wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 07:05 AM EST

PDB ID	:	7M6A
EMDB ID	:	EMD-23692
Title	:	High resolution structure of the membrane embedded skeletal muscle ryanodine receptor
Authors	:	Melville, Z.; Kim, K.; Clarke, O.B.; Marks, A.R.
Deposited on	:	2021-03-25
Resolution	:	3.36 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

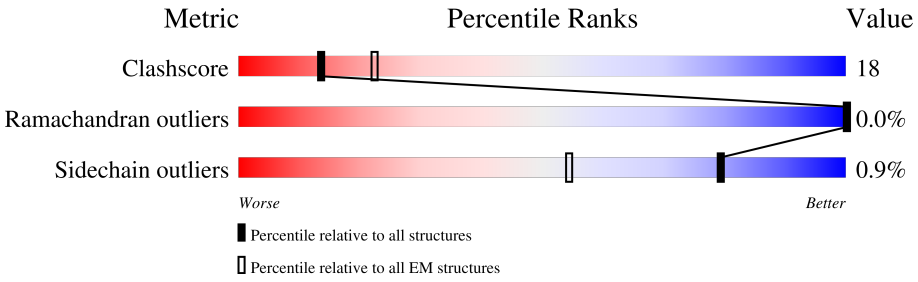
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.36 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	F	108	67% 29%
1	H	108	67% 30%
1	J	108	69% 28%
1	O	108	68% 28%
2	A	5037	11% 60% 25% 15%
2	B	5037	11% 60% 25% 15%
2	G	5037	11% 60% 25% 15%
2	I	5037	11% 60% 25% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 140632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

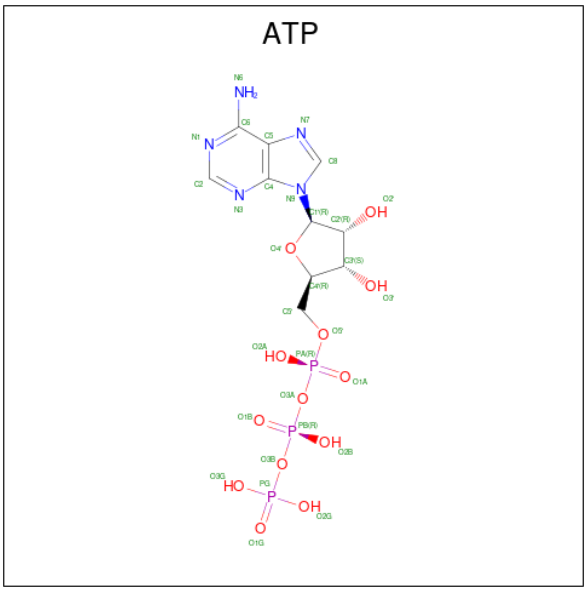
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	G	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	B	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	I	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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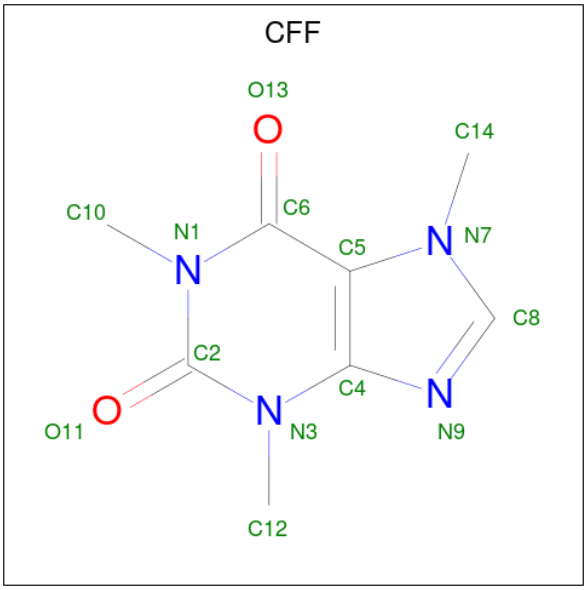
Mol	Chain	Residues	Atoms	AltConf
5	G	1	Total Zn 1 1	0
5	B	1	Total Zn 1 1	0
5	I	1	Total Zn 1 1	0

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



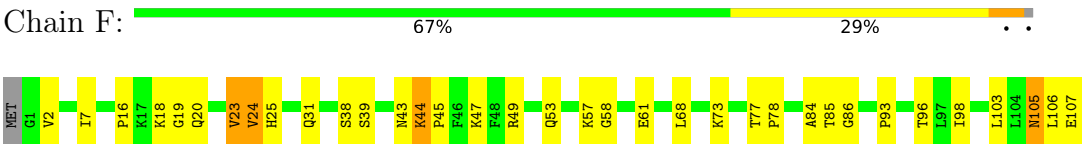
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 14 8 4 2	0
6	G	1	Total C N O 14 8 4 2	0
6	B	1	Total C N O 14 8 4 2	0
6	I	1	Total C N O 14 8 4 2	0

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.

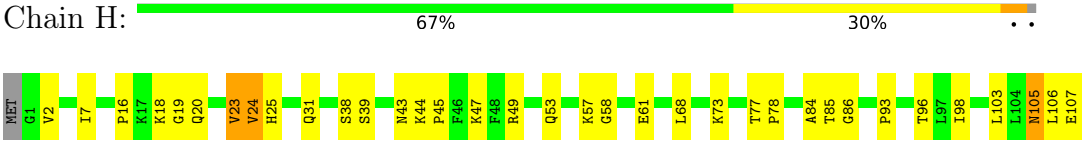
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



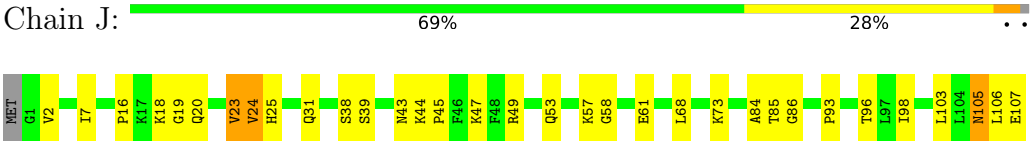
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



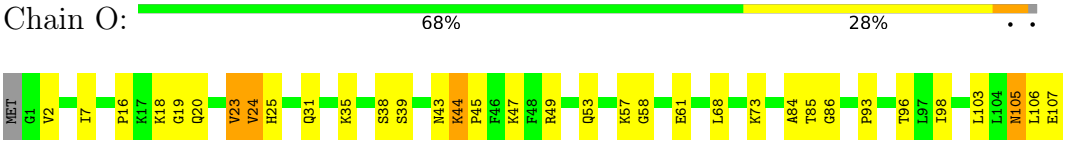
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:



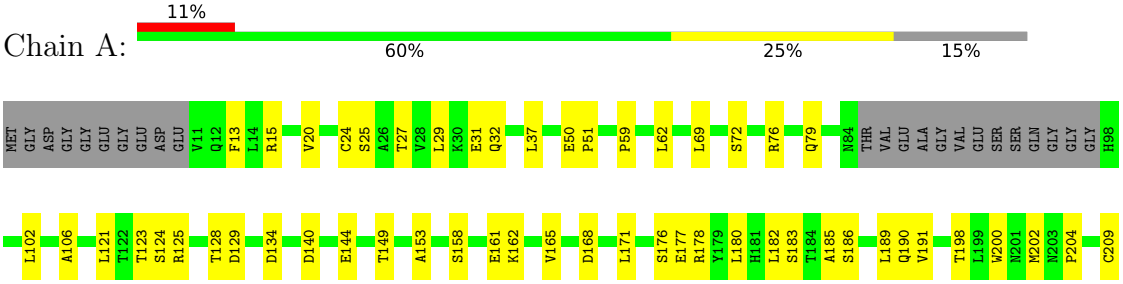
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

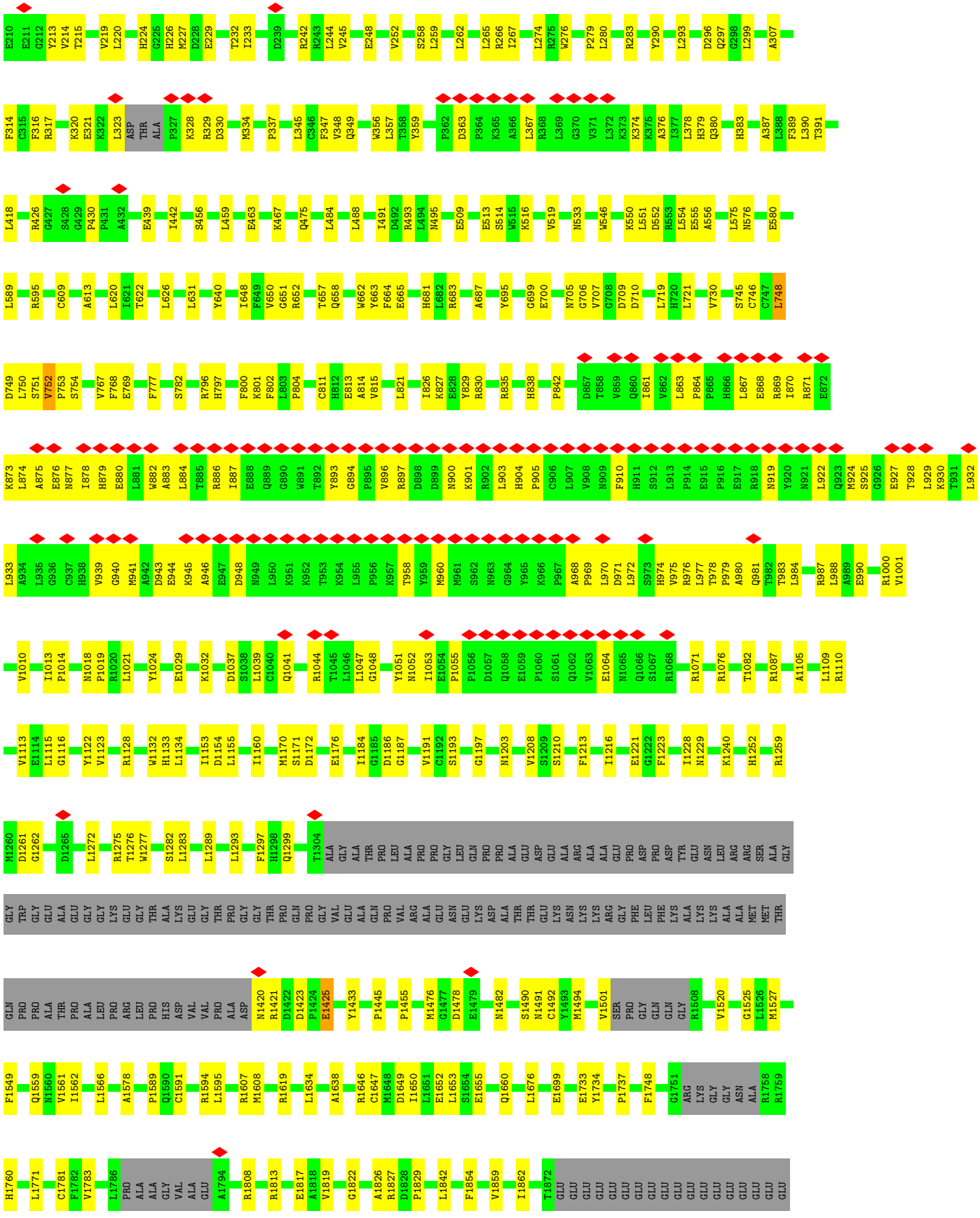
Chain O:

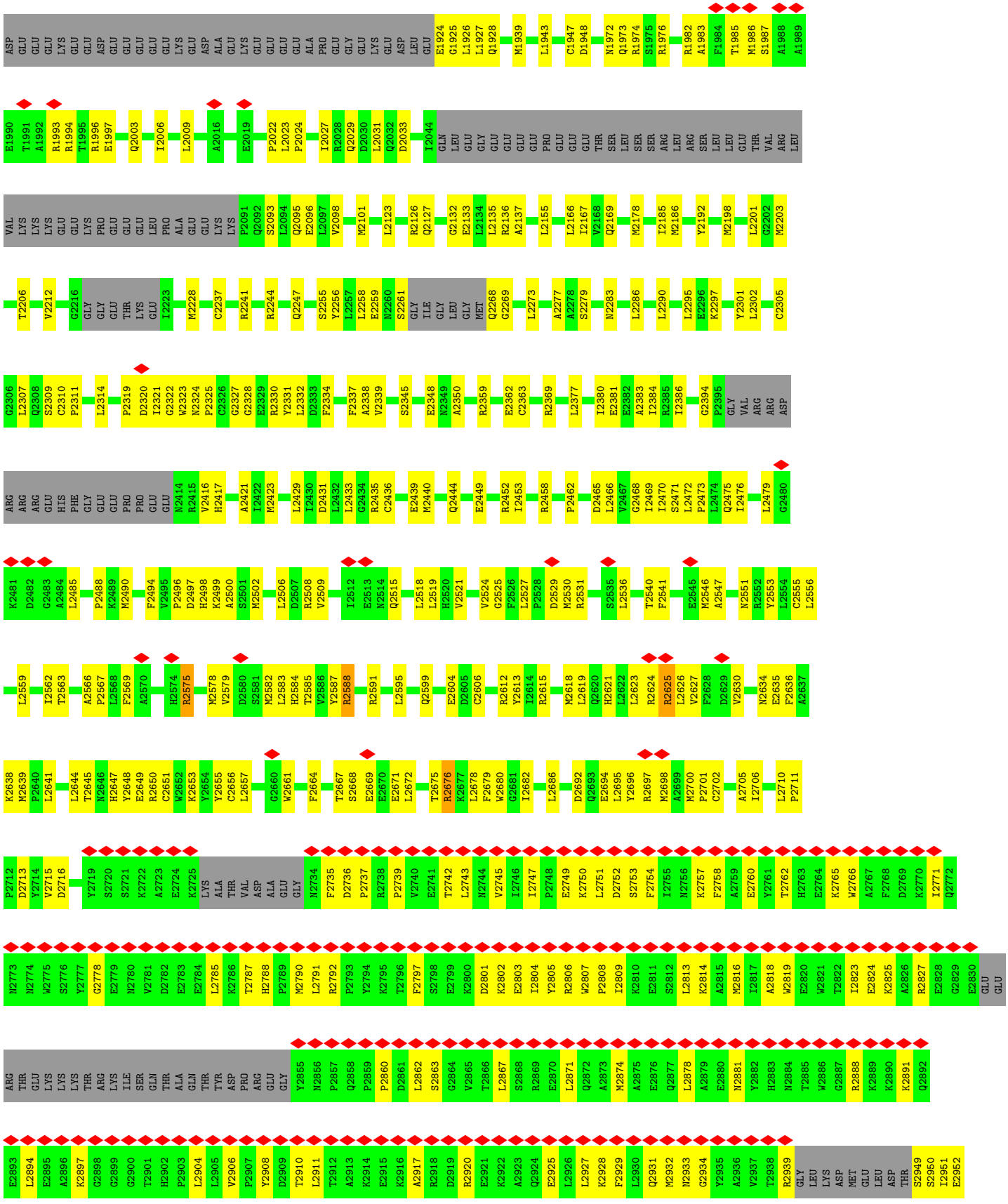


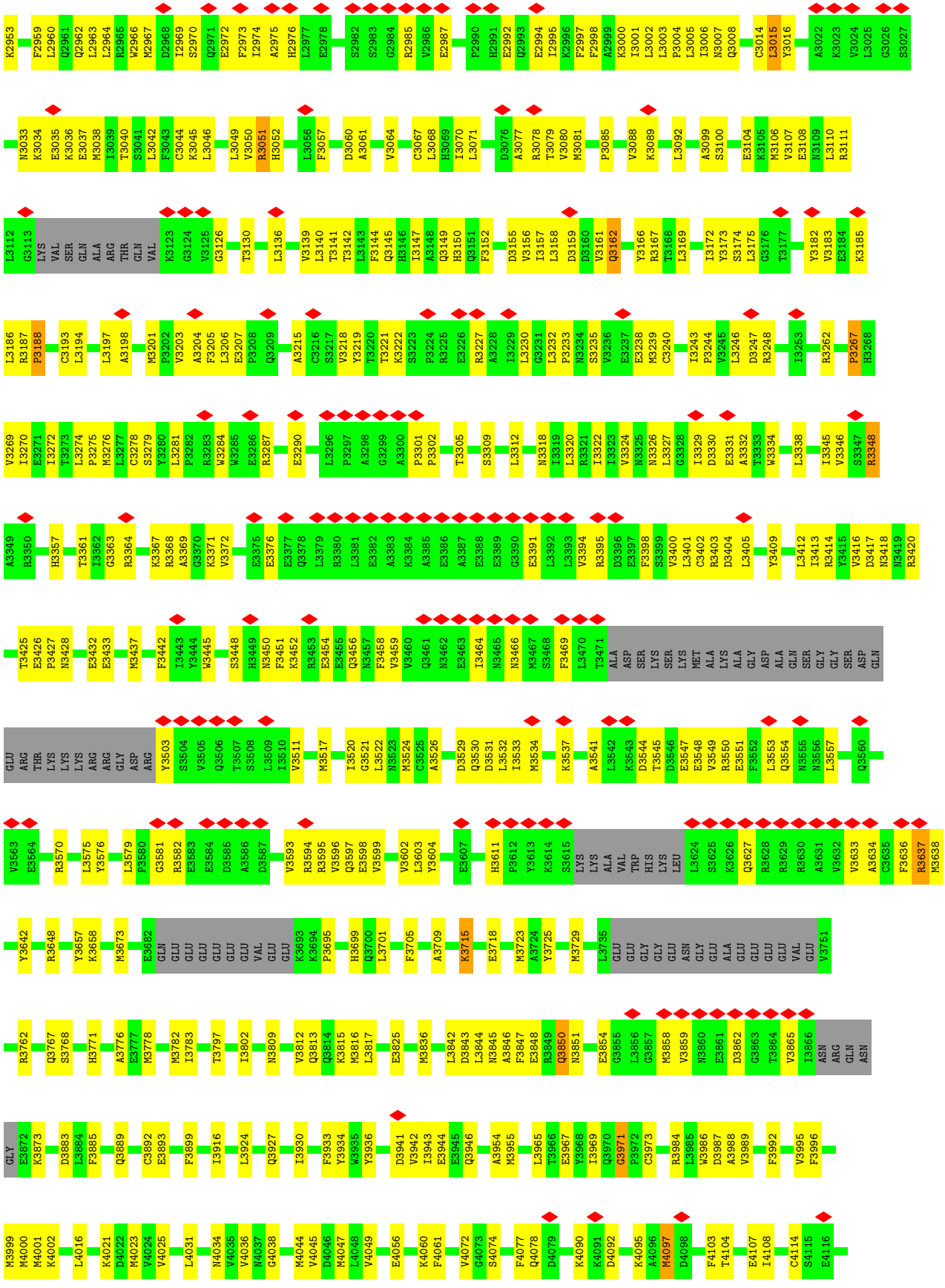
• Molecule 2: Ryanodine receptor 1

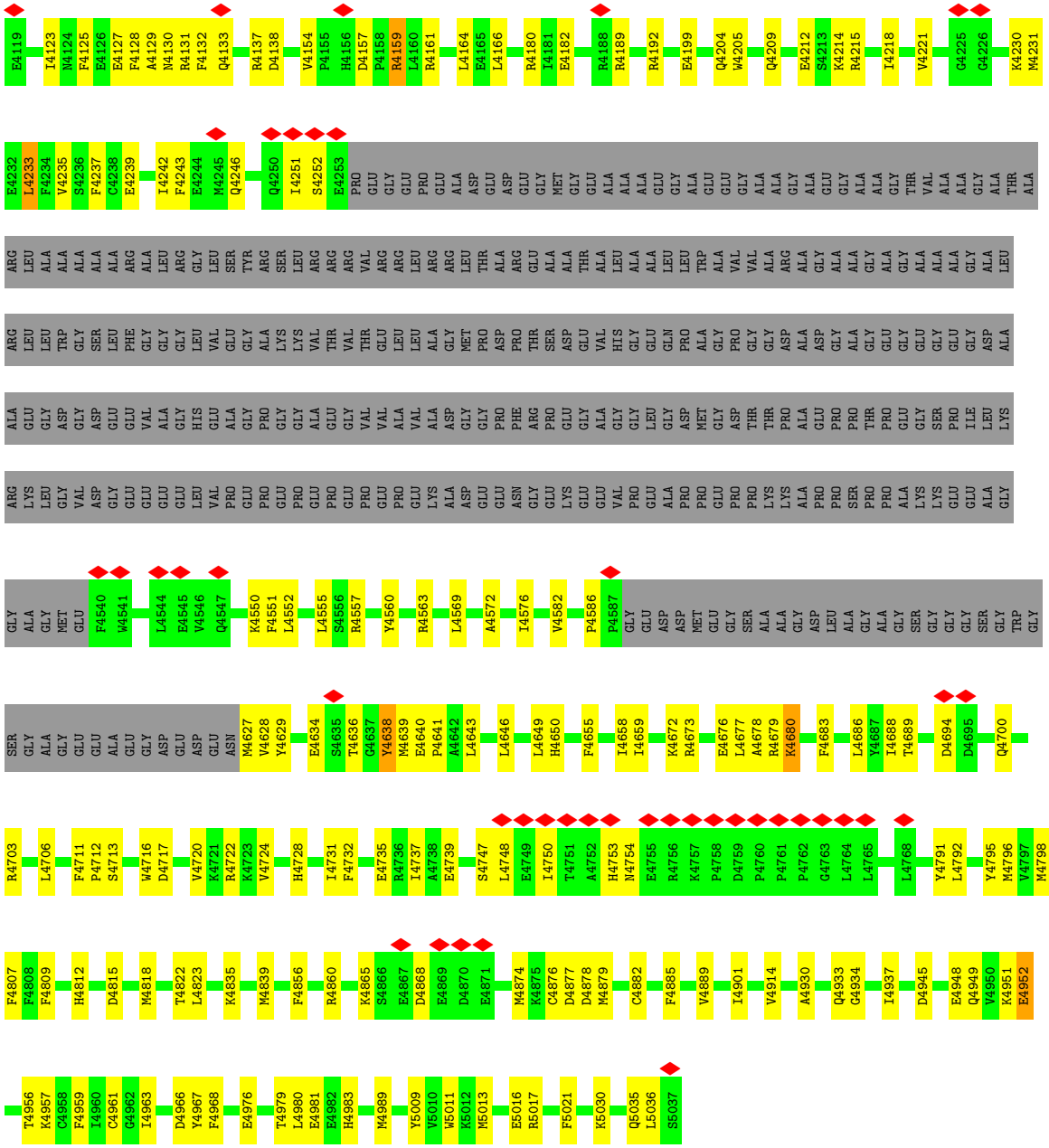
Chain A:





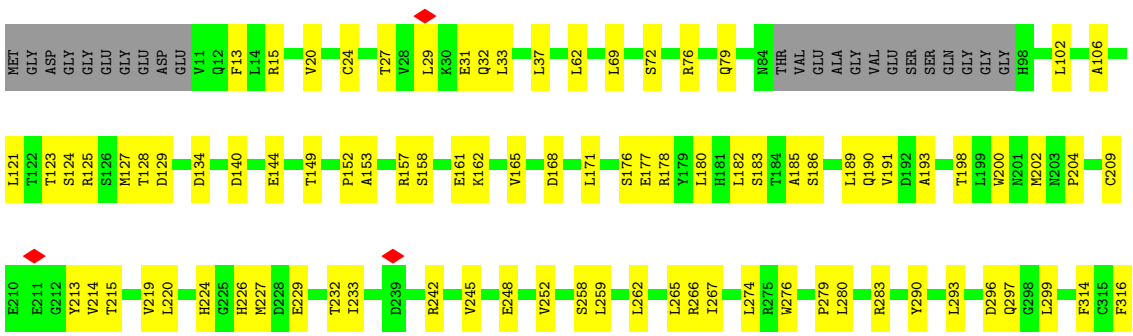

ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU
E1924 G1925 L1926 L1927 Q1928 M1939 L1943 C1947 D1948 N1972 Q1973 R1974 S1975 R1976 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989
E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 Q2003 I2006 L2009 A2016 E2019 P2022 L2023 P2024 I2027 R2028 Q2029 D2030 L2031 Q2032 D2033 I2044
GLN LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU
VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS
P2091 Q2092 S2093 L2094 Q2095 E2096 L2097 V2098 M2101 L2123 R2126 Q2127 G2132 E2133 L2134 L2135 R2136 A2137 L2155 L2166 I2167 V2168 Q2169 M2178 I2185 M2186 Y2192 M2198 L2201 G2202 M2203
T2206 V2212 G2216 GLY GLY GLU THR LYS GLU I2223 M2228 C2237 R2241 R2244 Q2247 S2255 Y2256 L2257 L2258 E2259 N2260 S2261 GLY ILE GLY LEU GLY MET Q2268 G2269 L2273 A2277 A2278 S2279 N2283 L2286 L2290 L2295 E2296 K2297 Y2301 L2302 C2305
G2306 L2307 Q2308 S2309 C2310 P2311 L2314 P2319 D2320 I2321 G2322 W2323 N2324 P2325 C2326 G2327 G2328 E2329 R2330 Y2331 L2332 D2333 F2334 F2337 A2338 V2339 S2345 E2348 N2349 A2350 R2359 E2362 C2363 R2369 L2377 I2380 E2381 E2382 A2383 I2384 R2385 I2386 G2394 P2395 GLY VAL ARG ARG ASP
ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 A2421 I2422 M2423 L2429 I2430 D2431 L2432 L2433 G2434 R2435 C2436 E2439 M2440 Q2444 E2449 R2452 I2453 R2458 P2462 D2465 L2466 V2467 G2468 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 L2479 G2480
K2481 D2482 G2483 A2484 L2485 P2488 K2489 M2490 F2494 V2495 P2496 D2497 H2498 K2499 A2500 S2501 M2502 L2506 D2507 R2508 V2509 I2512 E2513 N2514 Q2515 L2518 L2519 H2520 V2521 V2524 G2525 F2526 L2527 P2528 D2529 M2530 R2531 S2535 L2536 T2540 F2541 E2545 M2546 A2547 N2551 R2552 Y2553 L2554 C2555 L2556
L2559 I2562 T2563 A2566 P2567 L2568 F2569 A2570 H2574 R2575 M2578 V2579 D2580 S2581 M2582 L2583 H2584 T2585 V2586 Y2587 R2588 R2591 L2595 Q2599 E2604 D2605 C2606 R2612 Y2613 I2614 R2615 M2618 L2619 Q2620 H2621 L2622 L2623 R2624 R2625 L2626 V2627 F2628 D2629 V2630 N2634 E2635 F2636 A2637
K2638 M2639 P2640 L2641 L2644 T2645 N2646 H2647 Y2648 E2649 R2650 C2651 W2652 K2653 Y2654 Y2655 C2656 L2657 G2660 W2661 F2664 T2667 S2668 E2669 E2670 E2671 L2672 T2675 R2676 K2677 L2678 F2679 W2680 G2681 I2682 L2686 D2692 Q2693 E2694 L2695 Y2696 R2697 M2698 A2699 M2700 P2701 C2702 A2705 I2706 L2710 P2711
P2712 D2713 Y2714 V2715 D2716 Y2719 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772
N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU
ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892
E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR S2949 S2950 I2951 E2952

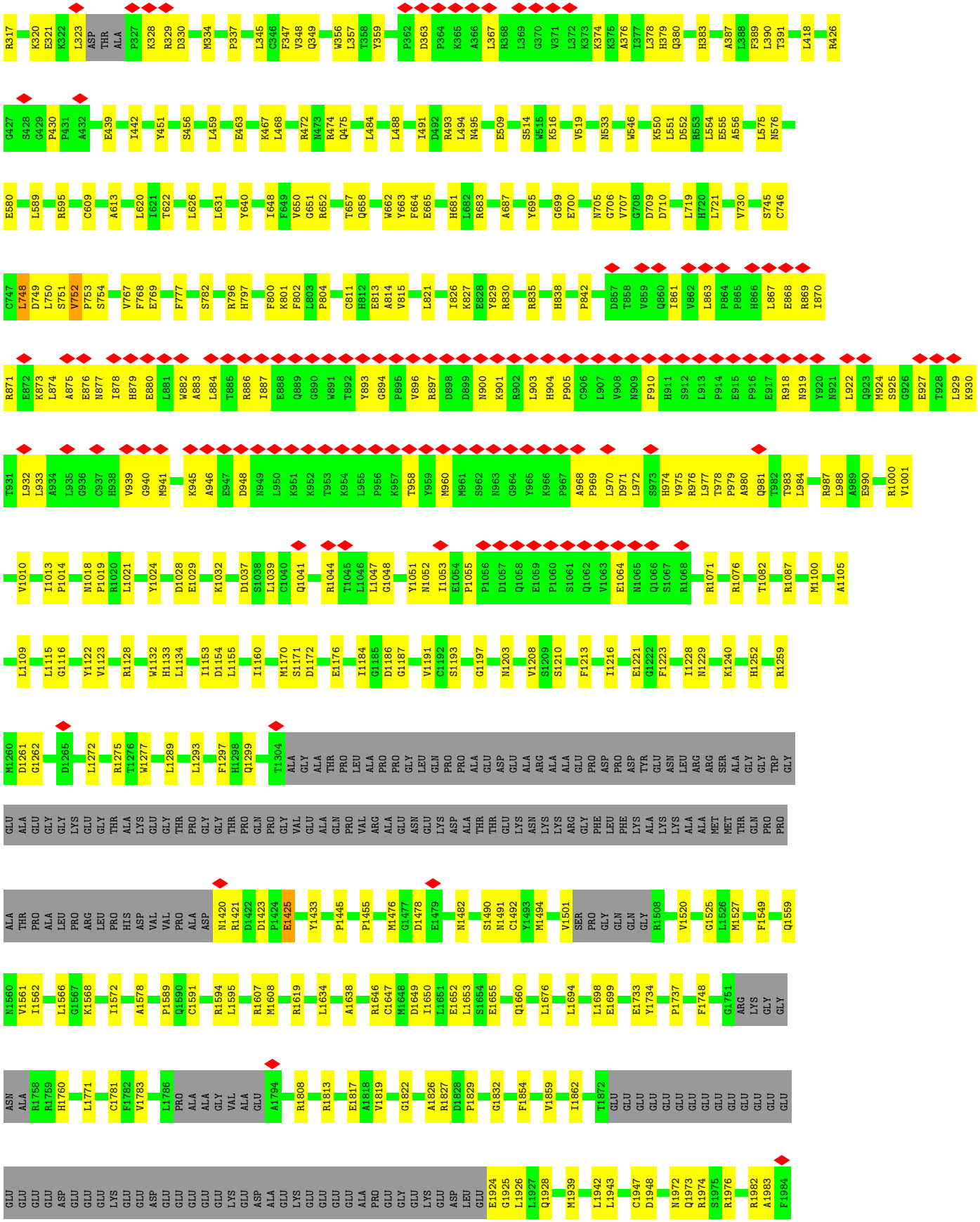




• Molecule 2: Ryanodine receptor 1

Chain G:

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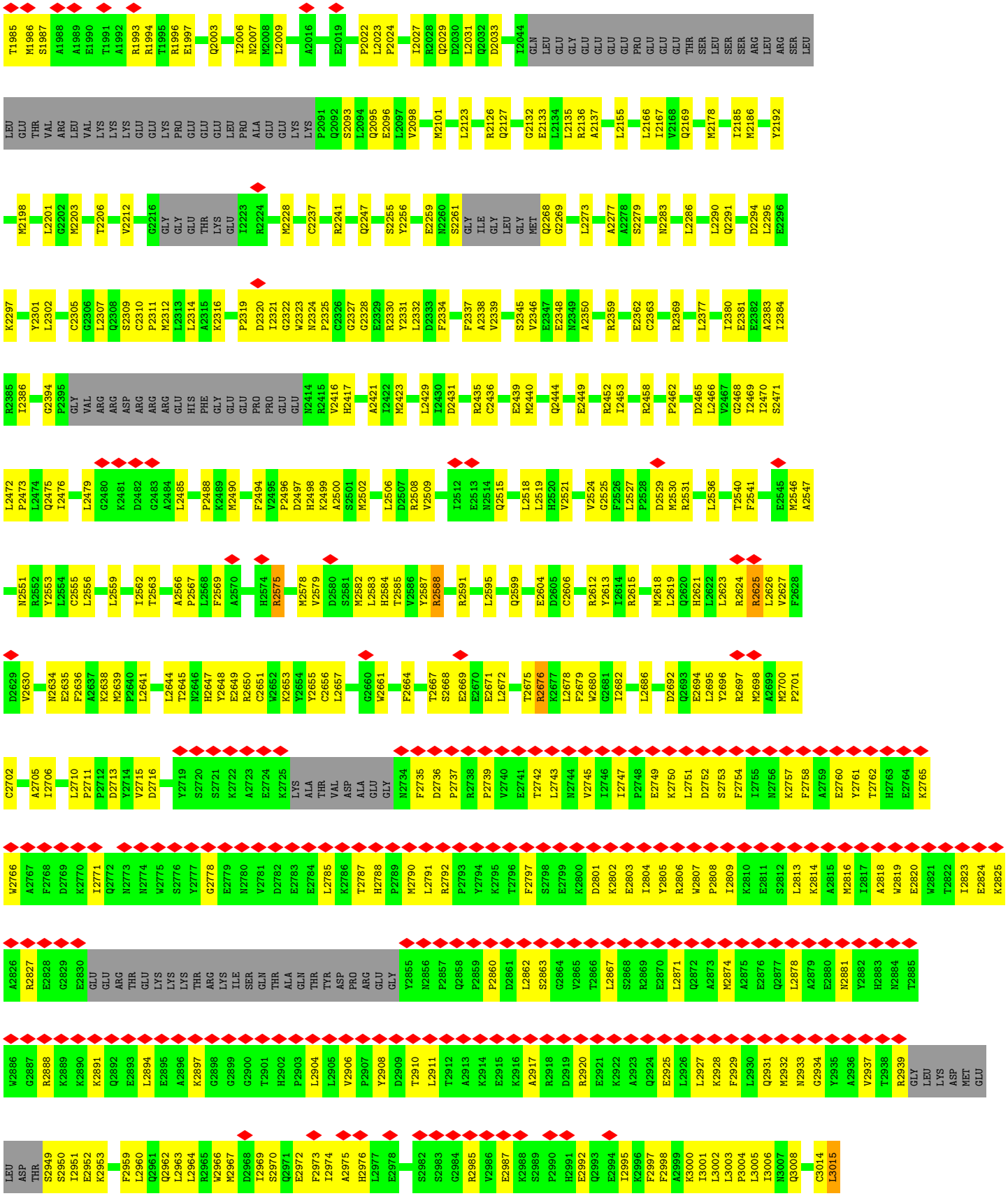
G427 S428 G429 P430 P431 A432 E439 T442 Y451 S456 L459 E463 K467 L468 R472 N473 R474 Q475 L484 L488 I491 D492 R493 L494 N495 E509 S514 W515 K516 V519 N533 W546 K550 L551 D552 R553 L554 E555 A556 L575 N576
E580 L589 R595 C609 A613 L620 T621 T622 L626 L631 Y640 I648 F649 V650 G651 R652 T657 Q658 W662 Y663 F664 E665 H681 L682 R683 A687 Y695 G699 E700 N705 G706 V707 G708 D709 D710 L719 H720 L721 V730 S745 C746
C747 L748 D749 L750 S751 V752 P753 S754 V767 F768 E769 F777 S782 R796 H797 F800 K801 F802 L803 P804 C811 H812 E813 A814 V815 L821 I826 K827 E828 Y829 R830 R835 H838 P842 D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870
R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930
T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 R987 L988 A989 E990 R1000 V1001
V1010 I1013 P1014 N1018 P1019 R1020 L1021 Y1024 D1028 E1029 K1032 D1037 S1038 L1039 C1040 Q1041 R1044 T1045 L1046 L1047 G1048 Y1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 R1071 R1076 T1082 R1087 M1100 A1105
L1109 L1115 G1116 Y1122 V1123 R1128 W1132 H1133 L1134 I1153 D1154 L1155 I1160 M1170 S1171 D1172 E1176 I1184 G1185 D1186 G1187 V1191 C1192 S1193 G1197 N1203 V1208 S1209 S1210 F1213 I1216 E1221 G1222 F1223 I1228 N1229 K1240 H1252 R1259
M1260 D1261 G1262 D1265 L1272 R1275 T1276 W1277 L1289 L1293 F1297 H1298 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY
GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO
ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 Y1433 P1445 P1455 M1476 G1477 D1478 E1479 N1482 S1490 N1491 C1492 Y1493 M1494 V1501 SER PRO GLY GLN GLN GLY R1508 V1520 G1525 L1526 M1527 F1549 Q1559
N1560 V1561 I1562 L1566 G1567 K1568 I1572 A1578 P1589 Q1590 C1591 R1594 L1595 R1607 M1608 R1619 L1634 A1638 R1646 C1647 M1648 D1649 I1650 L1651 E1652 L1653 S1654 E1655 Q1660 L1676 L1694 L1698 E1699 E1733 Y1734 P1737 F1748 G1751 ARG LYS GLY GLY
ASN ALA R1758 R1759 H1760 L1771 C1781 F1782 V1783 L1786 PRO ALA ALA GLY VAL ALA GLU A1794 R1808 R1813 E1817 A1818 V1819 G1822 A1826 R1827 D1828 P1829 G1832 F1854 V1859 I1862 T1872 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU GLU ASP GLU GLU GLU LYS GLU ASP GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU E1924 G1925 L1926 L1927 Q1928 M1939 L1942 L1943 C1947 D1948 N1972 Q1973 R1974 S1975 R1976 R1982 A1983 F1984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LEU GLU THR VAL ARG LEU VAL LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS P2091 Q2092 S2093 L2094 Q2095 E2096 L2097 V2098 M2101 L2123 R2126 Q2127 G2132 E2133 L2134 L2135 R2136 A2137 L2155 L2166 I2167 V2168 Q2169 M2178 I2185 M2186 Y2192
M2198 L2201 G2202 M2203 T2206 V2212 G2216 GLY GLY GLU THR LYS GLU I2223 R2224 M2228 C2237 R2241 Q2247 S2255 Y2256 E2259 N2260 S2261 GLY ILE GLY LEU GLY MET Q2268 G2269 L2273 A2277 A2278 S2279 N2283 L2286 L2290 Q2291 D2294 L2295 E2296
K2297 Y2301 L2302 C2305 G2306 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 K2316 P2319 D2320 I2321 G2322 W2323 N2324 P2325 C2326 G2327 G2328 E2329 R2330 Y2331 L2332 D2333 F2334 F2337 A2338 V2339 S2345 V2346 E2347 E2348 N2349 A2350 R2359 E2362 C2363 R2369 L2377 I2380 E2381 E2382 A2383 I2384
R2385 I2386 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 A2421 I2422 M2423 L2429 I2430 D2431 R2435 C2436 E2439 M2440 Q2444 E2449 R2452 I2453 R2458 P2462 D2465 L2466 V2467 G2468 I2469 I2470 S2471
L2472 P2473 L2474 Q2475 I2476 L2479 G2480 K2481 D2482 G2483 A2484 L2485 P2488 K2489 M2490 F2494 V2495 P2496 D2497 H2498 K2499 A2500 S2501 M2502 L2506 D2507 R2508 V2509 T2512 E2513 N2514 Q2515 L2518 L2519 H2520 V2521 V2524 G2525 F2526 L2527 P2528 D2529 M2530 R2531 L2536 T2540 F2541 E2545 M2546 A2547
N2551 R2552 Y2553 L2554 C2555 L2556 L2559 I2562 T2563 A2566 P2567 L2568 F2569 A2570 H2574 R2575 M2578 V2579 D2580 S2581 M2582 L2583 H2584 T2585 V2586 Y2587 R2588 R2591 L2595 Q2599 E2604 D2605 C2606 R2612 Y2613 I2614 R2615 M2618 L2619 Q2620 H2621 L2622 L2623 R2624 R2625 L2626 V2627 F2628
D2629 V2630 N2634 E2635 F2636 A2637 K2638 M2639 P2640 L2641 L2644 T2645 N2646 H2647 Y2648 E2649 R2650 C2651 W2652 K2653 Y2654 Y2655 C2656 L2657 G2660 W2661 F2664 T2667 S2668 E2669 E2670 E2671 L2672 T2675 R2676 K2677 L2678 F2679 W2680 G2681 I2682 L2686 D2692 Q2693 E2694 L2695 Y2696 R2697 M2698 A2699 M2700 P2701
C2702 A2705 I2706 L2710 P2711 P2712 D2713 Y2714 V2715 D2716 Y2719 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765
W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825
A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885
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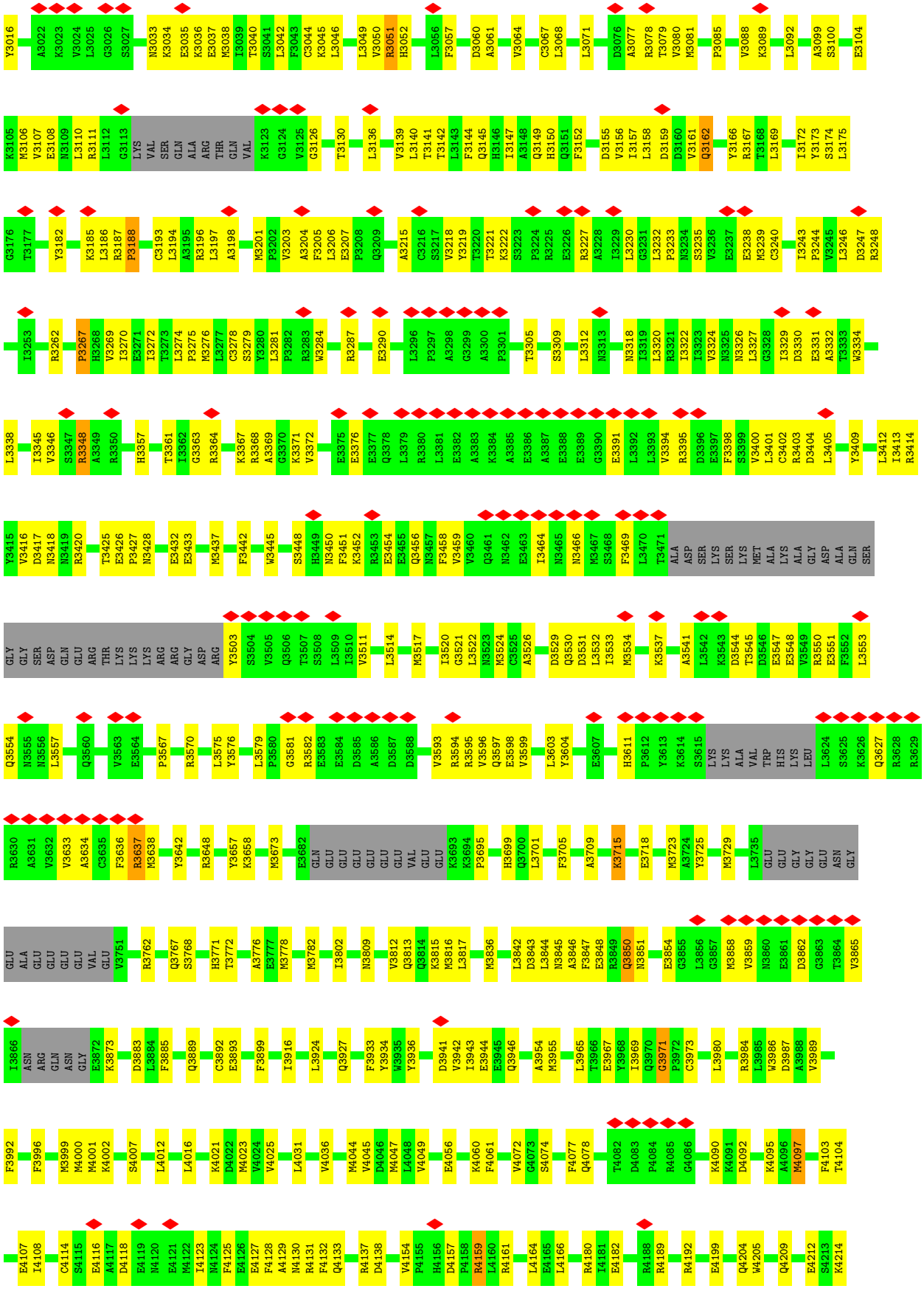
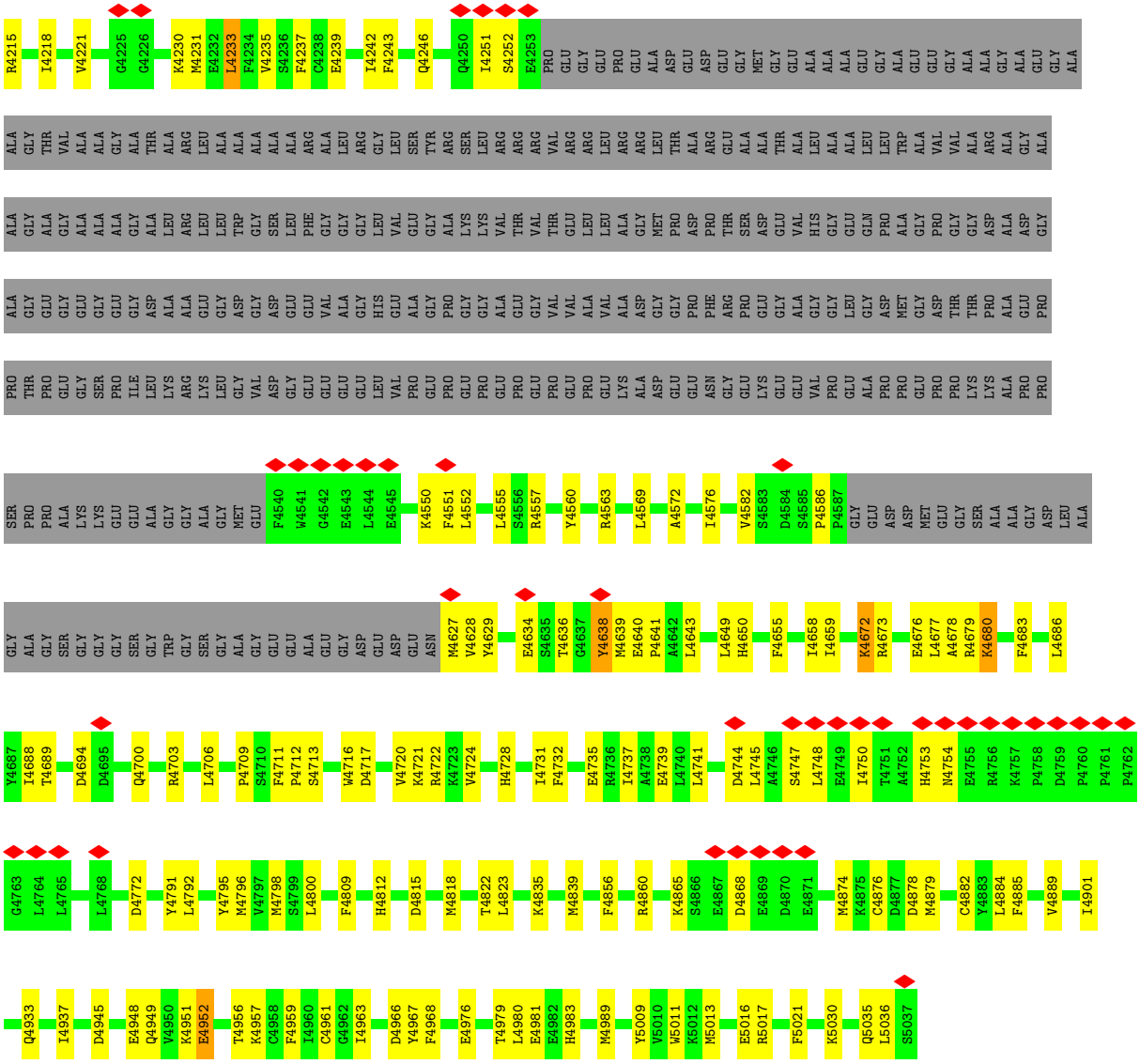
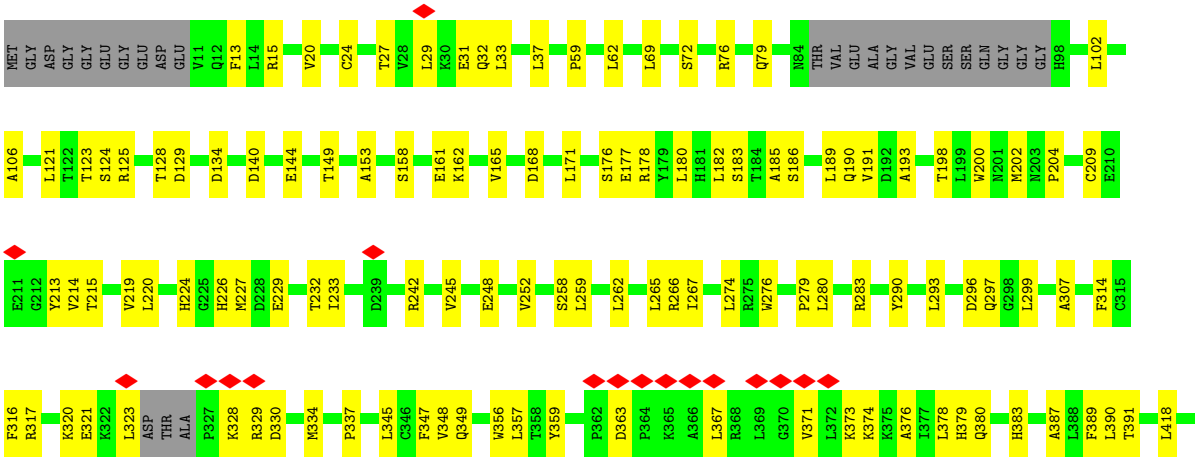
LEU ASP THR S2949 S2950 I2951 E2952 K2953 F2959 L2960 Q2961 Q2962 L2963 L2964 R2965 W2966 M2967 D2968 I2969 S2970 Q2971 E2972 F2973 I2974 A2975 H2976 L2977 E2978 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 E2994 I2995 K2996 F2997 F2998 A2999 K3000 I3001 L3002 L3003 P3004 L3005 I3006 N3007 Q3008 C3014 L3015





• Molecule 2: Ryanodine receptor 1

Chain B:

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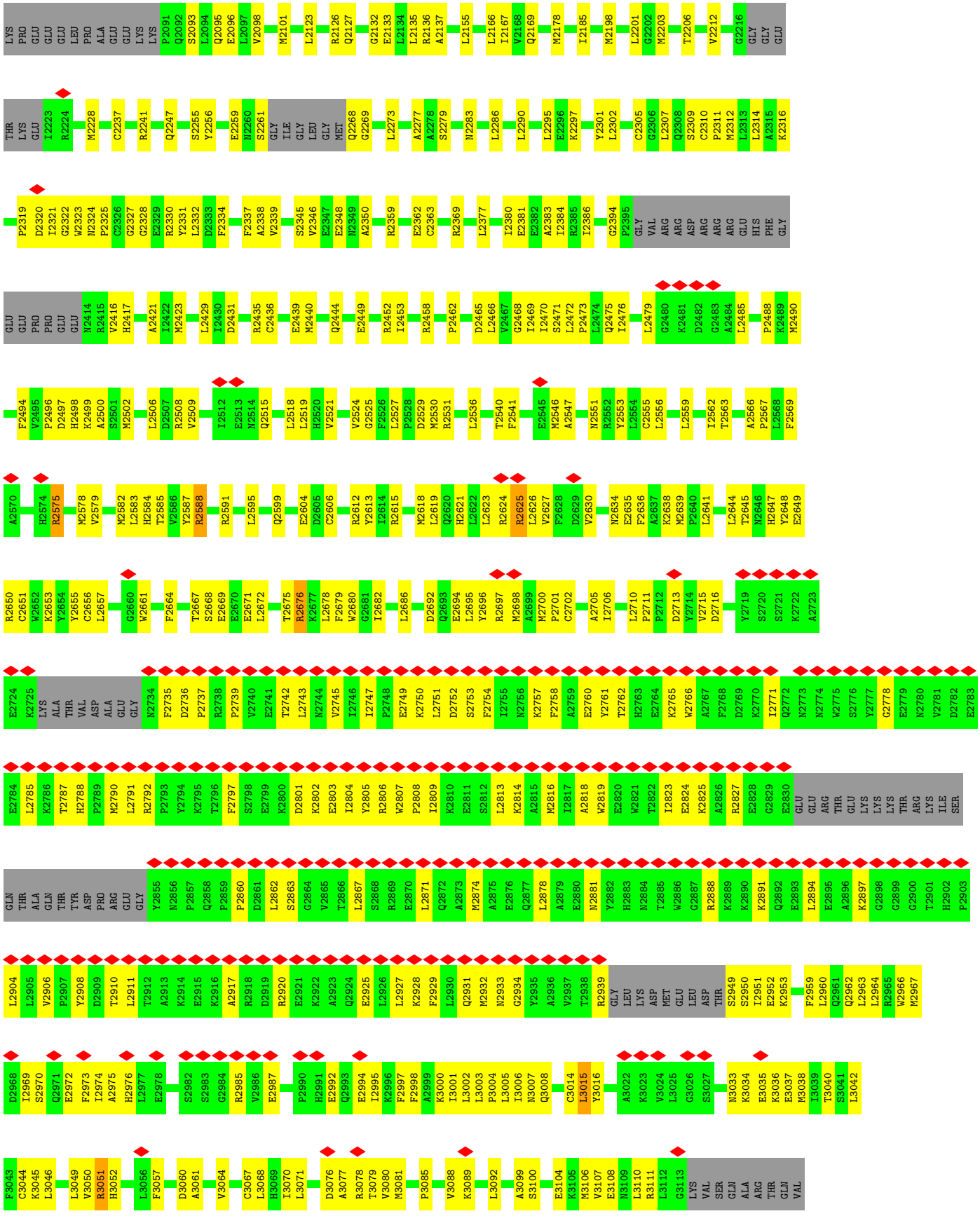
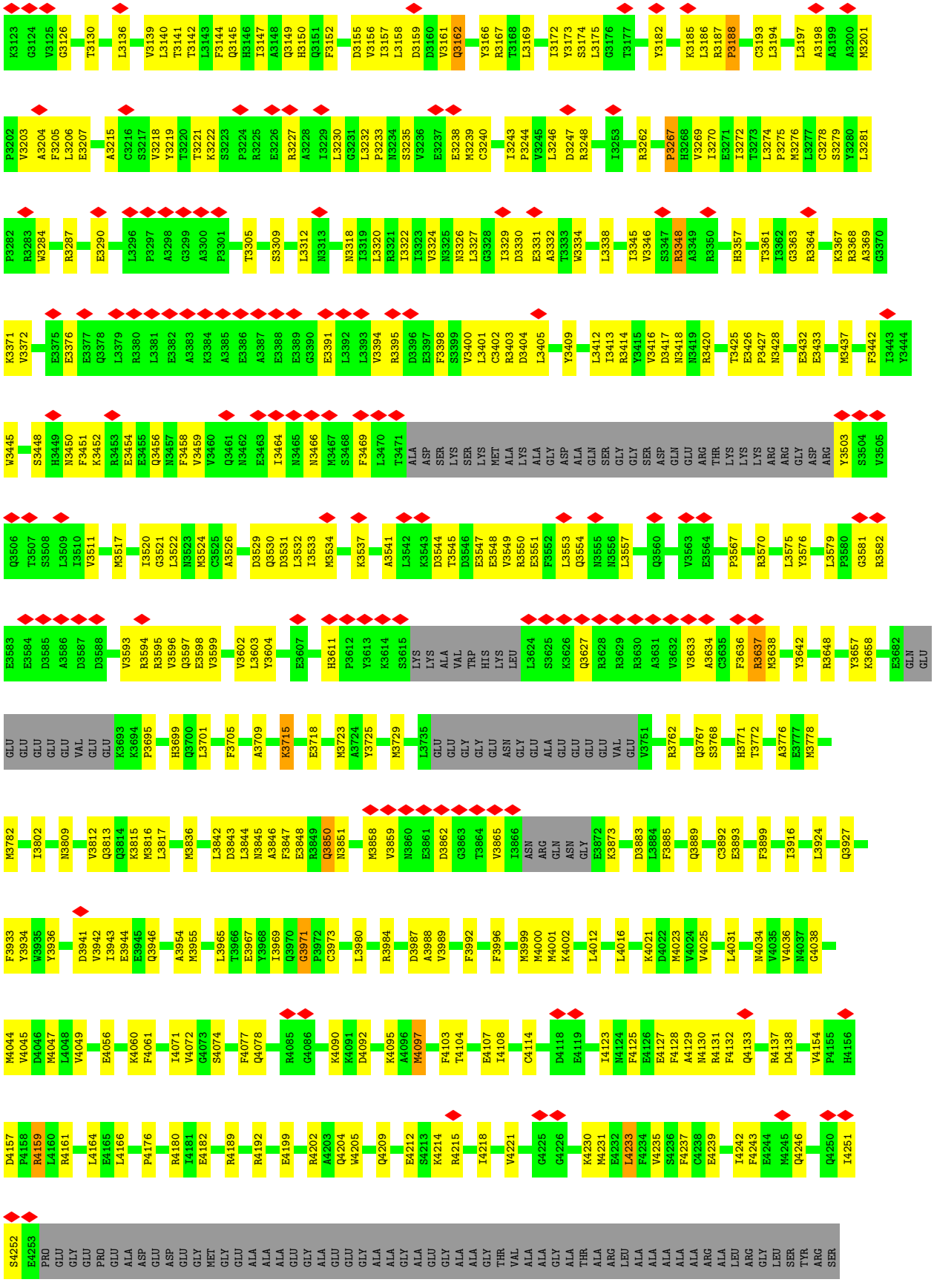
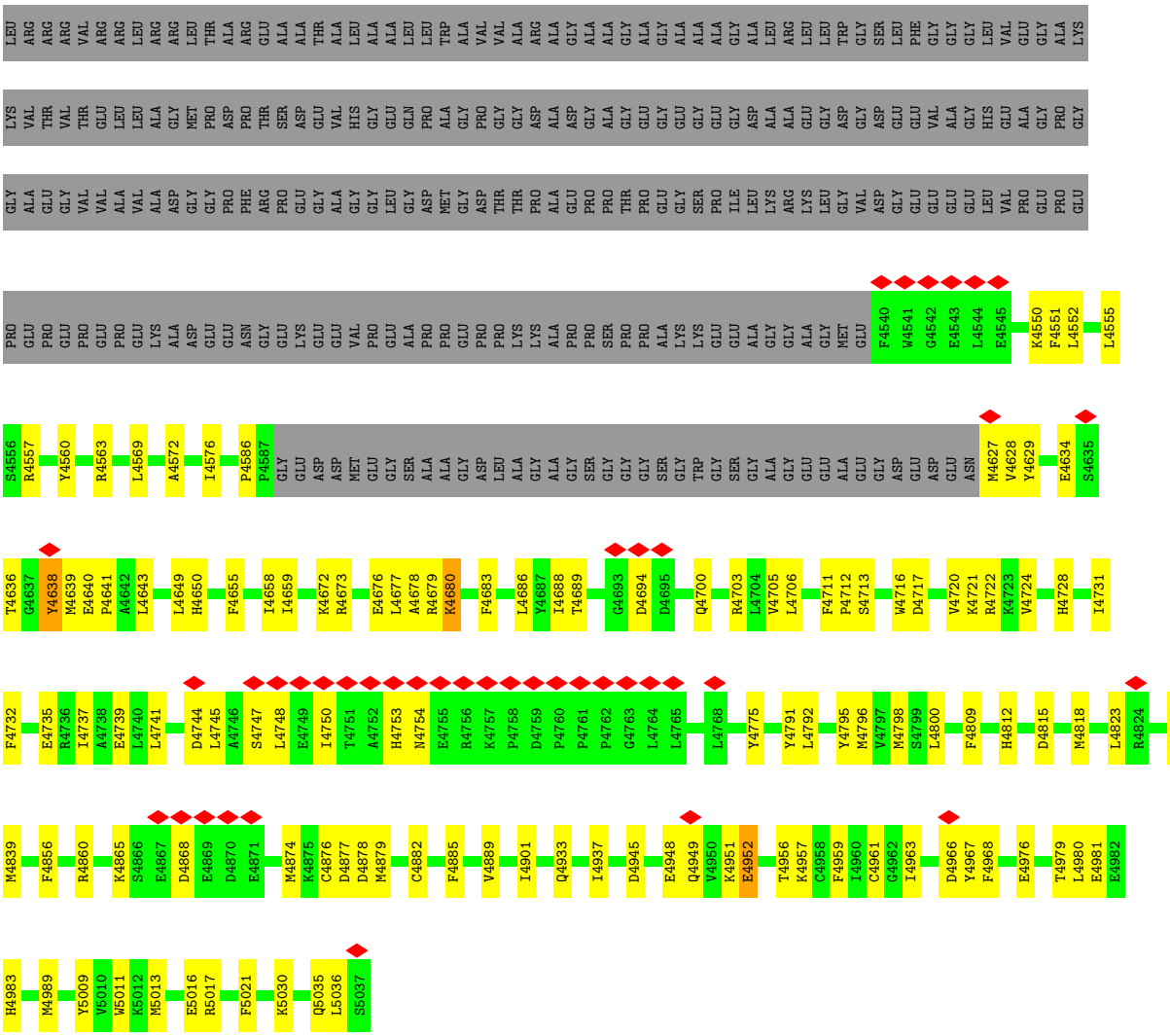
E580 L589 C609 A613 L620 I621 T622 L626 Y640 I648 F649 V650 G651 R652 T657 Q658 W662 Y663 F664 E665 H681 L682 R683 A687 Y695 G699 E700 N705 G706 V707 G708 D709 D710 L719 H720 L721 V730 S745 L748 D749 L750
S751 V752 P753 S754 V767 F768 E769 F777 S782 R796 H797 F800 K801 F802 L803 P804 C811 H812 E813 A814 V815 L821 I826 K827 E828 Y829 R830 R835 H838 P842 D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874
A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934
L935 G936 C937 H938 V939 G940 M941 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 R987 L988 A989 E990 R1000 V1001 V1010 I1013
P1014 N1018 P1019 R1020 L1021 Y1024 E1029 K1032 D1037 S1038 L1039 C1040 Q1041 R1044 T1045 L1046 L1047 G1048 Y1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 R1071 R1076 T1082 R1087 M1100 A1105 L1109 R1110 V1113
E1114 L1115 G1116 Y1122 V1123 R1128 W1132 H1133 L1134 I1153 D1154 L1155 I1160 M1170 S1171 D1172 E1176 I1184 G1185 D1186 G1187 V1191 C1192 S1193 G1197 N1203 V1208 S1209 S1210 F1213 I1216 E1221 G1222 F1223 I1228 N1229 K1240 E1251 H1252 R1259 M1260
D1261 G1262 D1265 L1272 R1275 T1276 W1277 S1282 L1289 L1293 F1297 H1298 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP
GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS ALA ALA MET MET THR GLN PRO
PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 Y1433 P1445 P1455 M1476 G1477 D1478 E1479 N1482 S1490 N1491 C1492 Y1493 M1494 V1501 SER PRO GLY GLN GLN GLY R1508 V1520 G1525 L1526 M1527 F1549
Q1559 N1560 V1561 I1562 A1578 C1591 R1594 L1595 R1607 M1608 R1619 L1634 A1638 R1646 C1647 M1648 D1649 I1650 L1651 E1652 L1653 S1654 E1655 Q1660 L1676 E1699 E1733 Y1734 P1737 F1748 G1751 ARG LYS GLY GLY ASN ALA R1758 R1759 H1760 L1771 C1781 F1782
V1783 L1786 PRO ALA ALA GLY VAL ALA GLU A1794 R1808 R1813 E1817 A1818 V1819 G1822 A1826 R1827 D1828 P1829 G1832 F1854 V1859 I1862 T1872 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU
GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU E1924 G1925 L1926 L1927 Q1928 M1939 L1943 C1947 D1948 N1972 Q1973 R1974 S1975 R1976 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 R1993 R1994 T1995 R1996 E1997
Q2003 I2006 L2009 D2014 E2015 A2016 E2019 P2022 L2023 P2024 I2027 R2028 Q2029 D2030 L2031 Q2032 D2033 I2044 GLN LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU

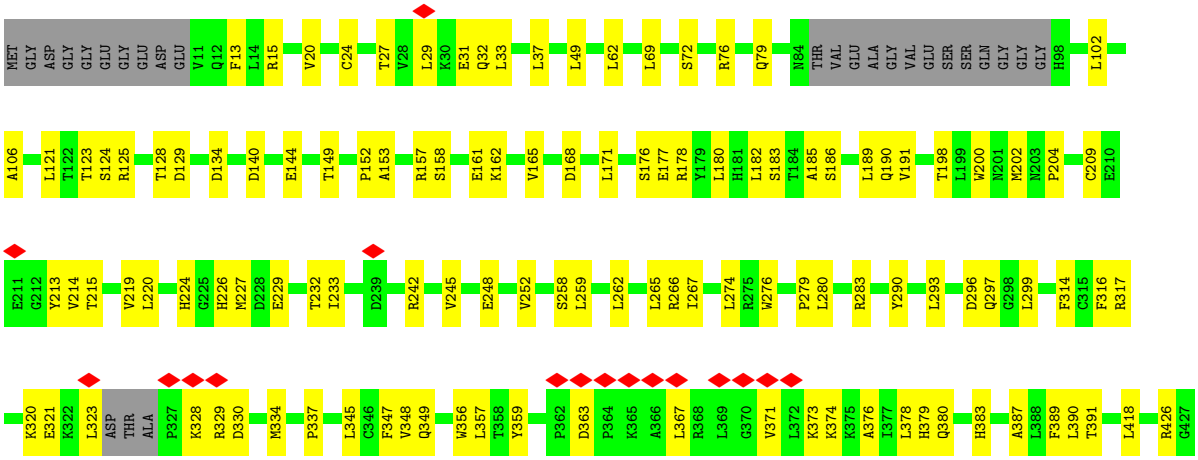


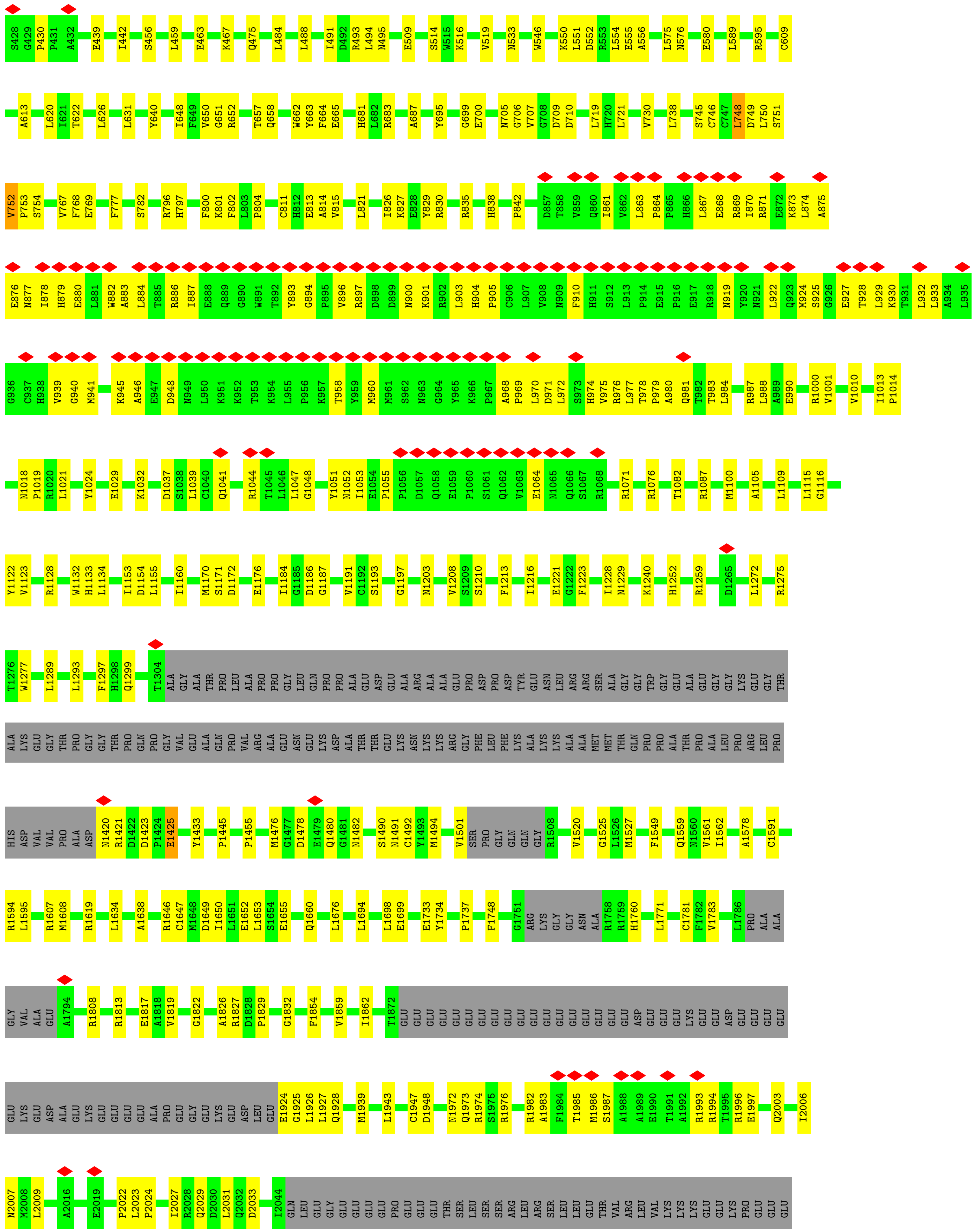




• Molecule 2: Ryanodine receptor 1

Chain I:

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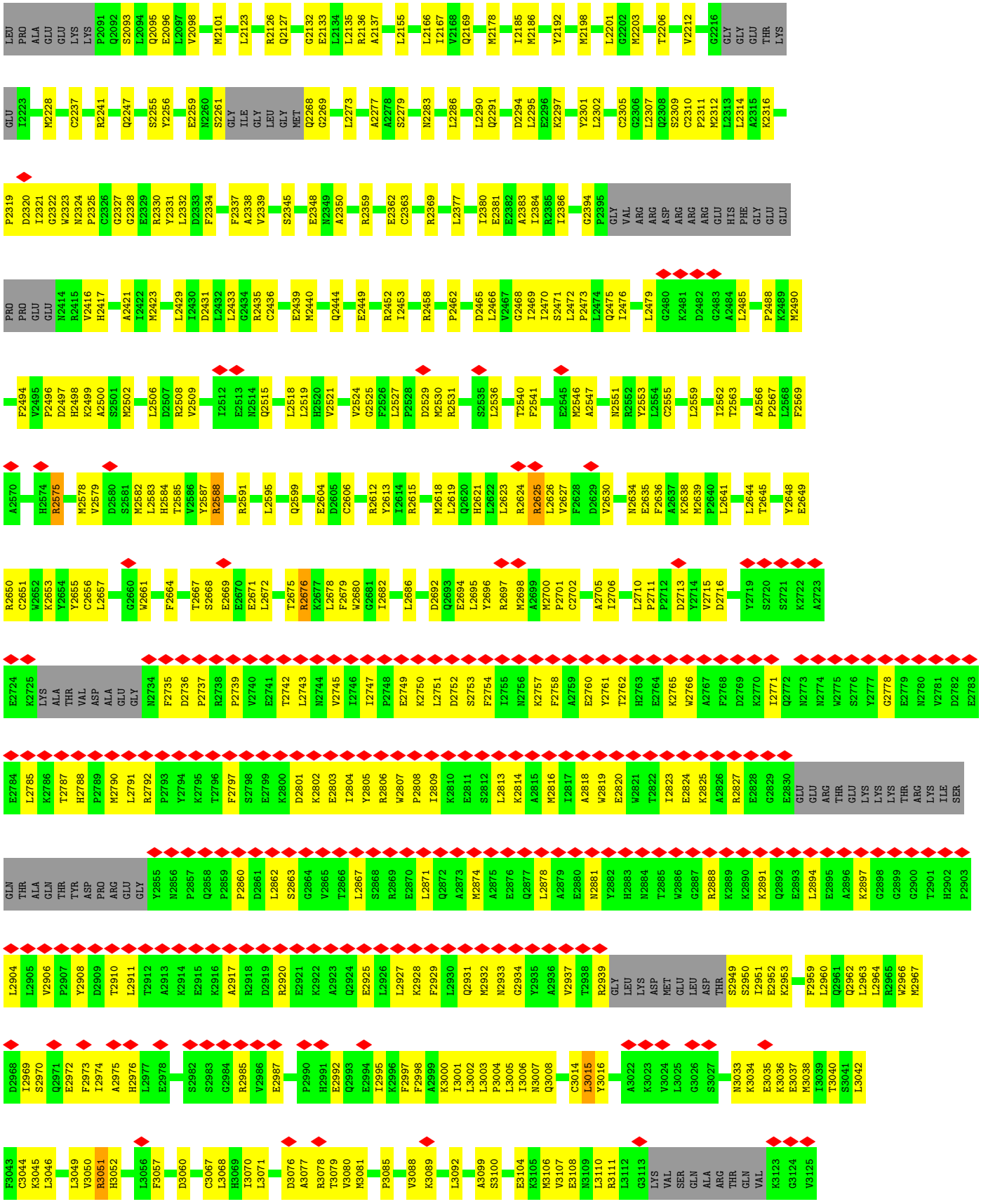
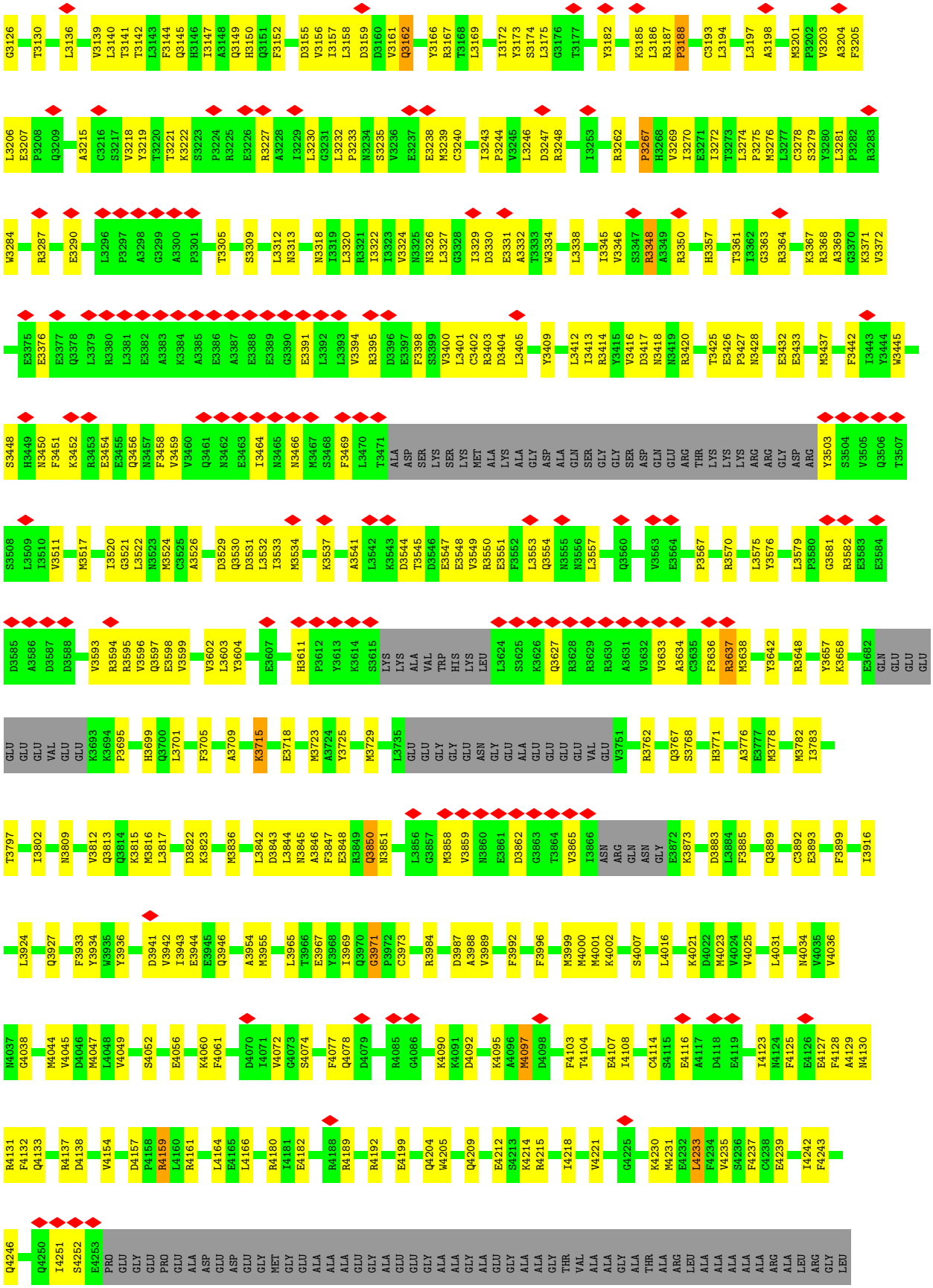
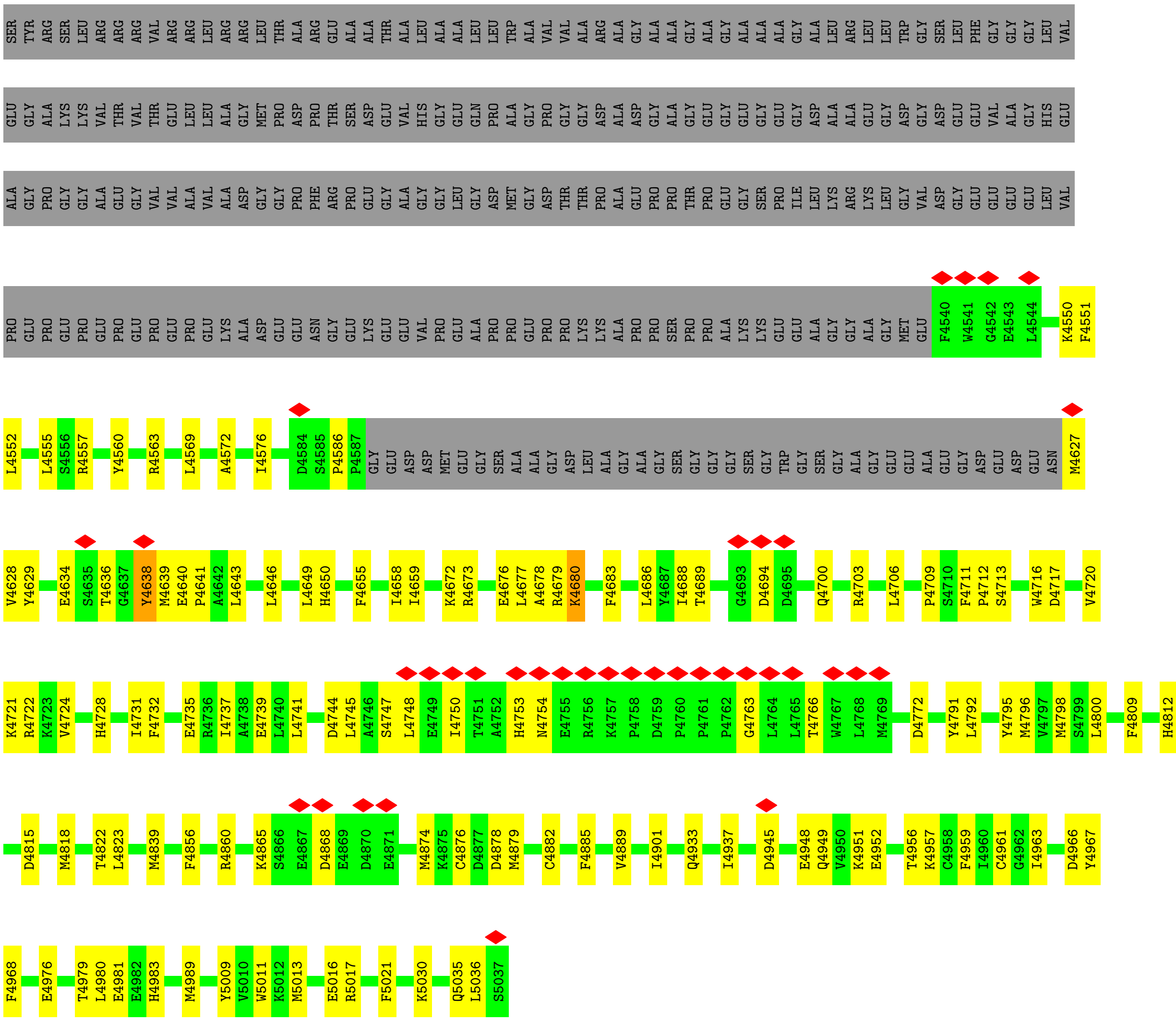
A613 L620 I621 T622 L626 L631 Y640 I648 F649 V650 G651 R652 T657 Q658 W662 Y663 F664 E665 H681 L682 R683 A687 Y695 G699 E700 N705 G706 V707 G708 D709 D710 L719 H720 L721 V730 L738 S745 C746 C747 L748 D749 L750 S751
V752 P753 S754 V767 F768 E769 F777 S782 R796 H797 F800 K801 F802 L803 P804 C811 H812 E813 A814 V815 L821 I826 K827 E828 Y829 R830 R835 H838 P842 D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875
E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935
G936 C937 H938 V939 G940 M941 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 R987 L988 A989 E990 R1000 V1001 V1010 I1013 P1014
N1018 P1019 R1020 L1021 Y1024 E1029 K1032 D1037 S1038 L1039 C1040 Q1041 R1044 T1045 L1046 L1047 G1048 Y1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 R1071 R1076 T1082 R1087 M1100 A1105 L1109 L1115 G1116
Y1122 V1123 R1128 W1132 H1133 L1134 I1153 D1154 L1155 I1160 M1170 S1171 D1172 E1176 I1184 G1185 D1186 G1187 V1191 C1192 S1193 G1197 N1203 V1208 S1209 S1210 F1213 I1216 E1221 G1222 F1223 I1228 N1229 K1240 H1252 R1259 D1265 L1272 R1275
T1276 W1277 L1289 L1293 F1297 H1298 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR
ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO
HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 Y1433 P1445 P1455 M1476 G1477 D1478 E1479 Q1480 G1481 N1482 S1490 N1491 C1492 Y1493 M1494 V1501 SER PRO GLY GLN GLN GLY R1508 V1520 G1525 L1526 M1527 F1549 Q1559 N1560 V1561 I1562 A1578 C1591
R1594 L1595 R1607 M1608 R1619 L1634 A1638 R1646 C1647 M1648 D1649 I1650 L1651 E1652 L1653 S1654 E1655 Q1660 L1676 L1694 L1698 E1699 E1733 Y1734 P1737 F1748 G1751 ARG LYS GLY GLY ASN ALA R1758 R1759 H1760 L1771 C1781 F1782 V1783 L1786 PRO ALA ALA
GLY VAL ALA GLU A1794 R1808 R1813 E1817 A1818 V1819 G1822 A1826 R1827 D1828 P1829 G1832 F1854 V1859 I1862 T1872 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU
GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU E1924 G1925 L1926 L1927 Q1928 M1939 L1943 C1947 D1948 N1972 Q1973 R1974 S1975 R1976 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 Q2003 I2006
N2007 M2008 L2009 A2016 E2019 P2022 L2023 P2024 I2027 R2028 Q2029 D2030 L2031 Q2032 D2033 I2044 GLN LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU



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GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU
ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL
PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4544 K4550 F4551
L4552 L4555 S4556 R4557 Y4560 R4563 L4569 A4572 I4576 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU ASN M4627
V4628 Y4629 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 A4642 L4643 L4646 L4649 H4650 F4655 I4658 I4659 K4672 R4673 E4676 L4677 A4678 R4679 K4680 F4683 L4686 Y4687 I4688 T4689 G4693 D4694 D4695 Q4700 R4703 L4706 P4709 S4710 F4711 P4712 S4713 W4716 D4717 V4720
K4721 R4722 K4723 V4724 H4728 I4731 F4732 E4735 R4736 I4737 A4738 E4739 L4740 L4741 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 D4772 Y4791 L4792 Y4795 M4796 V4797 M4798 S4799 L4800 F4809 H4812
D4815 M4818 T4822 L4823 M4839 F4856 R4860 K4865 S4866 E4867 D4868 E4869 D4870 E4871 M4874 K4875 C4876 D4877 D4878 M4879 C4882 F4885 V4889 I4901 Q4933 I4937 D4945 E4948 Q4949 V4950 K4951 E4952 T4956 K4957 C4958 F4959 I4960 C4961 G4962 I4963 D4966 Y4967
F4968 E4976 T4979 L4980 E4981 E4982 H4983 M4989 Y5009 V5010 W5011 K5012 M5013 E5016 R5017 F5021 K5030 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	53882	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 ($e^-/Å^2$)	58.34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.119	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.121	Depositor
Map size (Å)	425.472, 425.472, 425.472	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

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

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	F	0.78	0/834	0.70	1/1123 (0.1%)
1	H	0.78	0/834	0.71	1/1123 (0.1%)
1	J	0.78	0/834	0.70	1/1123 (0.1%)
1	O	0.78	0/834	0.70	1/1123 (0.1%)
2	A	0.46	1/35070 (0.0%)	0.55	31/47504 (0.1%)
2	B	0.46	1/35070 (0.0%)	0.55	31/47504 (0.1%)
2	G	0.46	1/35070 (0.0%)	0.55	32/47504 (0.1%)
2	I	0.46	1/35070 (0.0%)	0.55	31/47504 (0.1%)
All	All	0.47	4/143616 (0.0%)	0.56	129/194508 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	B	0	1
2	G	0	1
2	I	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3188	PRO	N-CD	-8.43	1.36	1.47
2	B	3188	PRO	N-CD	-8.43	1.36	1.47
2	I	3188	PRO	N-CD	-8.43	1.36	1.47
2	G	3188	PRO	N-CD	-8.37	1.36	1.47

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3850	GLN	CA-CB-CG	8.89	132.95	113.40
2	A	3850	GLN	CA-CB-CG	8.88	132.94	113.40
2	I	3850	GLN	CA-CB-CG	8.87	132.92	113.40
2	G	3850	GLN	CA-CB-CG	8.86	132.90	113.40
2	B	2676	ARG	CB-CG-CD	-8.82	88.66	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4638	TYR	Peptide
2	B	4638	TYR	Peptide
2	G	4638	TYR	Peptide
2	I	4638	TYR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	818	0	824	36	0
1	H	818	0	824	35	0
1	J	818	0	824	34	0
1	O	818	0	824	36	0
2	A	34293	0	33897	1228	0
2	B	34293	0	33897	1219	0
2	G	34293	0	33897	1242	0
2	I	34293	0	33897	1219	0
3	A	31	0	12	2	0
3	B	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1	0	0	0	0
6	A	14	0	10	1	0
6	B	14	0	10	1	0
6	G	14	0	10	1	0
6	I	14	0	10	1	0
All	All	140632	0	138972	4997	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 18.

The worst 5 of 4997 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3989:VAL:HG23	2:I:4023:MET:CE	1.38	1.52
2:B:3989:VAL:HG23	2:B:4023:MET:CE	1.38	1.51
2:A:3989:VAL:HG23	2:A:4023:MET:CE	1.38	1.49
2:G:3989:VAL:HG23	2:G:4023:MET:CE	1.38	1.49
2:G:2615:ARG:NH2	2:G:2618:MET:HE1	1.16	1.48

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	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	J	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	O	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	A	4260/5037 (85%)	4079 (96%)	179 (4%)	2 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	4260/5037 (85%)	4078 (96%)	180 (4%)	2 (0%)	100	100
2	G	4260/5037 (85%)	4080 (96%)	178 (4%)	2 (0%)	100	100
2	I	4260/5037 (85%)	4079 (96%)	179 (4%)	2 (0%)	100	100
All	All	17460/20580 (85%)	16720 (96%)	732 (4%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	801	LYS
2	G	801	LYS
2	B	801	LYS
2	I	801	LYS
2	A	3267	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	88/89 (99%)	78 (89%)	10 (11%)	5	22
1	H	88/89 (99%)	78 (89%)	10 (11%)	5	22
1	J	88/89 (99%)	78 (89%)	10 (11%)	5	22
1	O	88/89 (99%)	78 (89%)	10 (11%)	5	22
2	A	3738/4276 (87%)	3713 (99%)	25 (1%)	84	92
2	B	3738/4276 (87%)	3713 (99%)	25 (1%)	84	92
2	G	3738/4276 (87%)	3713 (99%)	25 (1%)	84	92
2	I	3738/4276 (87%)	3713 (99%)	25 (1%)	84	92
All	All	15304/17460 (88%)	15164 (99%)	140 (1%)	79	89

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	751	SER

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Mol	Chain	Res	Type
2	I	1128	ARG
2	I	4031	LEU
1	J	25	HIS
1	J	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	2127	GLN
2	I	2324	ASN
2	I	3052	HIS
2	G	2127	GLN
2	G	877	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	A	5304	-	8,15,15	2.29	2 (25%)	8,23,23	1.16	1 (12%)
3	ATP	A	5301	2	26,33,33	0.86	1 (3%)	31,52,52	1.60	5 (16%)
3	ATP	G	5301	2	26,33,33	0.86	1 (3%)	31,52,52	1.60	5 (16%)
3	ATP	I	5301	2	26,33,33	0.86	1 (3%)	31,52,52	1.60	5 (16%)
6	CFF	B	5304	-	8,15,15	2.29	2 (25%)	8,23,23	1.16	1 (12%)
3	ATP	B	5301	2	26,33,33	0.87	1 (3%)	31,52,52	1.60	5 (16%)
6	CFF	G	5304	-	8,15,15	2.29	2 (25%)	8,23,23	1.15	1 (12%)
6	CFF	I	5304	-	8,15,15	2.28	2 (25%)	8,23,23	1.15	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	A	5304	-	-	-	0/2/2/2
3	ATP	A	5301	2	-	3/18/38/38	0/3/3/3
3	ATP	G	5301	2	-	3/18/38/38	0/3/3/3
3	ATP	I	5301	2	-	3/18/38/38	0/3/3/3
6	CFF	B	5304	-	-	-	0/2/2/2
3	ATP	B	5301	2	-	3/18/38/38	0/3/3/3
6	CFF	G	5304	-	-	-	0/2/2/2
6	CFF	I	5304	-	-	-	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5304	CFF	C5-C4	4.36	1.45	1.39
6	G	5304	CFF	C5-C4	4.36	1.45	1.39
6	B	5304	CFF	C5-C4	4.36	1.45	1.39
6	I	5304	CFF	C5-C4	4.36	1.45	1.39
6	G	5304	CFF	C5-C6	4.33	1.48	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	5301	ATP	PA-O3A-PB	-4.22	118.35	132.83
3	A	5301	ATP	PA-O3A-PB	-4.21	118.38	132.83
3	B	5301	ATP	PA-O3A-PB	-4.21	118.38	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5301	ATP	PA-O3A-PB	-4.21	118.39	132.83
3	G	5301	ATP	PB-O3B-PG	-3.58	120.56	132.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O3A
3	G	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	I	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	PA-O3A-PB-O1B

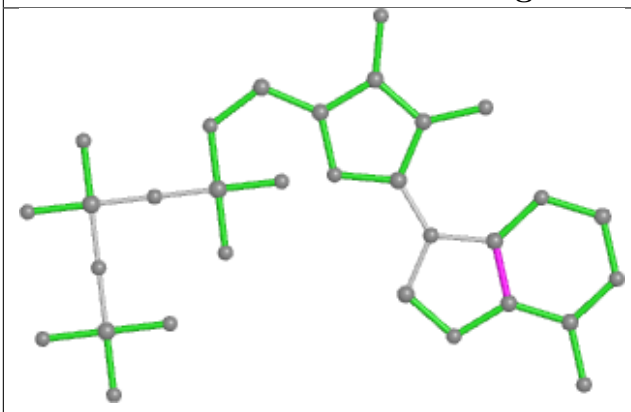
There are no ring outliers.

8 monomers are involved in 12 short contacts:

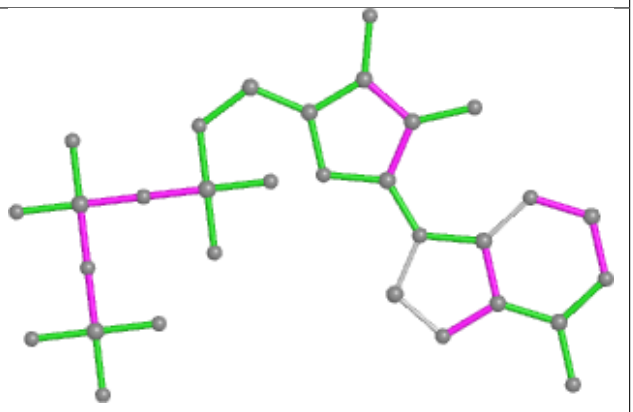
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5304	CFF	1	0
3	A	5301	ATP	2	0
3	G	5301	ATP	2	0
3	I	5301	ATP	2	0
6	B	5304	CFF	1	0
3	B	5301	ATP	2	0
6	G	5304	CFF	1	0
6	I	5304	CFF	1	0

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.

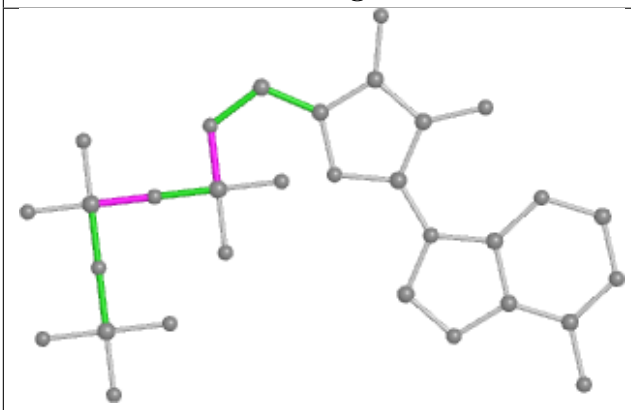
Ligand ATP A 5301



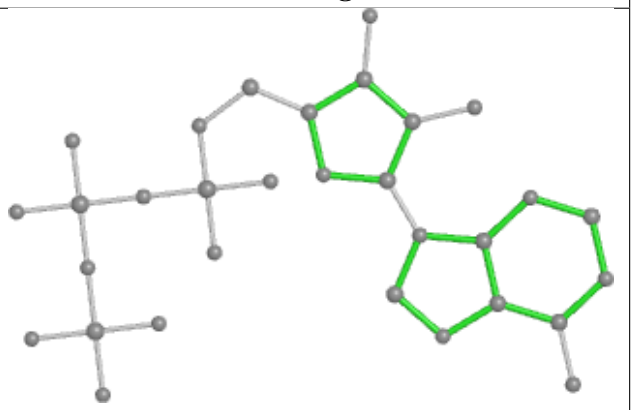
Bond lengths



Bond angles

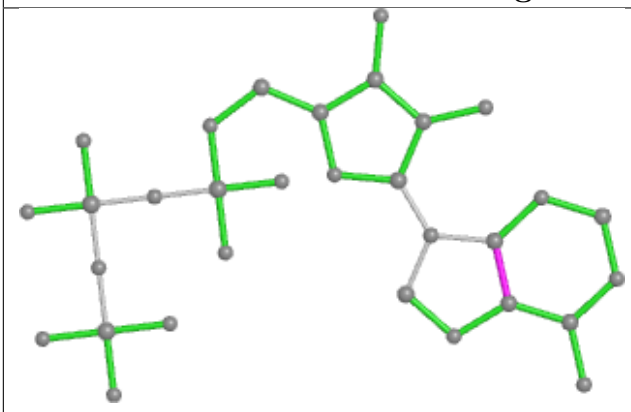


Torsions

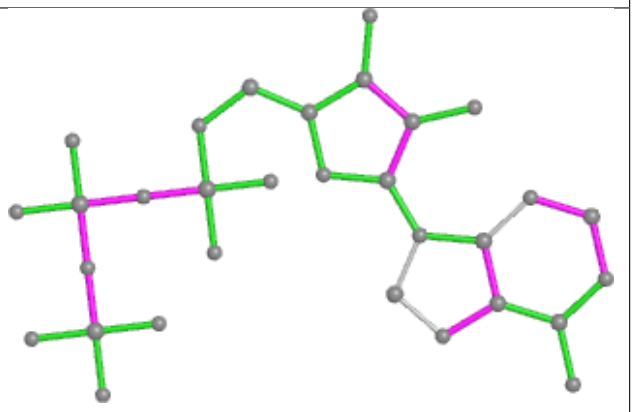


Rings

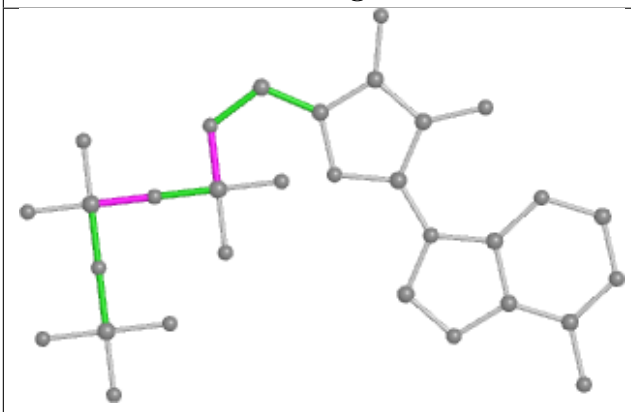
Ligand ATP G 5301



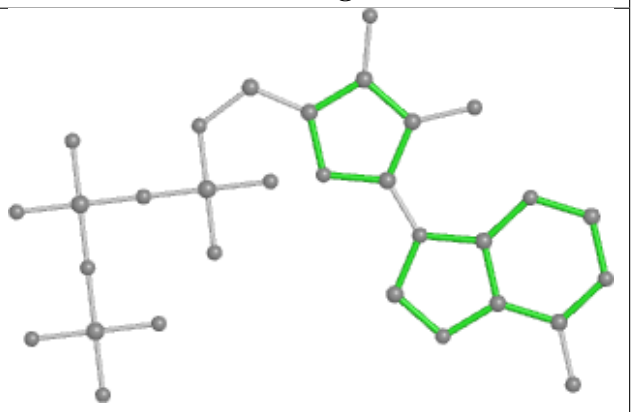
Bond lengths



Bond angles

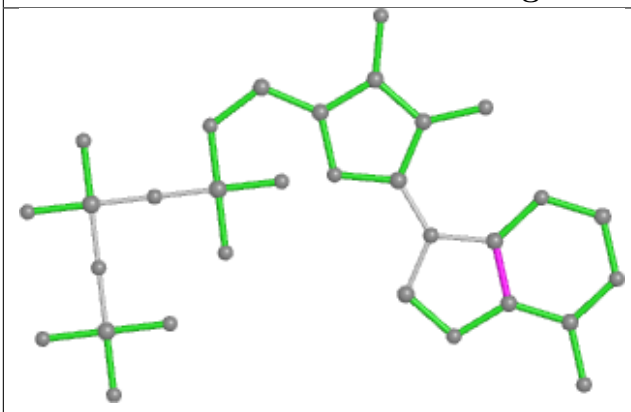


Torsions

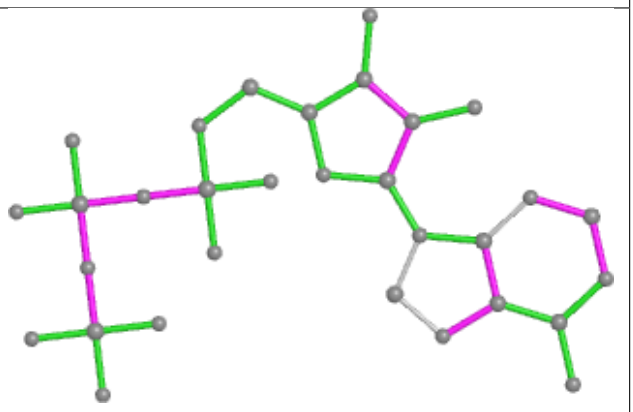


Rings

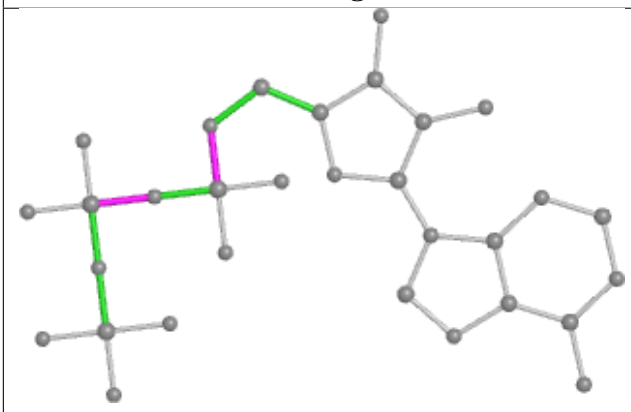
Ligand ATP I 5301



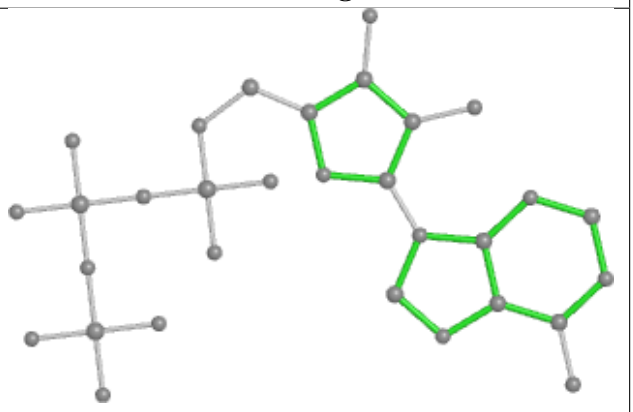
Bond lengths



Bond angles

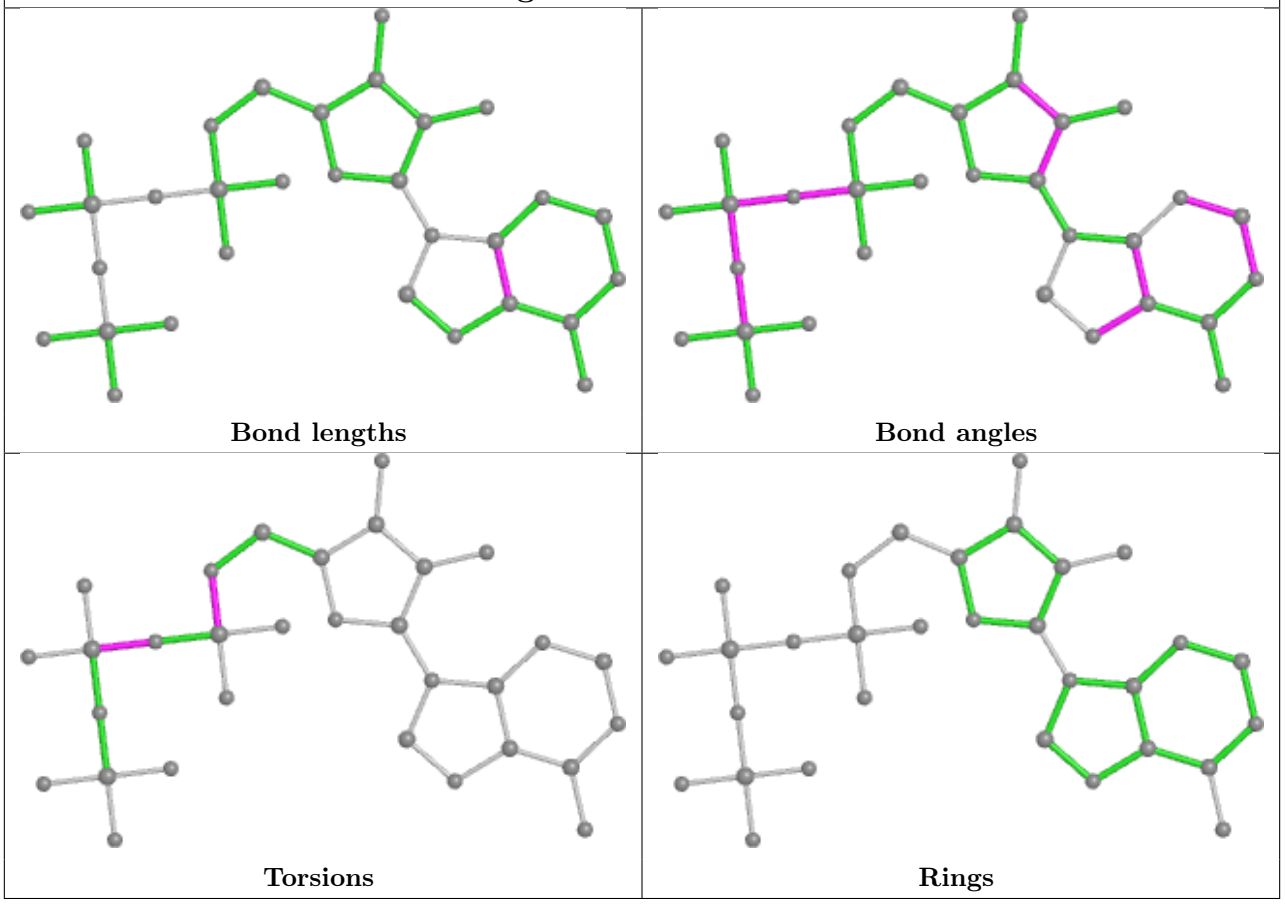


Torsions



Rings

Ligand ATP B 5301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

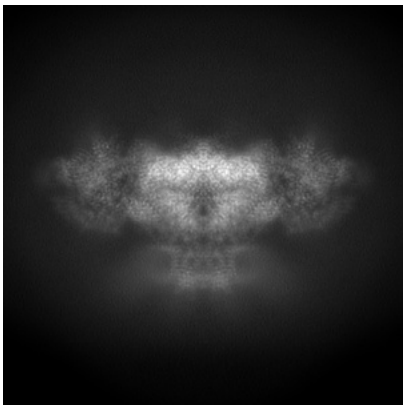
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23692. These allow visual inspection of the internal detail of the map and identification of artifacts.

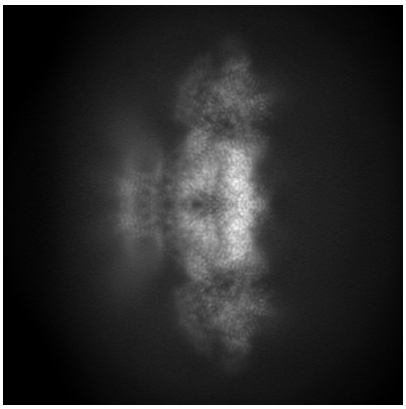
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

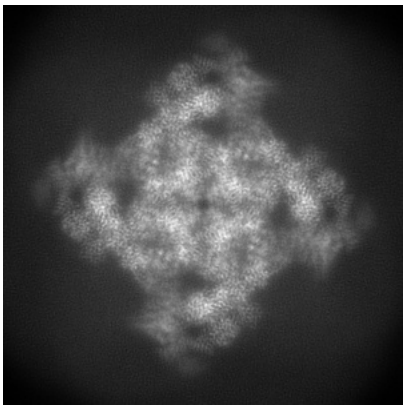
6.1.1 Primary map



X

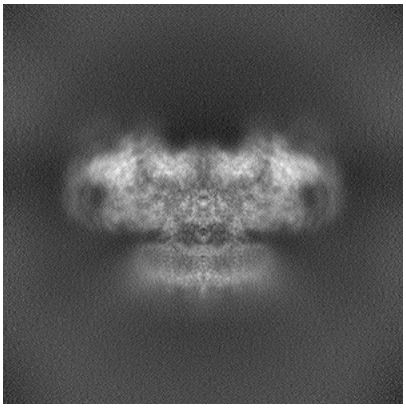


Y

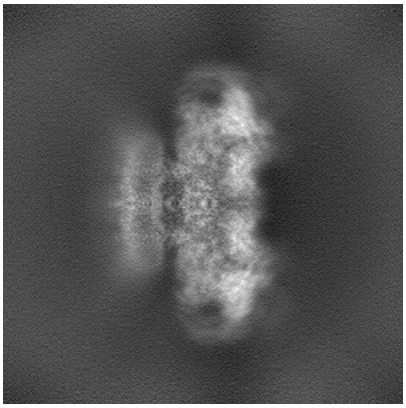


Z

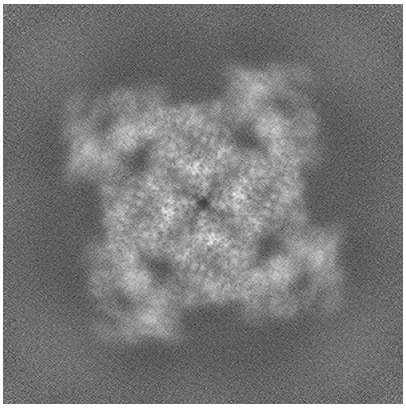
6.1.2 Raw map



X



Y

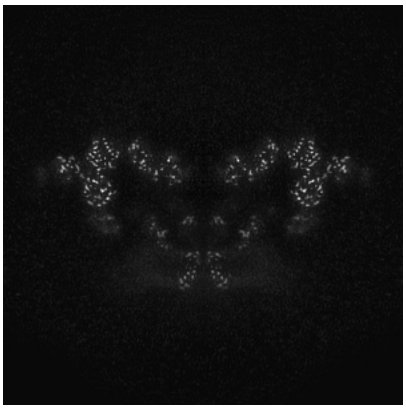


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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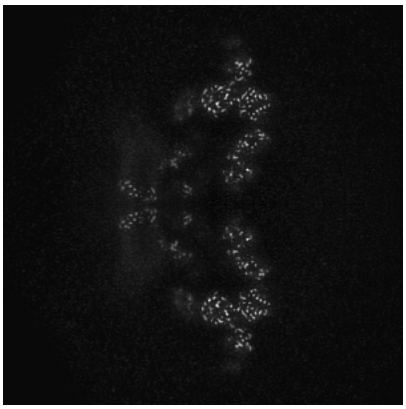
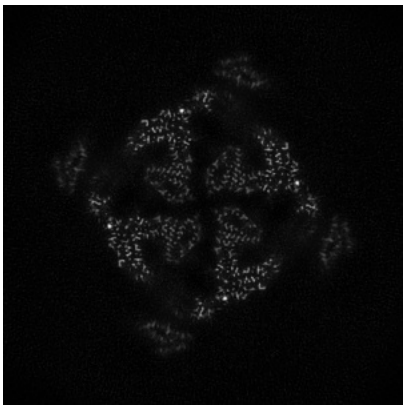
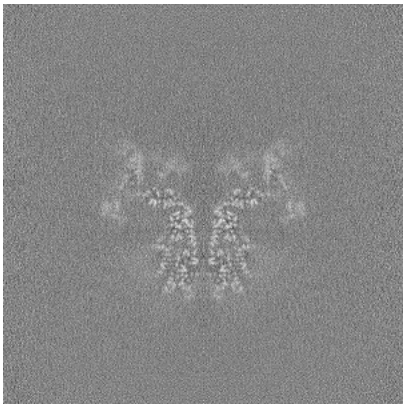


Y Index: 256



Z Index: 256

6.2.2 Raw map



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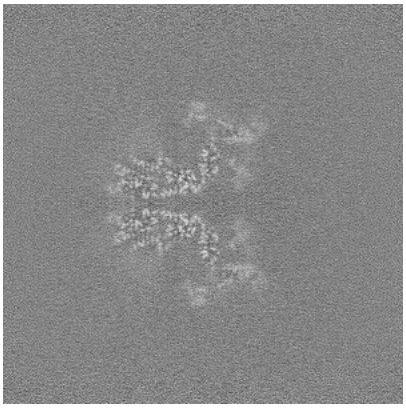
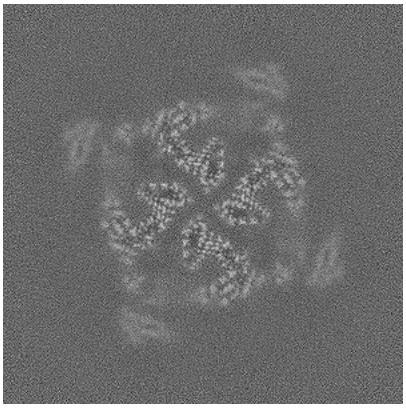


Y Index: 256

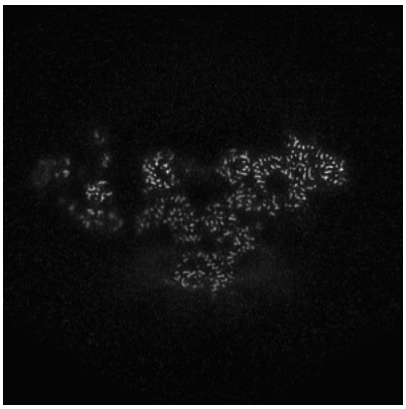


Z Index: 256

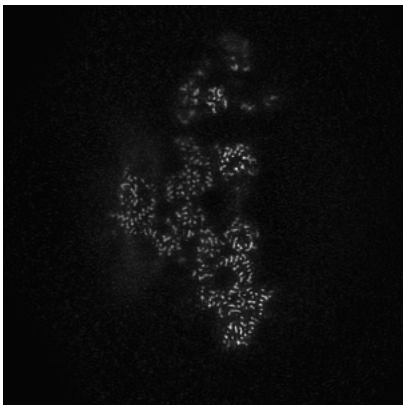
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

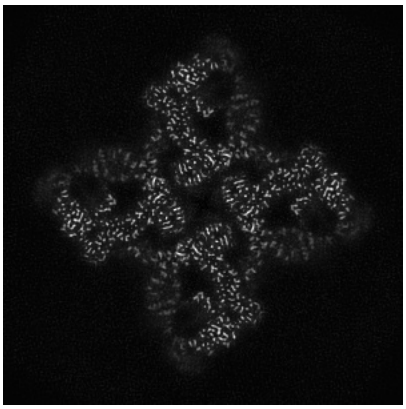
6.3.1 Primary map



X Index: 236

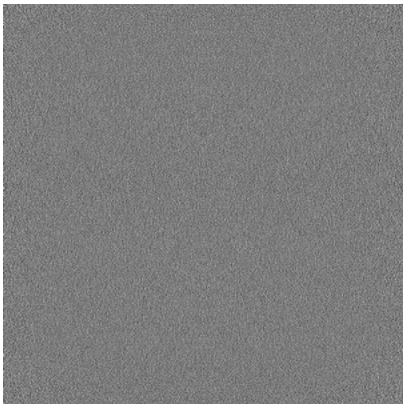


Y Index: 236

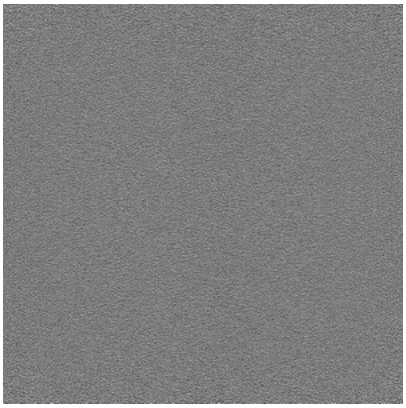


Z Index: 304

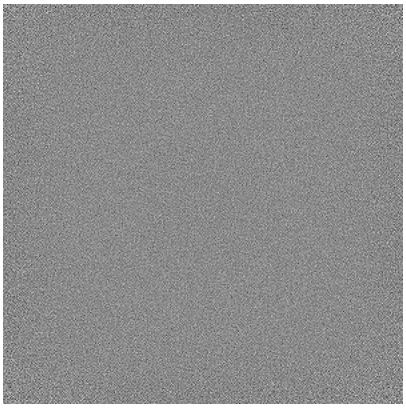
6.3.2 Raw map



X Index: 0



Y Index: 0

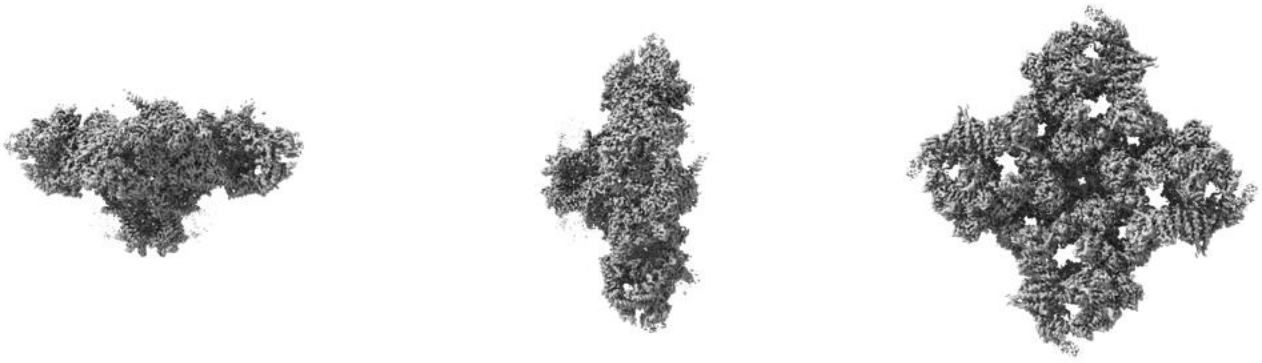


Z Index: 0

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

6.4 Orthogonal surface views (i)

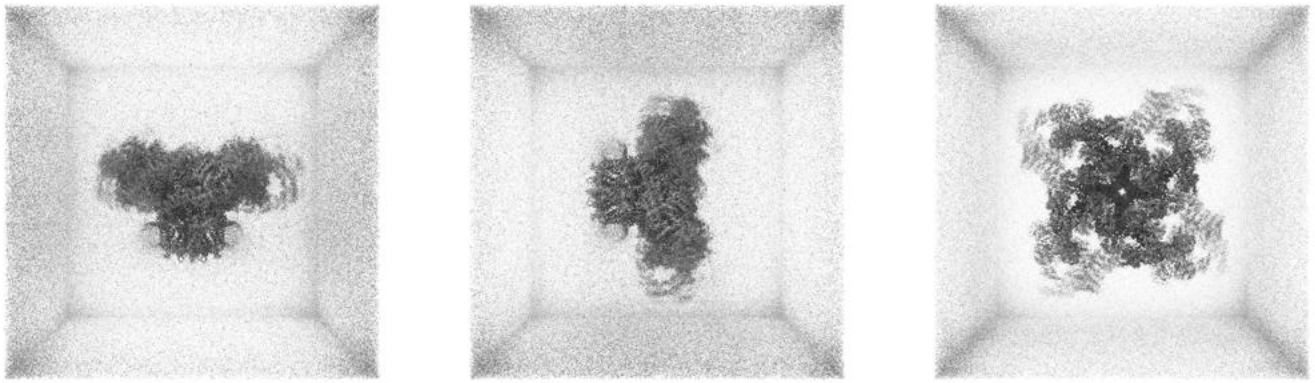
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.121. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

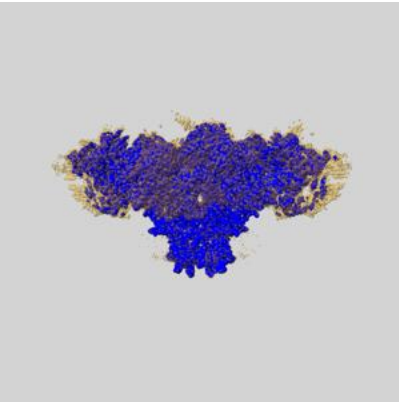
6.5 Mask visualisation (i)

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

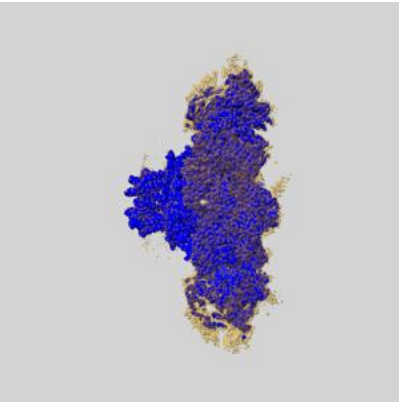
A mask typically either:

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

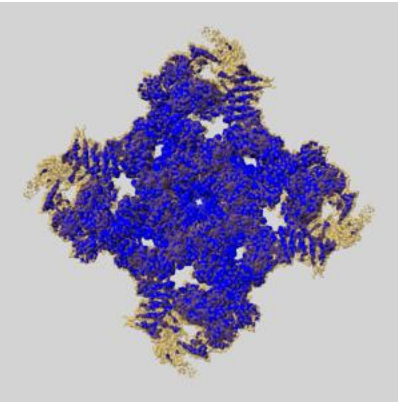
6.5.1 emd_23692_msk_1.map (i)



X



Y

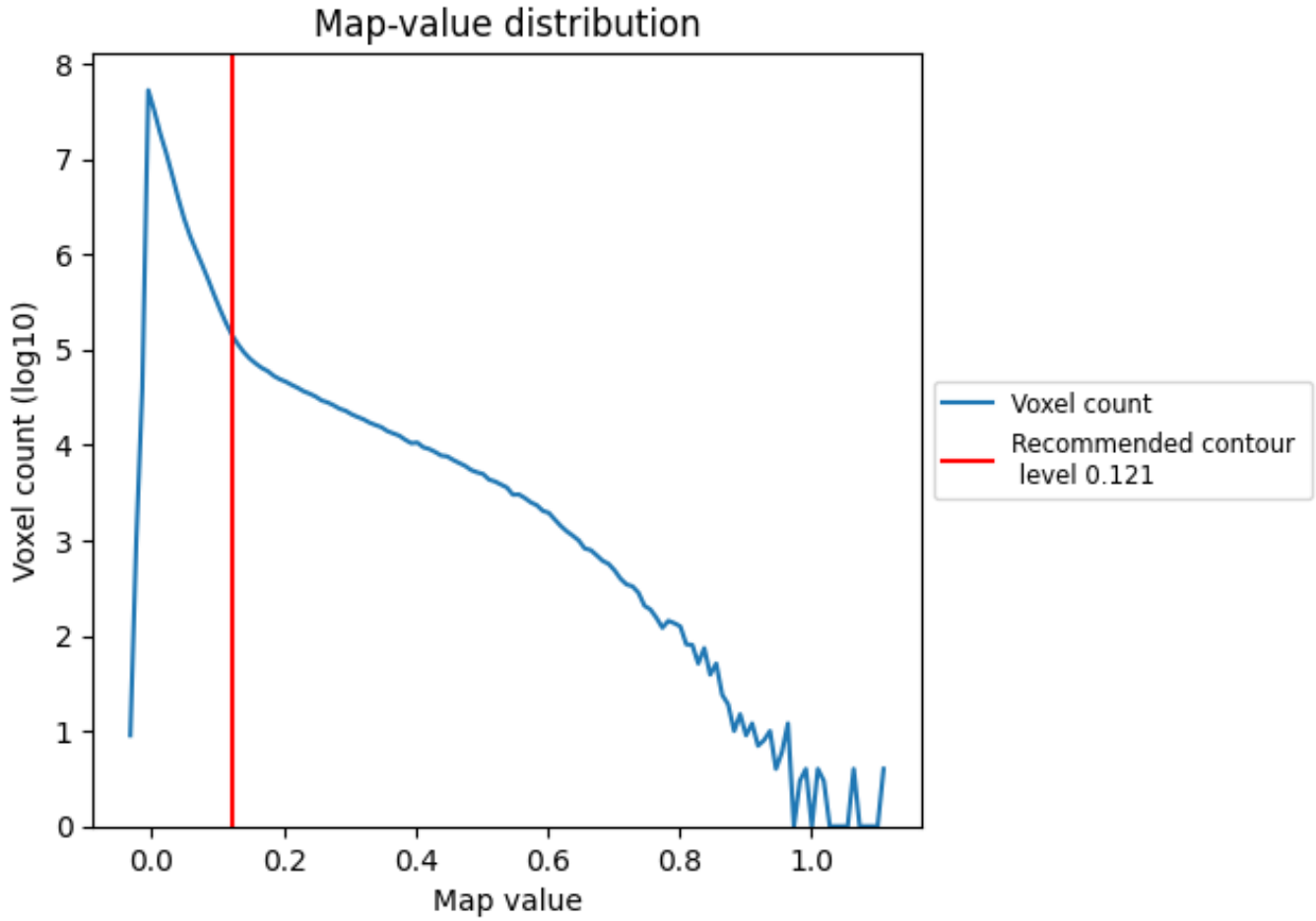


Z

7 Map analysis

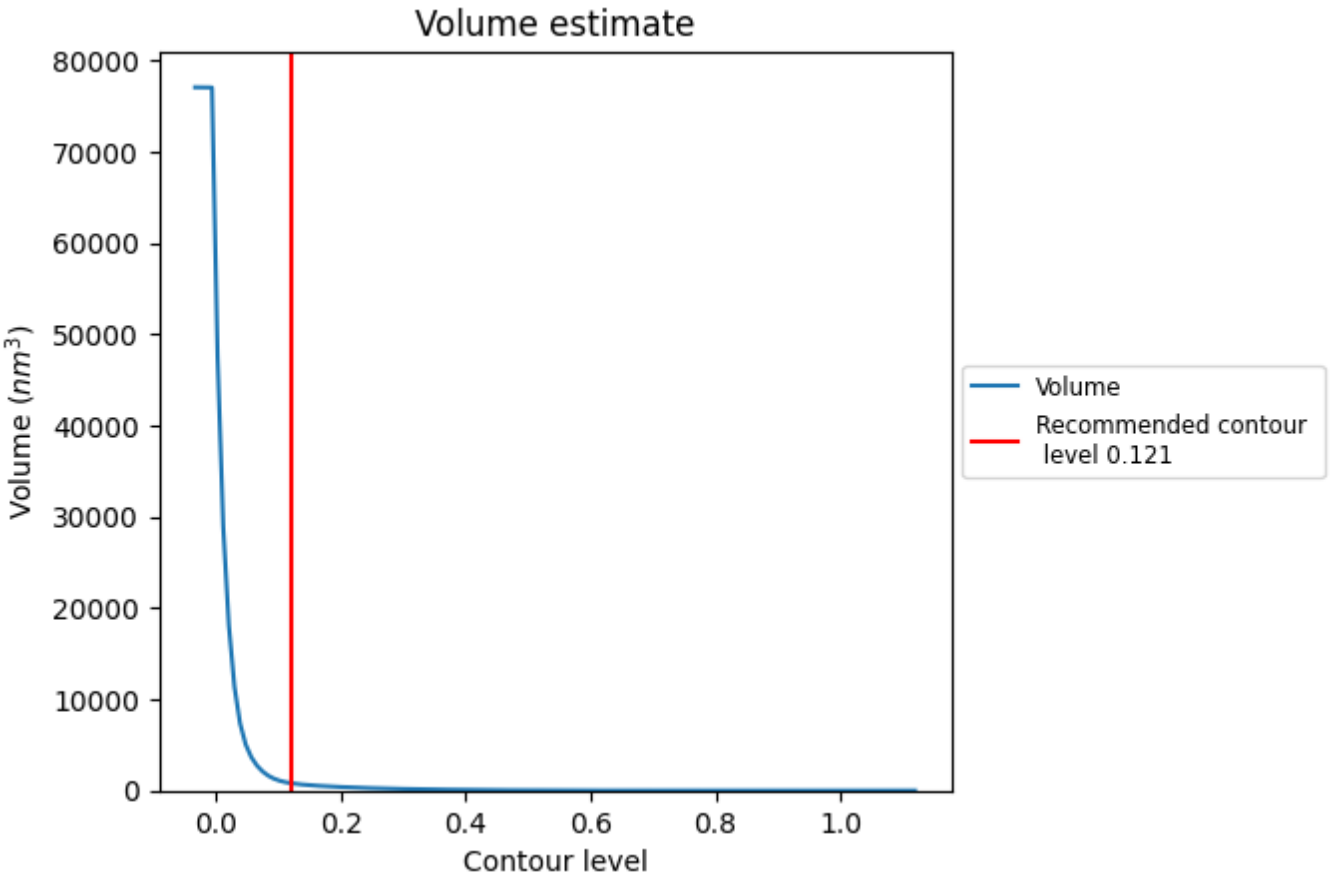
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

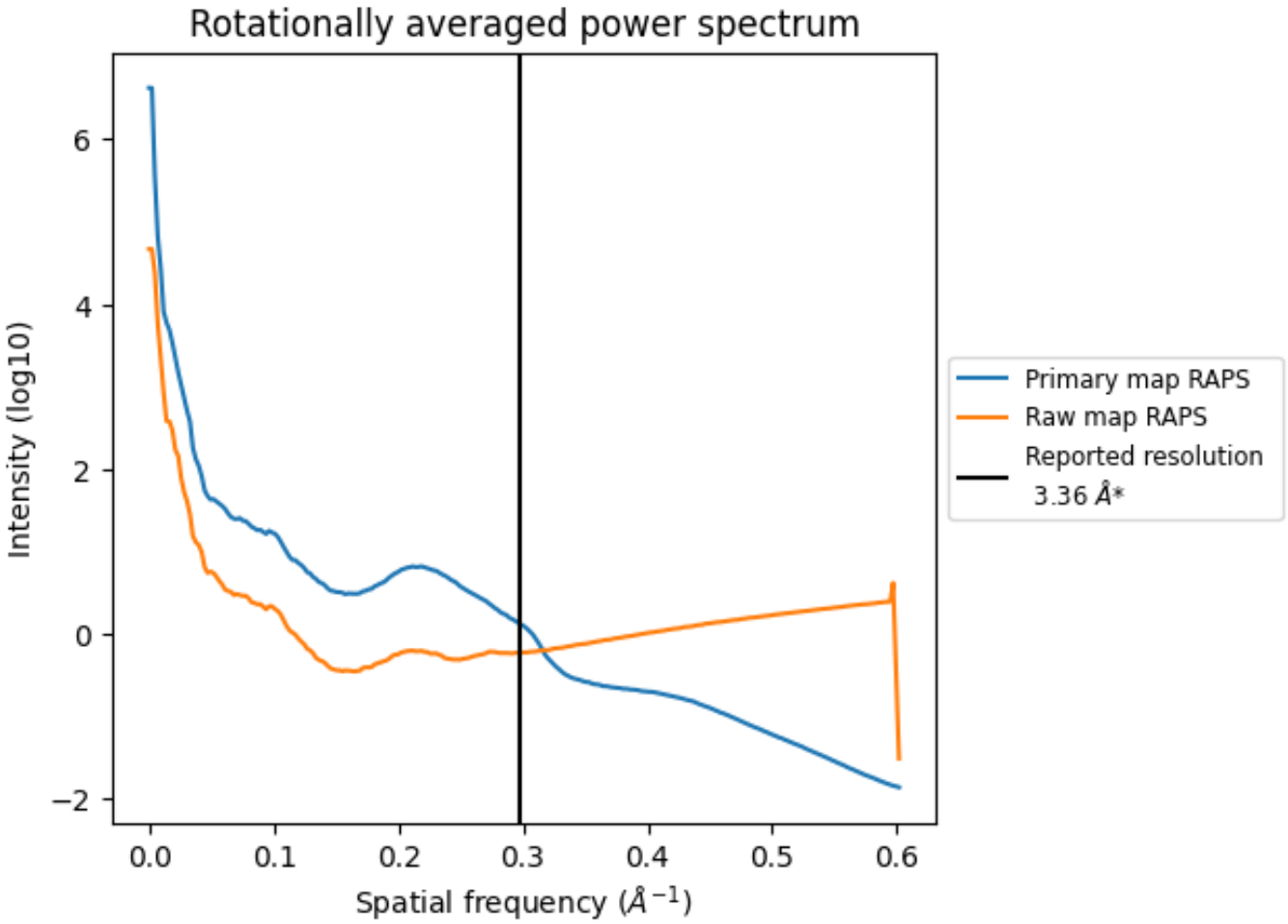
7.2 Volume estimate (i)



The volume at the recommended contour level is 808 nm^3; this corresponds to an approximate mass of 730 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)

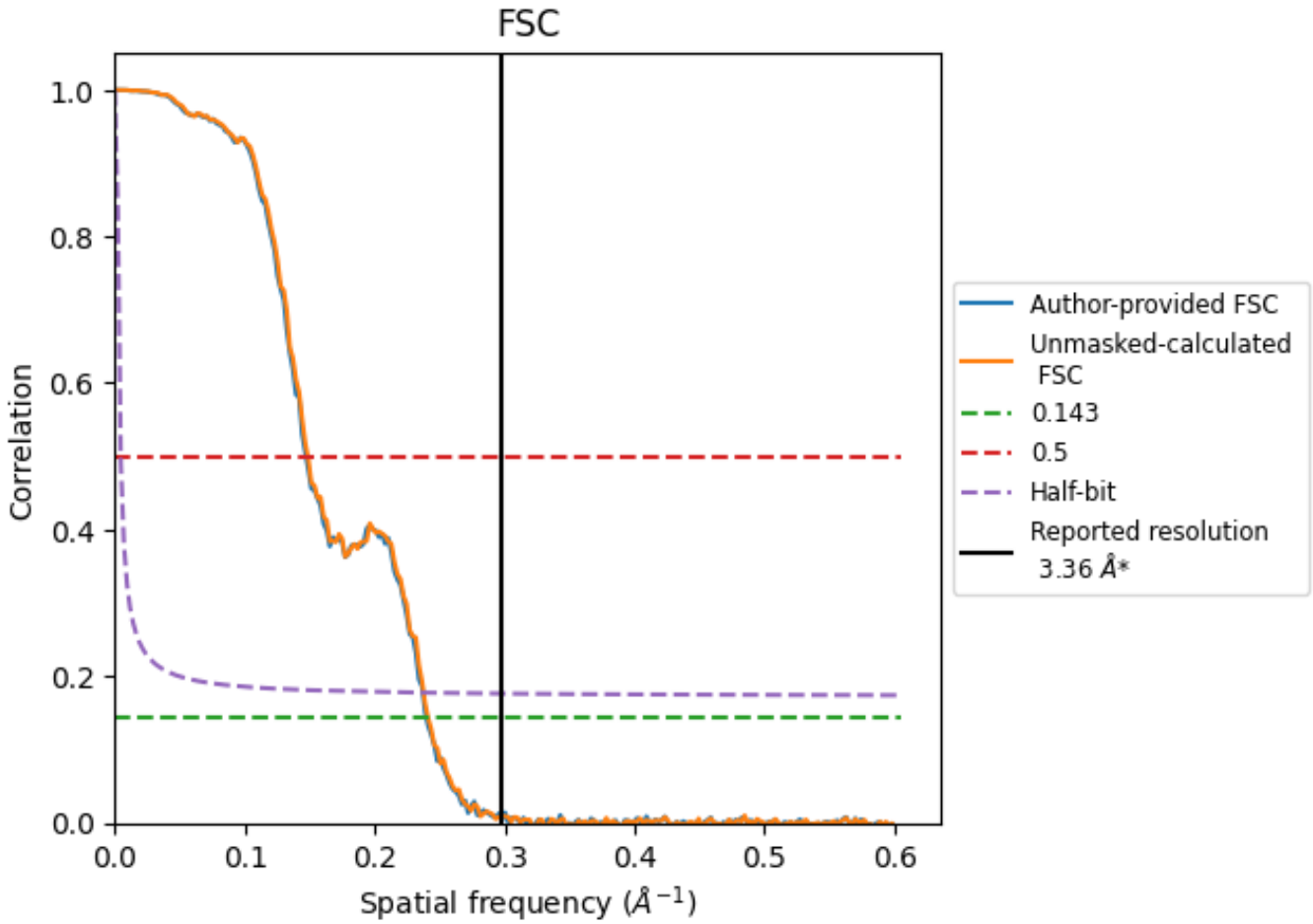


*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	4.17	6.79	4.22
Unmasked-calculated*	4.15	6.73	4.21

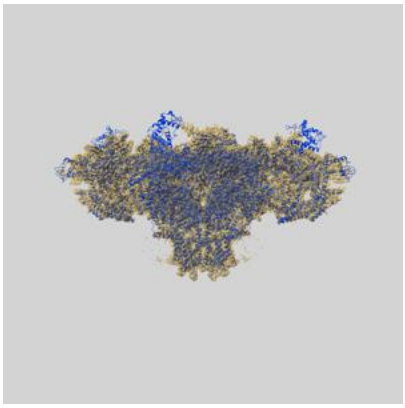
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.36 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.36 by more than 10 %

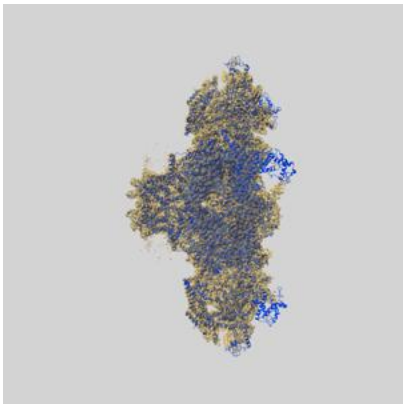
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23692 and PDB model 7M6A. Per-residue inclusion information can be found in section 3 on page 6.

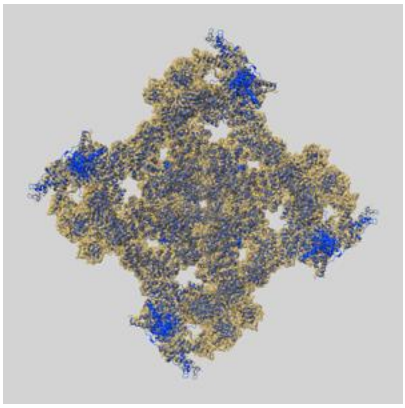
9.1 Map-model overlay



X



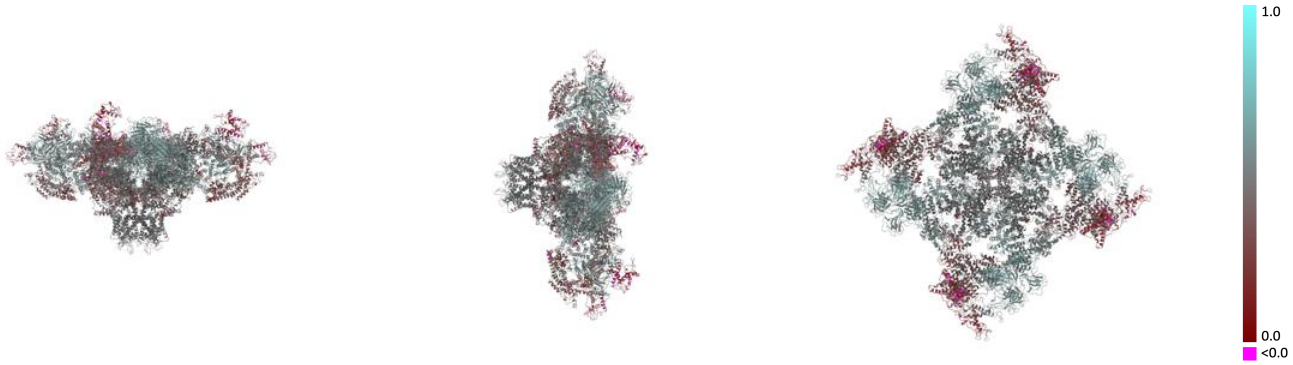
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

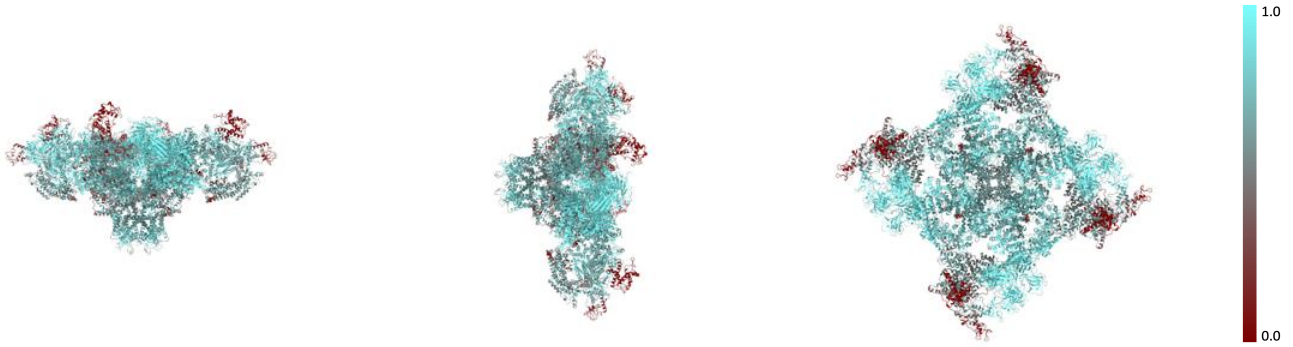
9.2 Q-score mapped to coordinate model



X Y Z

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

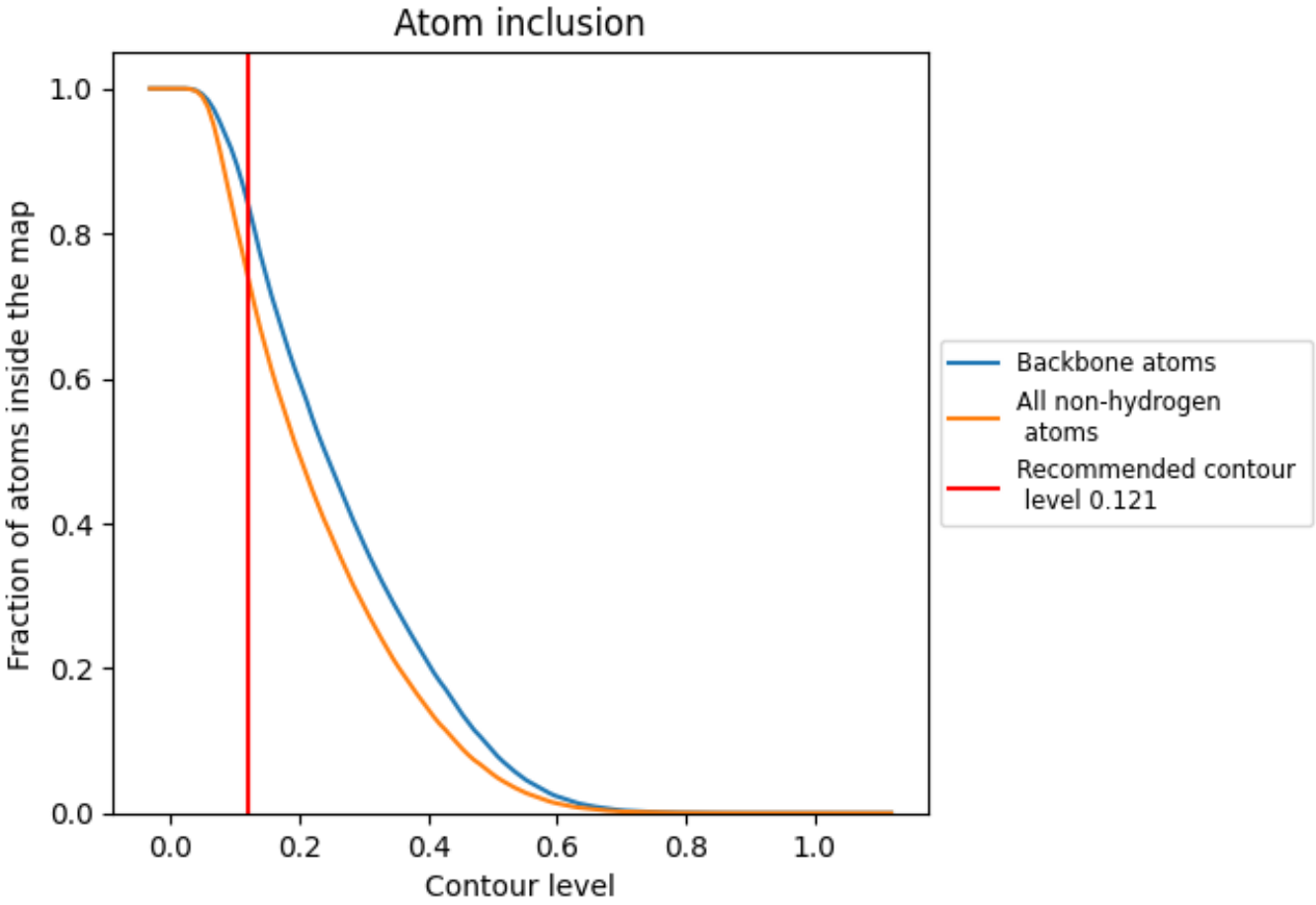
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.121).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7349	0.4570
A	0.7324	0.4580
B	0.7300	0.4530
F	0.8821	0.5530
G	0.7324	0.4540
H	0.8672	0.5530
I	0.7313	0.4530
J	0.8784	0.5500
O	0.8821	0.5520