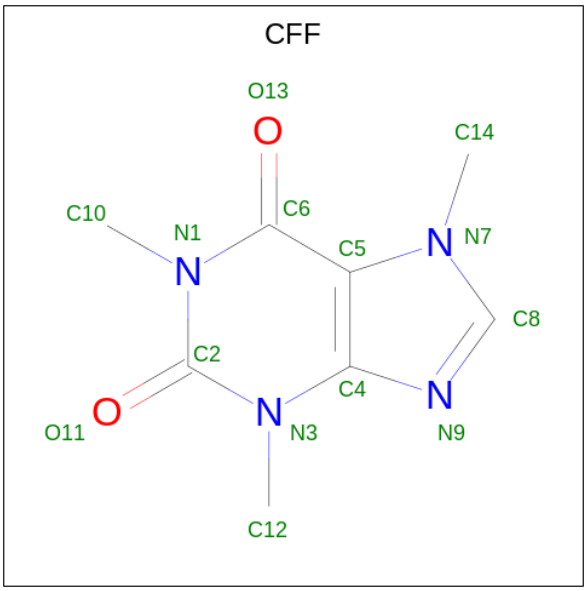


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



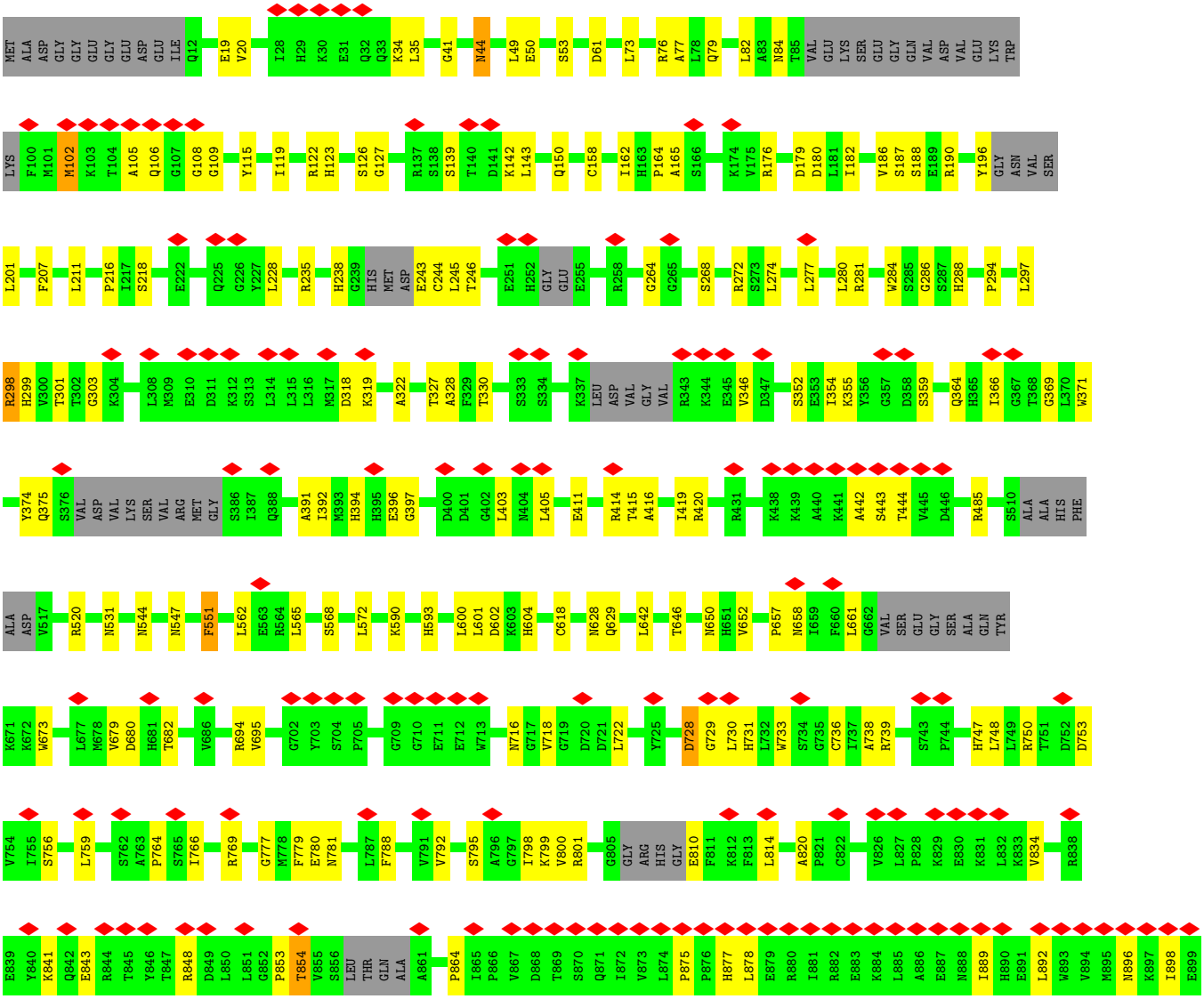
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	4	2	0
6	C	1	14	8	4	2	0
6	E	1	14	8	4	2	0
6	G	1	14	8	4	2	0

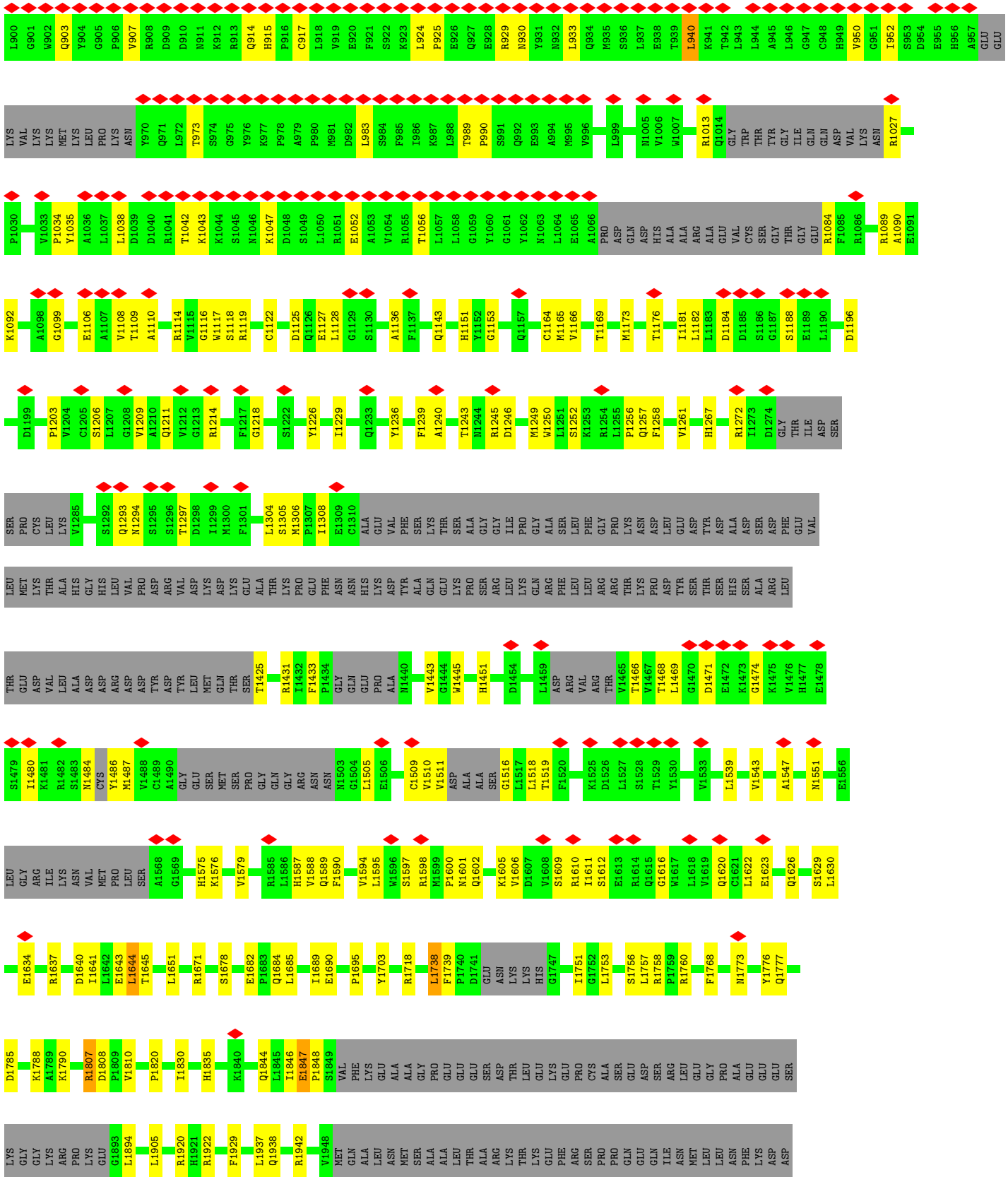
3 Residue-property plots (i)

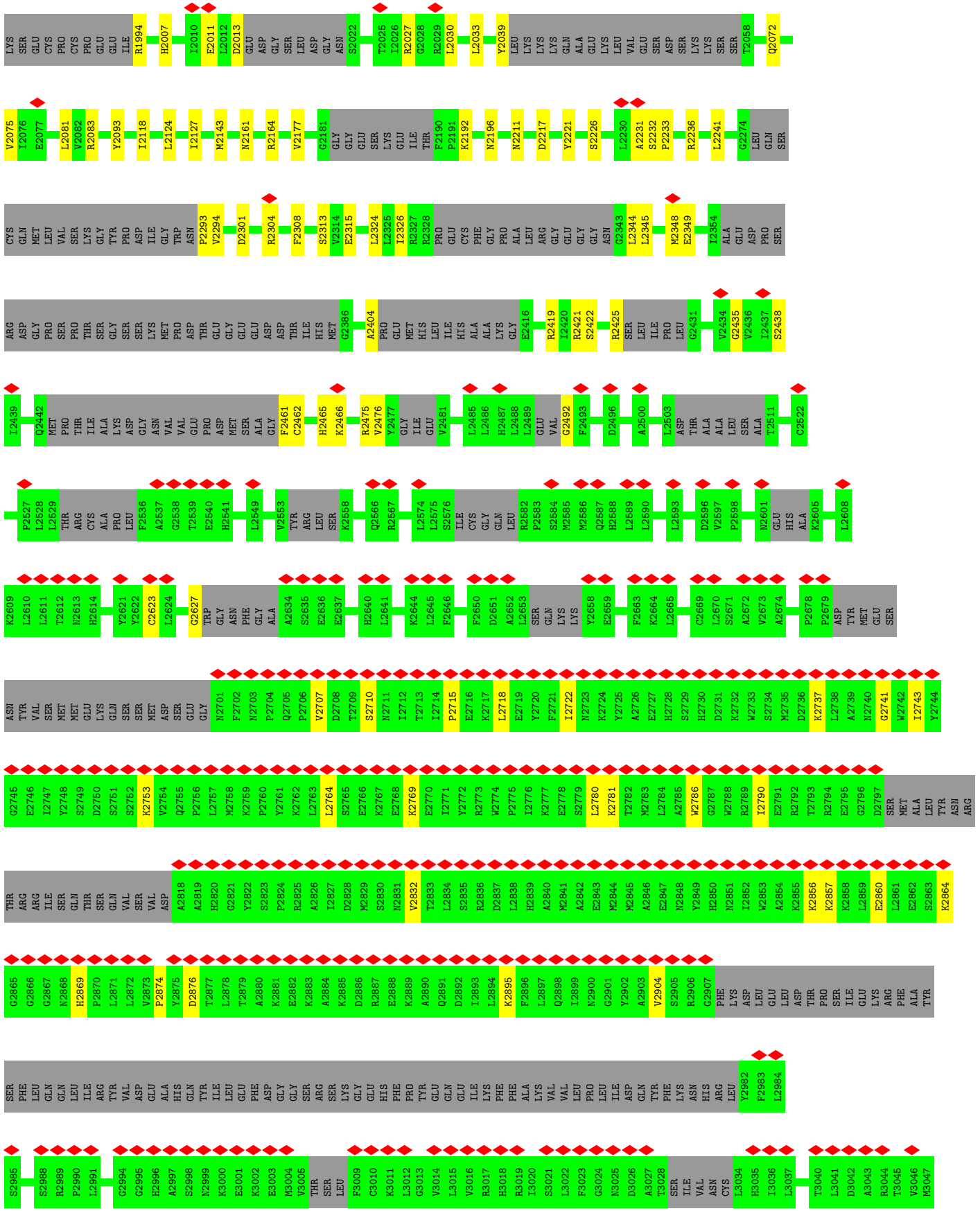
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

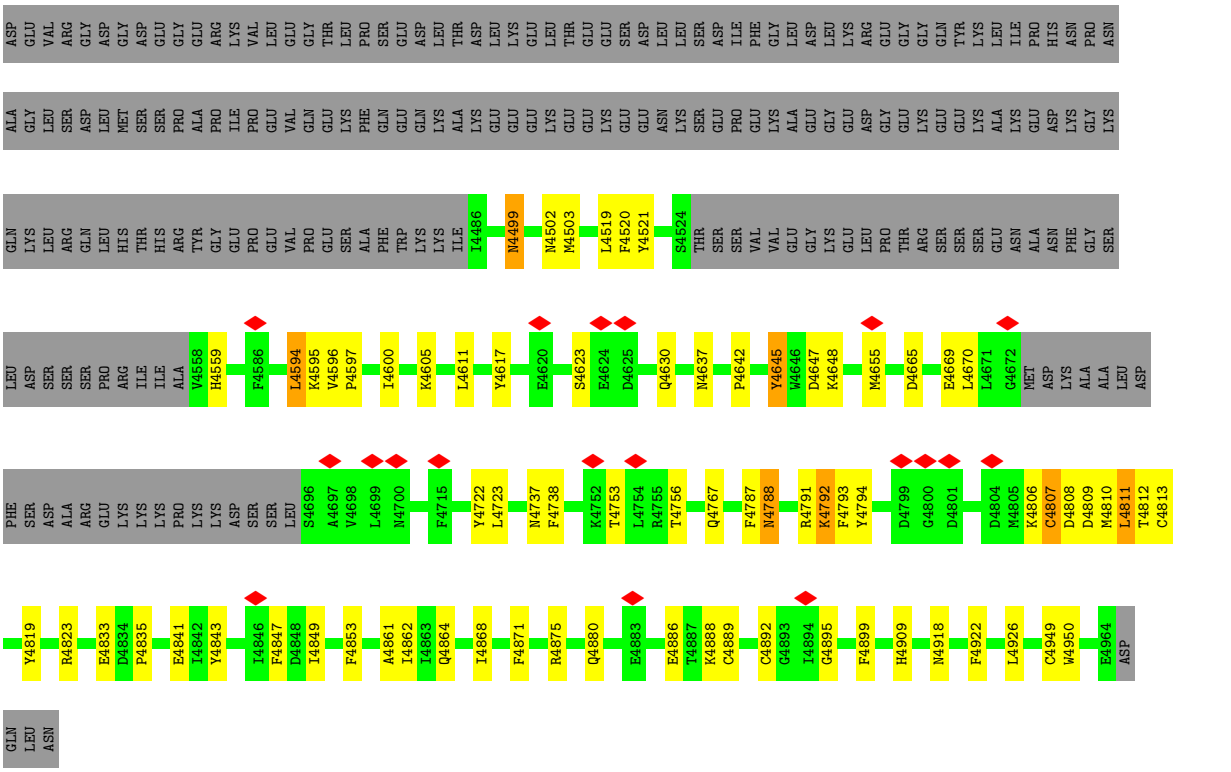
Chain A: 16% 57% 13% 30%




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 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 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 Q992 E993 A994 M995 V996 L999 N1005 V1006 W1007 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027
P1030 V1033 P1034 Y1035 A1036 L1037 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 A1098 G1099 E1106 A1107 V1108 T1109 A1110 R1114 V1115 G1116 W1117 S1118 R1119 C1122 D1125 Q1126 E1127 L1128 G1129 S1130 A1136 F1137 Q1143 H1151 Y1152 G1153 Q1157 C1164 M1165 V1166 T1169 M1173 T1176 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 D1196
D1199 P1203 V1204 C1205 S1206 L1207 G1208 V1209 A1210 Q1211 V1212 G1213 R1214 F1217 G1218 S1222 Y1226 I1229 Q1233 Y1236 F1239 A1240 T1243 N1244 R1245 D1246 M1249 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 F1258 V1261 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER
SER PRO CYS LEU LYS V1285 S1292 Q1293 N1294 S1295 S1296 T1297 D1298 I1299 M1300 F1301 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 TYR LEU MET GLN THR SER T1425 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 H1451 D1454 L1459 ASP ARG VAL ARG THR V1465 T1466 V1467 T1468 L1469 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478
S1479 I1480 R1481 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG ASN ASN N1503 G1504 L1505 E1506 C1509 V1510 V1511 ASP ALA ALA SER G1516 L1517 L1518 T1519 F1520 K1525 D1526 L1527 S1528 T1529 Y1530 V1533 L1539 V1543 A1547 N1551 E1556
LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 H1575 K1576 V1579 R1585 L1586 H1587 V1588 Q1589 F1590 V1594 L1595 W1596 S1597 R1598 M1599 P1600 N1601 Q1602 K1605 V1606 D1607 V1608 S1609 R1610 I1611 S1612 E1613 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 E1623 Q1626 S1629 L1630
E1634 R1637 D1640 I1641 L1642 E1643 L1644 T1645 L1651 R1671 S1678 E1682 P1683 Q1684 L1685 I1689 E1690 P1695 Y1703 R1718 L1738 F1739 P1740 D1741 GLU ASN LYS LYS HIS G1747 I1751 G1752 L1753 S1756 L1757 R1758 P1759 R1760 F1768 N1773 Y1776 Q1777
D1785 K1788 A1789 K1790 R1807 D1808 P1809 V1810 P1820 I1830 H1835 K1840 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 GLU GLU SER
LYS GLY GLY LYS ARG PRO LYS GLU G1893 L1894 L1905 R1920 H1921 R1922 F1929 L1937 Q1938 R1942 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

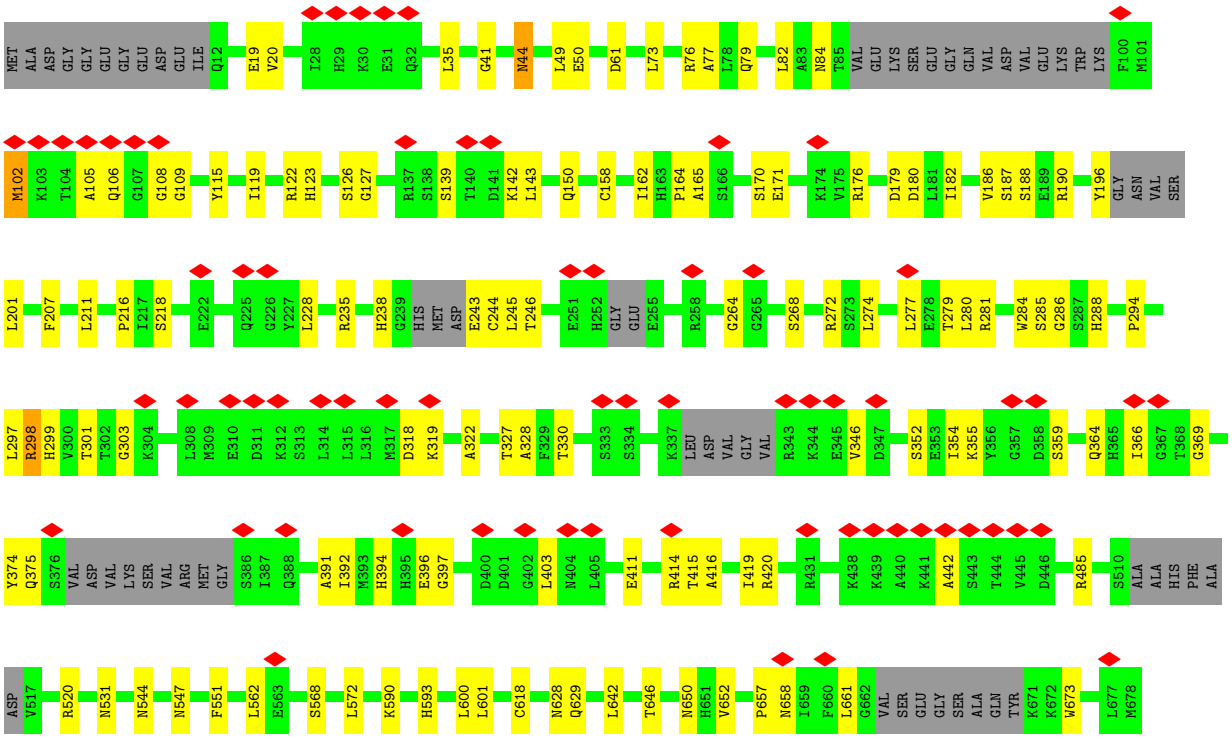

LYS SER GLU CYS PRO CYS PRO GLU GLU ILE R1994 H2007 I2010 E2011 L2012 D2013 GLU ASP GLY SER LEU ASP GLY ASN S2022 T2025 I2026 R2027 G2028 R2029 L2030 L2033 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 Q2072
V2075 I2076 E2077 L2081 V2082 R2083 Y2093 I2118 L2124 I2127 M2143 N2161 R2164 V2177 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191 K2192 N2196 N2211 D2217 Y2221 S2226 L2230 A2231 S2232 P2233 R2236 L2241 G2274 LEU GLN SER
CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 V2294 D2301 R2304 F2308 S2313 V2314 E2315 L2324 L2325 I2326 R2327 R2328 PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 L2344 L2345 M2348 E2349 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 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 R2419 I2420 R2421 S2422 R2425 SER LEU ILE PRO LEU G2431 V2434 G2435 V2436 I2437 S2438
I2439 Q2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 C2462 H2465 K2466 R2475 V2476 Y2477 GLY ILE GLU V2481 L2485 L2486 H2487 L2488 L2489 GLU VAL G2492 F2493 D2496 A2500 L2503 ASP THR ALA ALA LEU SER ALA T2511 C2522
P2527 L2528 L2529 THR ARG CYS ALA PRO LEU F2536 A2537 G2538 T2539 E2540 H2541 L2549 V2553 TYR ARG LEU SER K2558 Q2566 R2567 L2574 L2575 S2576 ILE CYS GLY GLN LEU R2582 P2583 S2584 M2585 M2586 Q2587 H2588 L2589 L2590 L2593 D2596 V2597 P2598 N2601 GLU HIS ALA K2605 L2608
K2609 L2610 L2611 T2612 N2613 H2614 Y2621 Y2622 C2623 L2624 G2627 TRP GLY ASN PHE GLY ALA A2634 S2635 E2636 E2637 H2640 L2641 K2644 L2645 F2646 F2650 D2651 A2652 L2653 SER GLN LYS LYS Y2658 E2659 F2663 K2664 L2665 C2669 L2670 S2671 A2672 V2673 A2674 P2678 P2679 ASP TYR MET GLU SER
ASN TYR VAL SER MET MET GLU LYS GLN SER 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 A2818 A2819 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 F2983 L2984
S2985 S2988 R2989 P2990 L2991 G2994 G2995 H2996 A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 G3013 V3014 L3015 V3016 R3017 H3018 R3019 I3020 S3021 L3022 F3023 G3024 N3025 D3026 A3027 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 T3040 L3041 D3042 A3043 R3044 T3045 V3046 M3047

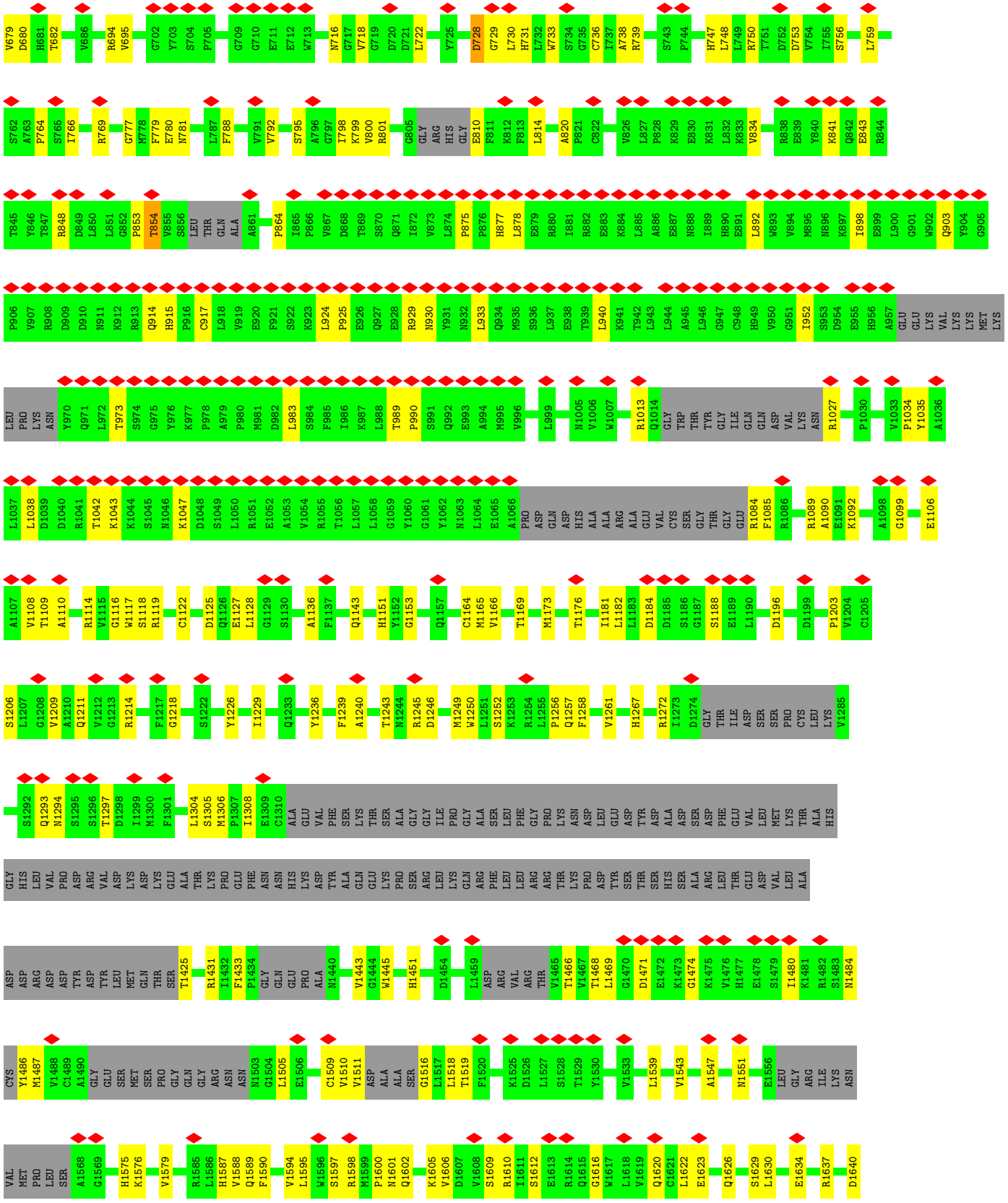
K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070 K3071 T3072 M3073 E3074 M3075 L3076 K3077 Q3078 G3079 Q3080 F3081 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107
S3108 L3109 F3110 E3111 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 E3150 R3151 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 HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE 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 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 GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL VAL ALA GLU VAL PHE ILE 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 LEU THR ASP THR LYS SER LYS MET SER LYS ALA ALA LYS VAL SER ASP GLN GLU ARG LYS LYS MET SER LYS ARG LYS ASP TYR 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 ILE ALA LEU ALA LYS ASN ARG PHE SER LEU 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 THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL 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 L3612 E3634 H3635 Y3636 L3641 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 K3680 E3684 F3687 L3688 Y3689 M3690 C3700
HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU VAL LYS S3714 Q3729 A3730 H3733 D3734 R3735 Q3743 L3760 K3761 G3769 K3777 Y3781 S3800 C3801 S3802 V3803 N3813 K3814 G3817 LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU K3829 Q3832 E3835 F3841
Q3845 L3846 L3847 Q3862 V3869 N3870 I3871 I3872 I3873 S3874 T3875 V3876 D3877 L3880 R3881 I3886 W3891 Y3892 Y3893 D3897 Q3904 R3905 N3906 A3910 Q3916 V3917 F3918 N3919 T3920 L3921 T3922 E3923 D3943 A3944 Q3956 Q3965 M3973 Q3976 L3983 N3990 N3993 G3994
V4005 E4006 S4007 V4011 L4015 L4022 K4023 L4024 K4025 D4026 L4027 S4030 D4031 T4032 F4033 D4037 P4038 D4039 G4040 K4041 G4042 R4047 M4053 E4054 S4055 H4056 Q4061 E4072 T4073 D4074 E4075 N4076 D4080 Y4081 E4082 E4083 F4084 V4085 K4086 R4087 F4088 H4089 K4093 D4094 I4095 L4102
N4105 E4108 H4109 M4110 D4113 T4114 R4115 L4116 Q4117 V4126 L4127 N4128 Y4129 F4130 Q4131 L4134 E4138 R4148 V4149 Y4150 K4170 F4175 N4179 G4182 E4183 K4184 E4185 K4186 L4189 F4190 V4191 N4192 L4203 I4207 SER GLU SER ASP LEU ASN GLU ARG SER ALA ASN LYS GLU
GLU SER GLU LYS GLU LYS PRO GLU GLY PRO ARG MET GLY PHE PHE SER LEU VAL THR VAL ARG SER ALA LEU ARG TYR ASN VAL LEU THR LEU MET ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS LYS VAL LEU LEU ALA ASN MET THR VAL ARG ASP MET
VAL THR ALA PHE PHE THR SER TYR TRP SER VAL PHE MET THR LEU LEU HIS PHE ALA ALA SER VAL SER ARG GLY PHE SER ARG ILE ILE GLY GLY LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS SER LYS ILE LYS LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN



- Molecule 1: RyR2

Chain C:

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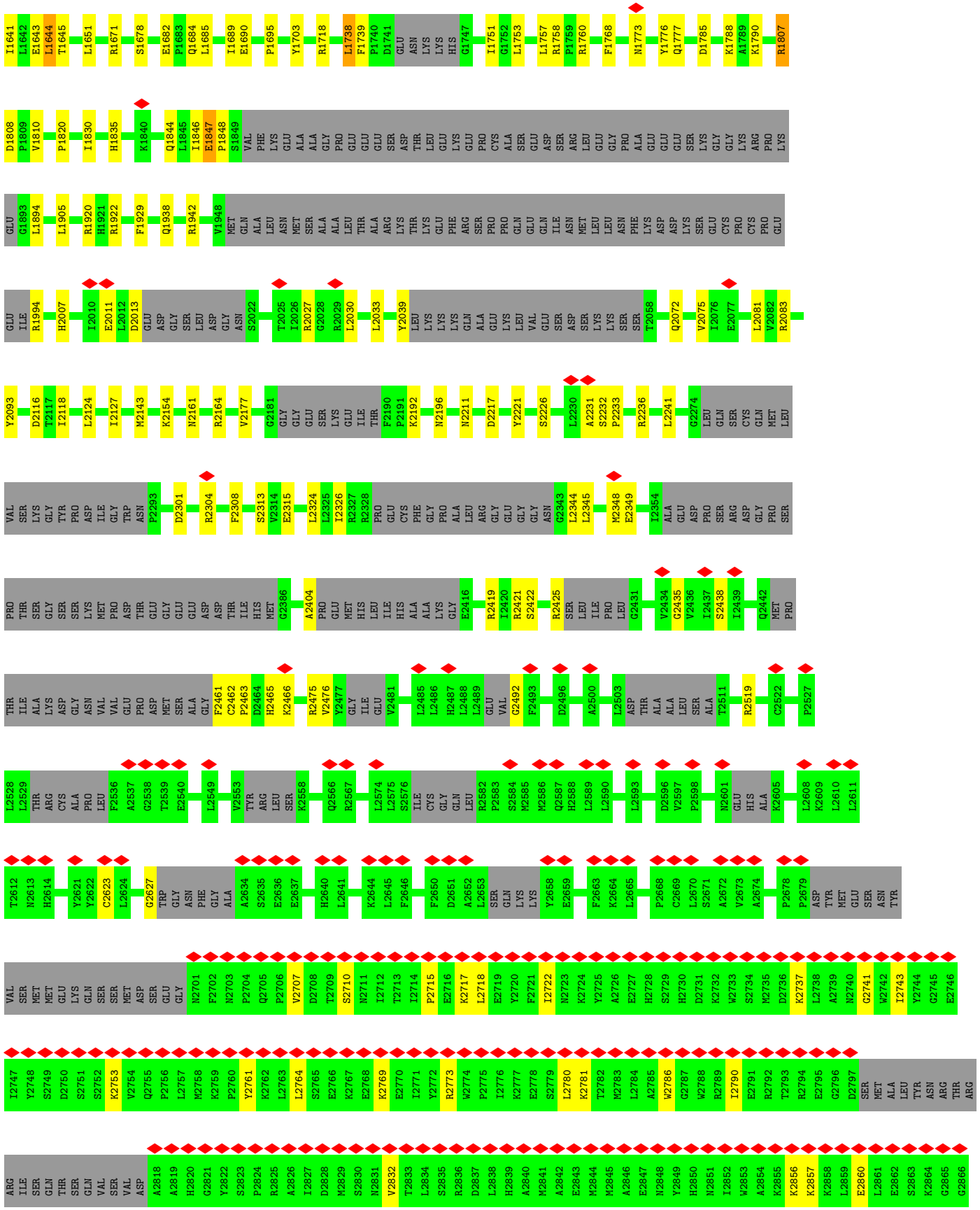
S762 A763 P764 S765 I766 R769 G777 W778 F779 E780 N781 L787 F788 V791 V792 S795 A796 G797 I798 K799 V800 R801 G805 GLY ARG HIS GLY E810 F811 K812 F813 L814 A820 P821 C822 V826 L827 P828 K829 E830 K831 L832 K833 V834 R838 E839 Y840 K841 Q842 E843 R844
T845 Y846 T847 R848 D849 L850 L851 G852 P853 T854 V855 S856 LEU THR GLN ALA A861 P864 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 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 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 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 Q992 E993 A994 M995 V996 L999 N1005 V1006 W1007 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 P1030 V1033 P1034 Y1035 A1036
L1037 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 A1098 G1099 E1106
A1107 V1108 T1109 A1110 R1114 V1115 G1116 W1117 S1118 R1119 C1122 D1125 Q1126 E1127 L1128 G1129 S1130 A1136 F1137 Q1143 H1151 Y1152 G1153 Q1157 C1164 M1165 V1166 T1169 M1173 T1176 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 D1196 D1199 P1203 V1204 C1205
S1206 L1207 G1208 V1209 A1210 Q1211 V1212 G1213 R1214 F1217 G1218 S1222 Y1226 I1229 Q1233 Y1236 F1239 A1240 T1243 N1244 R1245 D1246 M1249 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 F1258 V1261 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285
S1292 Q1293 N1294 S1295 S1296 T1297 D1298 I1299 M1300 F1301 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 TYR LEU MET GLN THR SER T1425 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 H1451 D1454 L1459 ASP ARG VAL ARG THR V1465 T1466 V1467 T1468 L1469 G1470 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 K1481 R1482 S1483 N1484
CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG ASN ASN N1503 G1504 L1505 E1506 C1509 V1510 V1511 ASP ALA ALA SER G1516 L1517 L1518 T1519 F1520 K1525 D1526 L1527 S1528 T1529 Y1530 V1533 L1539 V1543 A1547 N1551 E1556 LEU GLY ARG ILE LYS ASN
VAL MET PRO LEU SER A1568 G1569 H1575 K1576 V1579 R1585 L1586 H1587 V1588 Q1589 F1590 V1594 L1595 W1596 S1597 R1598 M1599 P1600 N1601 Q1602 K1605 V1606 D1607 V1608 S1609 R1610 I1611 S1612 E1613 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 G1621 L1622 E1623 Q1626 S1629 L1630 E1634 R1637 D1640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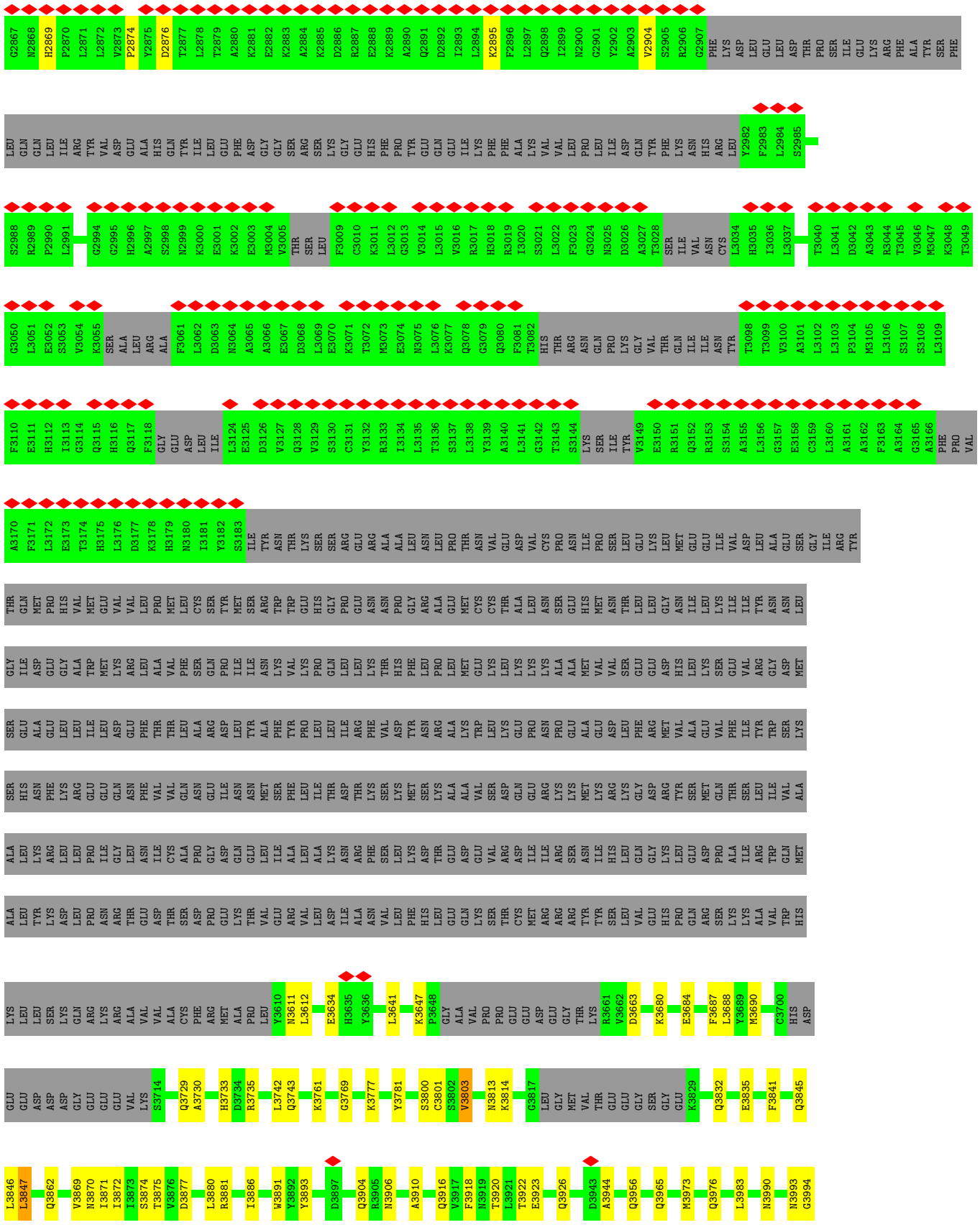
D1808 P1809 V1810 P1820 I1830 H1835 K1840 Q1844 L1845 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS
GLU G1893 L1894 L1905 R1920 H1921 R1922 F1929 Q1938 R1942 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 GLU GLN ILE ASN MET LEU LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU
GLU ILE R1994 H2007 I2010 E2011 L2012 D2013 GLU ASP GLY SER LEU ASP GLY ASN S2022 T2025 I2026 R2027 G2028 R2029 L2030 L2033 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 Q2072 V2075 I2076 E2077 L2081 V2082 R2083
Y2093 D2116 T2117 I2118 L2124 I2127 M2143 K2154 N2161 R2164 V2177 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191 K2192 N2196 N2211 D2217 Y2221 S2226 L2230 A2231 S2232 P2233 R2236 L2241 G2274 LEU GLN SER CYS GLN MET LEU
VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 D2301 R2304 F2308 S2313 V2314 E2315 L2324 L2325 I2326 R2327 R2328 PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 L2344 L2345 M2348 E2349 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 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 R2419 I2420 R2421 S2422 R2425 SER LEU ILE PRO LEU G2431 V2434 G2435 V2436 I2437 S2438 I2439 Q2442 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 L2485 L2486 H2487 L2488 L2489 GLU VAL G2492 F2493 D2496 A2500 L2503 ASP THR ALA ALA LEU SER ALA T2511 R2519 C2522 P2527
L2528 L2529 THR ARG CYS ALA PRO LEU F2536 A2537 G2538 T2539 E2540 L2549 V2553 TYR ARG LEU SER K2558 Q2566 R2567 L2574 L2575 S2576 ILE CYS GLY GLN LEU R2582 P2583 S2584 M2585 M2586 Q2587 H2588 L2589 L2590 L2593 D2596 V2597 P2598 N2601 GLU HIS ALA K2605 L2608 K2609 L2610 L2611
T2612 N2613 H2614 Y2621 Y2622 C2623 L2624 G2627 TRP GLY ASN PHE GLY ALA A2634 S2635 E2636 E2637 H2640 L2641 K2644 L2645 F2646 F2650 D2651 A2652 L2653 SER GLN LYS LYS Y2658 E2659 F2663 K2664 L2665 P2668 C2669 L2670 S2671 A2672 V2673 A2674 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 A2818 A2819 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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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 F2983 L2984 S2985
S2988 R2989 P2990 L2991 G2994 G2995 H2996 A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 G3013 V3014 L3015 V3016 R3017 H3018 R3019 I3020 S3021 L3022 F3023 G3024 N3025 D3026 A3027 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 T3040 L3041 D3042 A3043 R3044 T3045 V3046 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 K3077 Q3078 G3079 Q3080 F3081 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
F3110 E3111 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 E3150 R3151 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 LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET
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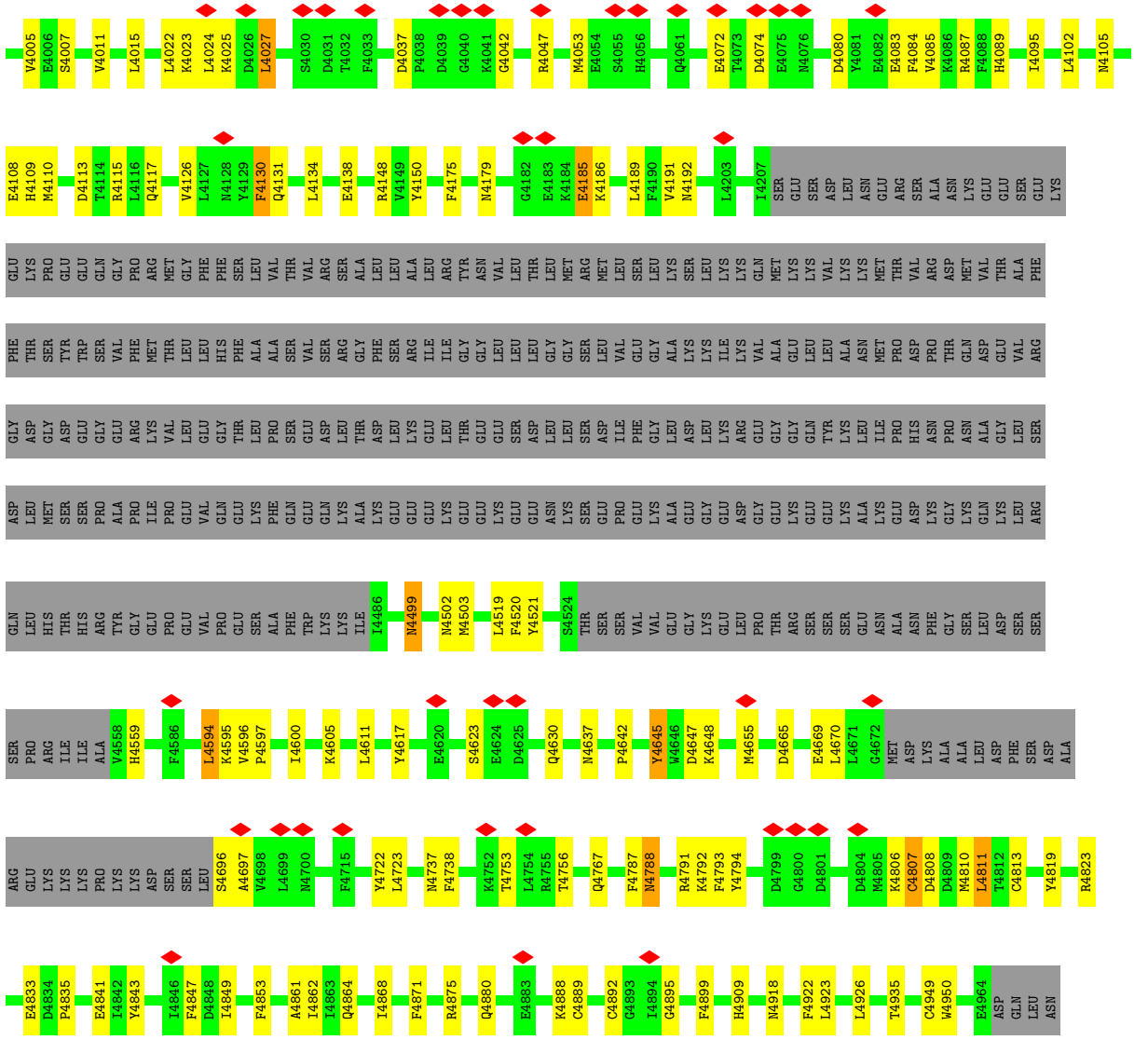
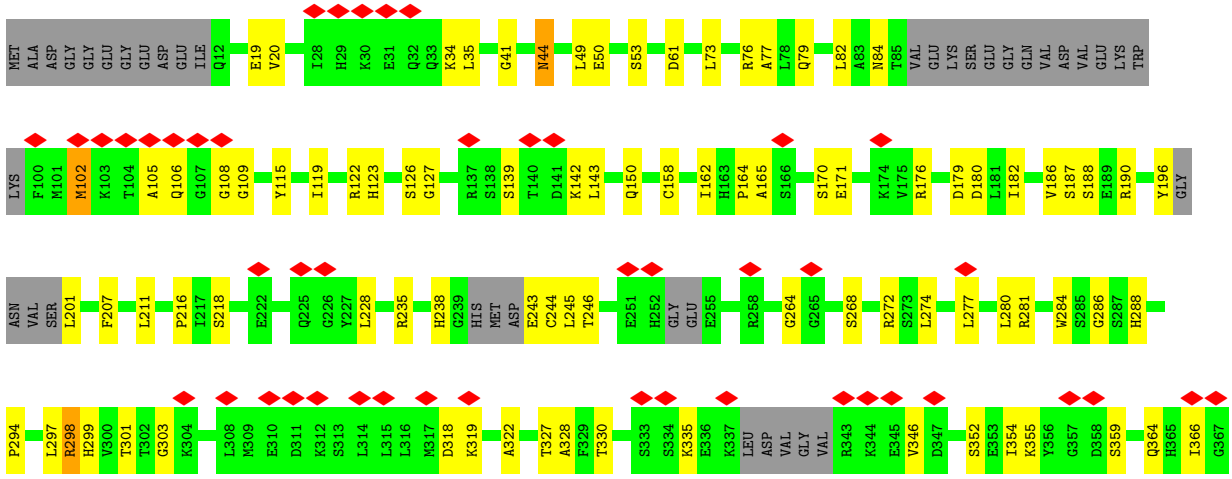
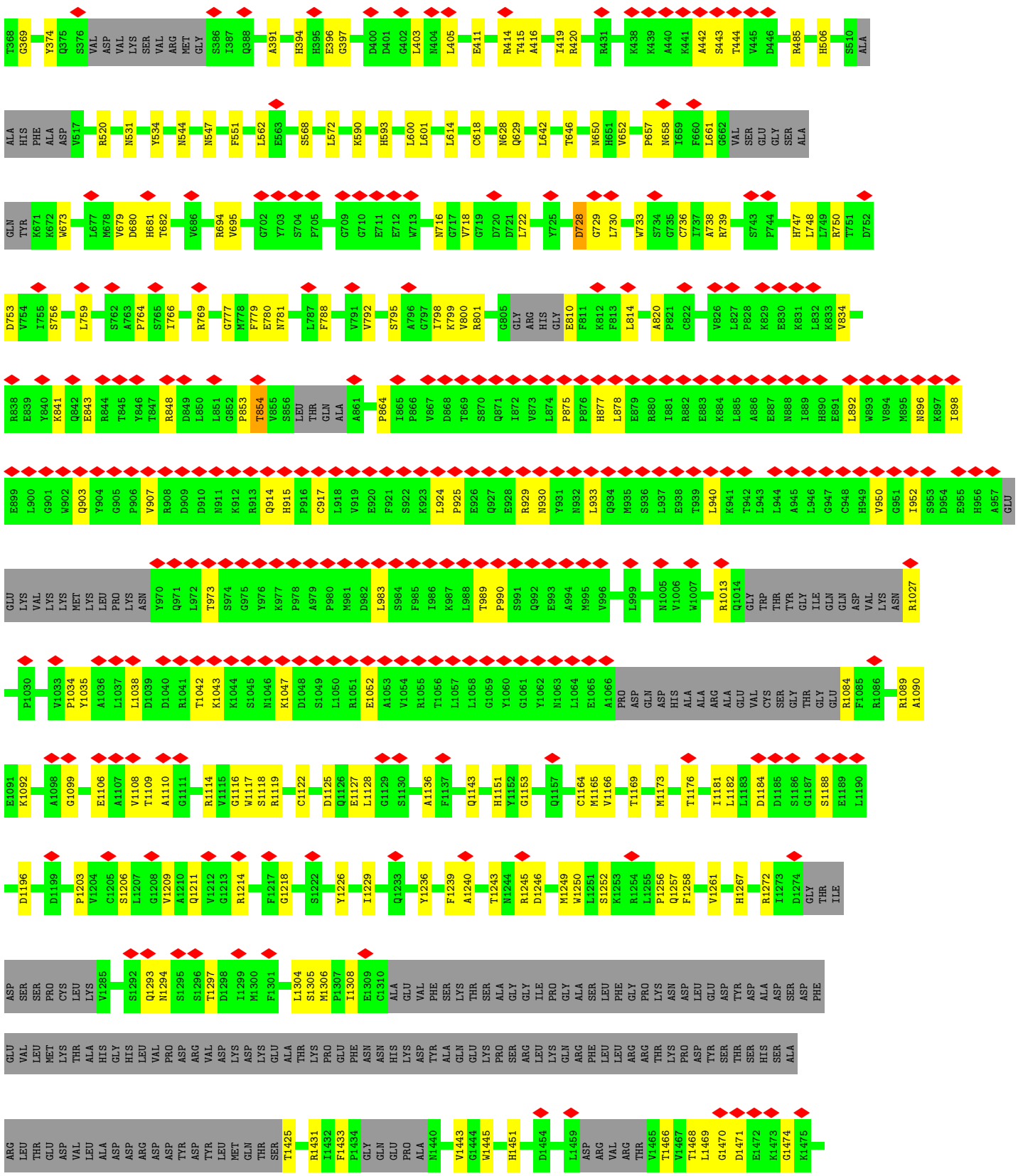
SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA
ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS 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 THR GLU ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL 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 L3612 E3634 H3635 Y3636 L3641 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 K3680 E3684 F3687 L3688 Y3689 M3690 C3700 HIS ASP
GLU GLU ASP ASP ASP GLY GLU GLU GLU VAL LYS S3714 Q3729 A3730 H3733 D3734 R3735 L3742 Q3743 K3761 G3769 K3777 Y3781 S3800 C3801 S3802 V3803 N3813 K3814 G3817 LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU K3829 Q3832 E3835 F3841 Q3845
L3846 L3847 Q3862 V3869 N3870 I3871 I3872 I3873 S3874 T3875 V3876 D3877 L3880 R3881 I3886 W3891 Y3892 Y3893 D3897 Q3904 R3905 N3906 A3910 Q3916 V3917 F3918 N3919 T3920 L3921 T3922 E3923 Q3926 D3943 A3944 Q3956 Q3965 M3973 Q3976 L3983 N3990 N3993 G3994



- Molecule 1: RyR2

Chain E:

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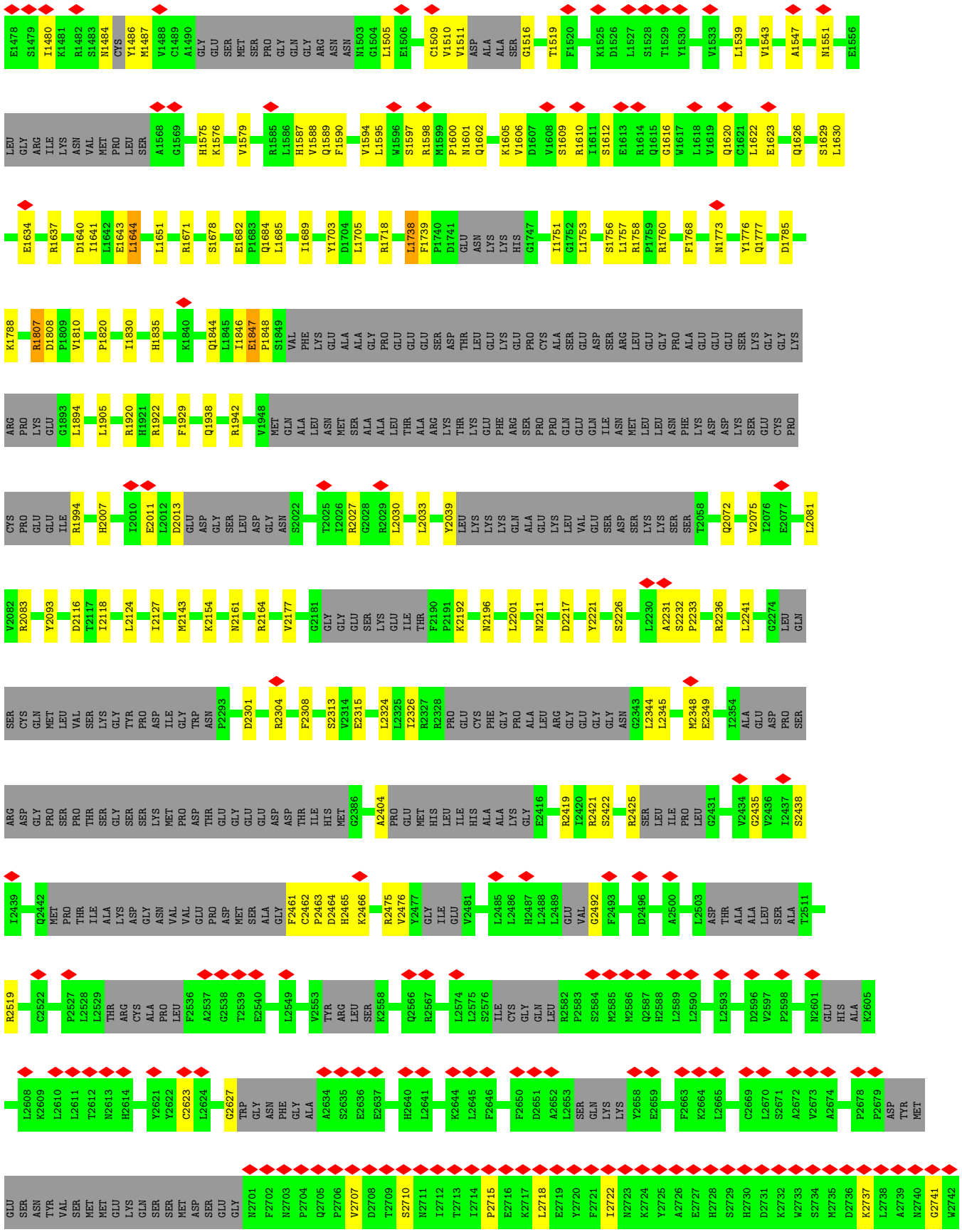
ALA HIS PHE ALA ASP V517 R520 N531 Y534 N544 N547 F551 L562 E563 S568 L572 K590 H593 L600 L601 L614 C618 N628 Q629 L642 T646 N650 H651 V652 P657 N658 I659 F660 L661 G662 VAL SER GLU GLY SER ALA
GLN TYR K671 K672 W673 L677 M678 V679 D680 H681 T682 V686 R694 V695 G702 Y703 S704 P705 G709 G710 E711 E712 W713 N716 G717 V718 G719 D720 D721 L722 Y725 D728 G729 L730 W733 S734 G735 C736 I737 A738 R739 S743 P744 H747 L748 L749 R750 T751 D752
D753 V754 I755 S756 L759 S762 A763 P764 S765 I766 R769 G777 M778 F779 E780 N781 L787 F788 V791 V792 S795 A796 G797 I798 K799 V800 R801 G805 GLY ARG HIS GLY E810 F811 K812 F813 L814 A820 P821 C822 V826 L827 P828 K829 E830 K831 L832 K833 V834
R838 E839 Y840 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 L850 L851 G852 P853 T854 V855 S856 LEU THR GLN ALA A861 P864 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 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 N930 Y931 N932 L933 Q934 N935 S936 L937 E938 T939 L940 K941 T942 L943 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 Q992 E993 A994 M995 V996 L999 N1005 V1006 W1007 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027
P1030 V1033 P1034 Y1035 A1036 L1037 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 A1098 G1099 E1106 A1107 V1108 T1109 A1110 G1111 R1114 V1115 G1116 W1117 S1118 R1119 C1122 D1125 Q1126 E1127 L1128 G1129 S1130 A1136 F1137 Q1143 H1151 Y1152 G1153 Q1157 C1164 M1165 V1166 T1169 M1173 T1176 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190
D1196 D1199 P1203 V1204 C1205 S1206 L1207 G1208 V1209 A1210 Q1211 V1212 G1213 R1214 F1217 G1218 S1222 Y1226 I1229 Q1233 Y1236 F1239 A1240 T1243 N1244 R1245 D1246 M1249 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 F1258 V1261 H1267 R1272 I1273 D1274 GLY THR ILE
ASP SER SER PRO CYS LEU LYS V1285 S1292 Q1293 N1294 S1295 S1296 T1297 D1298 I1299 M1300 F1301 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 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 TYR LEU MET GLN THR SER T1425 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 H1451 D1454 L1459 ASP ARG VAL ARG THR V1465 T1466 V1467 T1468 L1469 G1470 D1471 E1472 K1473 G1474 K1475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LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 H1575 K1576 V1579 R1585 L1586 H1587 V1588 Q1589 F1590 V1594 L1595 W1596 S1597 R1598 M1599 P1600 N1601 Q1602 K1605 V1606 D1607 V1608 S1609 R1610 I1611 S1612 E1613 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 E1623 Q1626 S1629 L1630
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K1788 R1807 D1808 P1809 V1810 P1820 I1830 H1835 K1840 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 GLU GLU SER LYS GLY GLY LYS
ARG PRO LYS GLU G1993 L1994 L1905 R1920 H1921 R1922 F1929 Q1938 R1942 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 H2007 I2010 E2011 L2012 D2013 GLU ASP GLY SER LEU ASP GLY ASN S2022 T2025 I2026 R2027 G2028 R2029 L2030 L2033 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2068 Q2072 V2075 I2076 E2077 L2081
V2082 R2083 Y2093 D2116 T2117 I2118 L2124 I2127 M2143 K2154 N2161 R2164 V2177 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191 K2192 N2196 L2201 N2211 D2217 Y2221 S2226 L2230 A2231 S2232 P2233 R2236 L2241 G2274 LEU GLN
SER CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 D2301 R2304 F2308 S2313 V2314 E2315 L2324 L2325 I2326 R2327 R2328 PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 L2344 L2345 M2348 E2349 I2354 ALA GLU ASP PRO SER
ARG ASP GLY PRO SER PRO THR THR SER GLY SER SER LYS MET PRO ASP THR GLU GLY GLU GLU ASP ASP THR ILE HIS MET G2386 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 R2419 I2420 R2421 S2422 R2425 SER LEU ILE PRO LEU G2431 V2434 G2435 V2436 I2437 S2438
I2439 Q2442 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 L2485 L2486 H2487 L2488 L2489 GLU VAL G2492 F2493 D2496 A2500 L2503 ASP THR ALA ALA LEU SER ALA T2511
R2519 C2522 P2527 L2528 L2529 THR ARG CYS ALA PRO LEU F2536 A2537 G2538 T2539 E2540 L2549 Y2553 TYR ARG LEU SER K2558 Q2566 R2567 L2574 L2575 S2576 ILE CYS GLY GLN LEU R2582 P2583 S2584 M2585 M2586 Q2587 H2588 L2589 L2590 L2593 D2596 V2597 P2598 N2601 GLU HIS ALA K2605
L2608 K2609 L2610 L2611 T2612 N2613 H2614 Y2621 Y2622 C2623 L2624 G2627 TRP GLY ASN PHE GLY ALA A2634 S2635 E2636 E2637 H2640 L2641 K2644 L2645 F2646 F2650 D2651 A2652 L2653 SER GLN LYS LYS Y2658 E2659 F2663 K2664 L2665 C2669 L2670 S2671 A2672 V2673 A2674 P2678 F2679 ASP TYR MET
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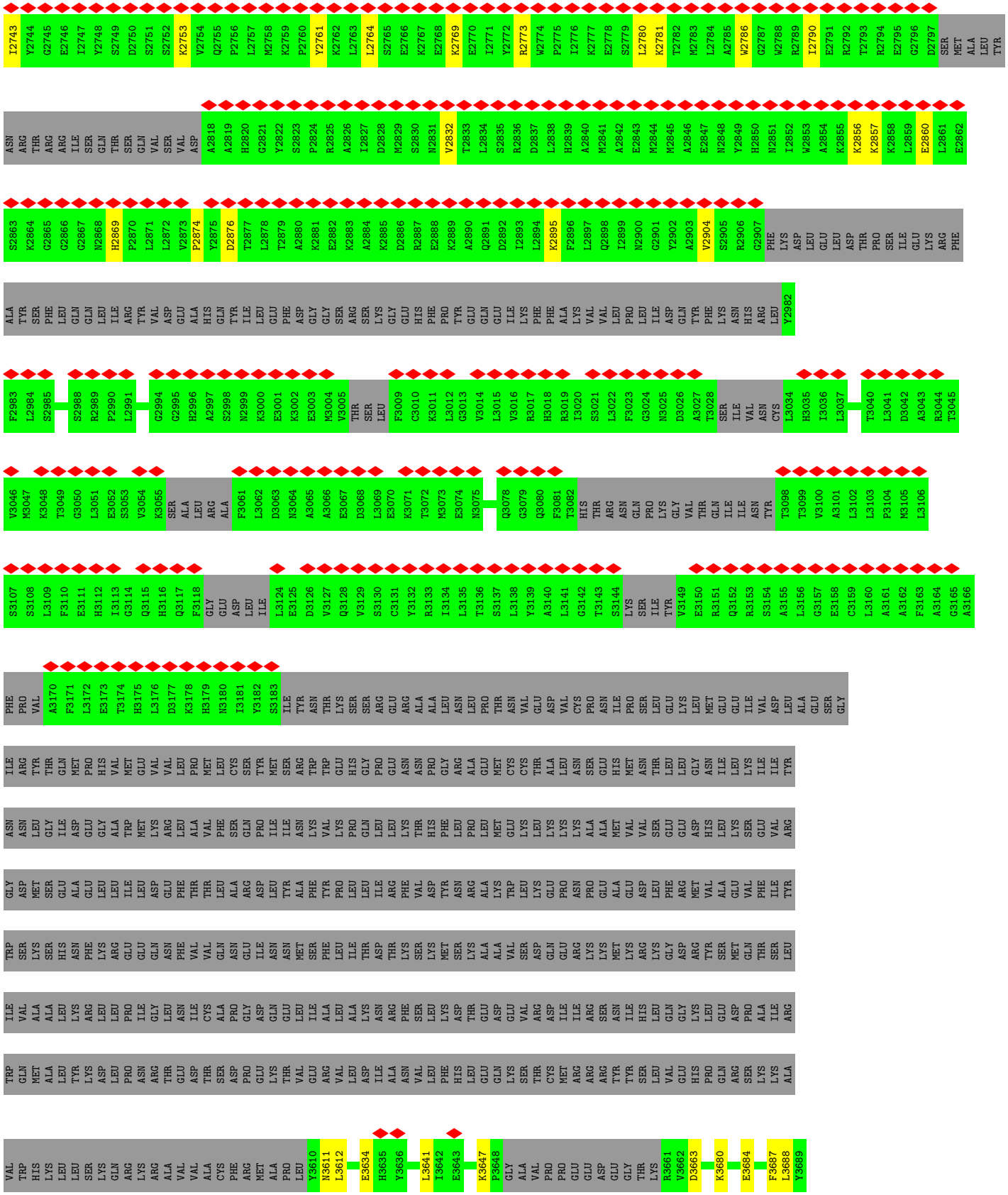
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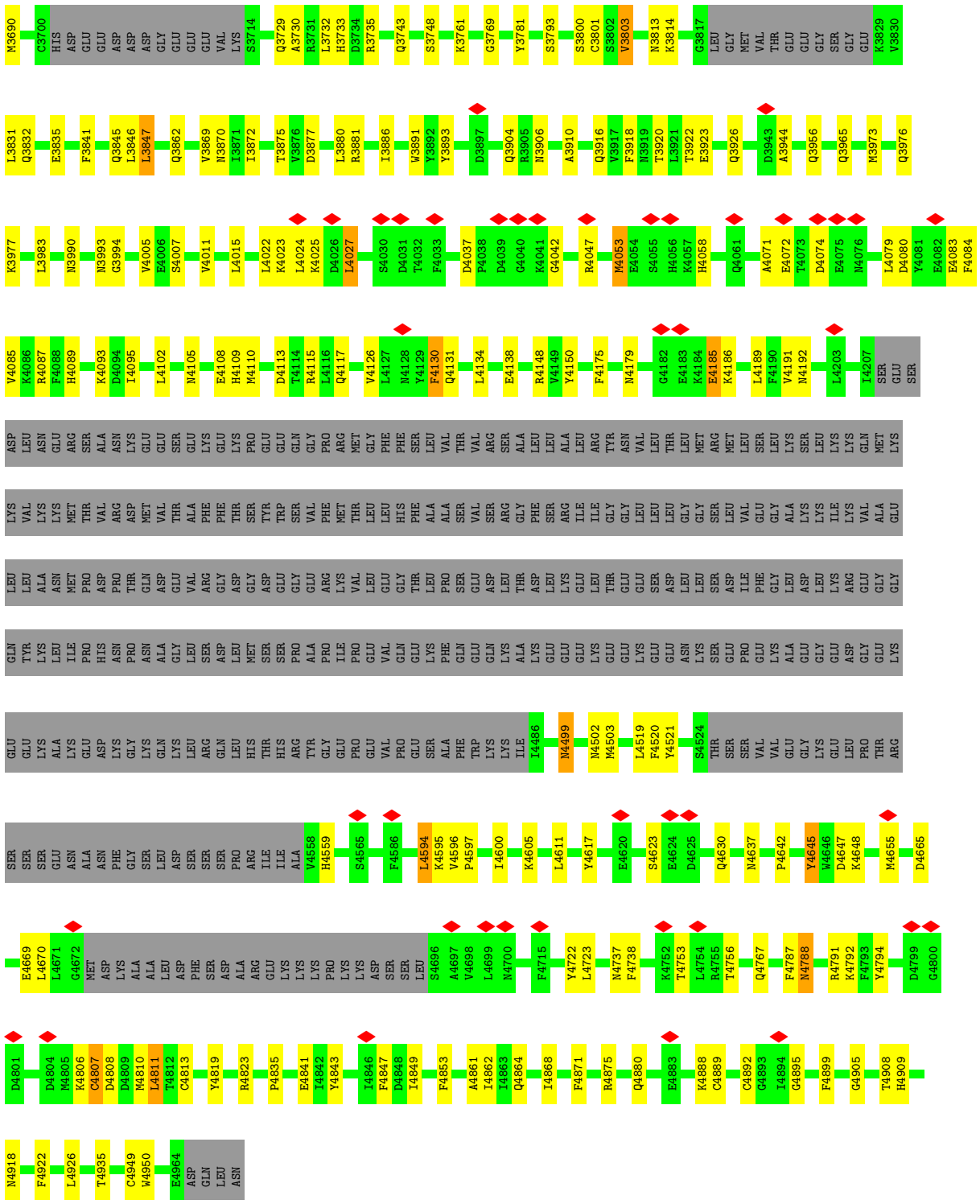
ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 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
F2983 L2984 S2985 S2988 R2989 P2990 L2991 G2994 G2995 H2996 A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 G3013 V3014 L3015 V3016 R3017 H3018 R3019 I3020 S3021 L3022 F3023 G3024 N3025 D3026 A3027 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 T3040 L3041 D3042 A3043 R3044 T3045
V3046 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 Q3078 G3079 Q3080 F3081 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 F3110 E3111 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 E3150 R3151 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 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 ASN 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 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 LYS GLU PRO ASN PRO GLU ALA GLU ASP ASP HIS LEU ILE ILE TYR
TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LYS ILE ILE THR ASP THR LYS SER MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY 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 ILE 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 GLU ASP PRO ALA ILE ILE ARG
TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER 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 L3612 E3634 H3635 Y3636 L3641 I3642 E3643 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 K3680 E3684 F3687 L3688 Y3689



- Molecule 1: RyR2

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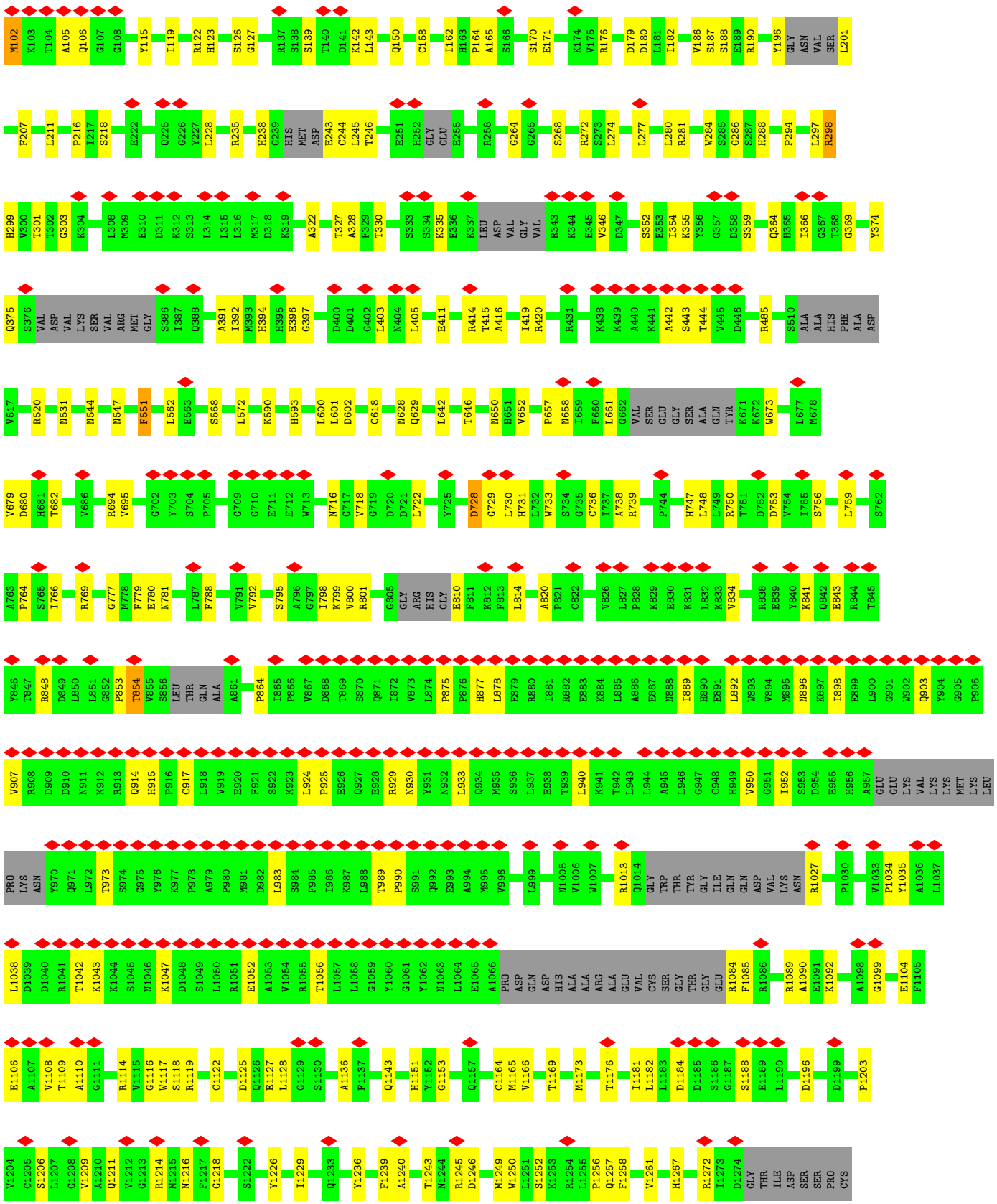
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PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 L999 N1005 V1006 W1007 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 P1030 V1033 P1034 Y1035 A1036 L1037
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E1106 A1107 V1108 T1109 A1110 G1111 R1114 V1115 G1116 W1117 S1118 R1119 C1122 D1125 Q1126 E1127 L1128 G1129 S1130 A1136 F1137 Q1143 H1151 Y1152 G1153 Q1157 C1164 M1165 V1166 T1169 M1173 T1176 I1181 L1182 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 D1196 D1199 P1203
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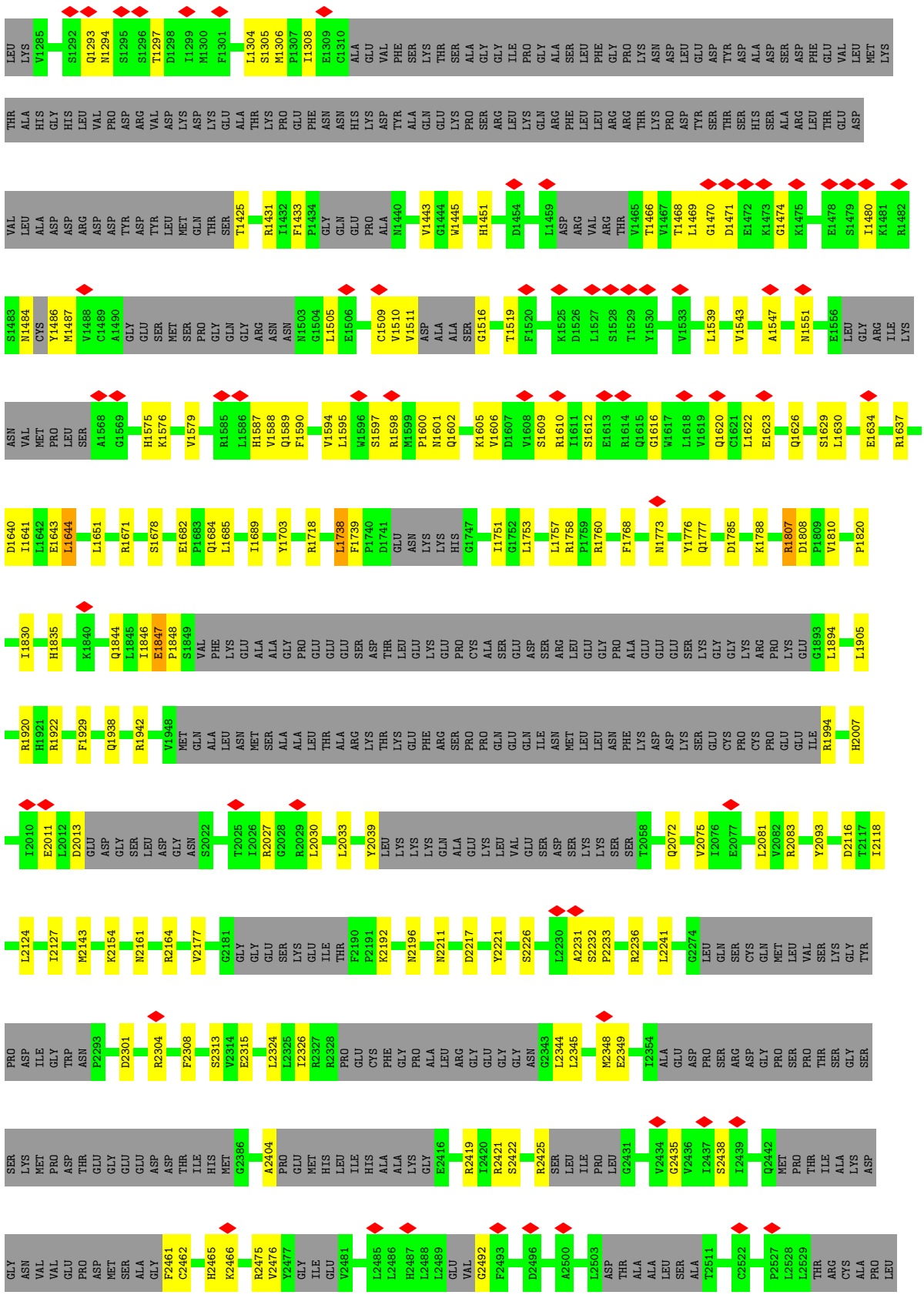
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THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP
VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 R1431 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 H1451 D1454 L1459 ASP ARG VAL ARG THR V1465 T1466 V1467 T1468 L1469 G1470 D1471 E1472 K1473 G1474 K1475 E1478 S1479 I1480 K1481 R1482
S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG ASN ASN N1503 G1504 L1505 E1506 C1509 V1510 V1511 ASP ALA ALA SER G1516 T1519 F1520 K1525 D1526 L1527 S1528 T1529 Y1530 V1533 L1539 V1543 A1547 N1551 E1556 LEU GLY ARG ILE LYS
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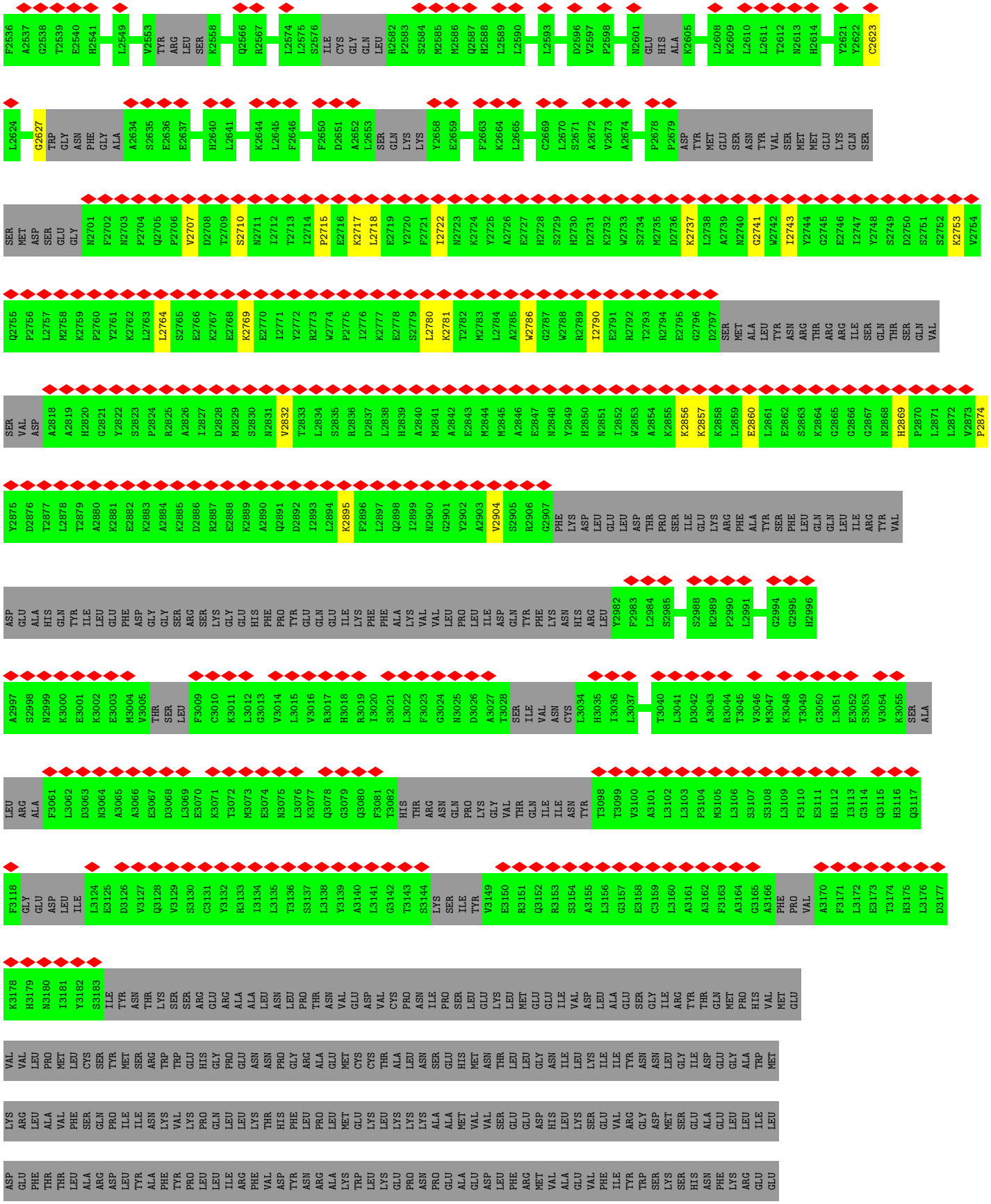
L2124 I2127 M2143 K2154 N2161 R2164 V2177 G2181 GLY GLY GLU SER LYS GLU ILE THR F2190 P2191 K2192 N2196 N2211 D2217 Y2221 S2226 L2230 A2231 S2232 P2233 R2236 L2241 G2274 LEU GLN SER CYS GLN MET LEU VAL SER LYS GLY TYR
PRO ASP ILE GLY TRP ASN P2293 D2301 R2304 F2308 S2313 V2314 E2315 L2324 L2325 I2326 R2327 R2328 PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 L2344 L2345 M2348 E2349 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 A2404 PRO GLU MET HIS LEU ILE HIS ALA ALA LYS GLY E2416 R2419 I2420 R2421 S2422 R2425 SER LEU ILE PRO LEU G2431 V2434 G2435 V2436 I2437 S2438 I2439 Q2442 MET PRO THR ILE ALA LYS ASP
GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 C2462 H2465 K2466 R2475 V2476 Y2477 GLY ILE GLU V2481 L2485 L2486 H2487 L2488 L2489 GLU VAL G2492 F2493 D2496 A2500 L2503 ASP THR ALA ALA LEU SER ALA T2511 C2522 P2527 L2528 L2529 THR ARG CYS ALA PRO LEU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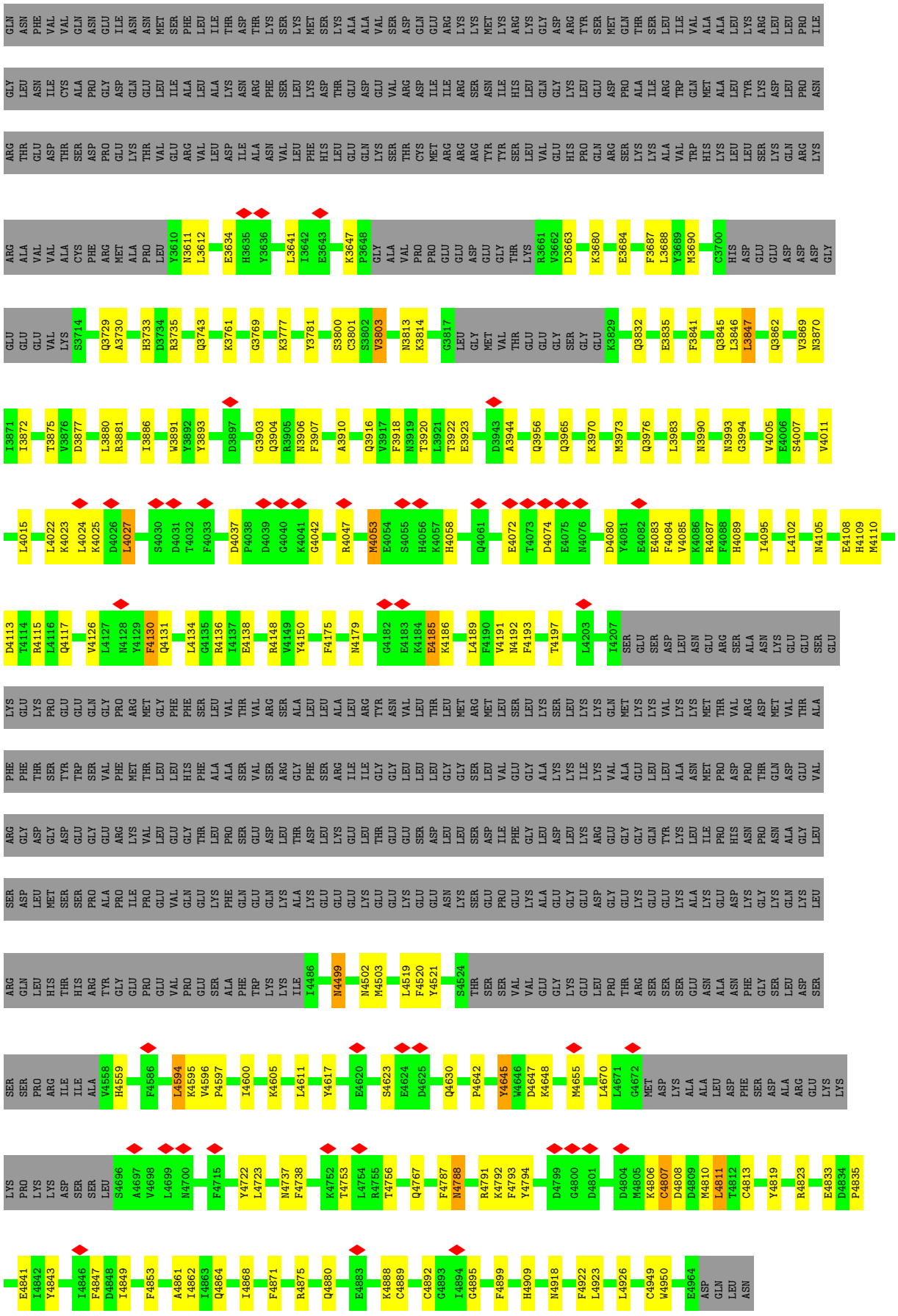
L2624 G2627 TRP GLY ASN PHE GLY ALA A2634 S2635 E2636 E2637 H2640 L2641 K2644 L2645 F2646 F2650 D2651 A2652 L2653 SER GLN LYS LYS Y2658 E2659 F2663 K2664 L2665 C2669 L2670 S2671 A2672 V2673 A2674 P2678 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER
SER MET ASP SER GLU GLY N2701 F2702 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 A2818 A2819 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 F2983 L2984 S2985 S2988 R2989 P2990 L2991 G2994 G2995 H2996
A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 G3013 V3014 L3015 V3016 R3017 H3018 R3019 I3020 S3021 L3022 F3023 G3024 N3025 D3026 A3027 T3028 SER ILE VAL ASN CYS L3034 H3035 I3036 L3037 T3040 L3041 D3042 A3043 R3044 T3045 V3046 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 S3077 Q3078 G3079 Q3080 F3081 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 F3110 E3111 H3112 I3113 G3114 Q3115 K3116 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 E3150 R3151 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 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 SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LEU LYS THR HIS PHE LEU PRO LEU MET VAL LYS SER 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 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 GLU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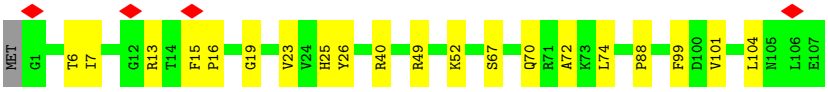
GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN
ARG THR GLU ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU 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 L3612 E3634 H3635 Y3636 L3641 T3642 E3643 K3647 P3648 GLY ALA VAL PRO PRO GLU VAL GLU ASP GLU GLY THR LYS R3661 V3662 D3663 K3680 E3684 F3687 L3688 Y3689 M3690 C3700 HIS ASP GLU GLU ASP ASP ASP GLY
GLU GLU GLU VAL LYS S3714 Q3729 A3730 H3733 D3734 R3735 Q3743 K3761 G3769 K3777 Y3781 S3800 C3801 S3802 V3803 N3813 K3814 G3817 LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU K3829 Q3832 E3835 F3841 Q3845 L3846 L3847 Q3862 V3869 N3870
I3871 I3872 T3875 V3876 D3877 L3880 R3881 I3886 W3891 Y3892 Y3893 D3897 G3903 Q3904 R3905 N3906 F3907 A3910 Q3916 V3917 F3918 N3919 T3920 L3921 T3922 E3923 D3943 A3944 Q3956 Q3965 K3970 M3973 Q3976 L3983 N3990 N3993 G3994 V4005 E4006 S4007 V4011
L4015 L4022 K4023 L4024 K4025 D4026 L4027 S4030 D4031 T4032 F4033 D4037 P4038 D4039 G4040 K4041 G4042 R4047 M4053 E4054 S4055 H4056 K4057 H4058 Q4061 E4072 T4073 D4074 E4075 N4076 D4080 Y4081 E4082 E4083 F4084 V4085 K4086 R4087 F4088 H4089 I4095 L4102 N4105 E4108 H4109 M4110
D4113 T4114 R4115 L4116 Q4117 V4126 L4127 N4128 Y4129 F4130 Q4131 L4134 G4135 R4136 I4137 E4138 R4148 V4149 Y4150 F4175 N4179 G4182 E4183 K4184 E4185 K4186 L4189 F4190 V4191 N4192 F4193 T4197 L4203 I4207 SER GLU SER ASP LEU ASN GLU ARG SER 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 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 THR ALA
PHE PHE THR SER TYR TRP SER VAL PHE MET THR LEU LEU HIS PHE ALA ALA SER VAL SER ARG GLY PHE SER ARG ILE ILE GLY GLY LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL
ARG GLY ASP GLY ASP GLU GLY GLY ARG LYS VAL LEU GLU GLY THR LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY 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 LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU GLU LYS GLU GLU GLU LYS GLU GLU ASN LYS SER GLU PRO GLU LYS ALA GLU GLY LYS GLU ASP GLY GLU LYS GLU GLN LYS LYS GLU ASP ASP LYS GLY LYS GLN LYS LEU
ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA PHE TRP LYS LYS ILE I4486 N4499 N4502 M4503 L4519 F4520 Y4521 S4524 THR SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG SER SER SER GLU ASN ALA ASN PHE GLY SER LEU ASP SER
SER SER PRO ARG ILE ILE ALA V4558 H4559 F4586 L4594 K4595 V4596 P4597 I4600 K4605 L4611 Y4617 E4620 S4623 E4624 D4625 Q4630 P4642 Y4645 W4646 D4647 K4648 M4655 L4670 L4671 G4672 MET ASP LYS ALA ALA LEU ASP PHE SER ASP ALA ARG GLU LYS LYS
LYS PRO LYS LYS ASP SER SER LEU S4696 A4697 V4698 L4699 N4700 F4715 Y4722 L4723 N4737 F4738 K4752 T4753 L4754 R4755 T4756 Q4767 F4787 N4788 R4791 K4792 F4793 Y4794 D4799 G4800 D4801 D4804 M4805 K4806 C4807 D4808 D4809 M4810 L4811 T4812 C4813 Y4819 R4823 E4833 D4834 P4835
E4841 I4842 Y4843 I4846 F4847 D4848 I4849 F4853 A4861 I4862 I4863 Q4864 I4868 F4871 R4875 Q4880 E4883 K4888 C4889 C4892 G4893 I4894 G4895 F4899 H4909 N4918 F4922 L4923 L4926 C4949 W4950 E4964 ASP GLN LEU ASN

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

Chain B:



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

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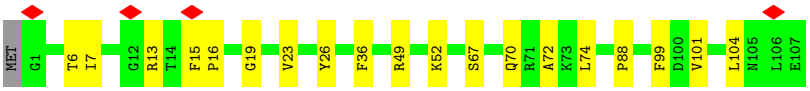
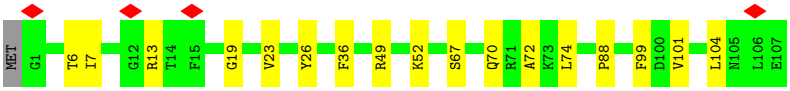


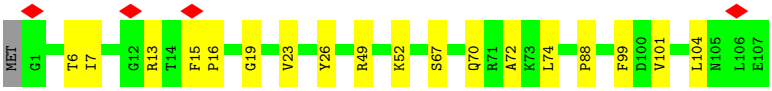
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	78841	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	0.089	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	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: CA, ATP, CFF, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.38	0/27073	0.62	12/36605 (0.0%)
1	C	0.38	0/27073	0.62	12/36605 (0.0%)
1	E	0.38	0/27073	0.62	12/36605 (0.0%)
1	G	0.38	0/27073	0.62	12/36605 (0.0%)
2	B	0.32	0/835	0.55	0/1123
2	D	0.32	0/835	0.55	0/1123
2	F	0.32	0/835	0.55	0/1123
2	H	0.32	0/835	0.55	0/1123
All	All	0.38	0/111632	0.62	48/150912 (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	25
1	C	0	25
1	E	0	25
1	G	0	25
All	All	0	100

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1644	LEU	CA-CB-CG	7.82	133.28	115.30
1	C	1644	LEU	CA-CB-CG	7.82	133.28	115.30
1	E	1644	LEU	CA-CB-CG	7.82	133.28	115.30
1	G	1644	LEU	CA-CB-CG	7.80	133.24	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3846	LEU	CA-CB-CG	6.67	130.65	115.30

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Peptide
1	A	142	LYS	Peptide
1	A	520	ARG	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	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	26577	0	25112	446	0
1	C	26577	0	25112	426	0
1	E	26577	0	25113	426	0
1	G	26577	0	25113	419	0
2	B	819	0	824	11	0
2	D	819	0	824	11	0
2	F	819	0	824	11	0
2	H	819	0	824	10	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	31	0	12	2	0
4	C	31	0	12	1	0
4	E	31	0	12	1	0
4	G	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	14	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
All	All	109772	0	103834	1565	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 7.

The worst 5 of 1565 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:E:4853:PHE:CZ	1:G:4823:ARG:HA	1.53	1.43
1:A:4823:ARG:HA	1:G:4853:PHE:CZ	1.54	1.42
1:C:4853:PHE:CZ	1:E:4823:ARG:HA	1.54	1.41
1:A:4853:PHE:CZ	1:C:4823:ARG:HA	1.54	1.40
1:A:4794:TYR:HD2	1:A:4807:CYS:CB	1.46	1.27

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%)	2912 (87%)	435 (13%)	9 (0%)	41	76
1	C	3356/4968 (68%)	2915 (87%)	432 (13%)	9 (0%)	41	76
1	E	3356/4968 (68%)	2910 (87%)	437 (13%)	9 (0%)	41	76
1	G	3356/4968 (68%)	2912 (87%)	435 (13%)	9 (0%)	41	76
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%)	94 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
All	All	13844/20304 (68%)	12025 (87%)	1783 (13%)	36 (0%)	44	76

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4595	LYS
1	A	4645	TYR
1	C	4595	LYS
1	C	4645	TYR
1	E	4595	LYS

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	2681/4355 (62%)	2641 (98%)	40 (2%)	65	80
1	C	2680/4355 (62%)	2643 (99%)	37 (1%)	67	80
1	E	2682/4355 (62%)	2643 (98%)	39 (2%)	65	80
1	G	2681/4355 (62%)	2642 (98%)	39 (2%)	65	80
2	B	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	D	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	F	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	H	88/89 (99%)	87 (99%)	1 (1%)	73	84
All	All	11076/17776 (62%)	10917 (99%)	159 (1%)	68	80

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4792	LYS
1	G	3870	ASN
1	G	44	ASN
1	G	950	VAL

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Mol	Chain	Res	Type
1	G	4185	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	745	ASN
1	E	3990	ASN
1	E	1149	ASN
1	E	1941	GLN
1	G	84	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	CFF	E	5103	-	8,15,15	2.62	3 (37%)	8,23,23	1.29	1 (12%)
4	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.45	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	A	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.45	4 (12%)
4	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.45	5 (16%)
6	CFF	C	5103	-	8,15,15	2.61	3 (37%)	8,23,23	1.30	1 (12%)
4	ATP	C	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.45	4 (12%)
6	CFF	G	5103	-	8,15,15	2.63	3 (37%)	8,23,23	1.30	1 (12%)
6	CFF	A	5103	-	8,15,15	2.62	3 (37%)	8,23,23	1.30	1 (12%)

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
6	CFF	E	5103	-	-	-	0/2/2/2
4	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
4	ATP	A	5101	-	-	4/18/38/38	0/3/3/3
4	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
4	ATP	C	5101	-	-	4/18/38/38	0/3/3/3
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	A	5103	-	-	-	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5103	CFF	C5-C4	-4.74	1.33	1.39
6	E	5103	CFF	C5-C4	-4.74	1.33	1.39
6	G	5103	CFF	C5-C4	-4.74	1.33	1.39
6	C	5103	CFF	C5-C4	-4.69	1.33	1.39
6	G	5103	CFF	C6-N1	-4.58	1.31	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	C	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	E	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	G	5101	ATP	PA-O3A-PB	-3.52	120.74	132.83
4	A	5101	ATP	PB-O3B-PG	-3.13	122.08	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5101	ATP	PB-O3A-PA-O1A
4	A	5101	ATP	PB-O3A-PA-O2A
4	C	5101	ATP	PB-O3A-PA-O1A
4	C	5101	ATP	PB-O3A-PA-O2A
4	E	5101	ATP	PB-O3A-PA-O1A

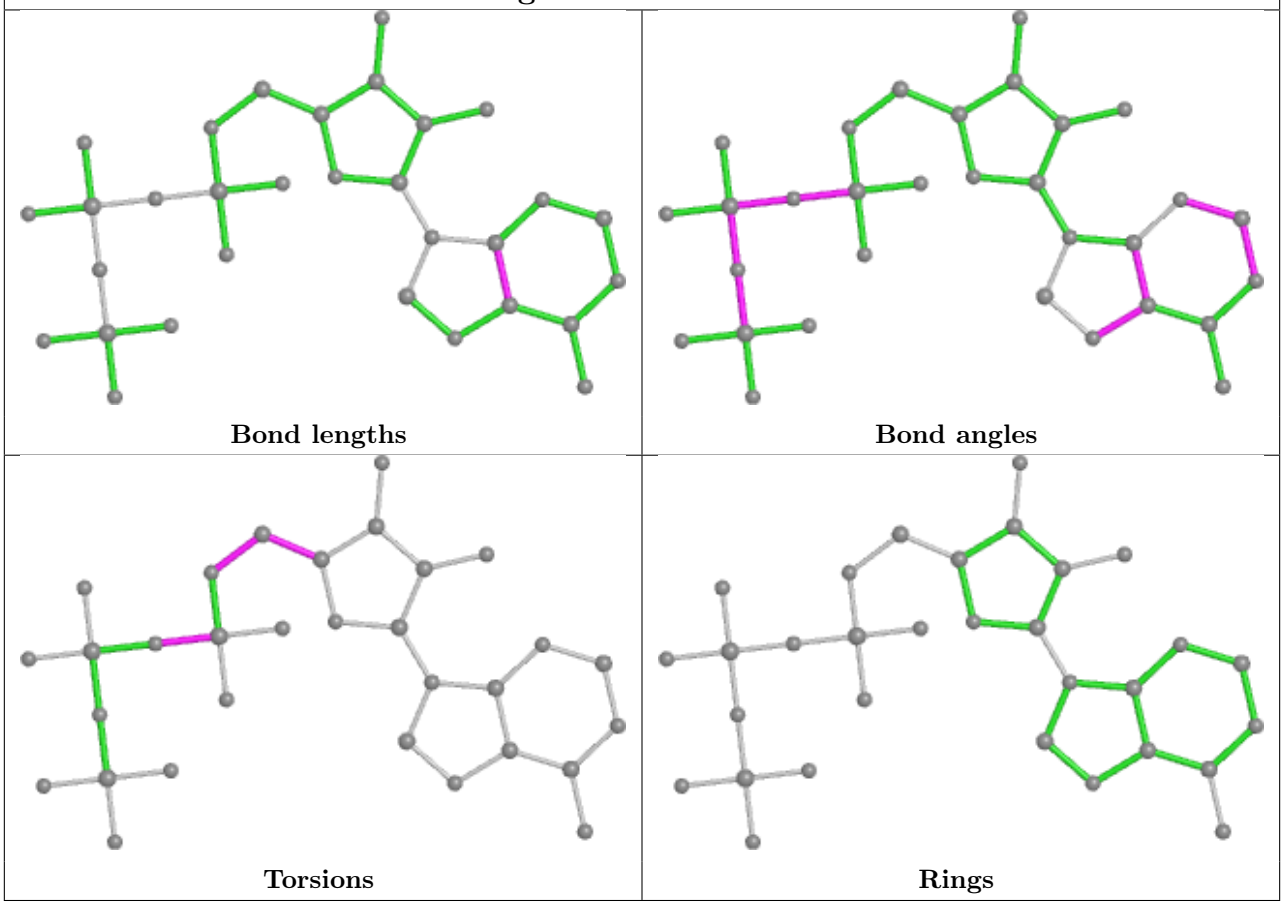
There are no ring outliers.

4 monomers are involved in 5 short contacts:

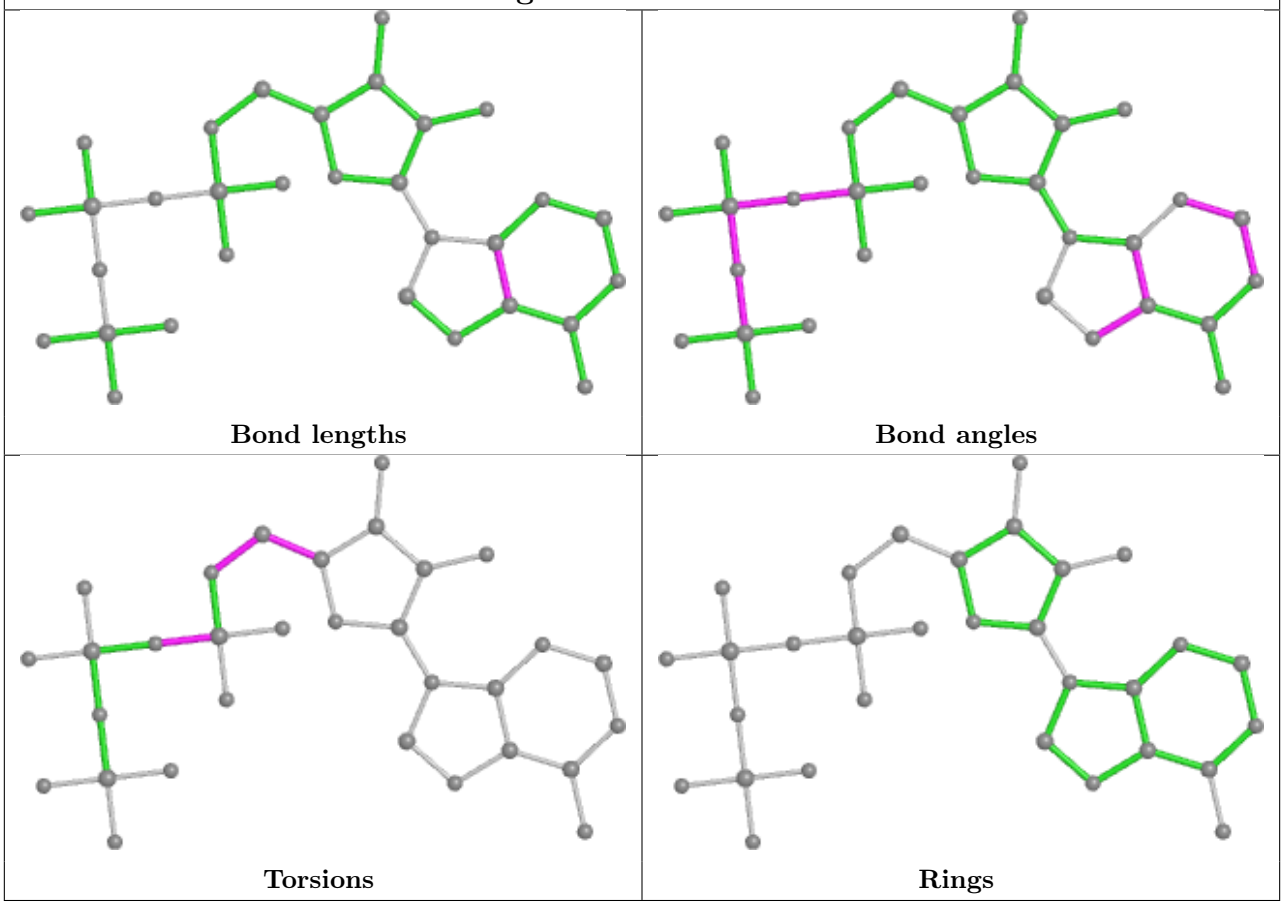
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5101	ATP	1	0
4	A	5101	ATP	2	0
4	G	5101	ATP	1	0
4	C	5101	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

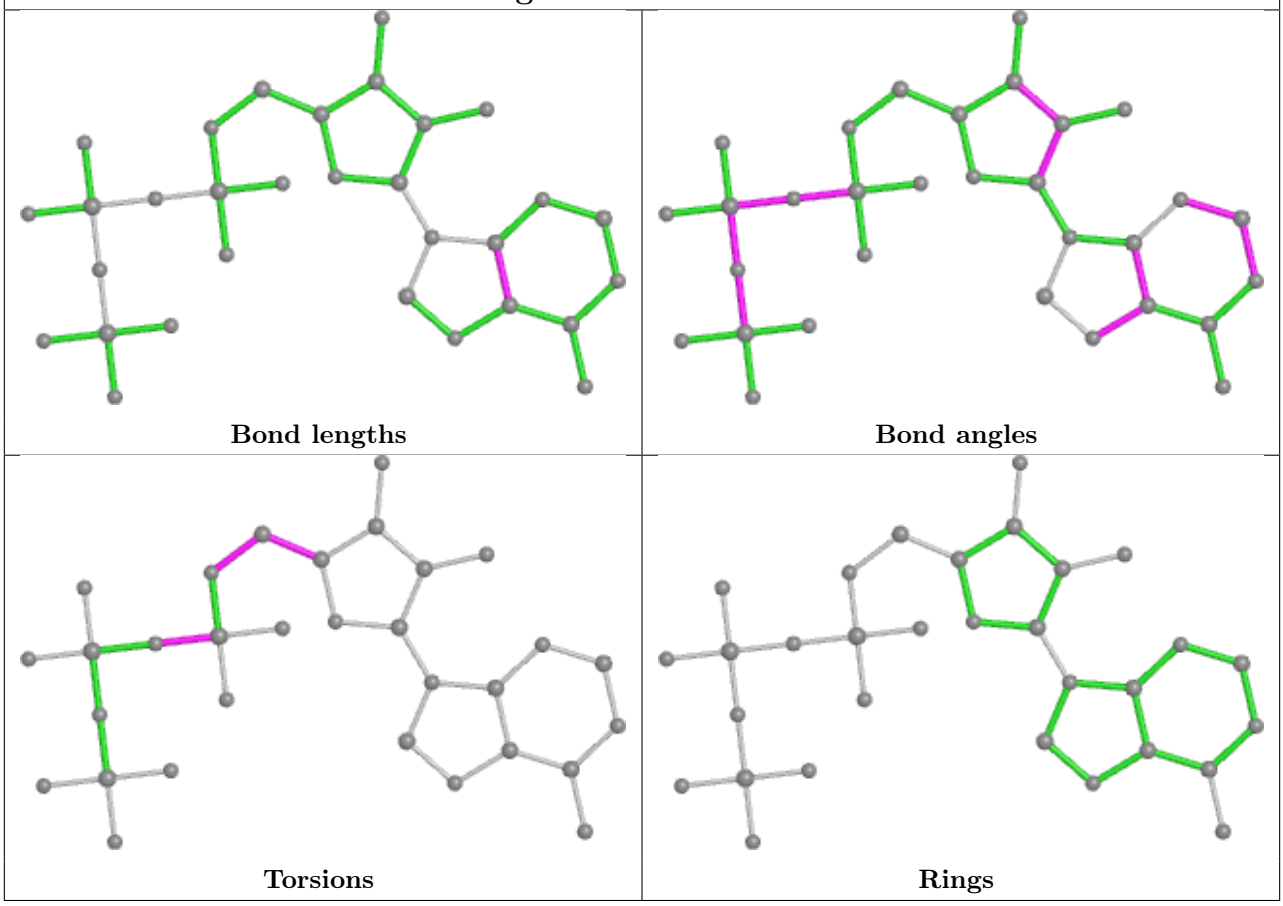
Ligand ATP E 5101

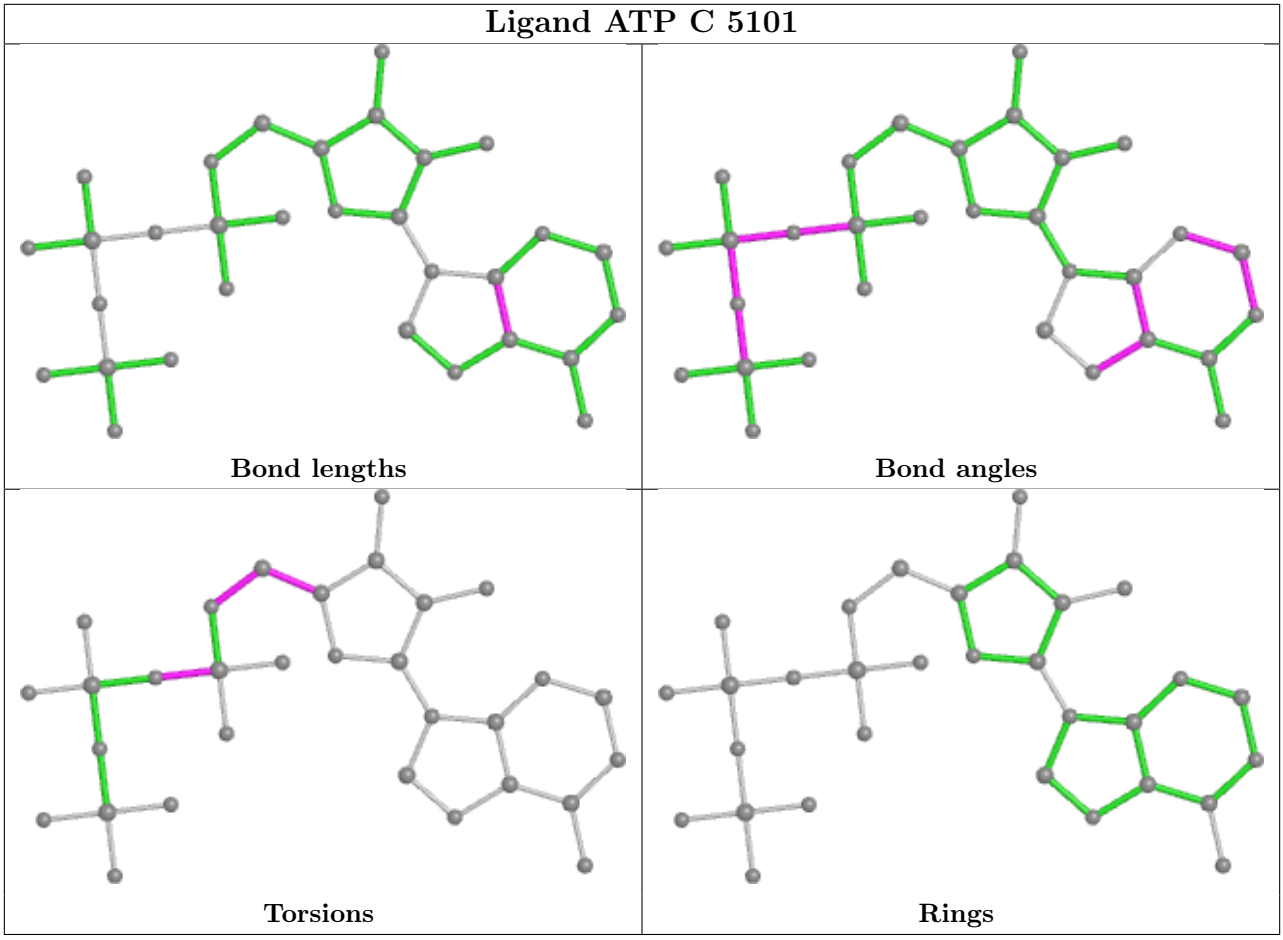


Ligand ATP A 5101



Ligand ATP G 5101





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.

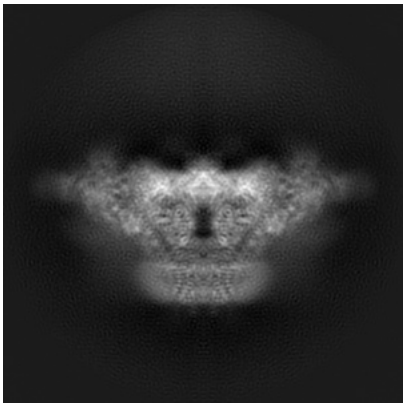
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9831. These allow visual inspection of the internal detail of the map and identification of artifacts.

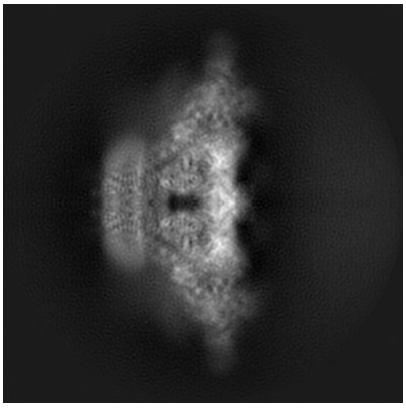
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

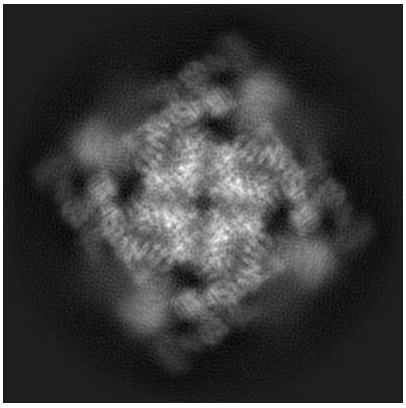
6.1.1 Primary map



X



Y

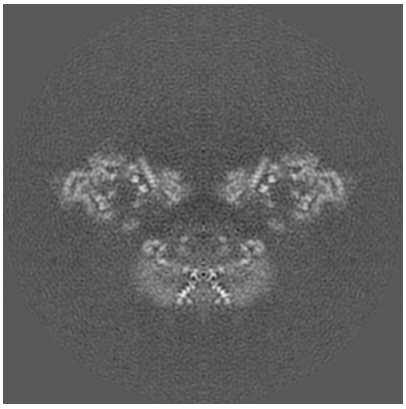


Z

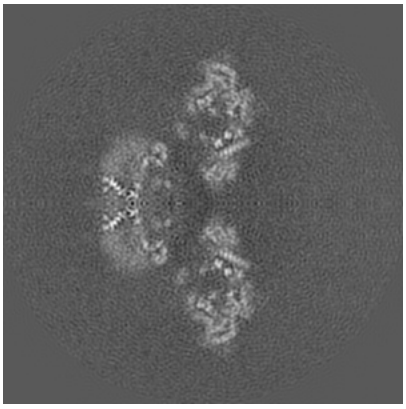
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

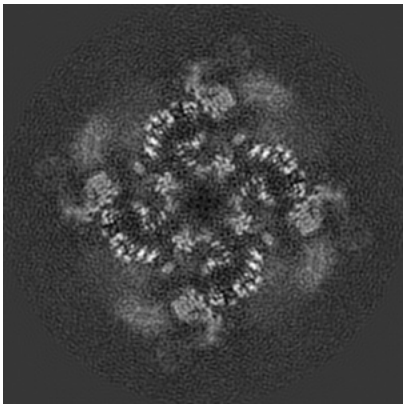
6.2.1 Primary map



X Index: 200



Y Index: 200

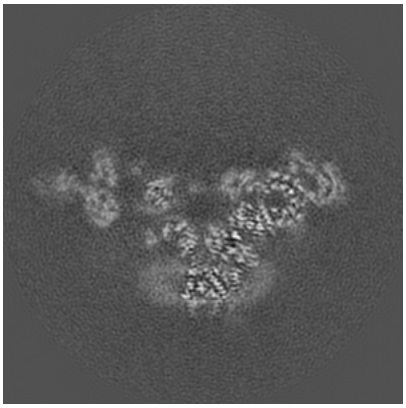


Z Index: 200

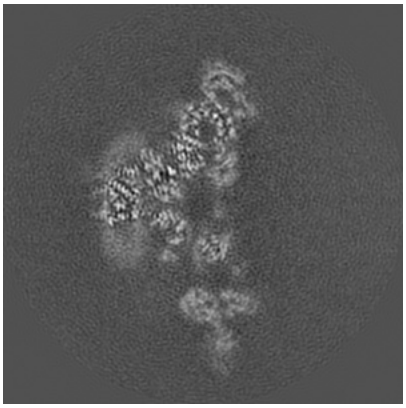
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

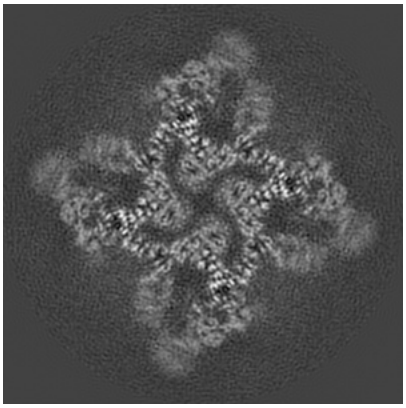
6.3.1 Primary map



X Index: 186



Y Index: 214

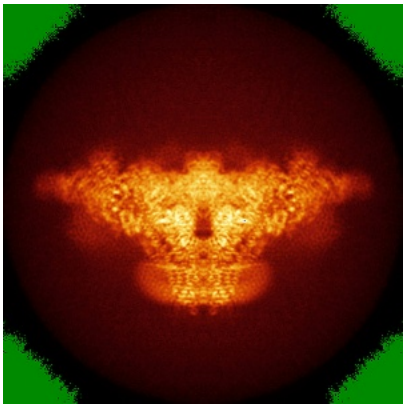


Z Index: 217

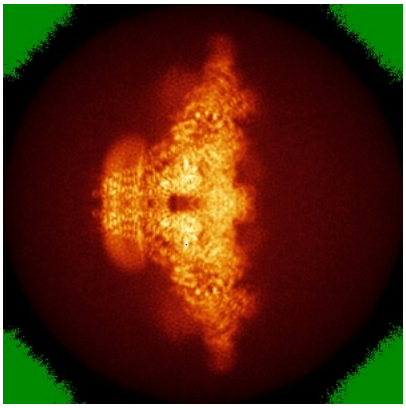
The images above show the largest variance slices of the map in three orthogonal directions.

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

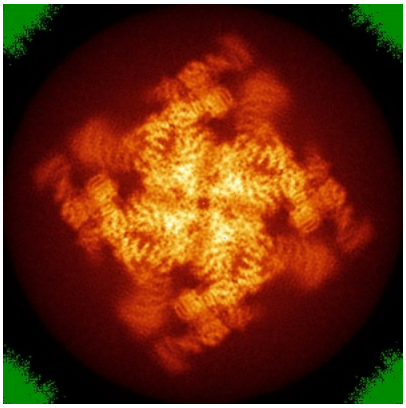
6.4.1 Primary map



X



Y

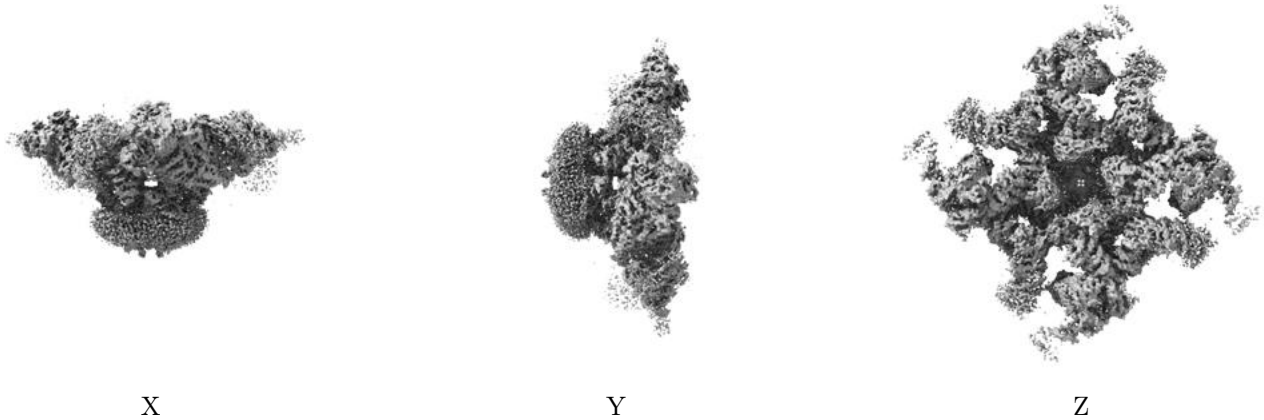


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

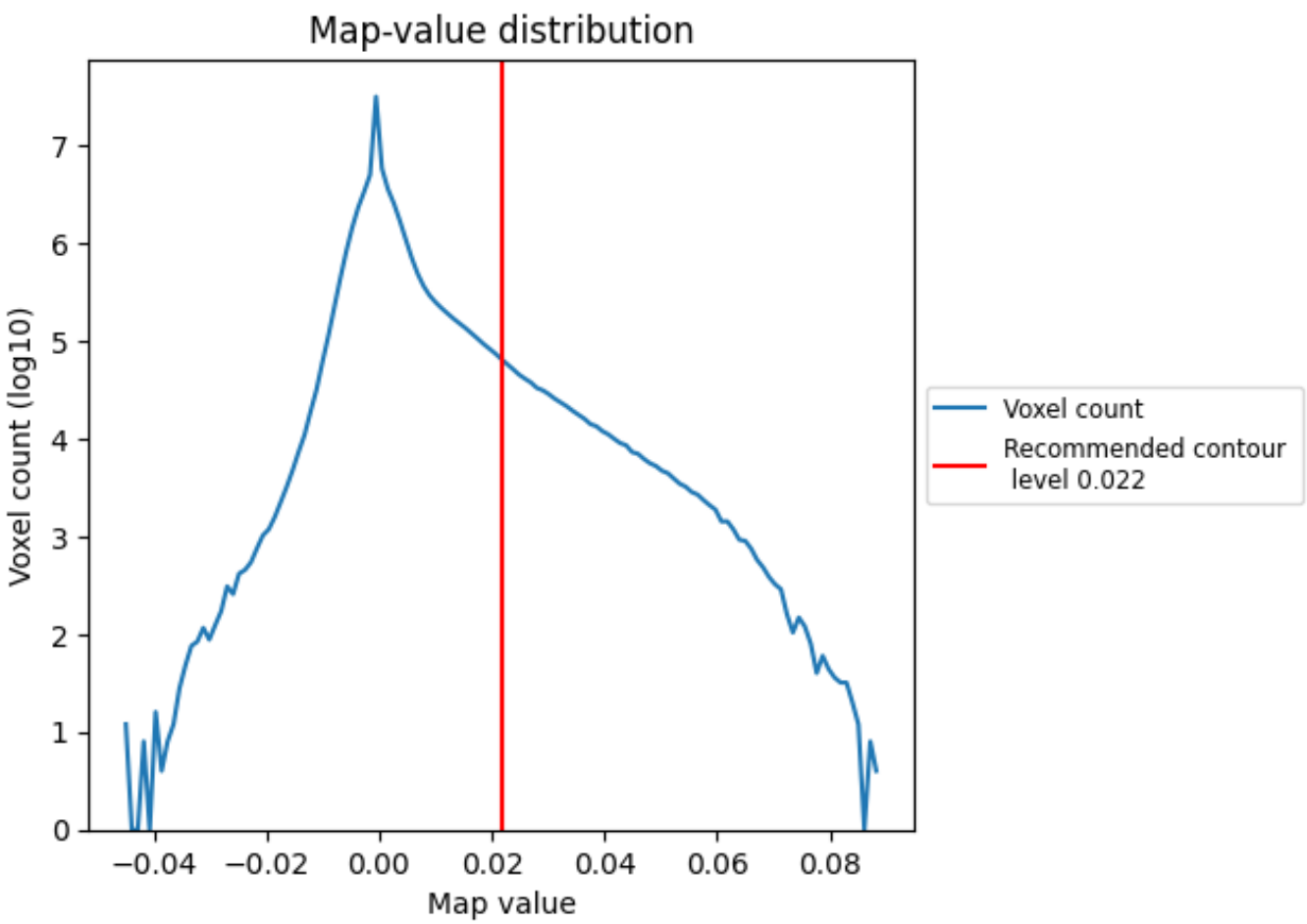
6.6 Mask visualisation (i)

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

7 Map analysis (i)

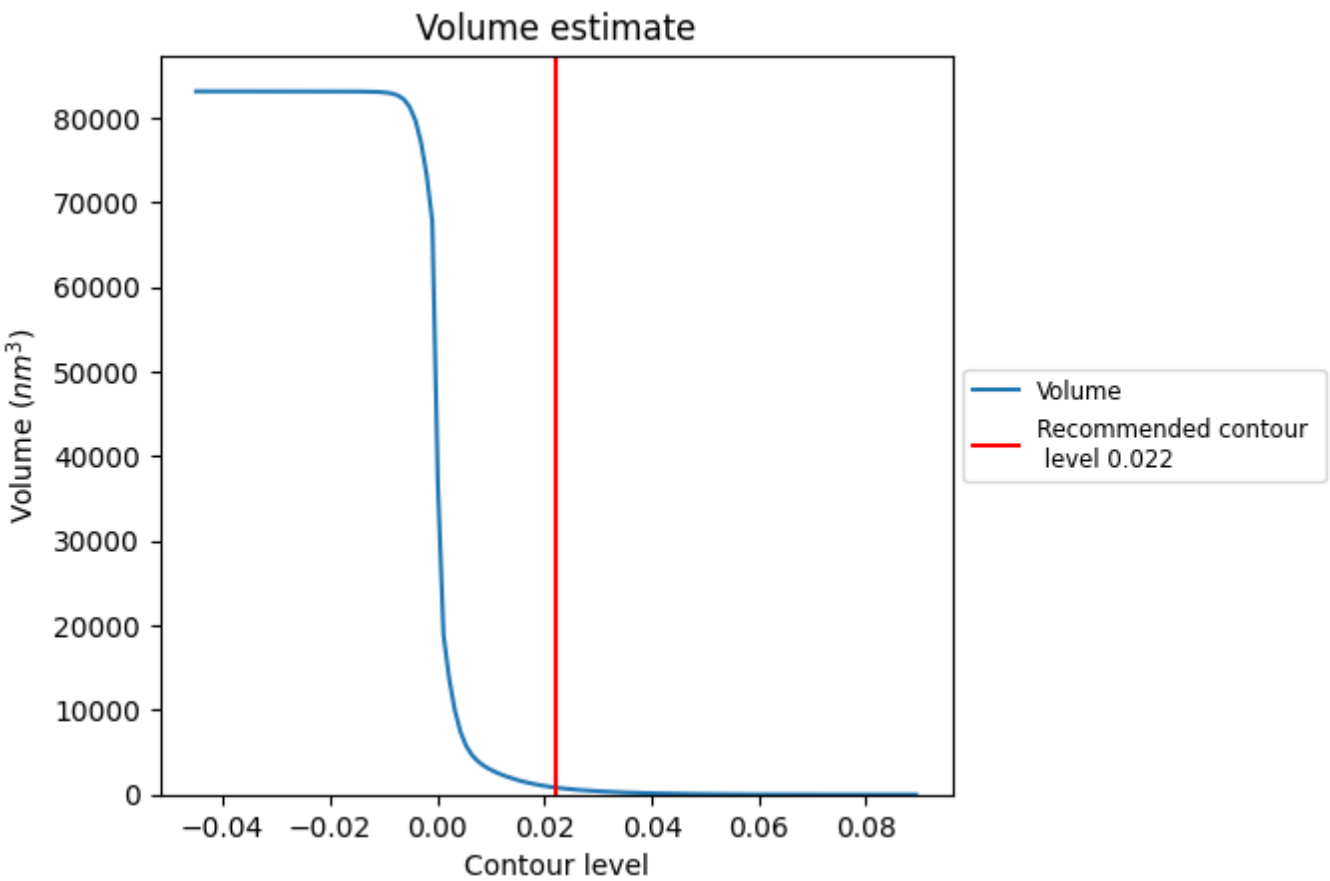
This section contains the results of statistical analysis of the map.

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.

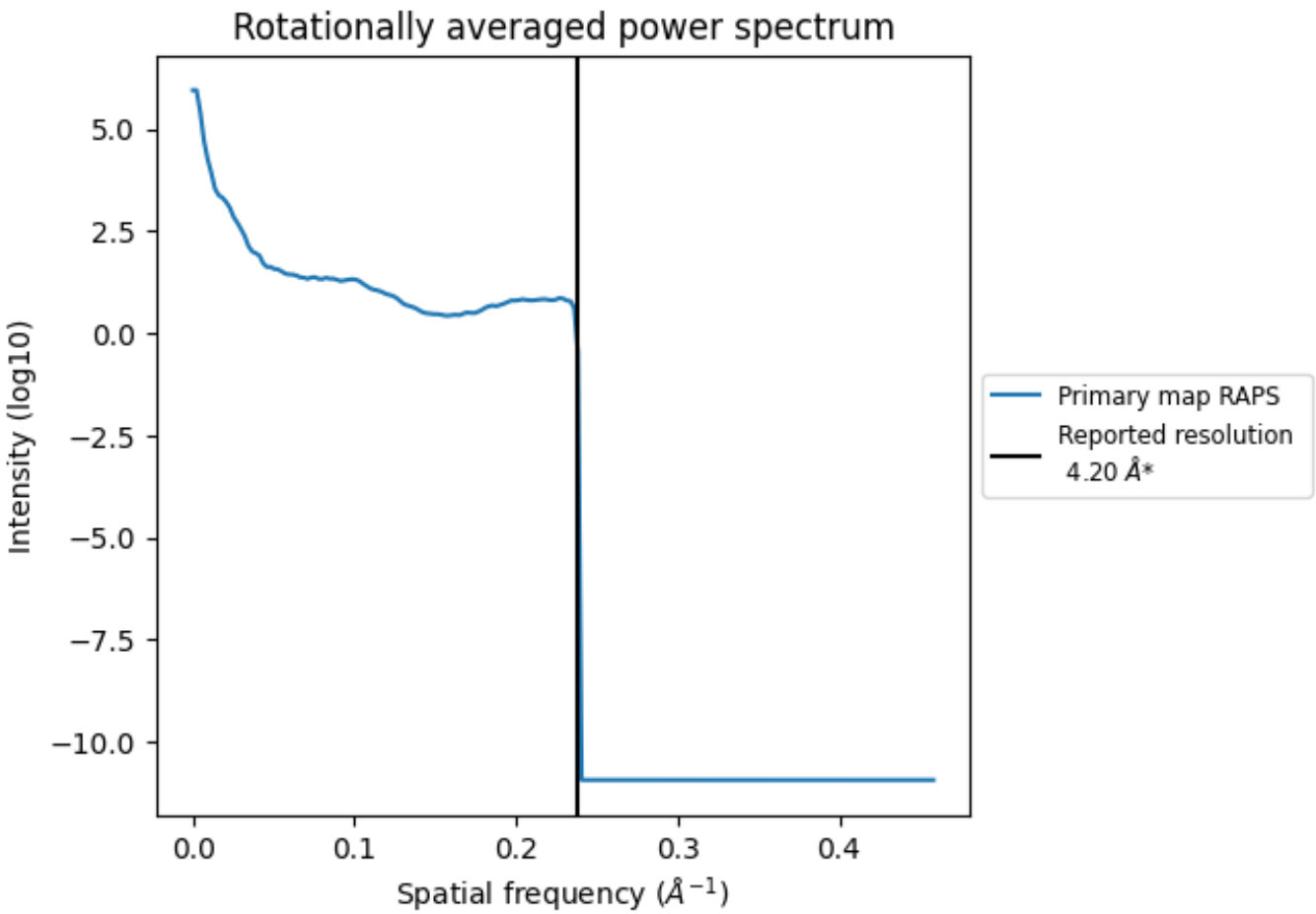
7.2 Volume estimate (i)



The volume at the recommended contour level is 836 nm^3; this corresponds to an approximate mass of 755 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)

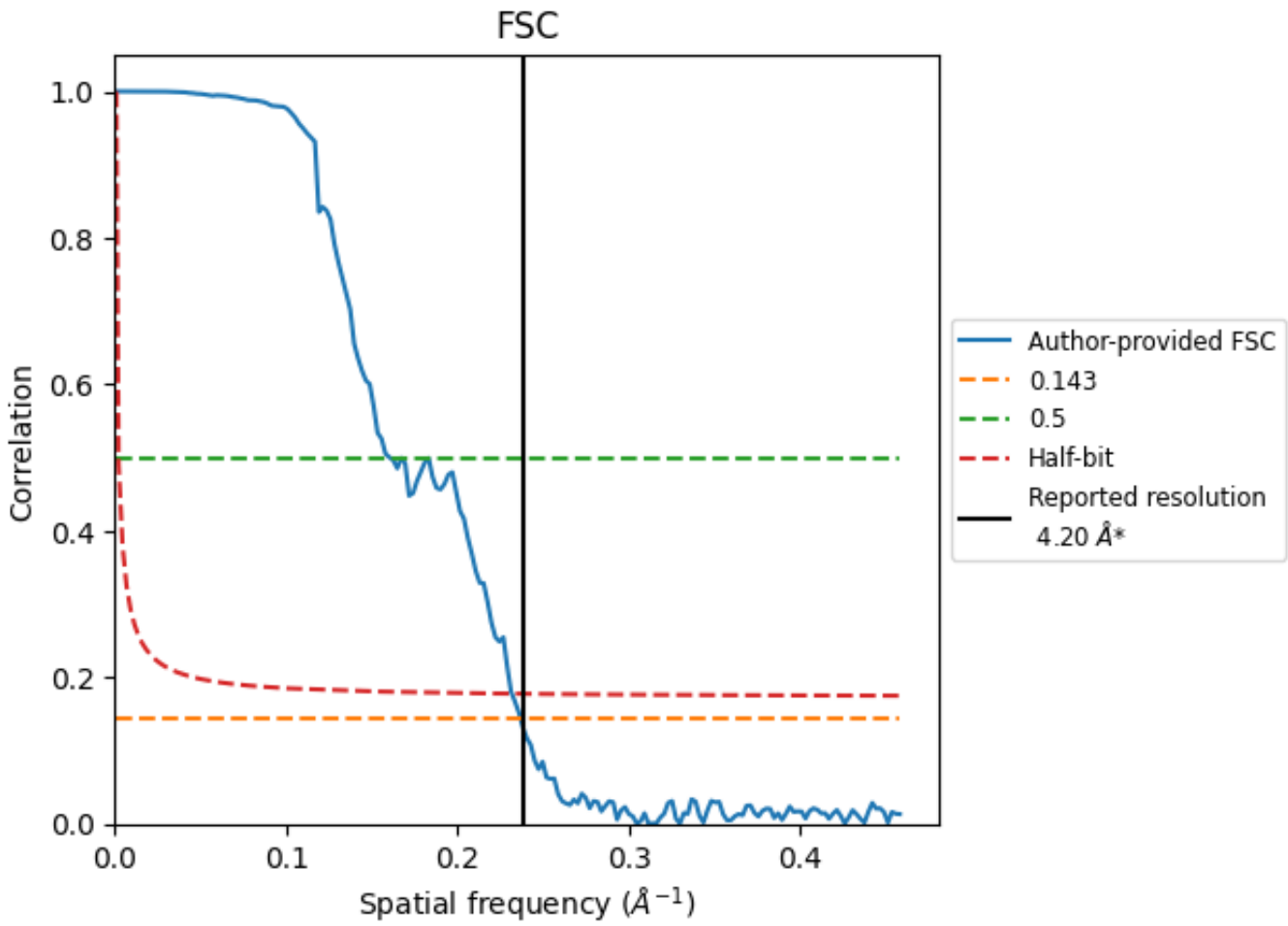


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (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 0.238 Å^{-1}

8.2 Resolution estimates (i)

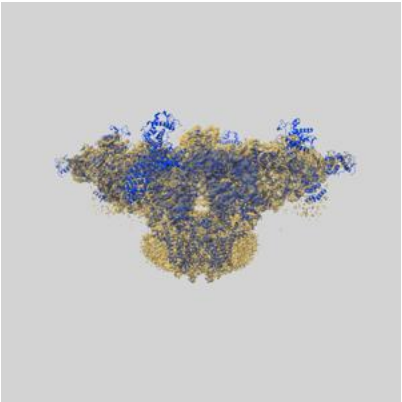
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	6.23	4.31
Unmasked-calculated*	-	-	-

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

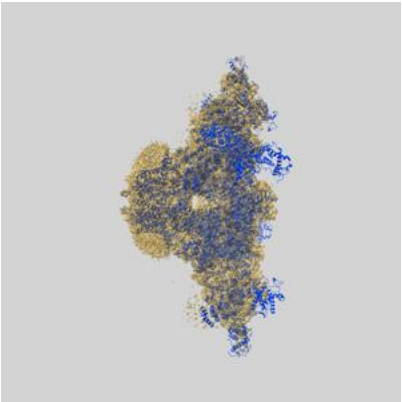
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9831 and PDB model 6JI0. Per-residue inclusion information can be found in section 3 on page 6.

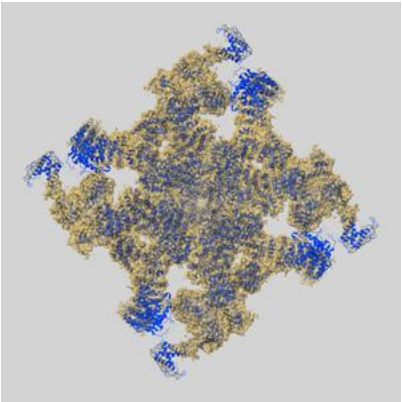
9.1 Map-model overlay (i)



X



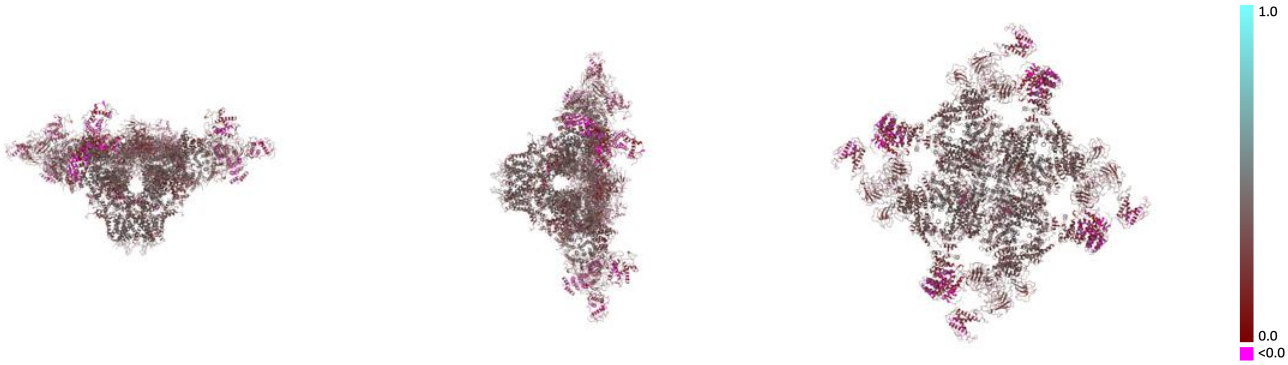
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

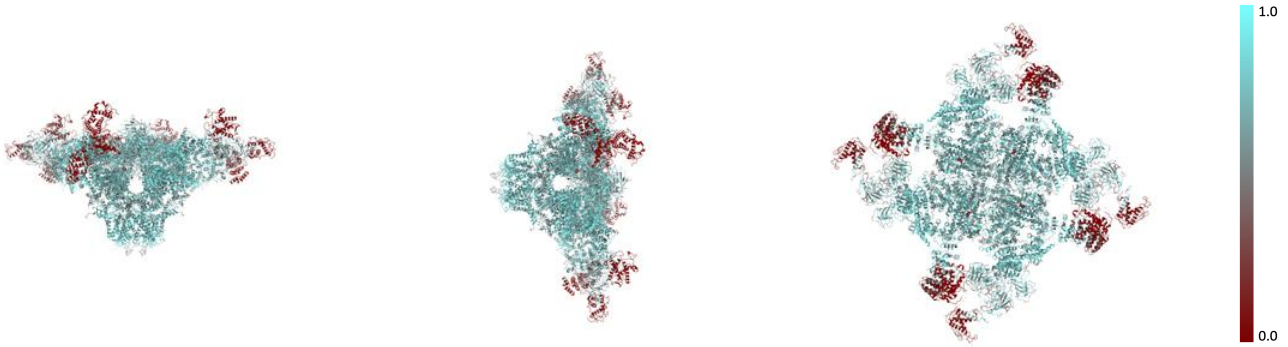
9.2 Q-score mapped to coordinate model (i)



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.

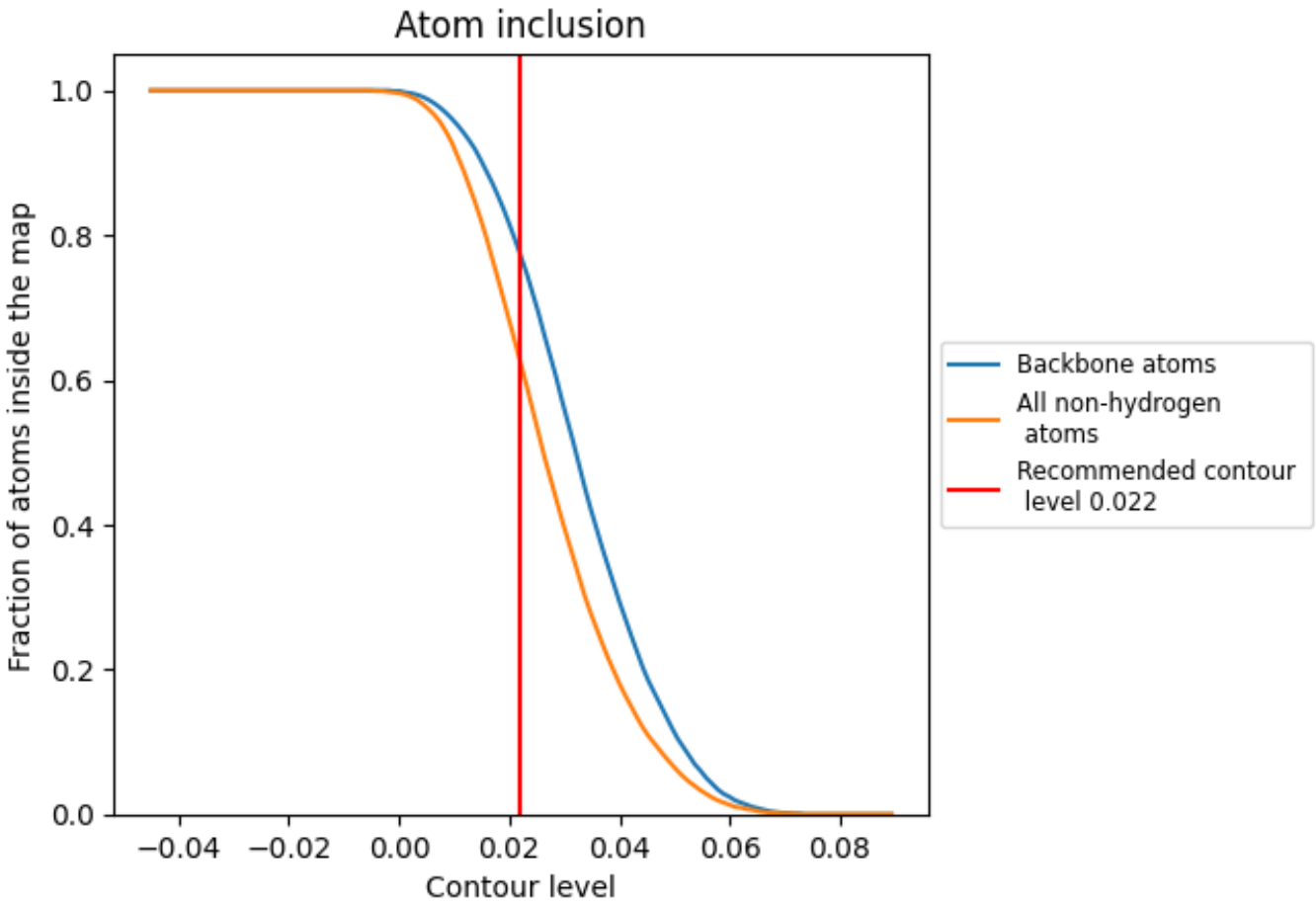
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 63% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.3220
A	0.6250	0.3220
B	0.6630	0.3270
C	0.6250	0.3220
D	0.6630	0.3280
E	0.6250	0.3210
F	0.6630	0.3250
G	0.6250	0.3210
H	0.6650	0.3240