wwPDB EM Validation Summary Report (i)

Oct 14, 2024 – 07:57 PM EDT

PDB ID	:	8UQ4
EMDB ID	:	EMD-42460
Title	:	Structure of human RyR2-S2808D in the subprimed state in the presence of H2O2/NOC-12/GSH
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-10-23
Resolution	:	3.64 Å(reported)
Based on initial model	:	7UA5

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 (i)) were used in the production of this report:

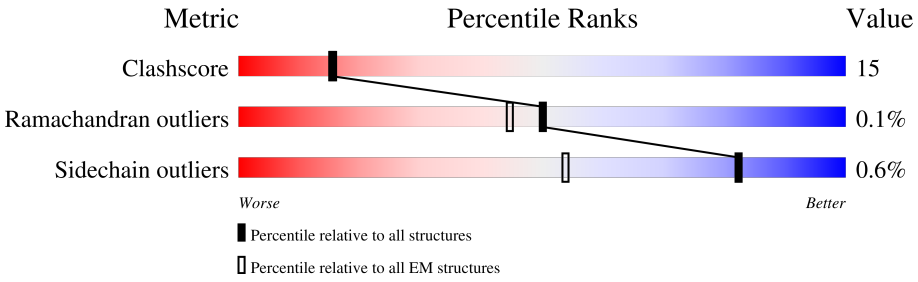
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4967	14% 58% 27% 15%
1	B	4967	14% 58% 27% 15%
1	C	4967	14% 58% 26% 15%
1	D	4967	14% 58% 26% 15%
2	E	108	80% 19%
2	F	108	80% 19%
2	G	108	79% 19%
2	H	108	80% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 138608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0
1	B	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0
1	C	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0
1	D	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

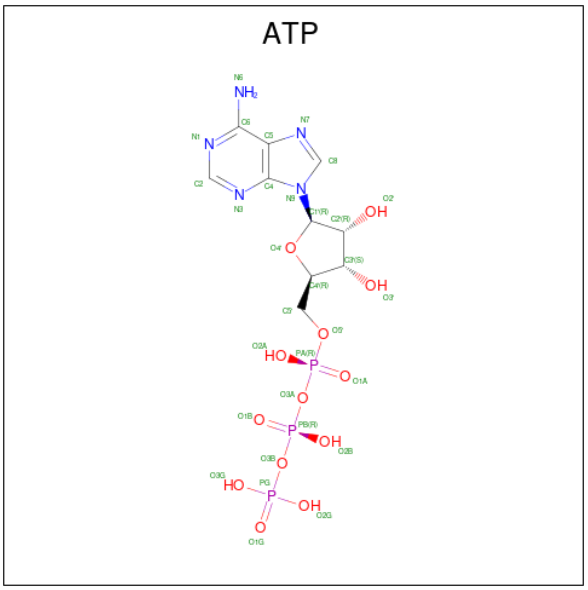
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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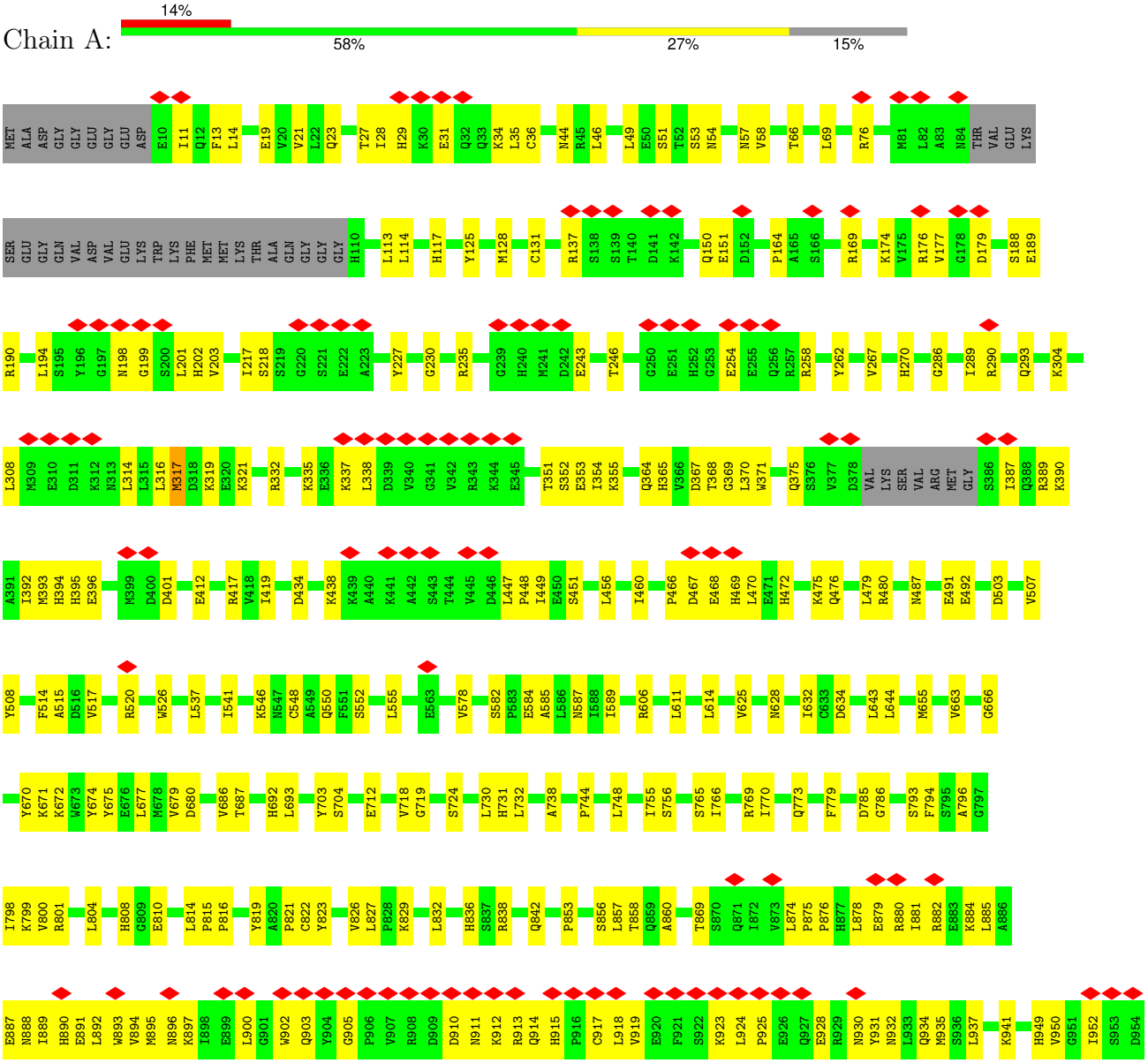
Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

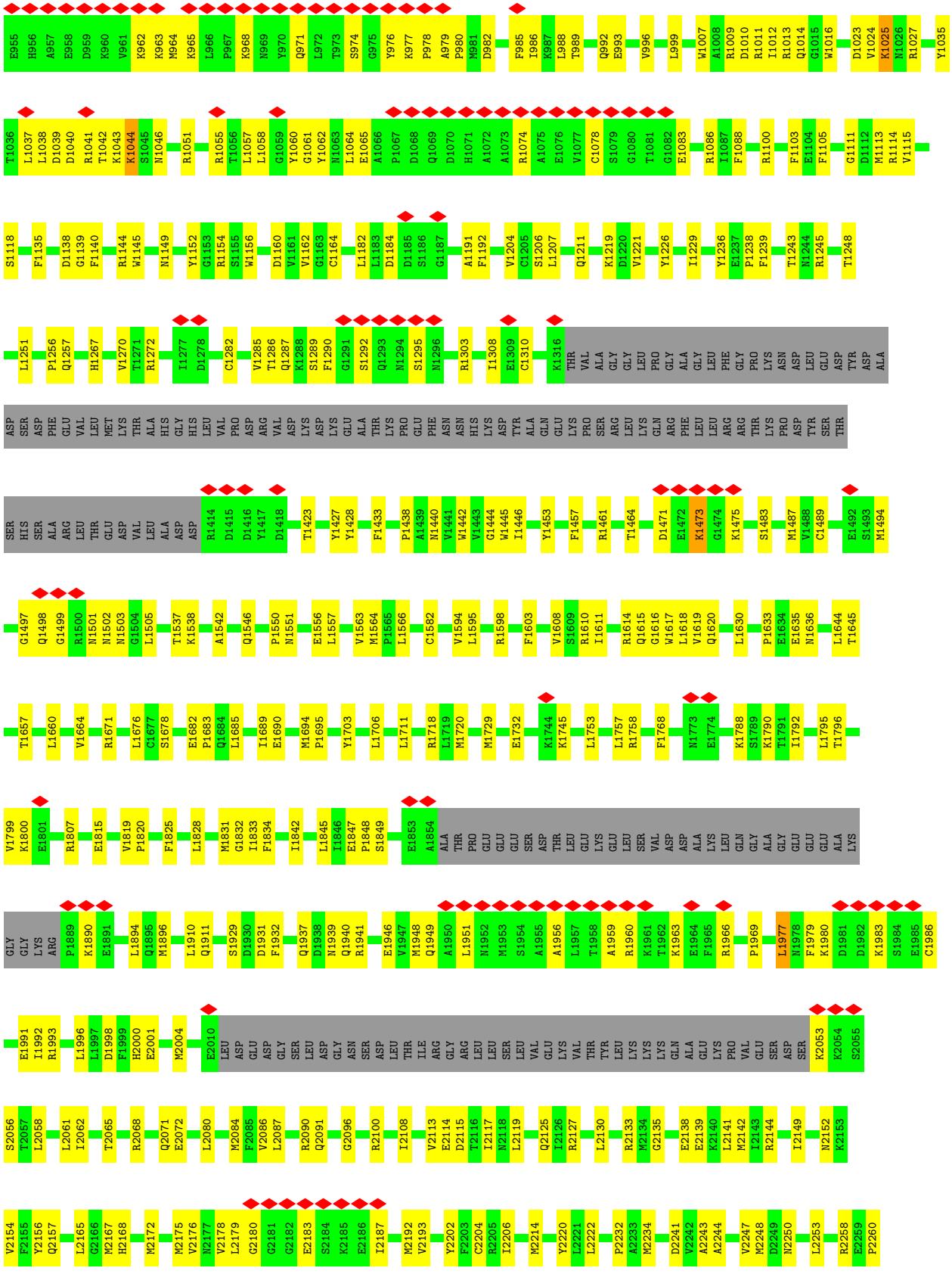
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ryanodine receptor 2

Chain A:

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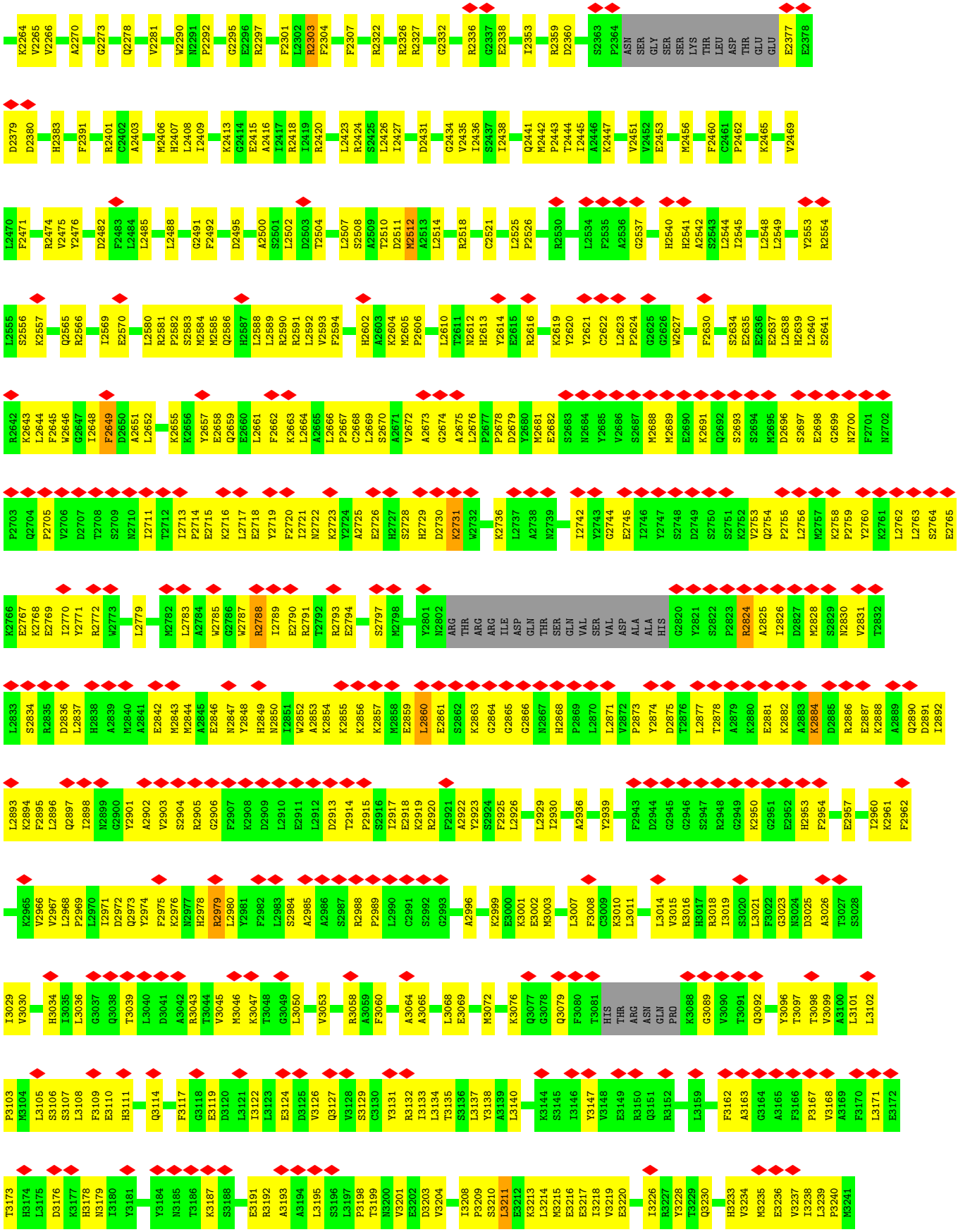
T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 R1051 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1086 I1087 F1088 R1100 F1103 E1104 F1105 G1111 D1112 M1113 R1114 V1115
S1118 F1135 D1138 G1139 F1140 R1144 W1145 N1149 Y1152 G1153 R1154 S1155 W1156 D1160 V1161 V1162 G1163 C1164 L1182 L1183 D1184 D1185 S1186 G1187 A1191 F1192 V1204 C1205 S1206 L1207 Q1211 K1219 D1220 V1221 Y1226 I1229 Y1236 E1237 P1238 F1239 T1243 N1244 R1245 T1248
L1251 P1256 Q1257 H1267 V1270 T1271 R1272 I1277 D1278 C1282 V1285 T1286 Q1287 K1288 S1289 F1290 G1291 S1292 Q1293 N1294 S1295 N1296 R1303 I1308 E1309 C1310 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY 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 R1414 D1415 D1416 Y1417 D1418 T1423 Y1427 Y1428 F1433 P1438 A1439 N1440 V1441 W1442 V1443 G1444 W1445 I1446 Y1453 F1457 R1461 T1464 D1471 E1472 K1473 G1474 K1475 S1483 M1487 V1488 C1489 E1492 S1493 M1494
G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 T1537 K1538 A1542 Q1546 P1550 N1551 E1556 L1557 V1563 M1564 P1565 L1566 C1582 V1594 L1595 R1598 F1603 V1608 S1609 R1610 I1611 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 L1630 P1633 E1634 E1635 N1636 L1644 T1645
T1657 L1660 V1664 R1671 L1676 C1677 S1678 E1682 P1683 Q1684 L1685 I1689 E1690 M1694 P1695 Y1703 L1706 L1711 R1718 L1719 M1720 M1729 E1732 K1744 K1745 L1753 L1757 R1758 F1768 N1773 E1774 K1788 S1789 K1790 T1791 I1792 L1795 T1796
V1799 K1800 E1801 R1807 E1815 V1819 P1820 F1825 L1828 M1831 G1832 I1833 F1834 I1842 L1845 I1846 E1847 P1848 S1849 E1853 A1854 ALA THR PRO GLU GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS
GLY GLY LYS ARG P1869 K1890 E1891 L1894 Q1896 M1896 L1910 Q1911 S1929 D1930 D1931 F1932 Q1937 D1938 N1939 Q1940 R1941 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 E1964 F1965 R1966 P1969 L1977 N1978 F1979 K1980 D1981 D1982 K1983 S1984 E1985 C1986
E1991 I1992 R1993 L1996 L1997 D1998 F1999 H2000 E2001 M2004 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055
S2056 T2057 L2058 L2061 I2062 T2065 R2068 Q2071 E2072 L2080 M2084 F2085 V2086 L2087 R2090 Q2091 G2096 R2100 I2108 V2113 E2114 D2115 T2116 I2117 N2118 L2119 Q2125 I2126 R2127 L2130 R2133 M2134 G2135 E2138 E2139 K2140 L2141 M2142 I2143 R2144 I2149 N2152 K2153
V2154 F2155 Y2156 Q2157 L2165 G2166 M2167 H2168 M2172 M2175 V2176 N2177 V2178 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 M2192 V2193 Y2202 F2203 C2204 R2205 I2206 M2214 Y2220 L2221 L2222 P2232 A2233 M2234 D2241 V2242 A2243 A2244 V2247 M2248 D2249 N2250 L2253 R2258 E2259 P2260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D2379 D2380 H2383 F2391 R2401 C2402 A2403 M2406 H2407 L2408 I2409 K2413 G2414 E2415 A2416 I2417 R2418 I2419 R2420 L2423 R2424 S2425 L2426 I2427 D2431 G2434 V2435 I2436 S2437 I2438 Q2441 M2442 P2443 T2444 I2445 A2446 K2447 V2451 V2452 E2453 M2456 F2460 C2461 P2462 K2465 V2469
L2470 F2471 R2474 V2475 Y2476 D2482 F2483 L2484 L2485 L2488 G2491 F2492 D2495 A2500 S2501 L2502 D2503 T2504 L2507 S2508 A2509 T2510 D2511 M2512 A2513 L2514 R2518 C2521 L2525 P2526 R2530 L2534 F2535 A2536 G2537 H2540 H2541 A2542 S2543 L2544 I2545 L2548 L2549 Y2553 R2554
L2555 S2556 K2557 Q2565 R2566 I2569 E2570 L2580 R2581 P2582 S2583 M2584 M2585 Q2586 H2587 L2588 L2589 R2590 R2591 L2592 V2593 F2594 H2602 A2603 K2604 M2605 P2606 L2610 T2611 N2612 H2613 Y2614 E2615 R2616 K2619 Y2620 Y2621 C2622 L2623 P2624 G2625 G2626 W2627 F2630 S2634 E2635 E2636 E2637 L2638 H2639 L2640 S2641
R2642 K2643 L2644 F2645 W2646 G2647 I2648 F2649 D2650 A2651 L2652 K2655 K2656 Y2657 E2658 Q2659 E2660 L2661 F2662 K2663 L2664 A2665 L2666 P2667 C2668 L2669 S2670 A2671 V2672 A2673 G2674 A2675 L2676 P2677 P2678 D2679 Y2680 M2681 E2682 S2683 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702
P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 N2722 K2723 Y2724 A2725 E2726 H2727 S2728 H2729 D2730 K2731 W2732 K2736 L2737 A2738 N2739 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765
K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 L2779 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 S2797 M2798 Y2801 N2802 ARG THR ARG ARG ILE ASP GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832
L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 H2849 N2850 I2851 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 V2872 P2873 Y2874 D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892
L2893 K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 K2919 R2920 F2921 A2922 Y2923 S2924 F2925 L2926 L2929 I2930 A2936 Y2939 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 E2957 I2960 K2961 F2962
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I3029 V3030 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 V3053 R3058 A3059 F3060 A3064 A3065 L3068 E3069 M3072 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 Y3096 T3097 T3098 V3099 A3100 L3101 L3102
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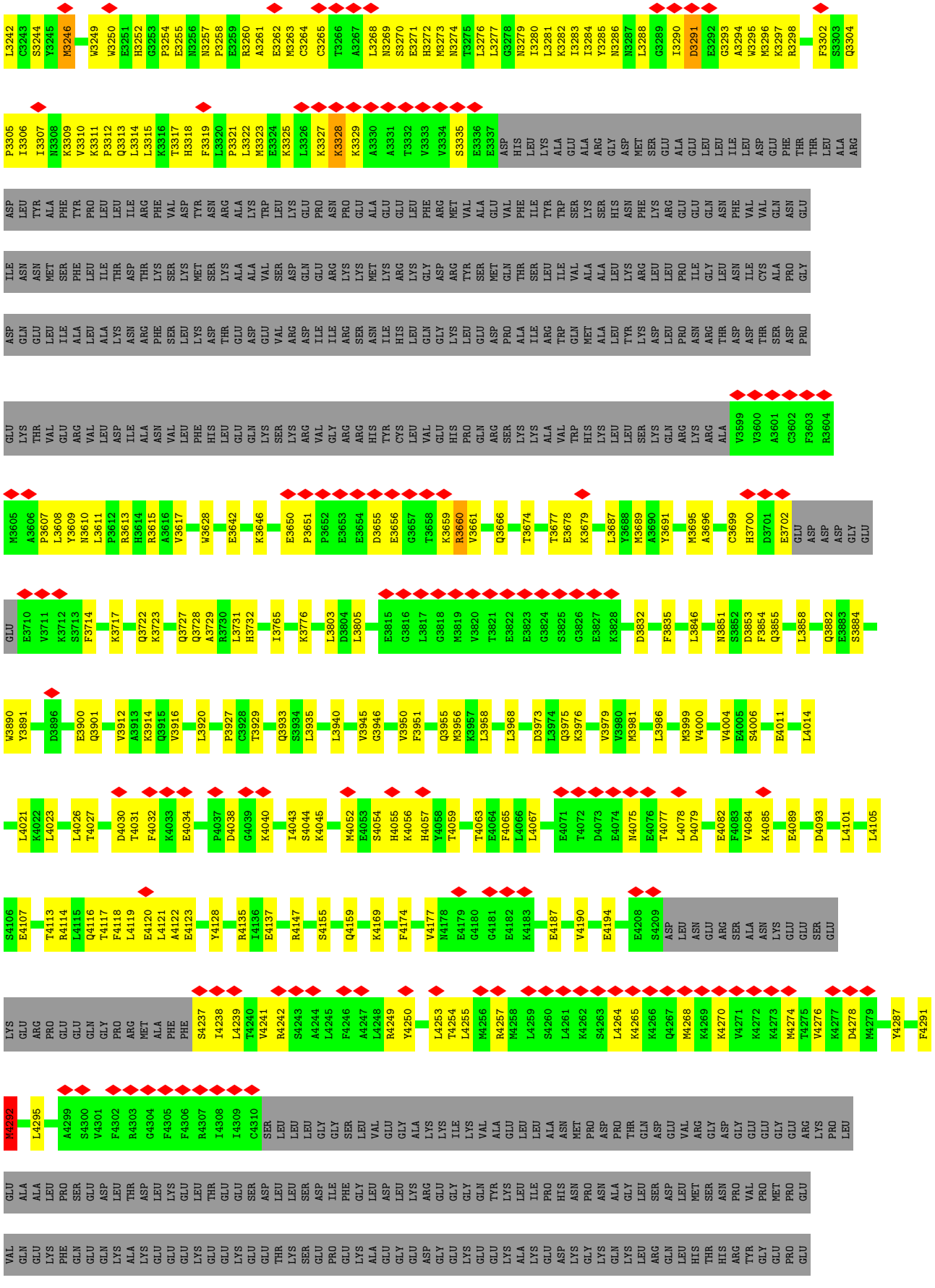
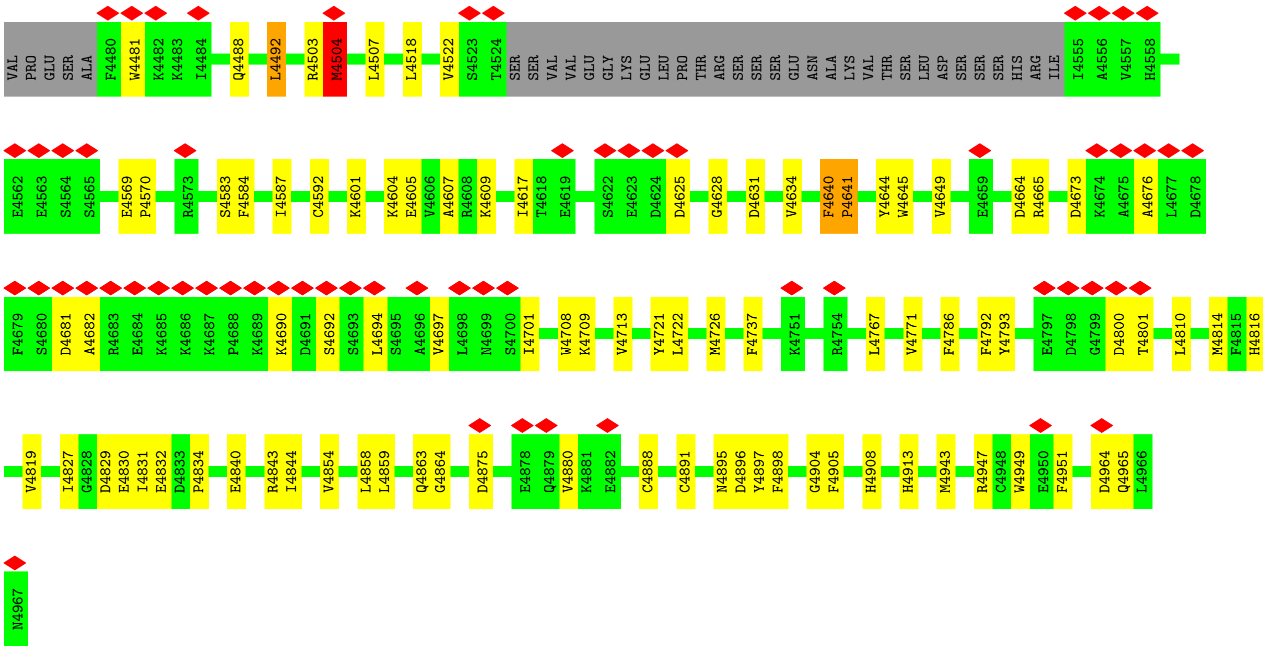
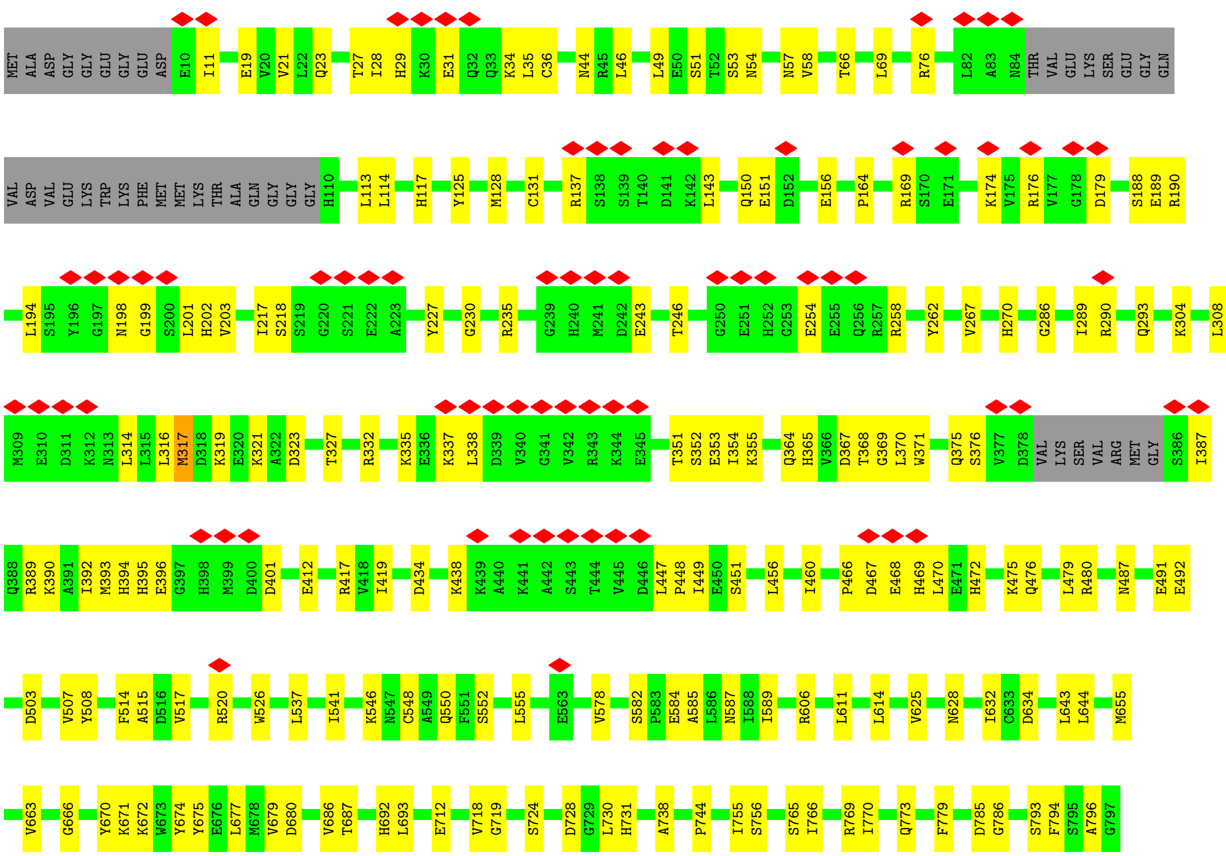
T3173 H3174 L3175 D3176 K3177 H3178 N3179 I3180 Y3181 Y3184 N3185 T3186 K3187 S3188 E3191 R3192 A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 V3201 E3202 D3203 V3204 I3208 P3209 S3210 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 I3226 R3227 Y3228 T3229 Q3230 H3233 V3234 M3235 E3236 V3237 I3238 L3239 P3240 M3241

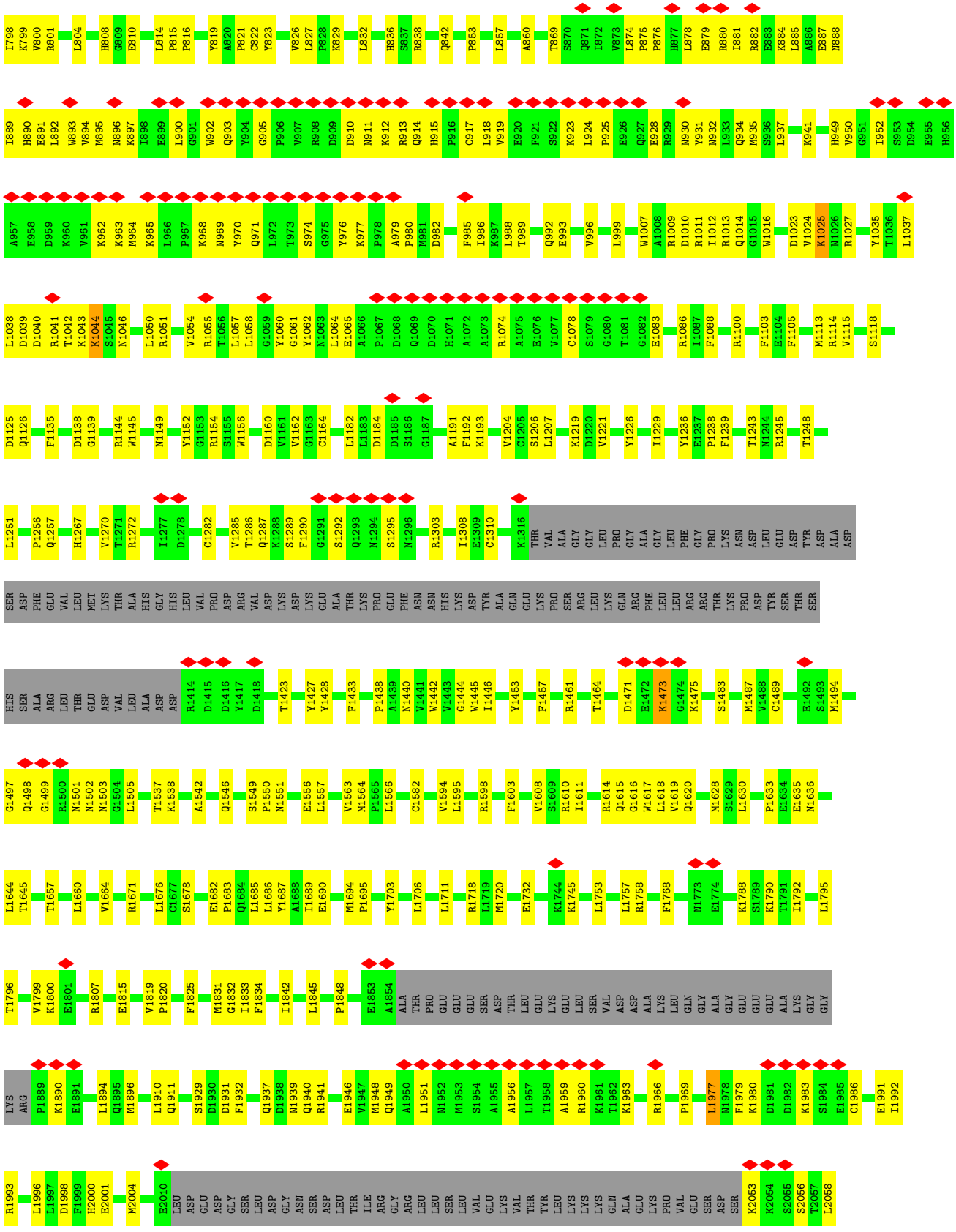




- Molecule 1: Ryanodine receptor 2

Chain B:

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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 K941 H949 V950 G951 I952 S953 D954 E955 H956
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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 R1414 D1415 D1416 Y1417 D1418 T1423 Y1427 Y1428 F1433 P1438 A1439 N1440 W1441 W1442 V1443 G1444 W1445 I1446 Y1453 F1457 R1461 T1464 D1471 E1472 K1473 G1474 K1475 S1483 M1487 V1488 C1489 E1492 S1493 M1494
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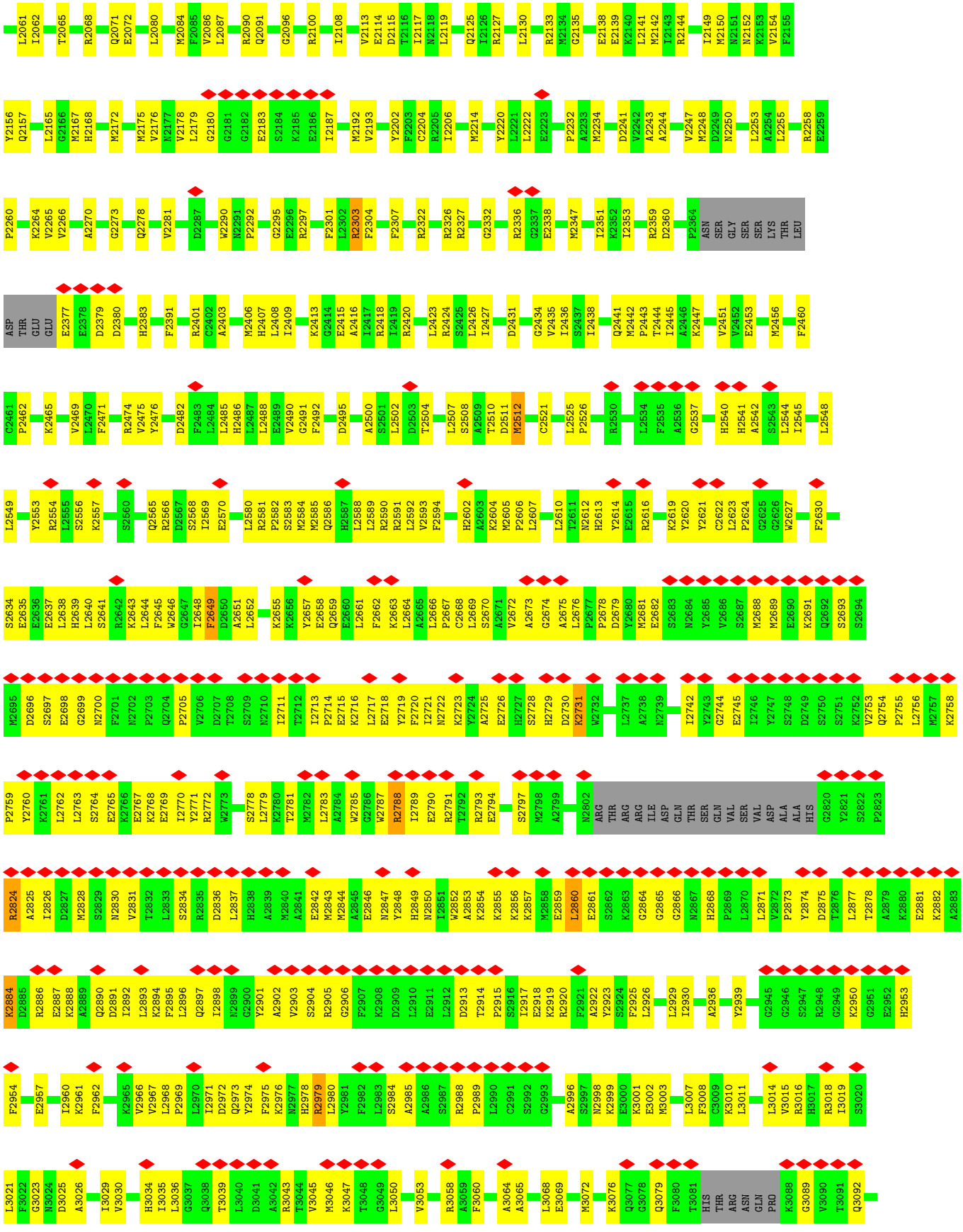
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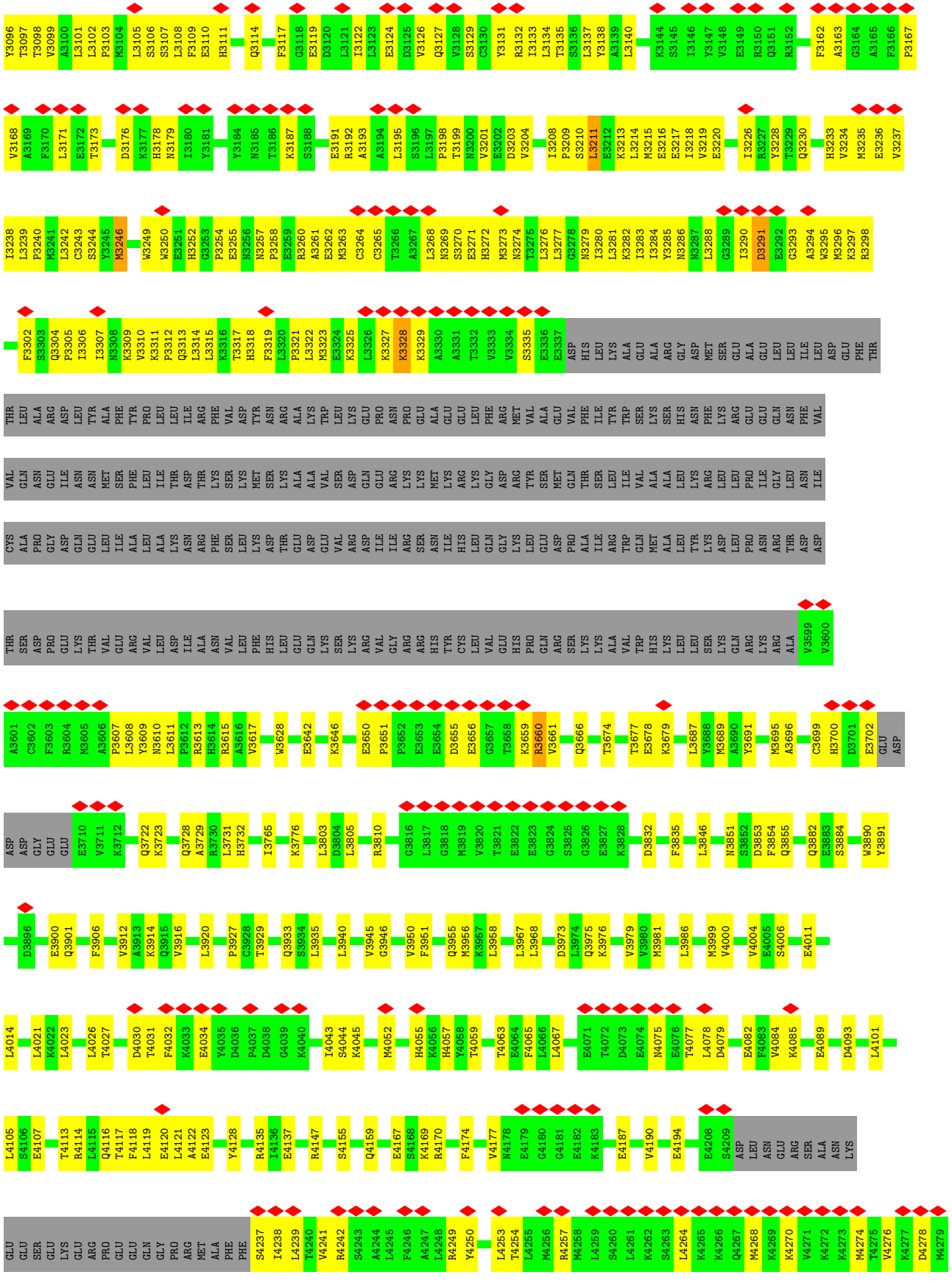
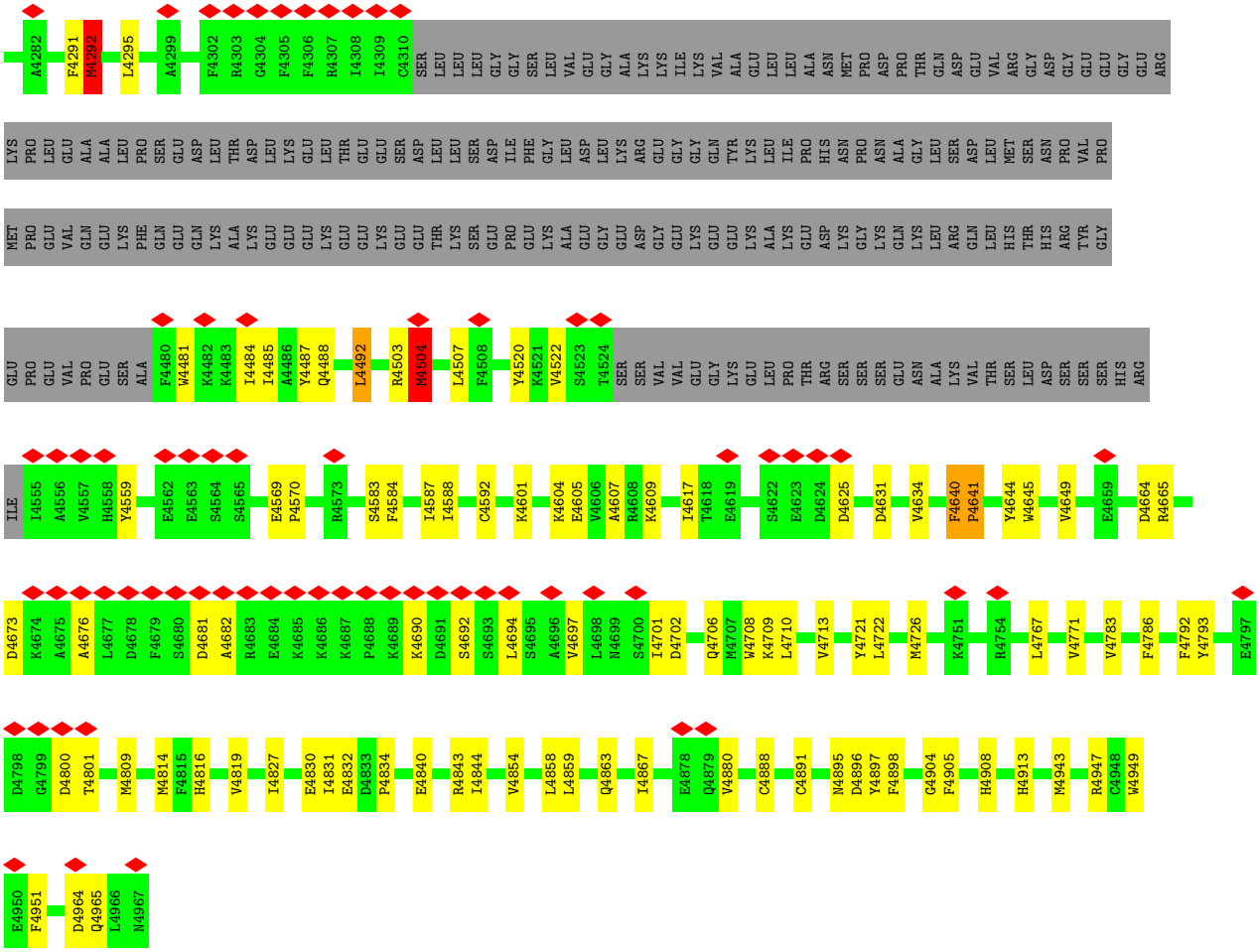
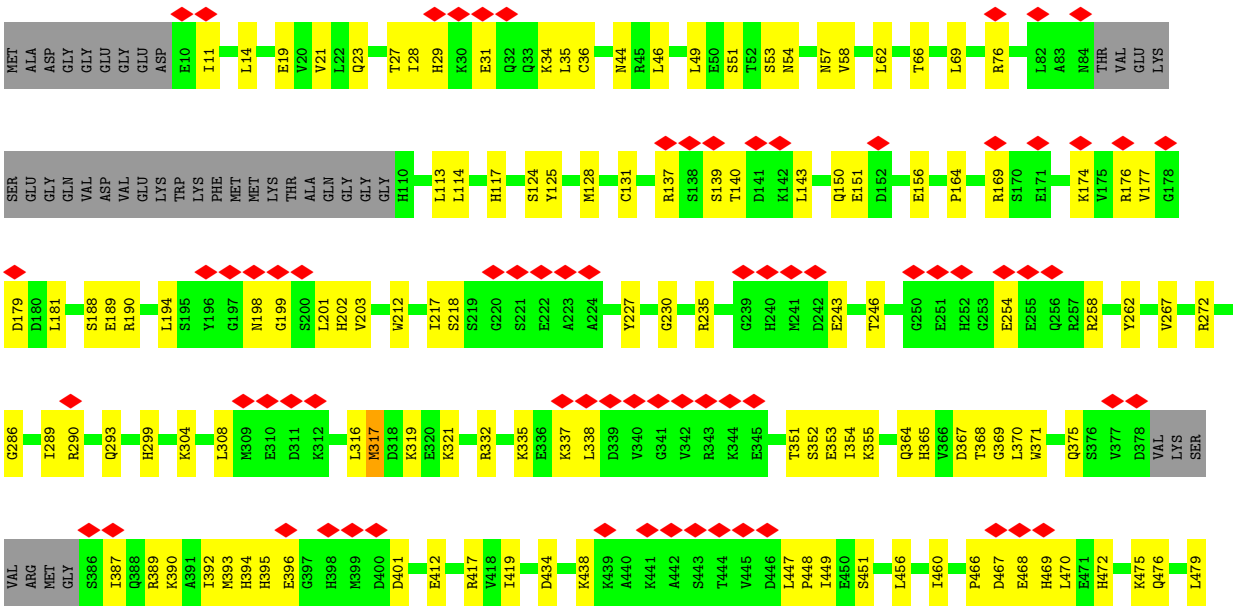
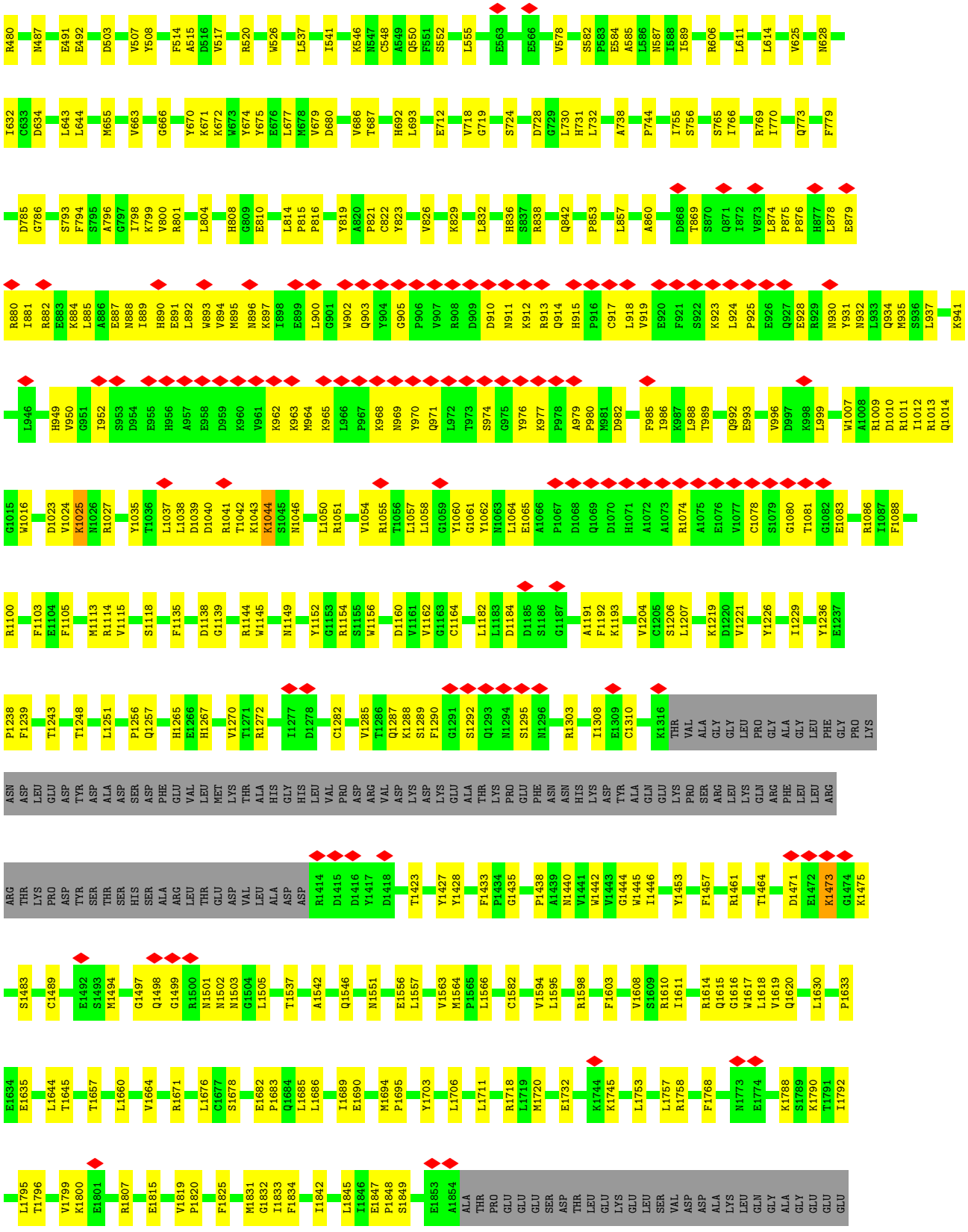




• Molecule 1: Ryanodine receptor 2

Chain C:

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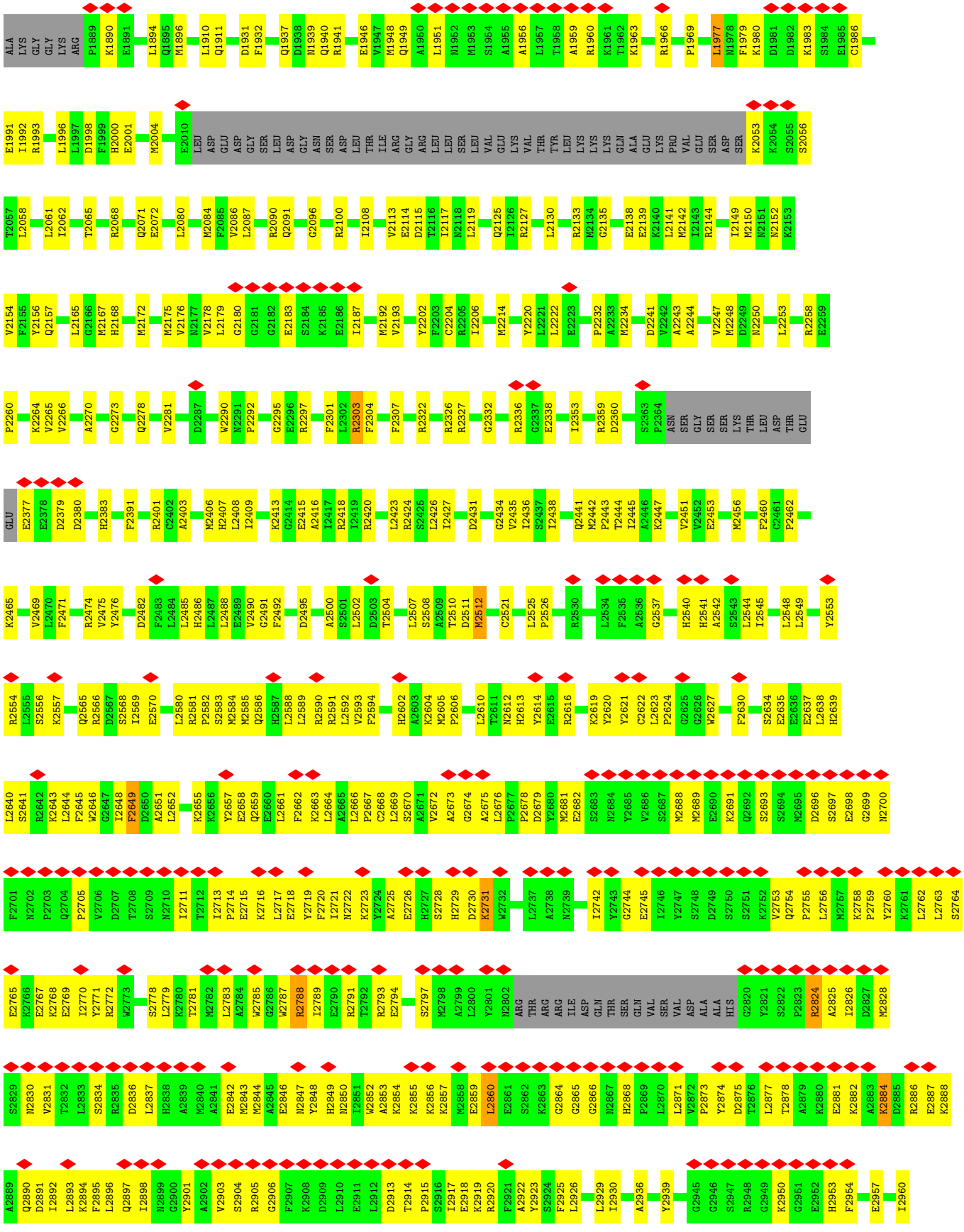

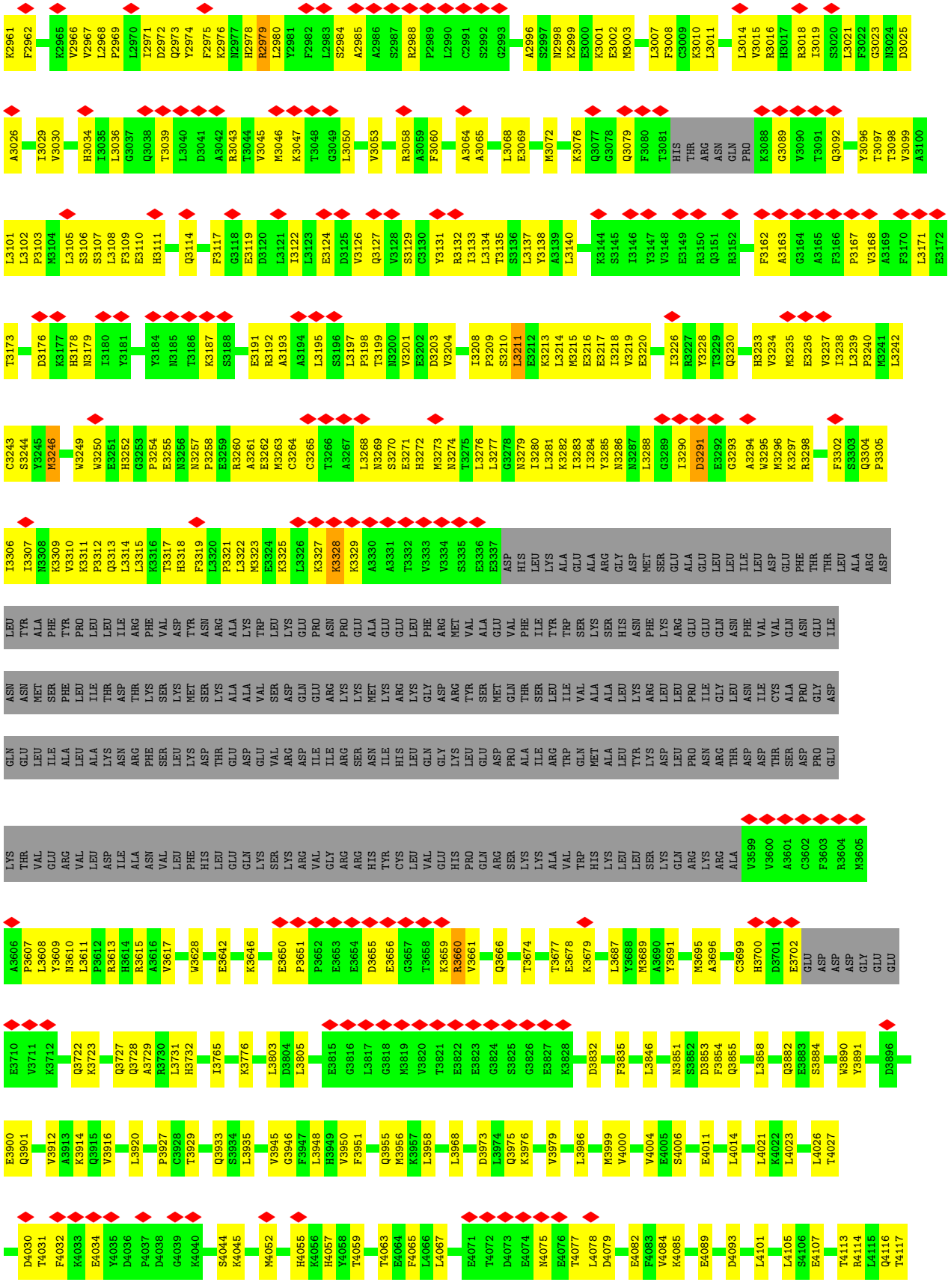
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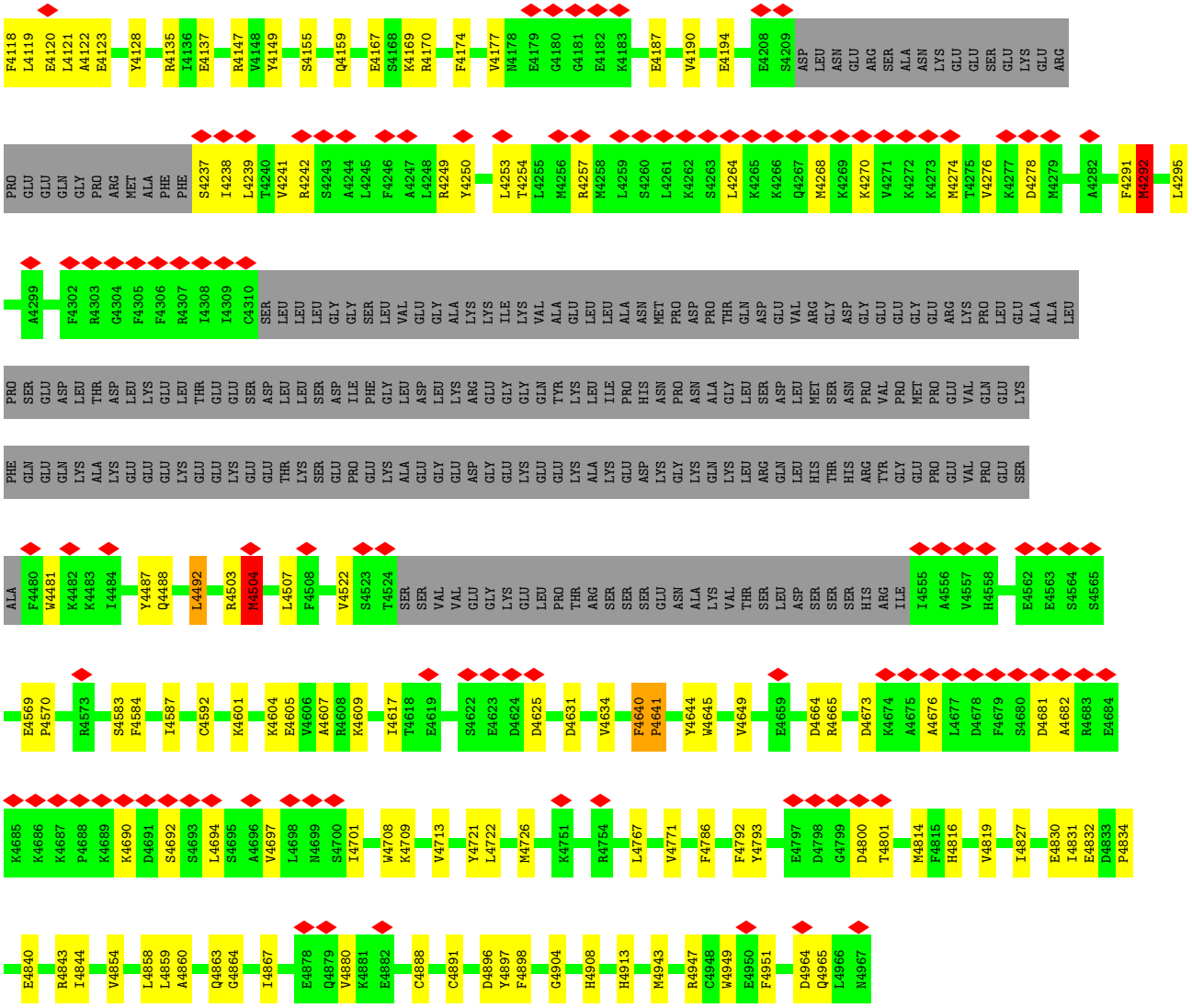
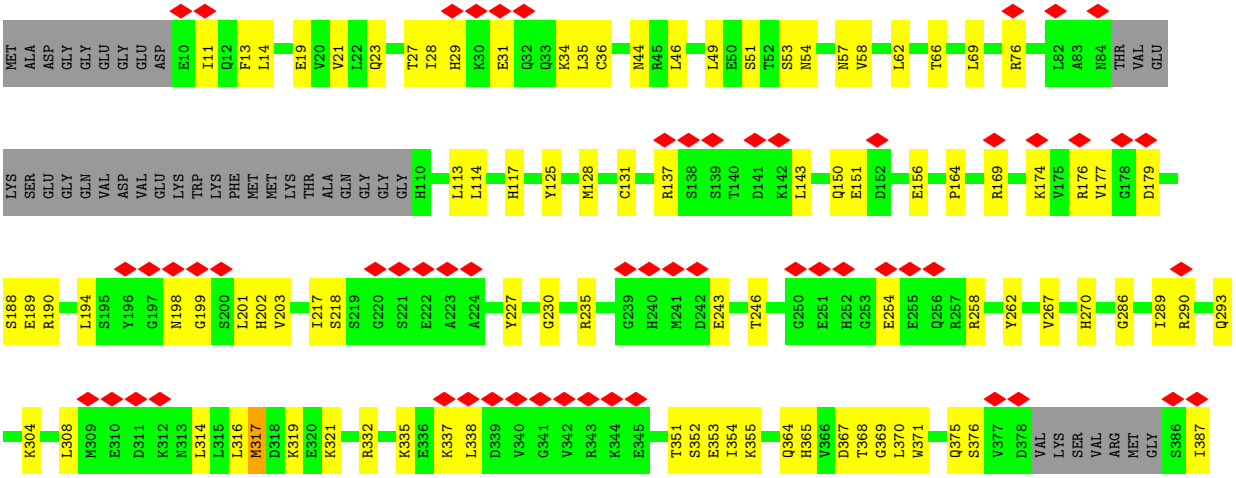
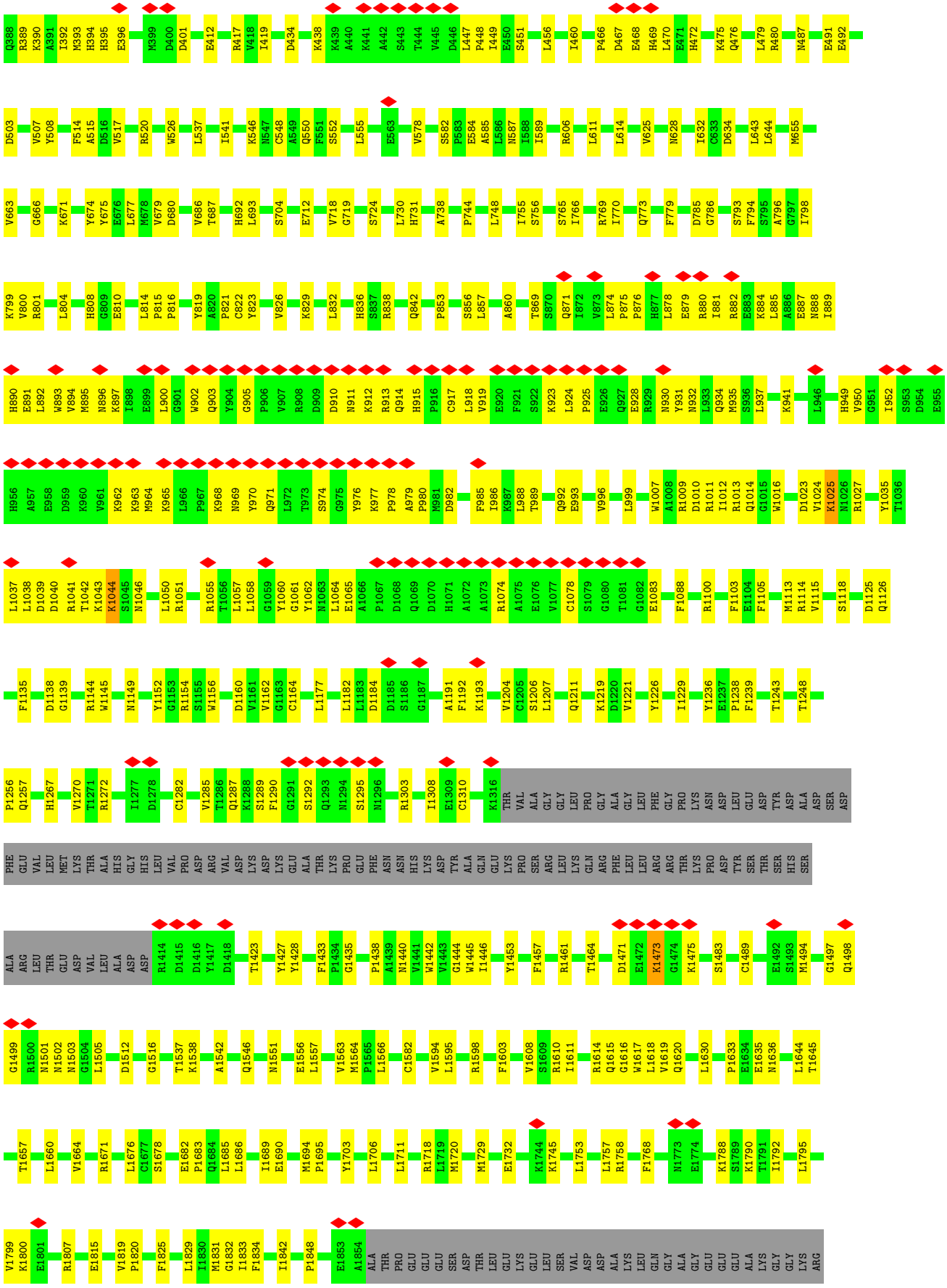


• Molecule 1: Ryanodine receptor 2

Chain D:

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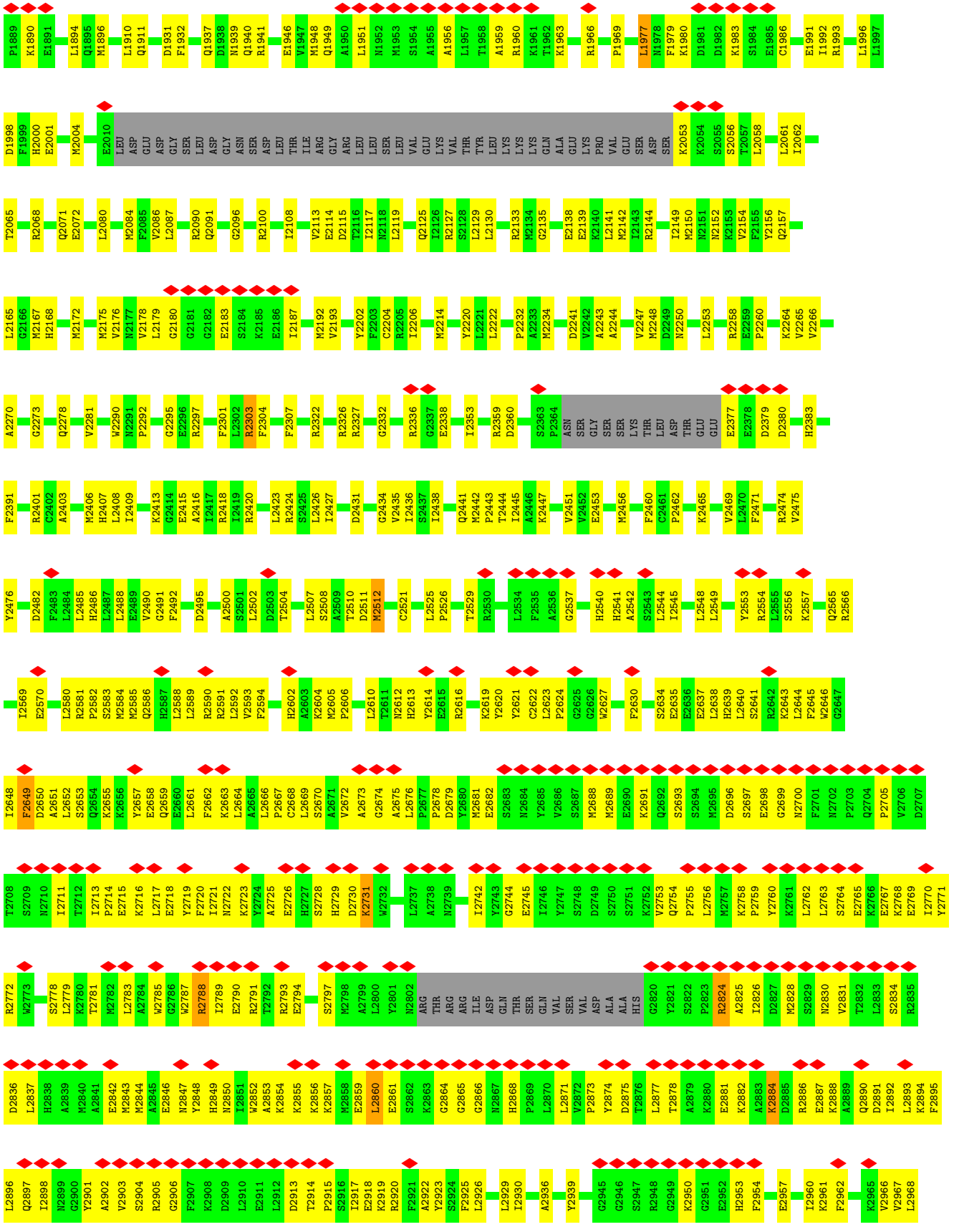
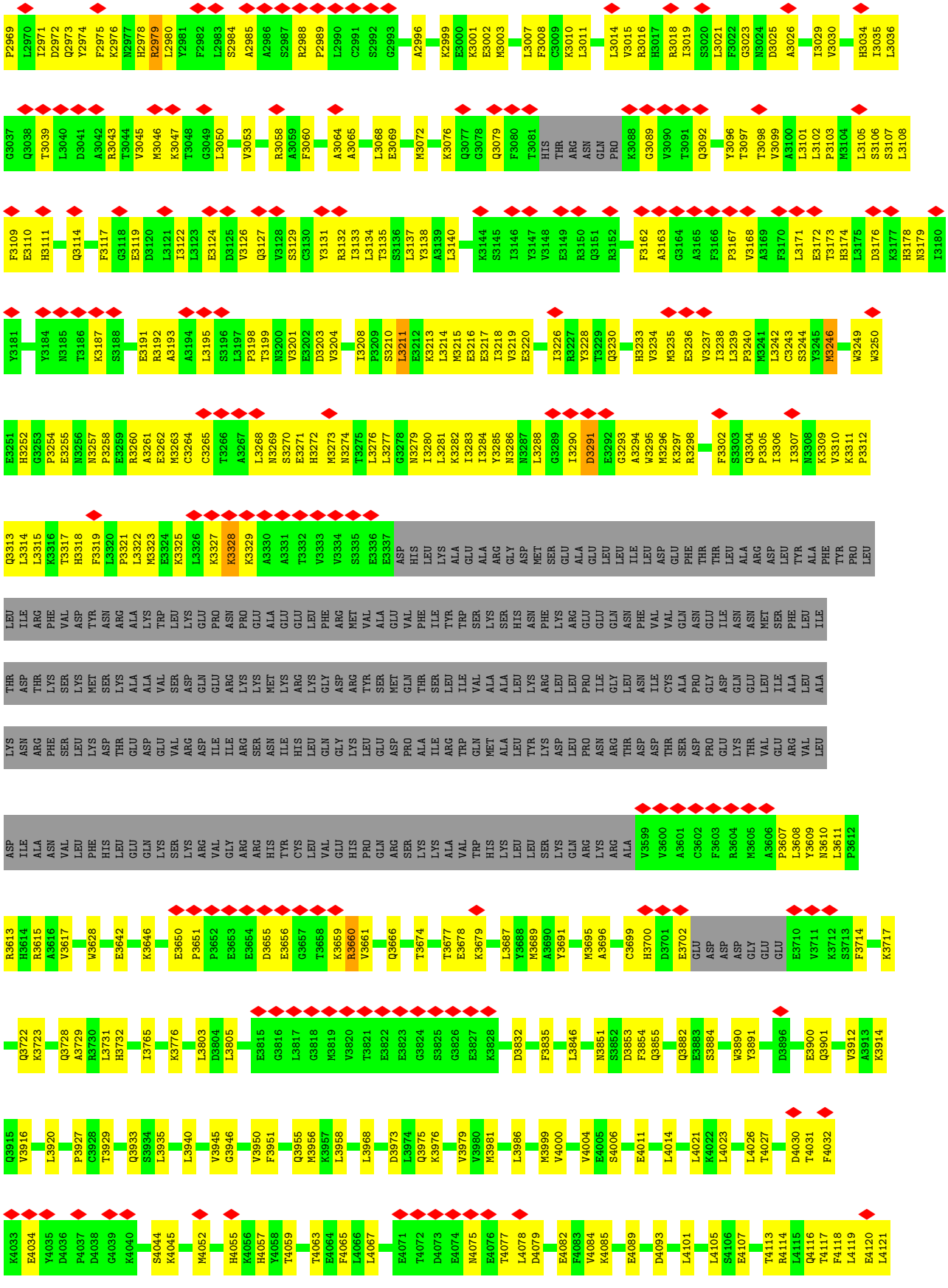
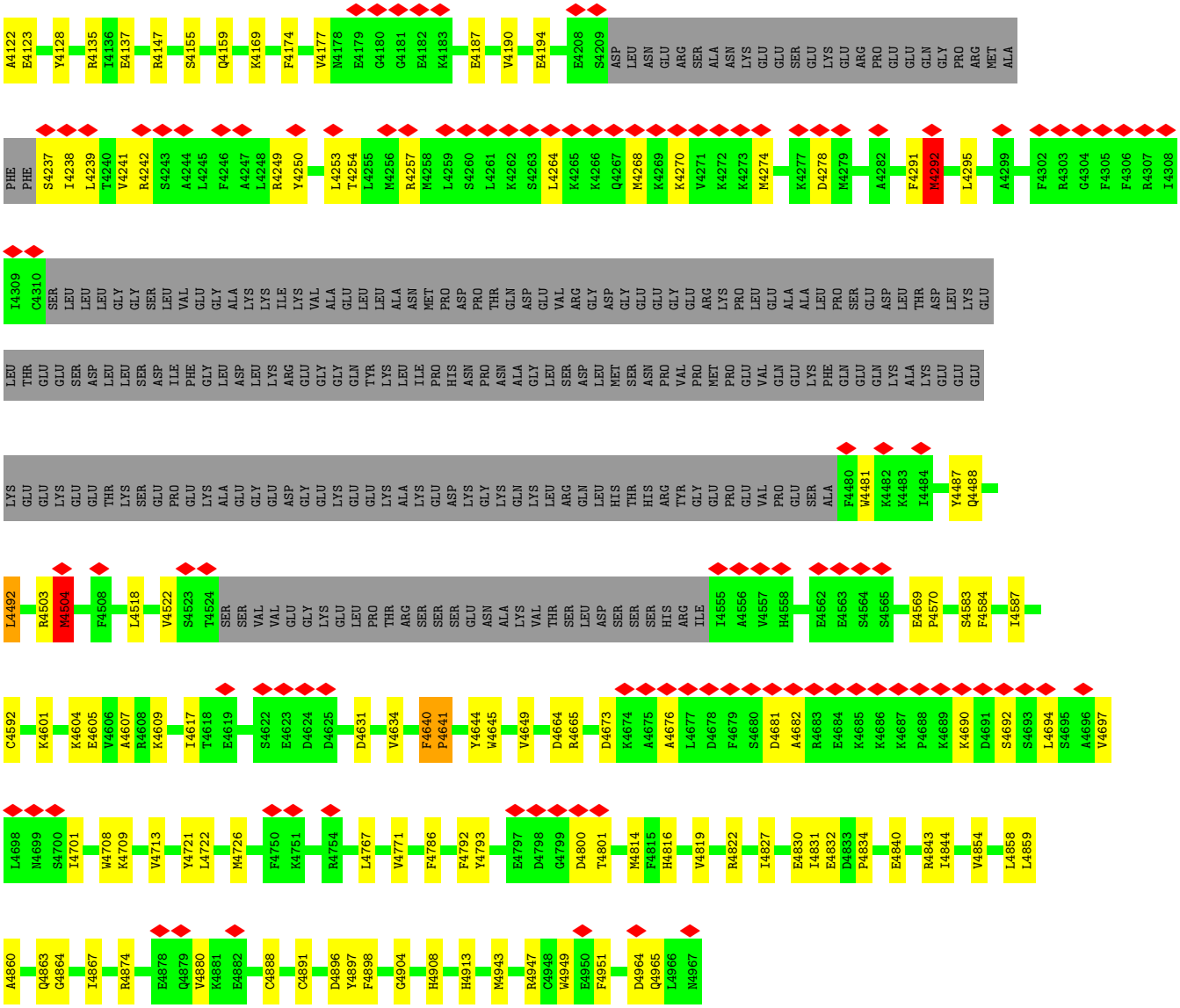
L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 L1050 R1051 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 F1088 R1100 F1103 E1104 F1105 M1113 R1114 V1115 S1118 D1125 Q1126
F1135 D1138 G1139 R1144 W1145 N1149 Y1152 G1153 R1154 S1155 W1156 D1160 V1161 V1162 G1163 C1164 L1177 L1182 L1183 D1184 D1185 S1186 G1187 A1191 F1192 K1193 V1204 C1205 S1206 L1207 Q1211 K1219 D1220 V1221 Y1226 I1229 Y1236 E1237 P1238 F1239 T1243 T1248
P1256 Q1257 H1267 V1270 T1271 R1272 I1277 D1278 C1282 V1285 T1286 Q1287 K1288 S1289 F1290 G1291 S1292 Q1293 N1294 S1295 N1296 R1303 I1308 E1309 C1310 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY 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 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 R1414 D1415 D1416 Y1417 D1418 T1423 Y1427 Y1428 F1433 P1434 G1435 P1438 A1439 N1440 V1441 W1442 V1443 G1444 W1445 I1446 Y1453 F1457 R1461 T1464 D1471 E1472 K1473 G1474 K1475 S1483 C1489 E1492 S1493 M1494 G1497 Q1498
G1499 R1500 N1501 N1502 N1503 G1504 L1505 D1512 G1516 T1537 K1538 A1542 Q1546 N1551 E1556 L1557 V1563 M1564 P1565 L1566 C1582 V1594 L1595 R1598 F1603 V1608 S1609 R1610 I1611 R1614 Q1615 G1616 W1617 L1618 V1619 Q1620 L1630 P1633 E1634 E1635 N1636 L1644 T1645
T1657 L1660 V1664 R1671 L1676 C1677 S1678 E1682 P1683 Q1684 L1685 L1686 I1689 E1690 M1694 P1695 Y1703 L1706 L1711 R1718 L1719 M1720 M1729 E1732 K1744 K1745 L1753 L1757 R1758 F1768 N1773 E1774 K1788 S1789 K1790 T1791 I1792 L1795
V1799 K1800 E1801 R1807 E1815 V1819 P1820 F1825 L1829 I1830 M1831 G1832 I1833 F1834 I1842 P1848 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU GLU ALA LYS GLY GLY LYS ARG

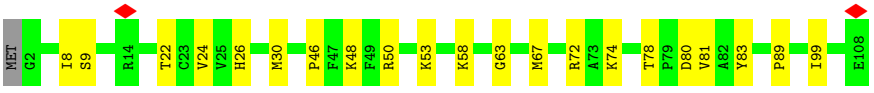






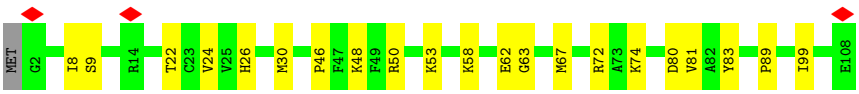
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



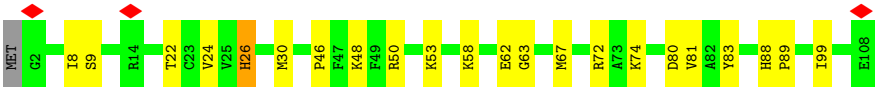
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



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

Chain G:



• 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	19753	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	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.474	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/34511	0.51	9/46614 (0.0%)
1	B	0.27	0/34511	0.51	9/46614 (0.0%)
1	C	0.27	0/34511	0.51	9/46614 (0.0%)
1	D	0.27	0/34511	0.51	9/46614 (0.0%)
2	E	0.29	0/834	0.51	0/1123
2	F	0.29	0/834	0.51	0/1123
2	G	0.29	0/834	0.51	0/1123
2	H	0.29	0/834	0.51	0/1123
All	All	0.27	0/141380	0.51	36/190948 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4292	MET	CB-CG-SD	7.58	135.13	112.40
1	C	4292	MET	CB-CG-SD	7.57	135.12	112.40
1	D	4292	MET	CB-CG-SD	7.57	135.10	112.40
1	A	4292	MET	CB-CG-SD	7.55	135.05	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4292	MET	CA-CB-CG	5.87	123.29	113.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2988	ARG	Peptide
1	A	4504	MET	Peptide
1	A	4640	PHE	Peptide
1	B	2988	ARG	Peptide
1	B	4504	MET	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	33771	0	33455	1002	0
1	B	33771	0	33455	1005	0
1	C	33771	0	33455	992	0
1	D	33771	0	33455	992	0
2	E	818	0	821	20	0
2	F	818	0	821	18	0
2	G	818	0	821	19	0
2	H	818	0	821	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	4	0
4	B	62	0	24	4	0
4	C	62	0	24	4	0
4	D	62	0	24	4	0
All	All	138608	0	137200	4003	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 15.

The worst 5 of 4003 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:B:1611:ILE:HD11	1:B:1618:LEU:HB2	1.49	0.93
1:D:1611:ILE:HD11	1:D:1618:LEU:HB2	1.49	0.92
1:A:1611:ILE:HD11	1:A:1618:LEU:HB2	1.49	0.91
1:C:1611:ILE:HD11	1:C:1618:LEU:HB2	1.49	0.90
1:B:2905:ARG:HE	1:B:2906:GLY:H	1.22	0.88

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	4198/4967 (84%)	4054 (97%)	140 (3%)	4 (0%)	48	78
1	B	4198/4967 (84%)	4055 (97%)	139 (3%)	4 (0%)	48	78
1	C	4198/4967 (84%)	4053 (96%)	141 (3%)	4 (0%)	48	78
1	D	4198/4967 (84%)	4053 (96%)	141 (3%)	4 (0%)	48	78
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17212/20300 (85%)	16623 (97%)	573 (3%)	16 (0%)	50	78

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3927	PRO
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO

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Mol	Chain	Res	Type
1	C	3927	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	A	3708/4358 (85%)	3684 (99%)	24 (1%)	84 91
1	B	3708/4358 (85%)	3684 (99%)	24 (1%)	84 91
1	C	3708/4358 (85%)	3684 (99%)	24 (1%)	84 91
1	D	3708/4358 (85%)	3684 (99%)	24 (1%)	84 91
2	E	88/89 (99%)	88 (100%)	0	100 100
2	F	88/89 (99%)	88 (100%)	0	100 100
2	G	88/89 (99%)	87 (99%)	1 (1%)	70 81
2	H	88/89 (99%)	88 (100%)	0	100 100
All	All	15184/17788 (85%)	15087 (99%)	97 (1%)	82 91

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2731	LYS
1	C	4504	MET
1	C	2824	ARG
1	C	3328	LYS
1	D	1044	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2849	HIS
1	C	4863	GLN
1	C	2868	HIS
1	C	3179	ASN

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Mol	Chain	Res	Type
1	D	477	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	ATP	B	5002	-	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
4	ATP	D	5002	-	28,33,33	0.67	0	34,52,52	0.66	1 (2%)
4	ATP	A	5003	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
4	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	D	5003	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
4	ATP	B	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	A	5002	-	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
4	ATP	C	5002	-	28,33,33	0.67	0	34,52,52	0.67	1 (2%)

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
4	ATP	B	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	3/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	3/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	3/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	3/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	10/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	10/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5003	ATP	C5-C6-N6	2.32	123.84	120.31
4	B	5003	ATP	C5-C6-N6	2.30	123.81	120.31
4	D	5003	ATP	C5-C6-N6	2.30	123.81	120.31
4	C	5002	ATP	C5-C6-N6	2.30	123.81	120.31
4	D	5002	ATP	C5-C6-N6	2.28	123.79	120.31

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	PB-O3B-PG-O3G
4	B	5002	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	ATP	1	0
4	D	5002	ATP	1	0
4	A	5003	ATP	3	0
4	C	5003	ATP	3	0

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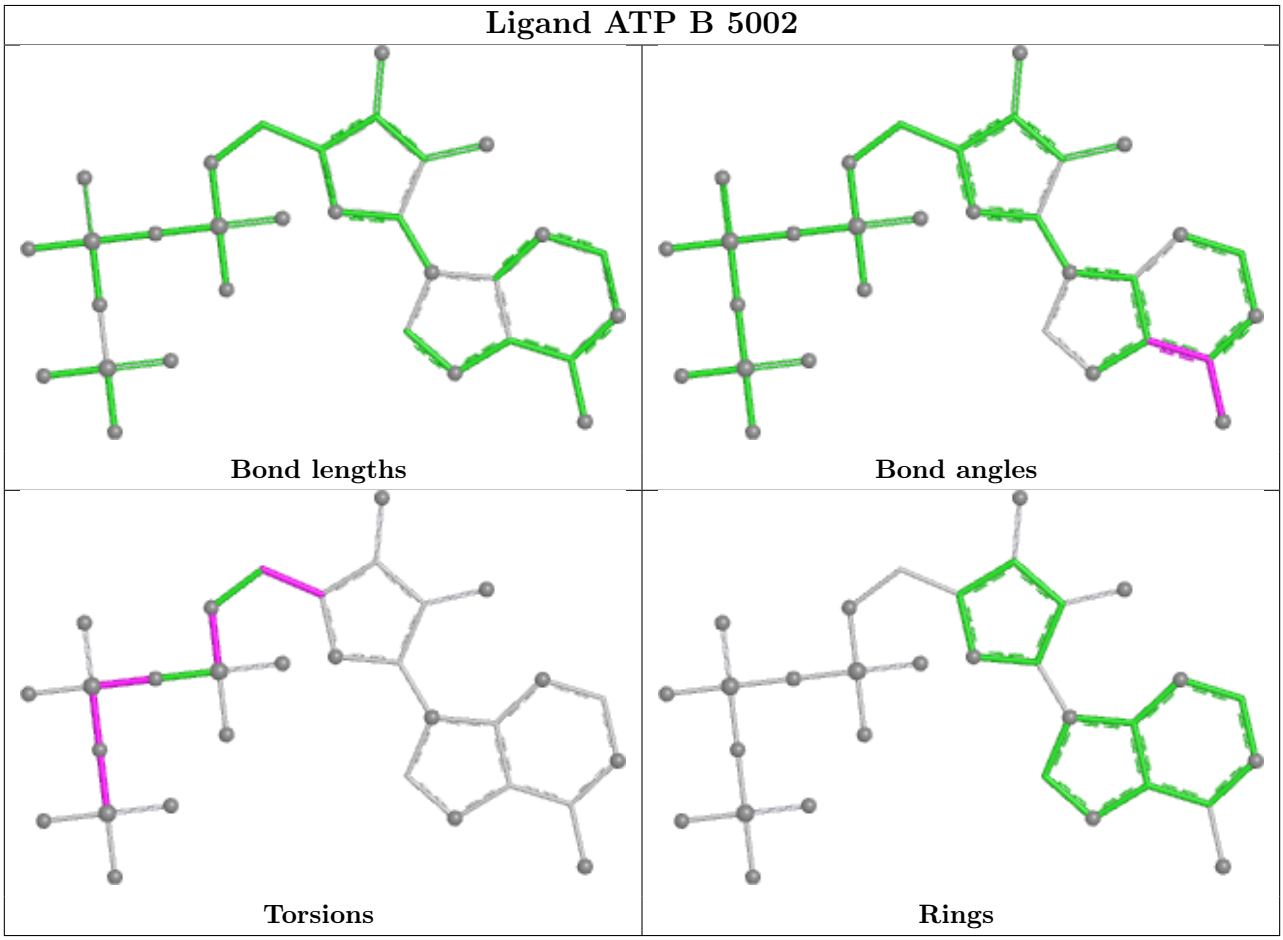
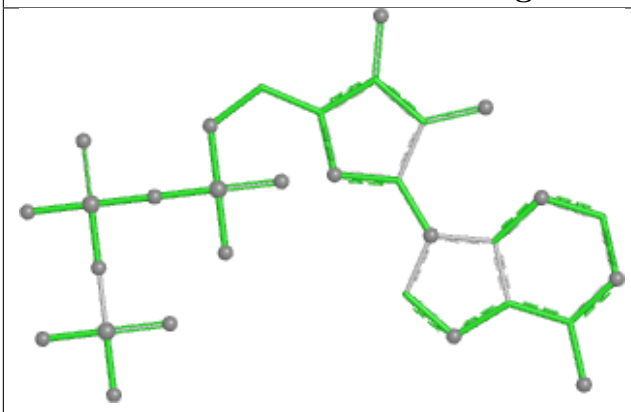
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5003	ATP	3	0
4	B	5003	ATP	3	0
4	A	5002	ATP	1	0
4	C	5002	ATP	1	0

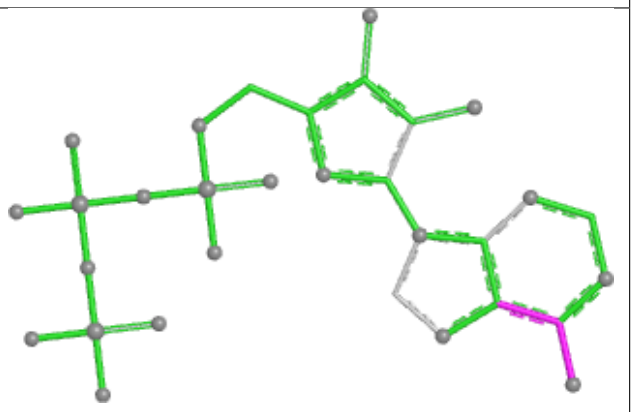
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



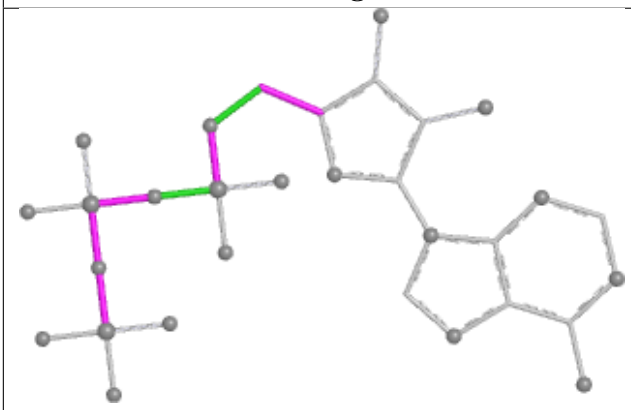
Ligand ATP D 5002



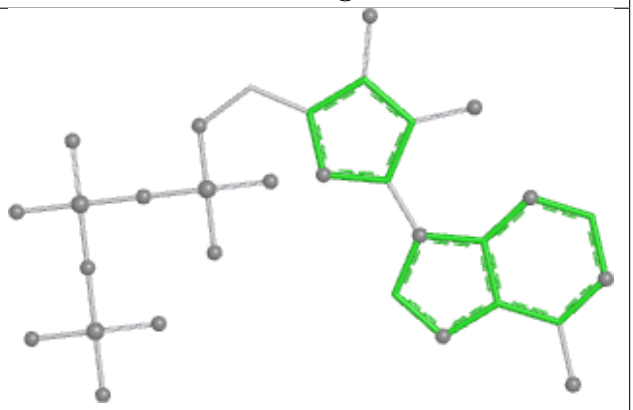
Bond lengths



Bond angles

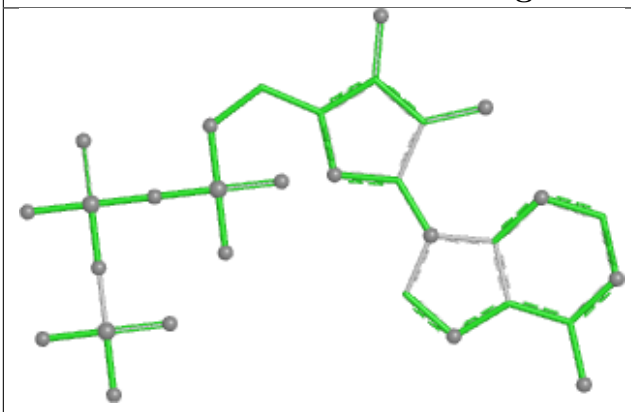


Torsions

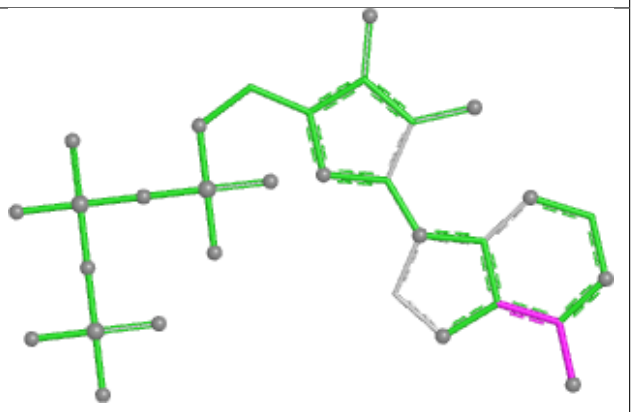


Rings

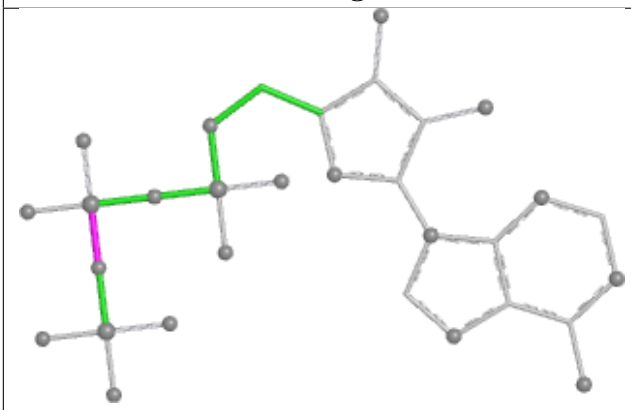
Ligand ATP A 5003



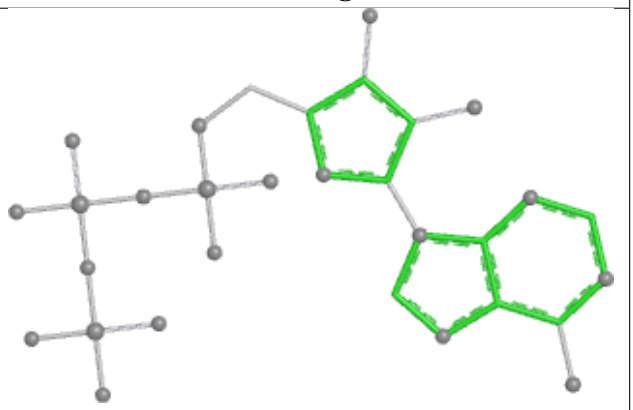
Bond lengths



Bond angles

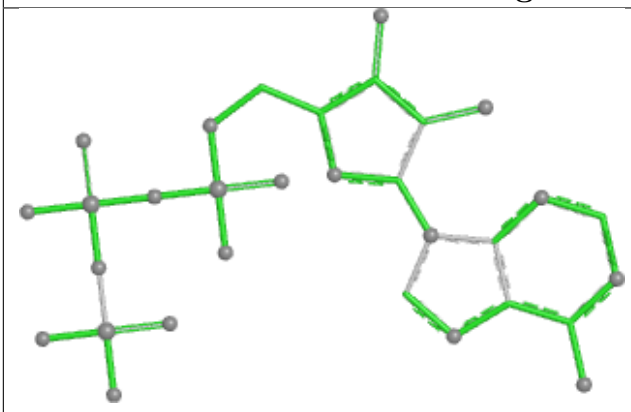


Torsions

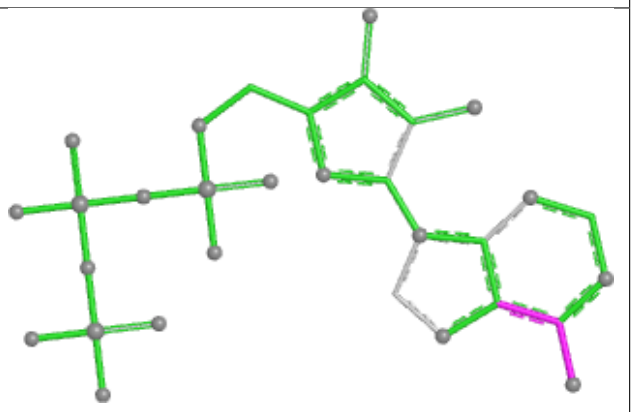


Rings

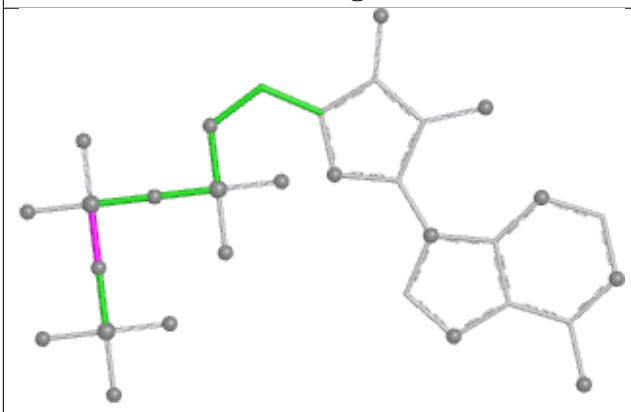
Ligand ATP C 5003



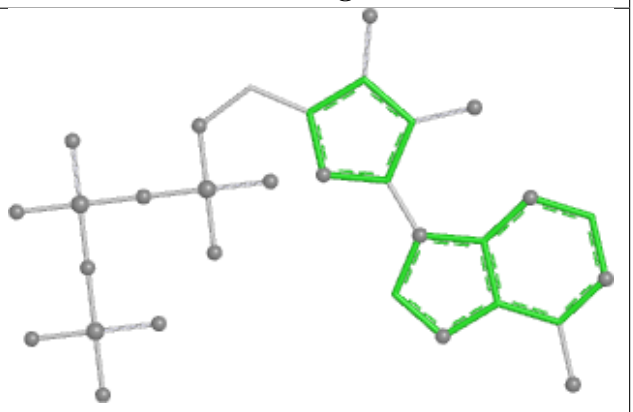
Bond lengths



Bond angles

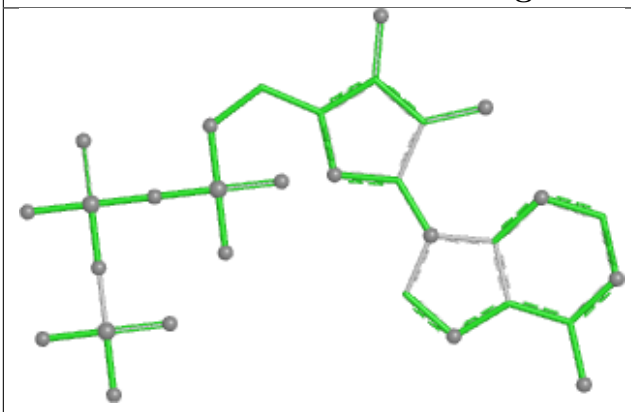


Torsions

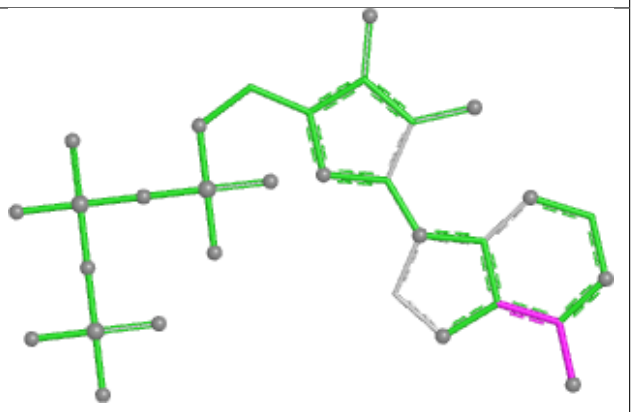


Rings

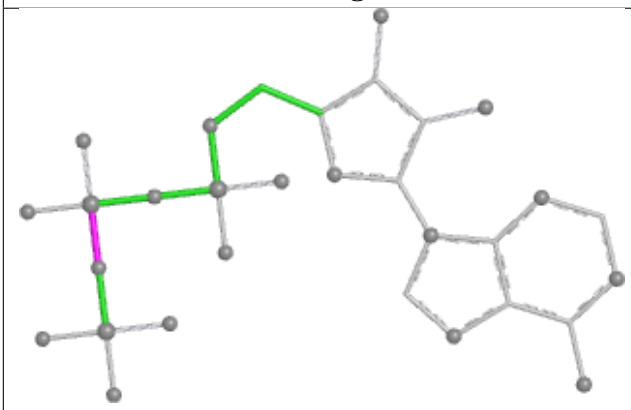
Ligand ATP D 5003



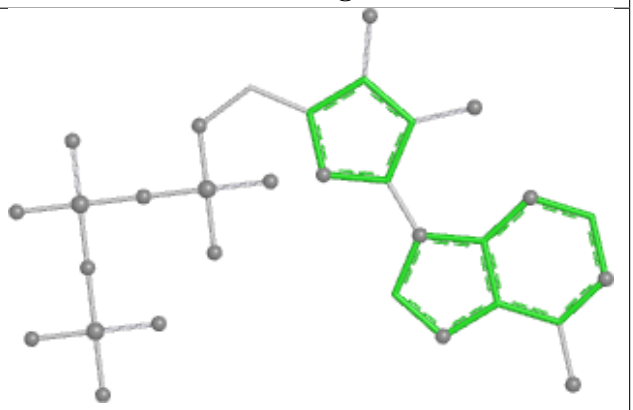
Bond lengths



Bond angles

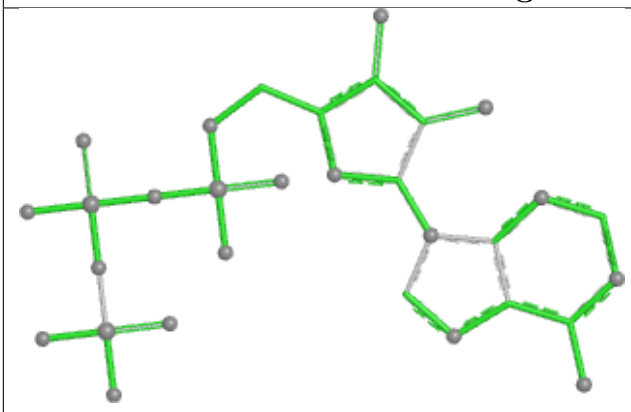


Torsions

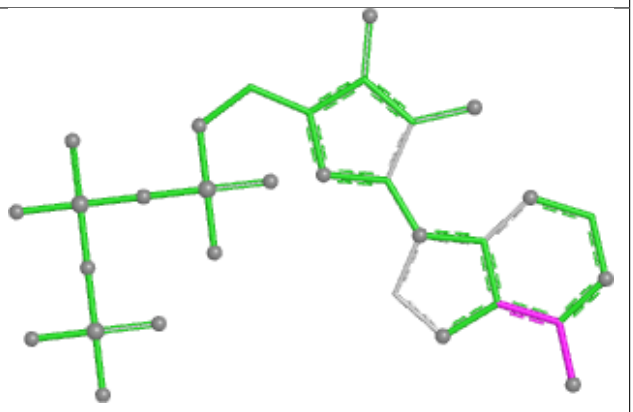


Rings

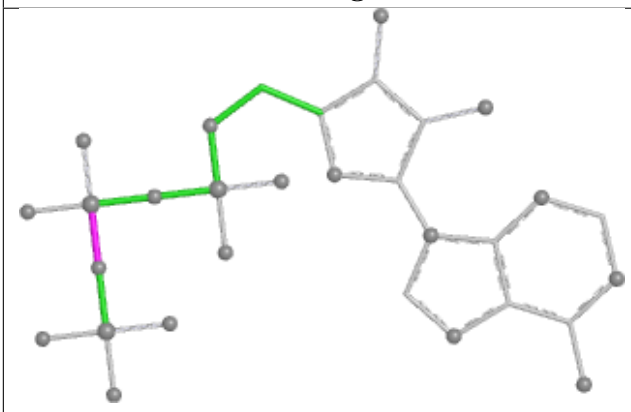
Ligand ATP B 5003



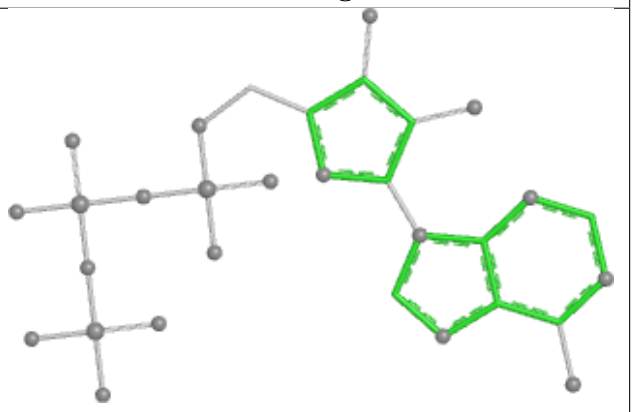
Bond lengths



Bond angles

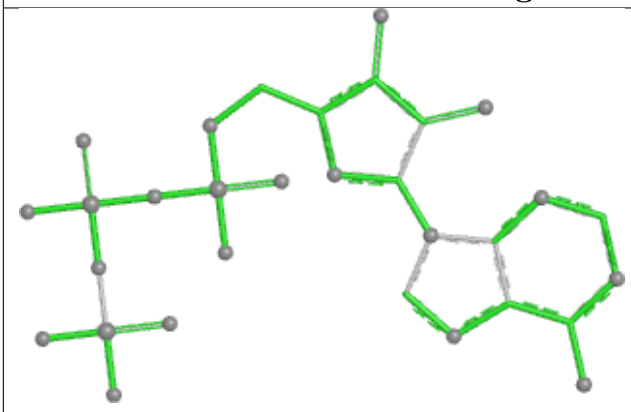


Torsions

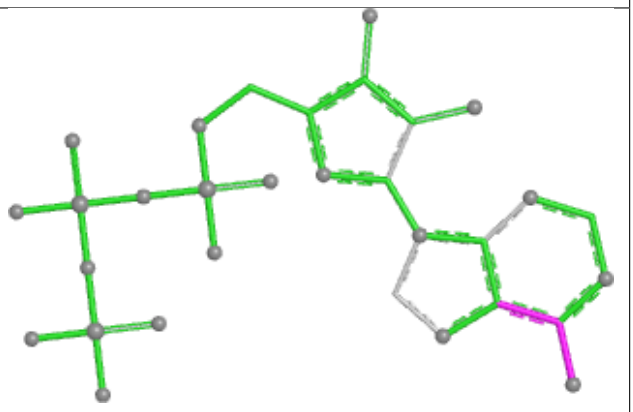


Rings

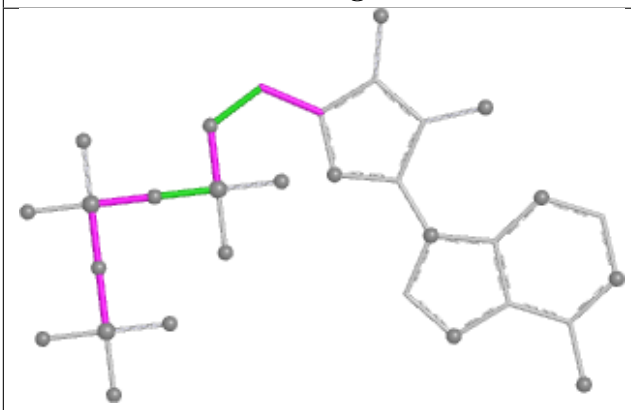
Ligand ATP A 5002



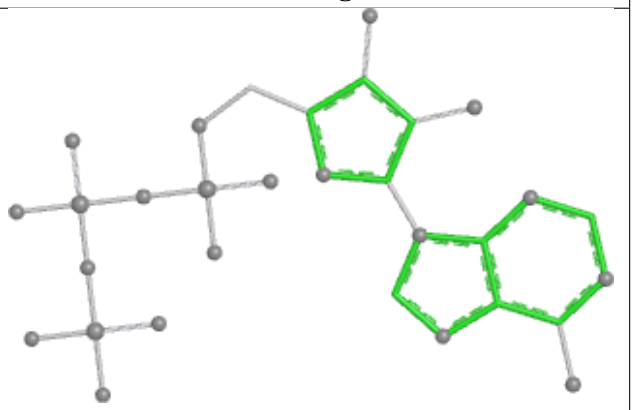
Bond lengths



Bond angles

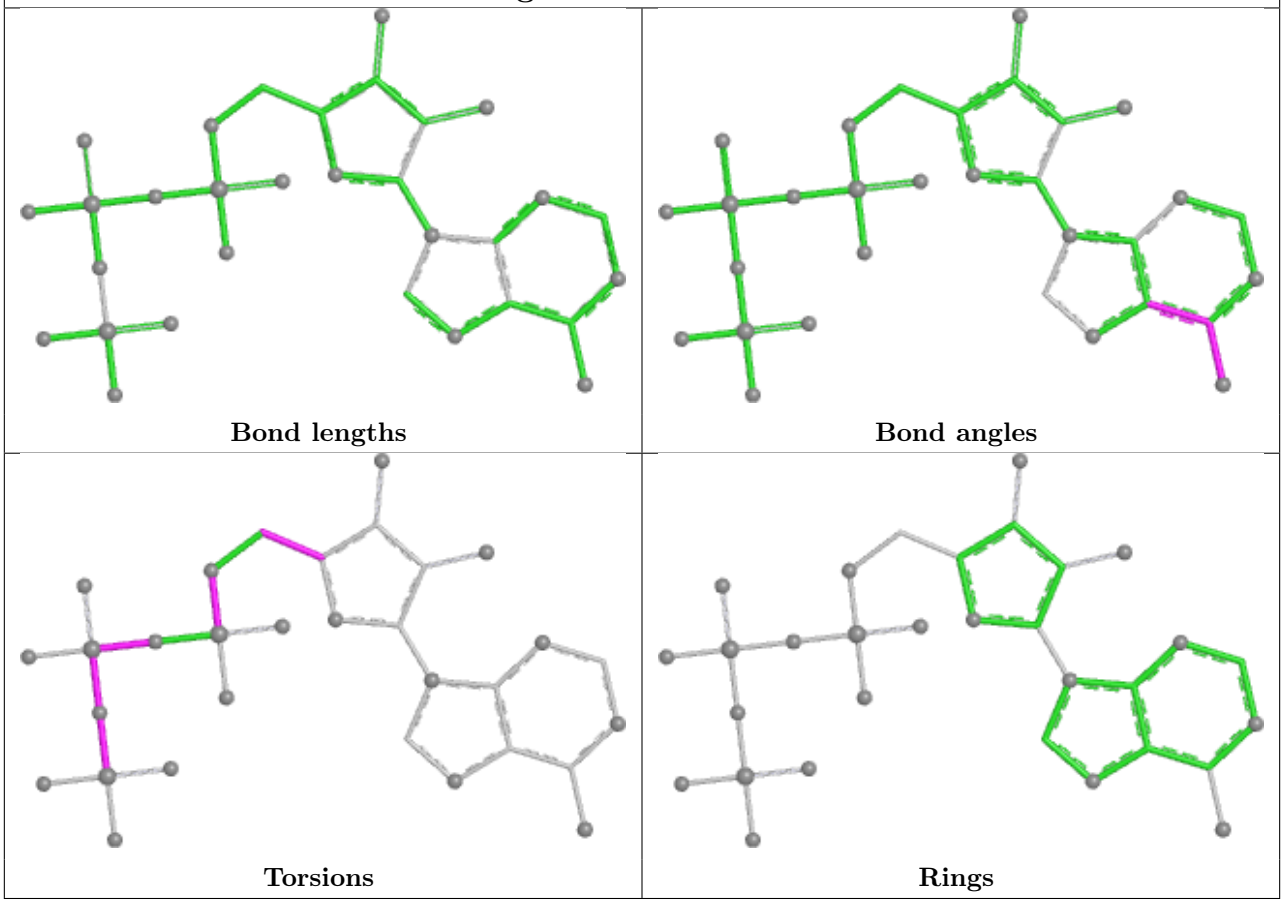


Torsions



Rings

Ligand ATP C 5002



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.

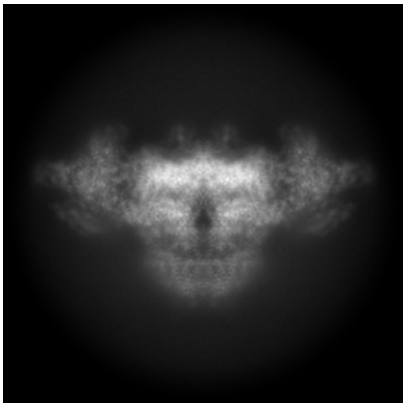
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42460. These allow visual inspection of the internal detail of the map and identification of artifacts.

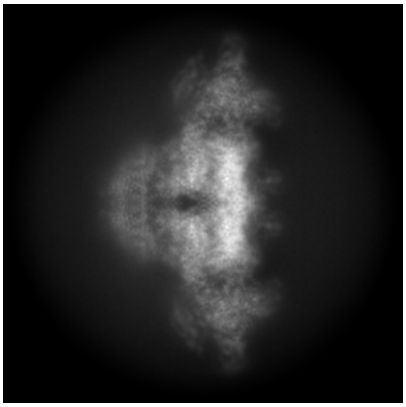
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

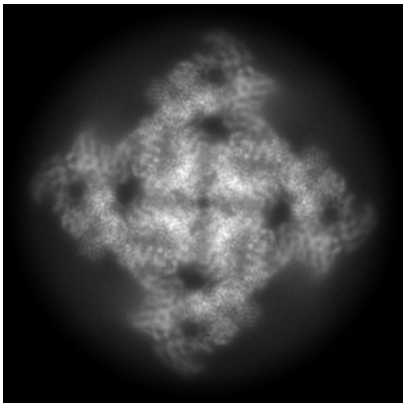
6.1.1 Primary map



X



Y

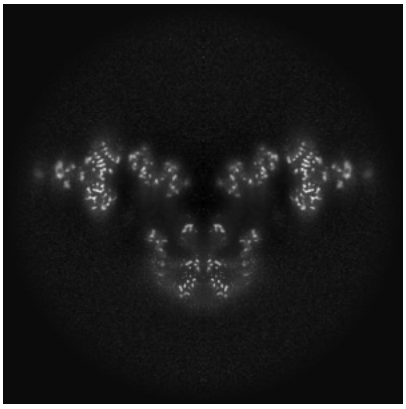


Z

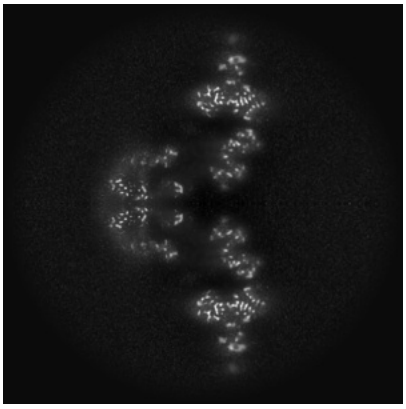
The images above show the map projected in three orthogonal directions.

6.2 Central slices

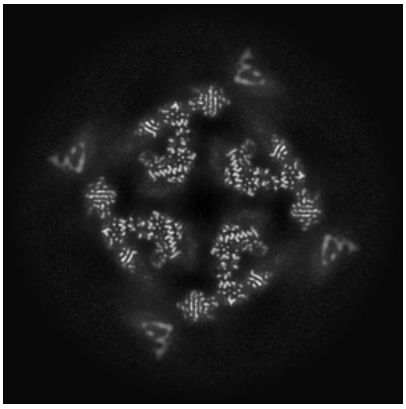
6.2.1 Primary map



X Index: 256



Y Index: 256

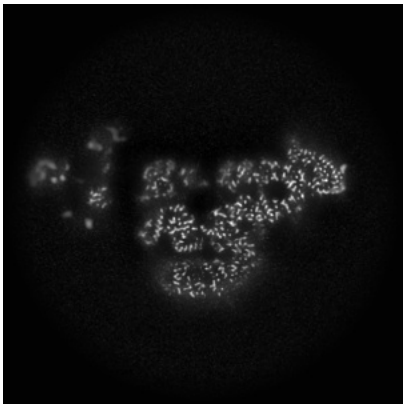


Z Index: 256

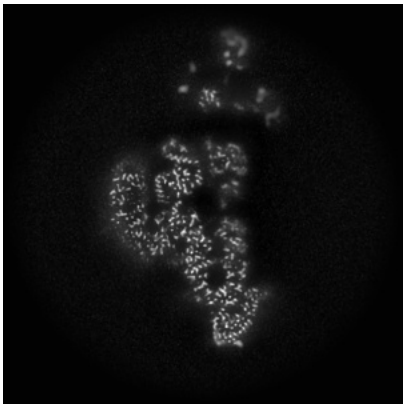
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

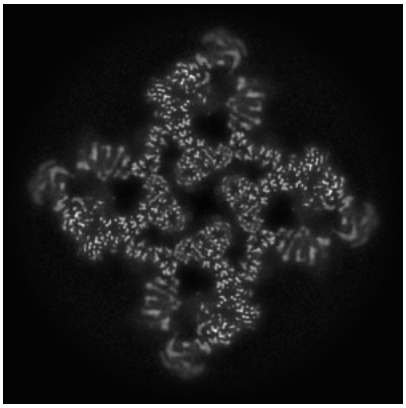
6.3.1 Primary map



X Index: 233



Y Index: 233

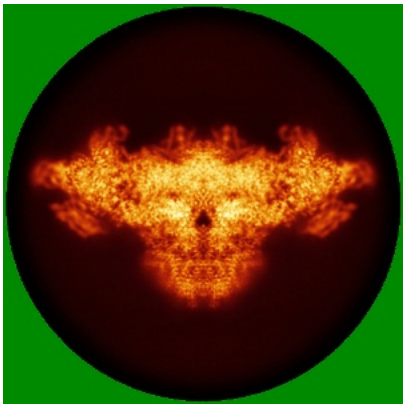


Z Index: 290

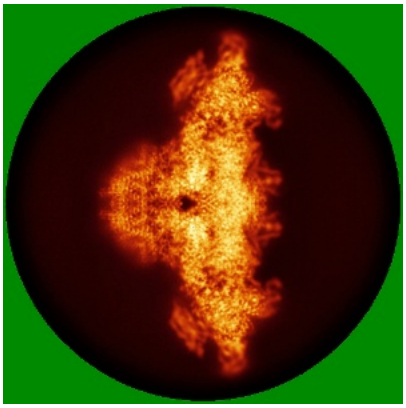
The images above show the largest variance slices of the map in three orthogonal directions.

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

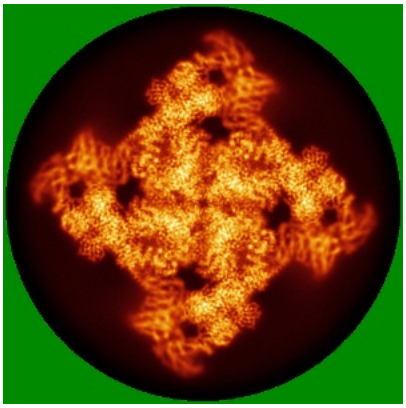
6.4.1 Primary map



X



Y

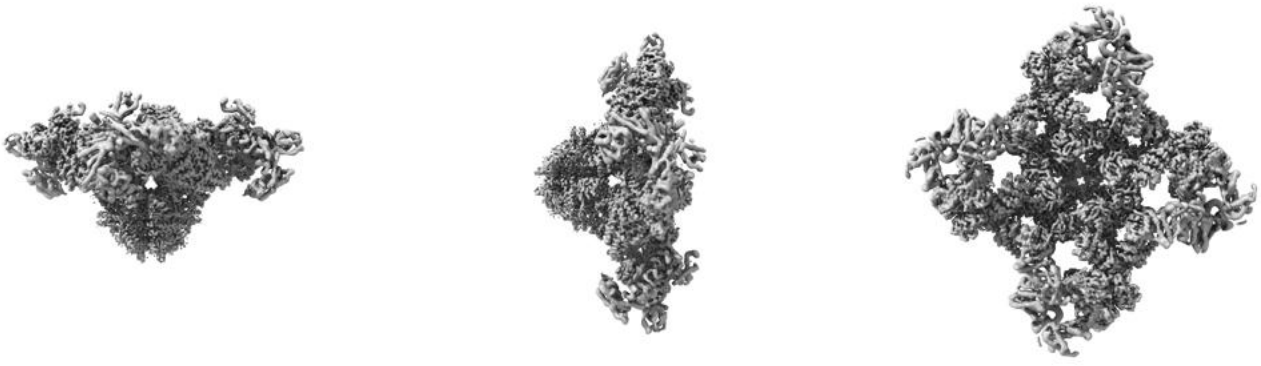


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

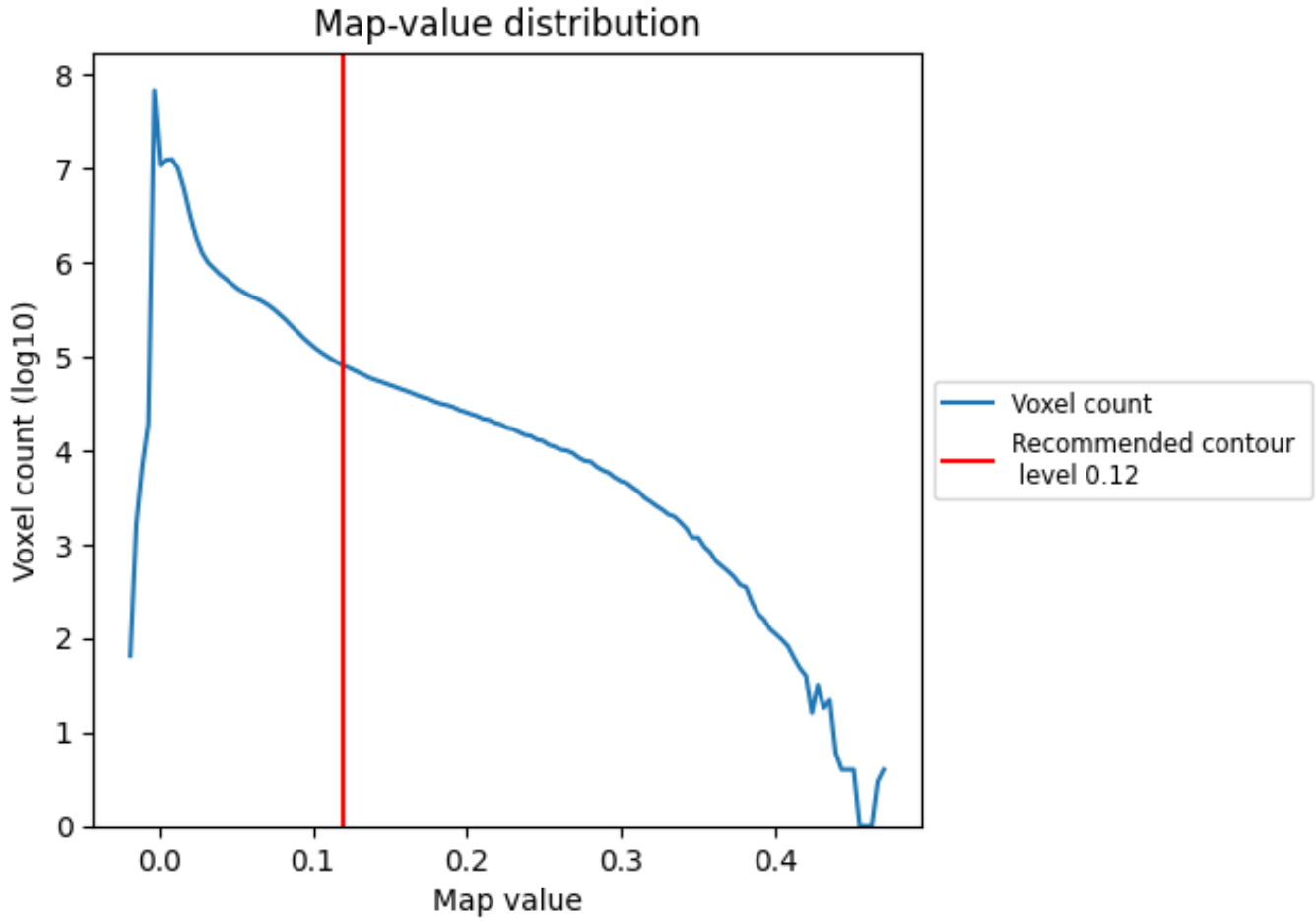
6.6 Mask visualisation (i)

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

7 Map analysis

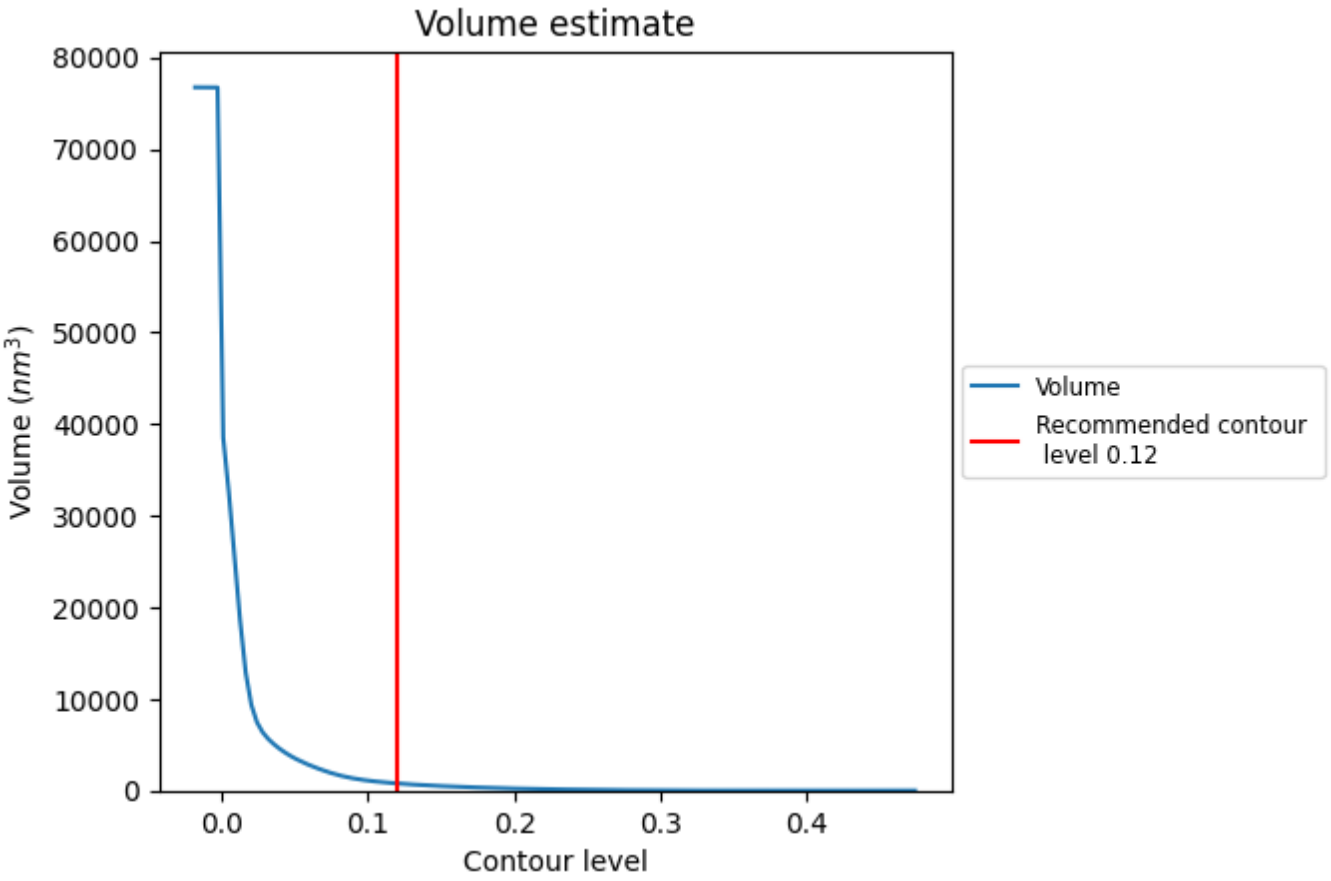
This section contains the results of statistical analysis of the map.

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.

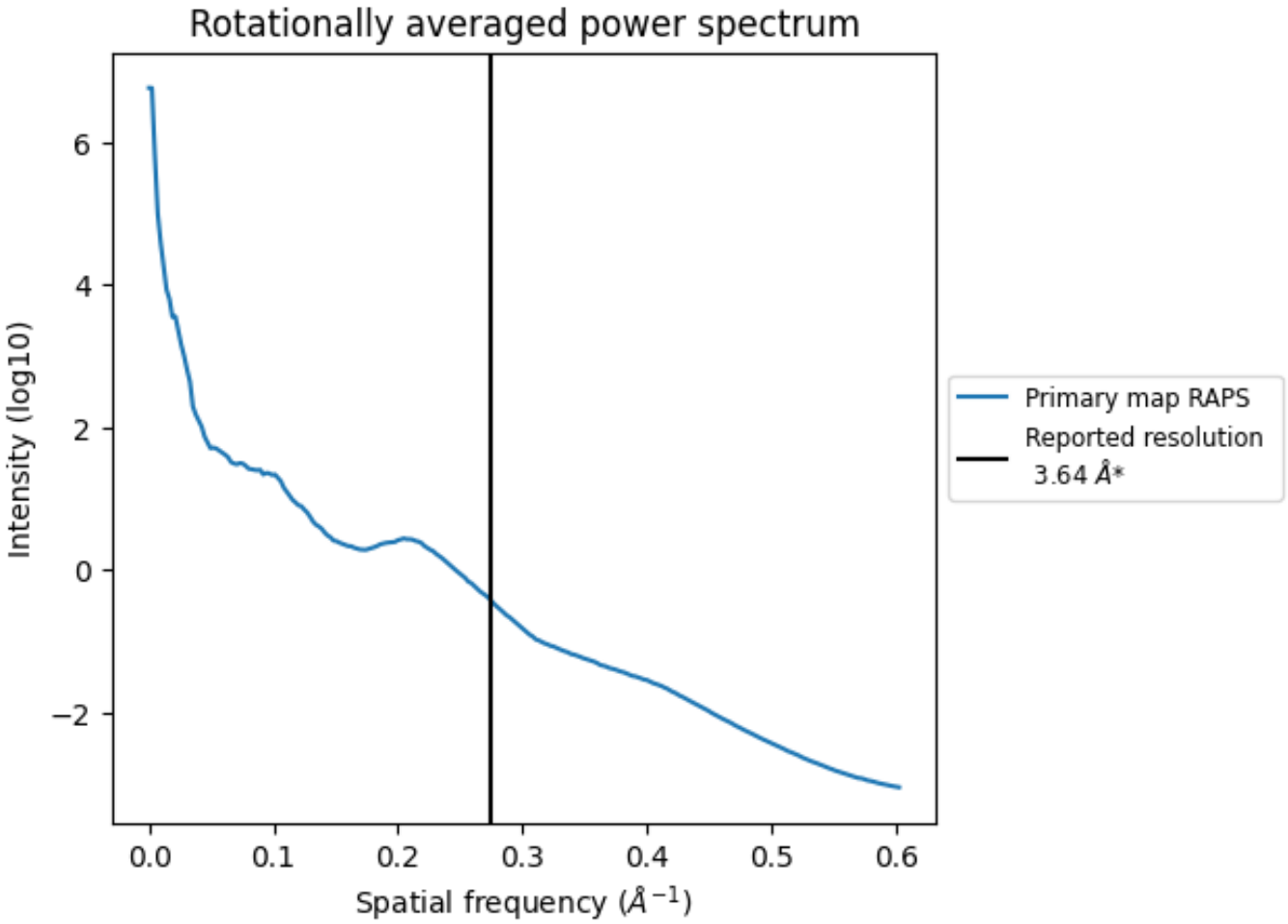
7.2 Volume estimate (i)



The volume at the recommended contour level is 778 nm^3; this corresponds to an approximate mass of 703 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 0.275 Å^{-1}

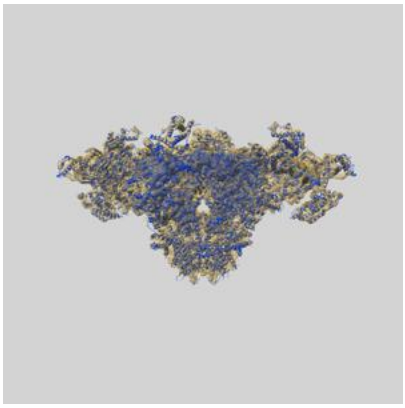
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

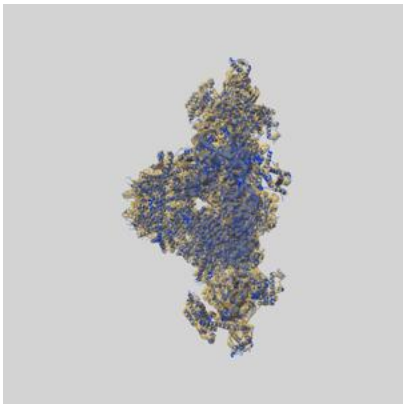
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42460 and PDB model 8UQ4. Per-residue inclusion information can be found in section 3 on page 6.

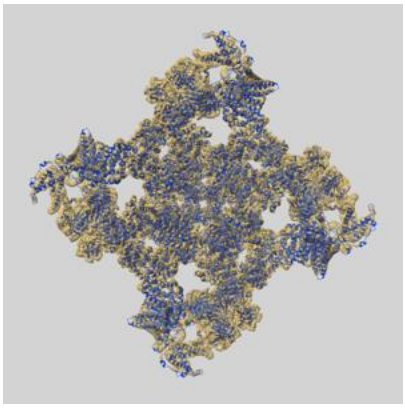
9.1 Map-model overlay



X



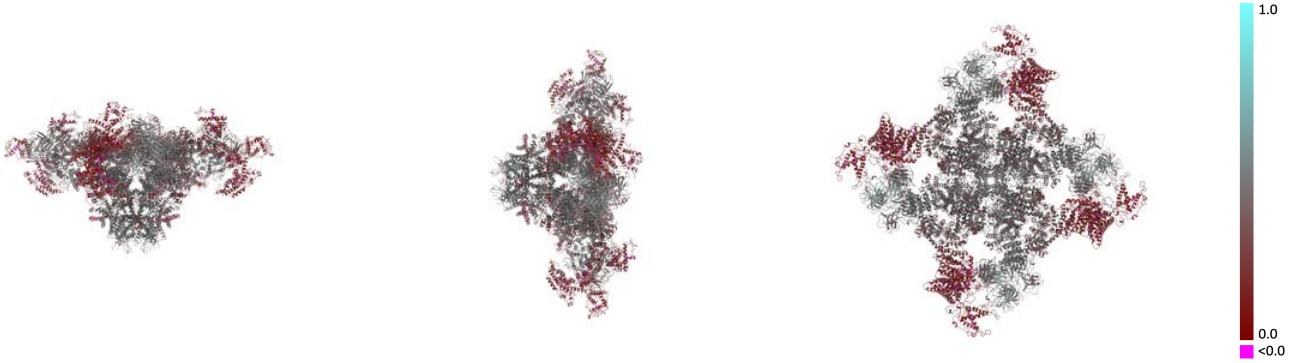
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

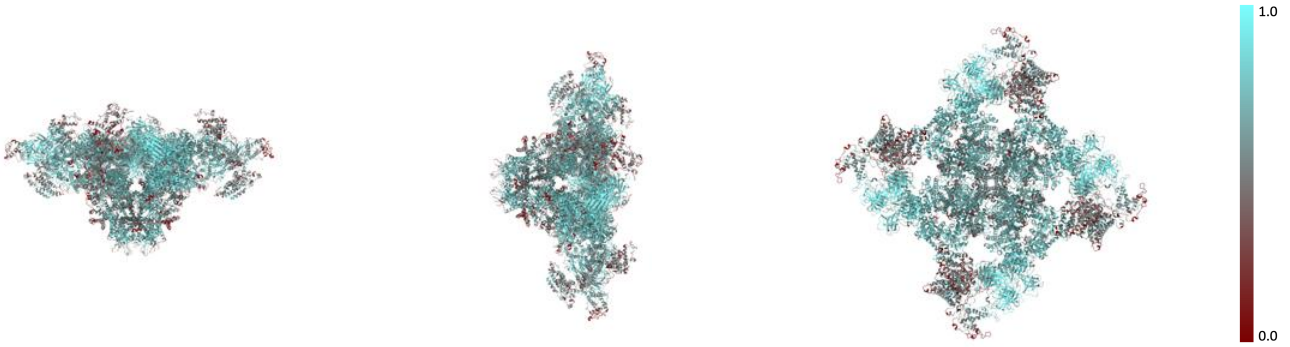
9.2 Q-score mapped to coordinate model



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.

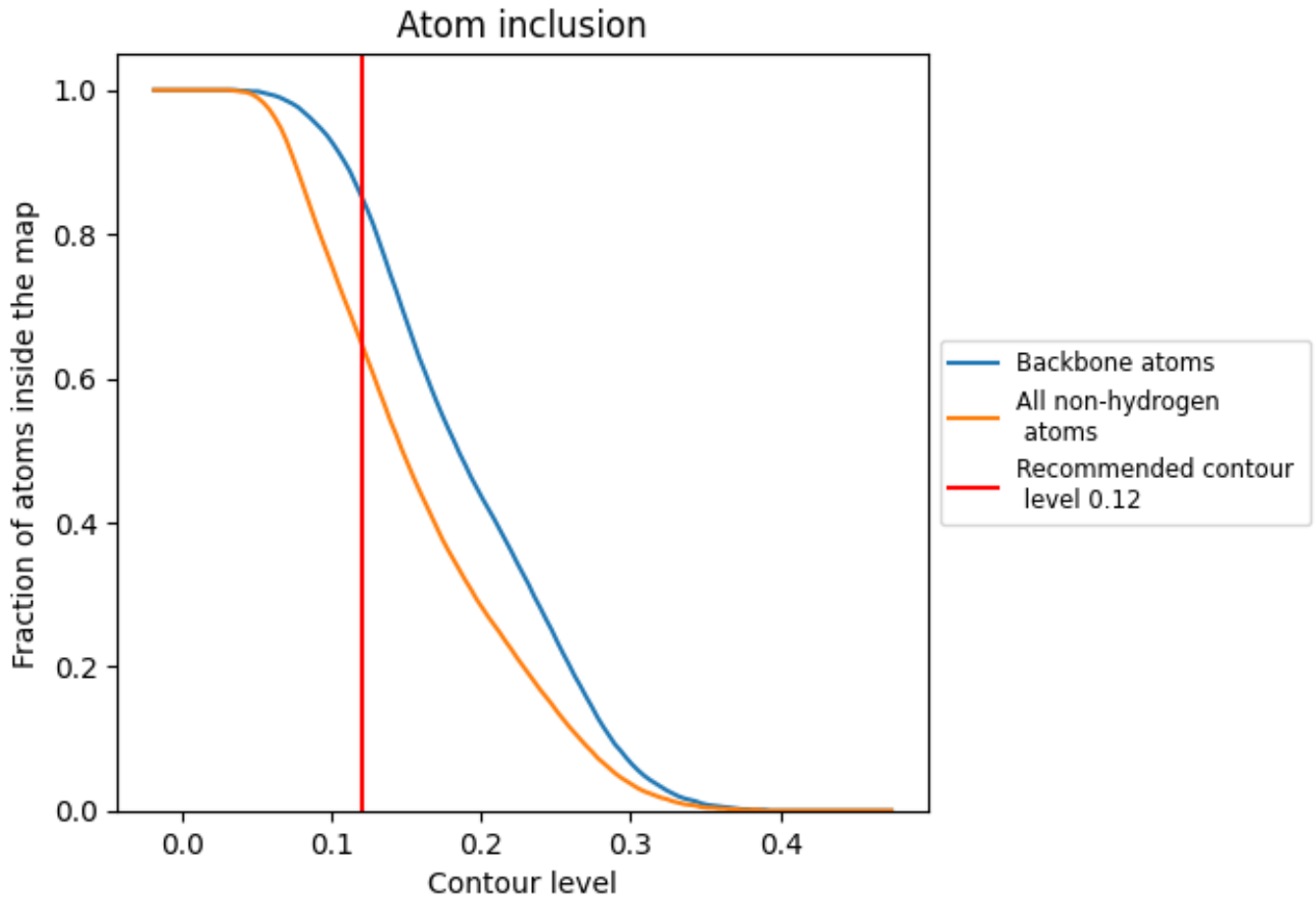
9.3 Atom inclusion mapped to coordinate model



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.3650
A	0.6440	0.3620
B	0.6450	0.3630
C	0.6450	0.3630
D	0.6450	0.3630
E	0.7900	0.4640
F	0.7960	0.4670
G	0.7990	0.4680
H	0.7930	0.4670