# wwPDB EM Validation Summary Report (i)

Oct 28, 2024 – 05:39 PM EDT

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|---|---|---|
| PDB ID | : | 8UXH |
| EMDB ID | : | EMD-42764 |
| Title | : | Structure of PKA phosphorylated human RyR2-R420W in the primed state in the presence of calcium |
| Authors | : | Miotto, M.C.; Marks, A.R. |
| Deposited on | : | 2023-11-09 |
| Resolution | : | 3.52 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.

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The following versions of software and data (see references (1)) were used in the production of this report:

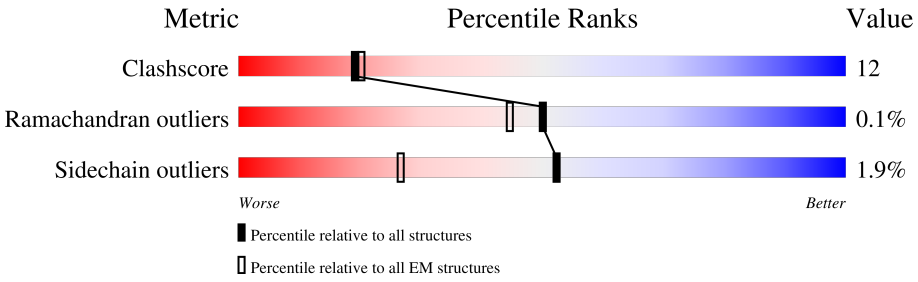
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| 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 3.52 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 | 10% 57% 23% • 19% |
| 1 | B | 4967 | 10% 57% 23% • 19% |
| 1 | C | 4967 | 10% 57% 23% • 19% |
| 1 | D | 4967 | 11% 57% 22% • 19% |
| 2 | E | 108 | 77% 22% • |
| 2 | F | 108 | 79% 20% • |
| 2 | G | 108 | 78% 21% • |
| 2 | H | 108 | 78% 21% • |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 131656 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 | 4004 | Total<br>32032 | C<br>20411 | N<br>5451 | O<br>5955 | S<br>215 | 2 | 0 |
| 1 | B | 4004 | Total<br>32032 | C<br>20411 | N<br>5451 | O<br>5955 | S<br>215 | 2 | 0 |
| 1 | C | 4004 | Total<br>32032 | C<br>20411 | N<br>5451 | O<br>5955 | S<br>215 | 2 | 0 |
| 1 | D | 4004 | Total<br>32032 | C<br>20411 | N<br>5451 | O<br>5955 | S<br>215 | 2 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 420 | TRP | ARG | variant | UNP Q92736 |
| B | 420 | TRP | ARG | variant | UNP Q92736 |
| C | 420 | TRP | ARG | variant | UNP Q92736 |
| D | 420 | TRP | ARG | variant | UNP Q92736 |

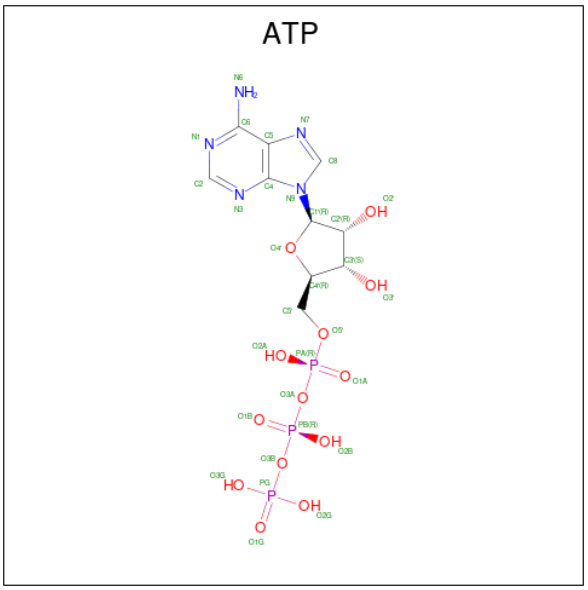
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | E | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |
| 2 | F | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |
| 2 | G | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>4 | 0 | 0 |
| 2 | H | 107 | Total<br>818 | C<br>516 | N<br>144 | O<br>154 | S<br>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<br>1 1 | 0 |
| 3 | B | 1 | Total Zn<br>1 1 | 0 |
| 3 | C | 1 | Total Zn<br>1 1 | 0 |
| 3 | D | 1 | Total Zn<br>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<br>31 10 5 13 3 | 0 |
| 4 | A | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | B | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | B | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | C | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | C | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | D | 1 | Total C N O P<br>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 | |

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

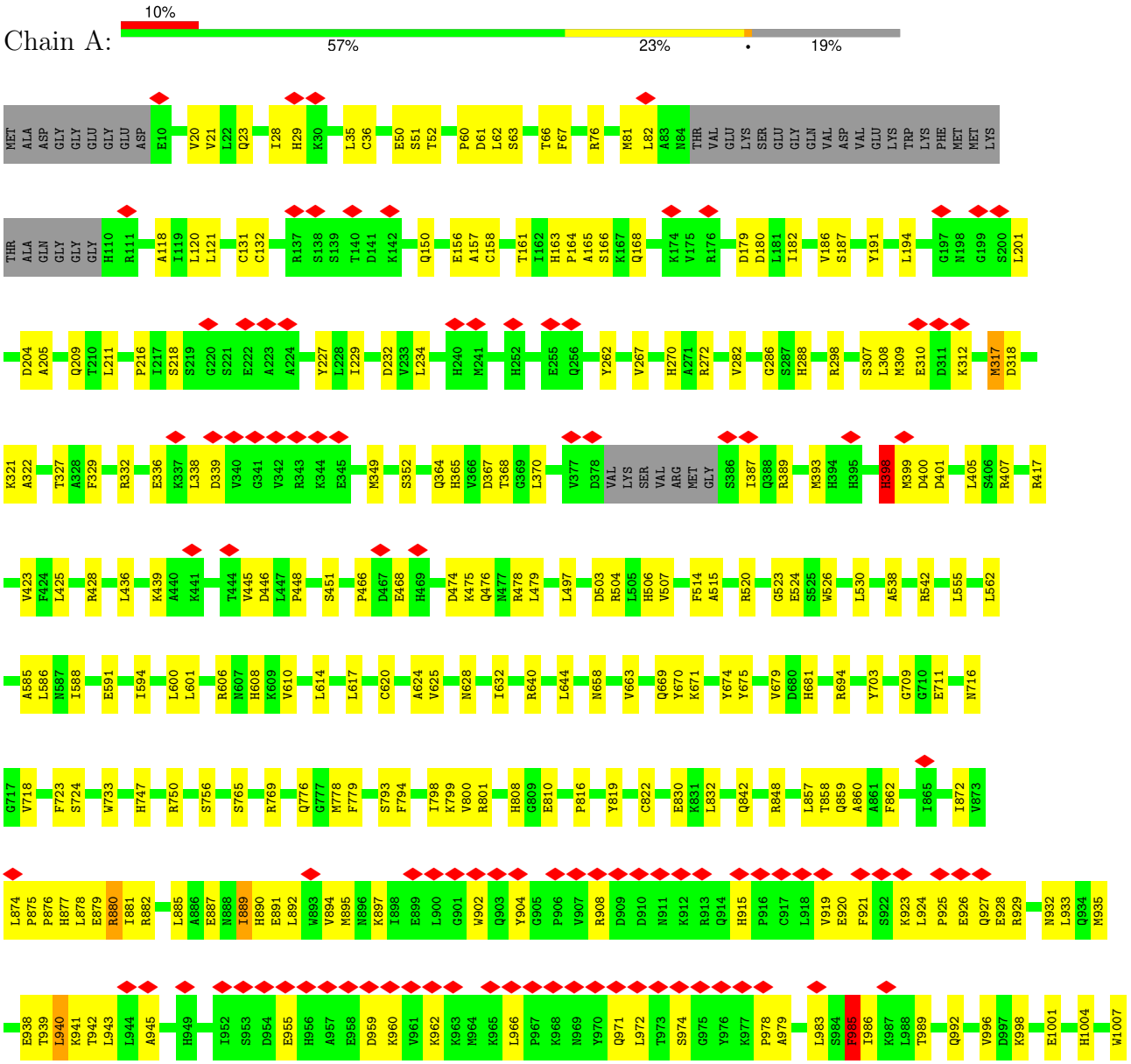
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 5 | A | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 5 | B | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 5 | C | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 5 | D | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |

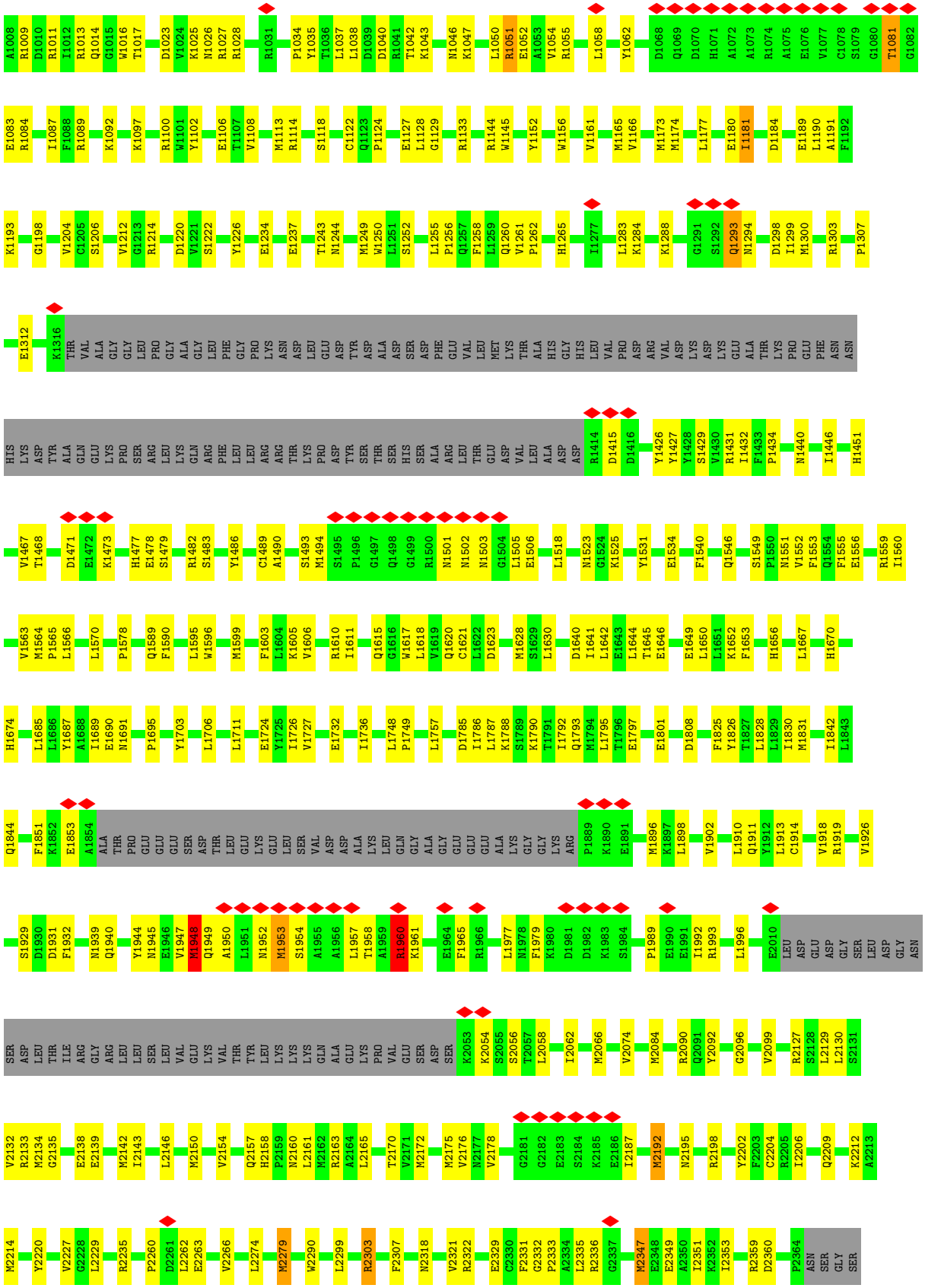
# 3 Residue-property plots (i)

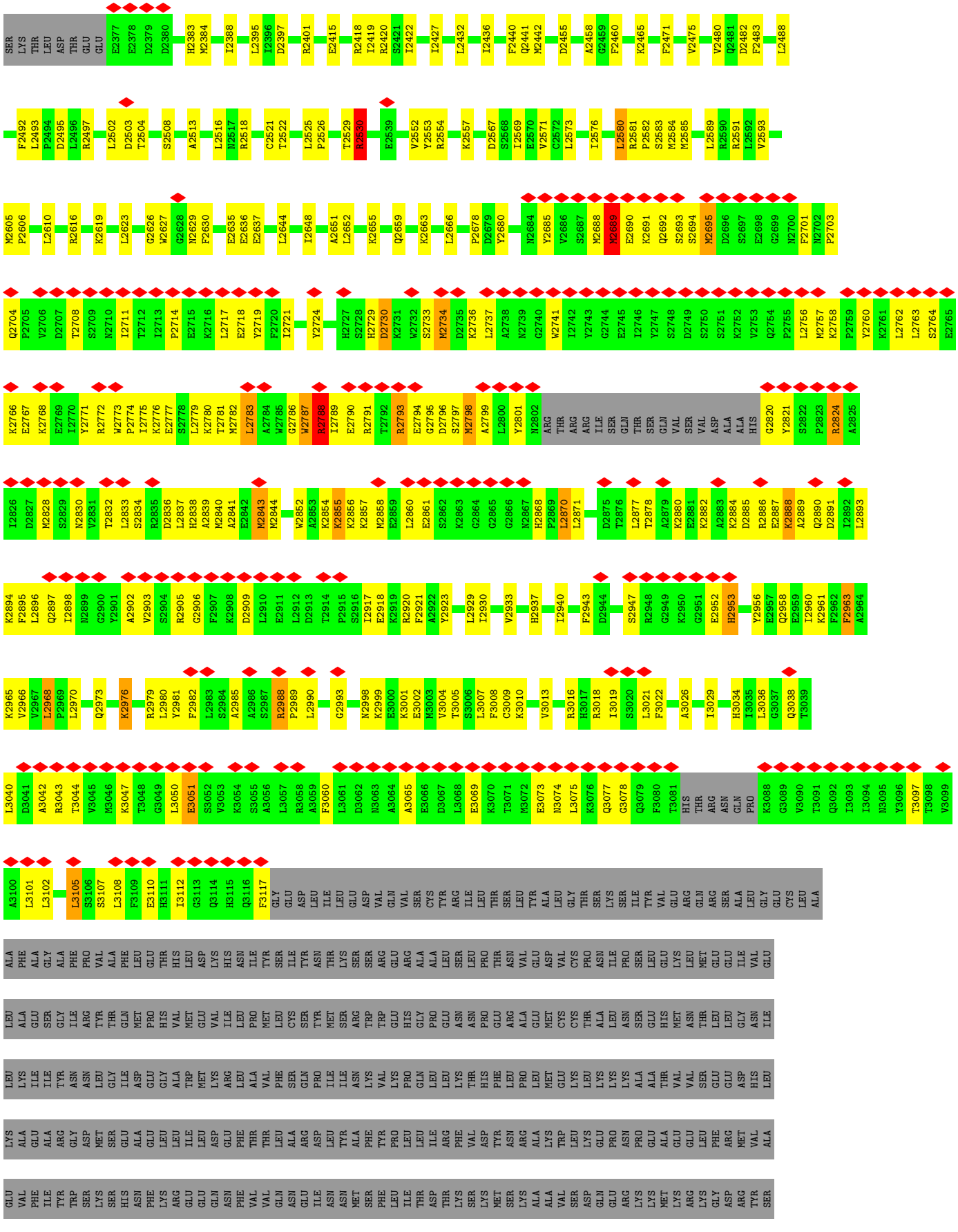
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

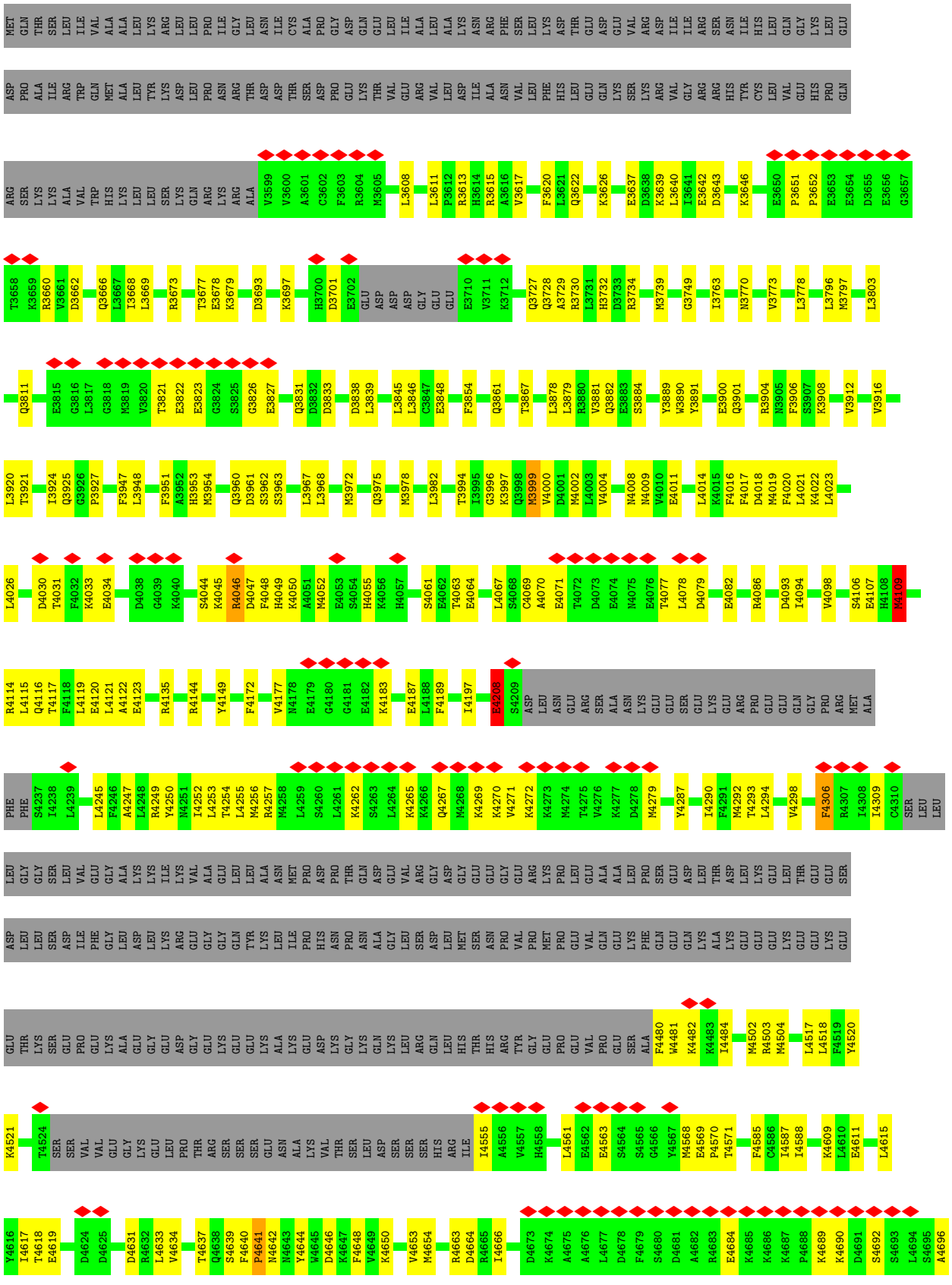
- Molecule 1: Ryanodine receptor 2

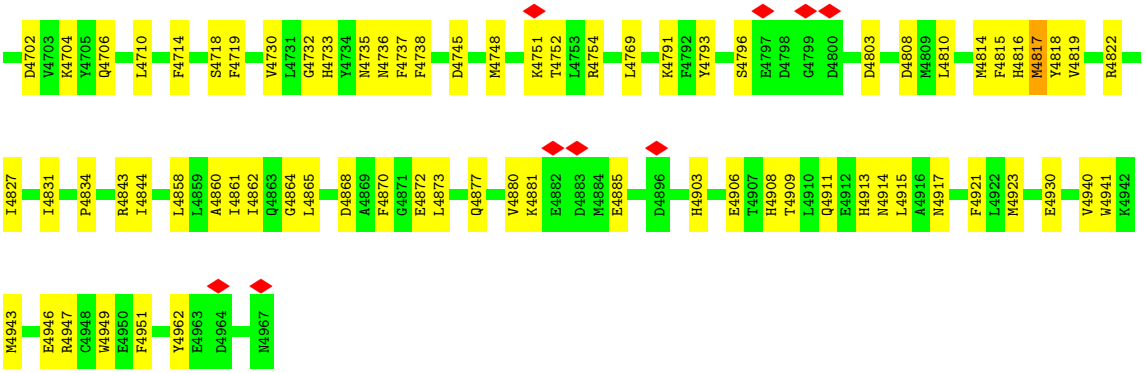
Chain A:




A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 D1023 V1024 K1025 N1026 R1027 R1028 R1031 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 N1046 K1047 L1050 R1051 E1052 A1053 V1054 R1055 L1058 Y1062 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082
E1083 R1084 I1087 F1088 R1089 K1092 K1097 R1100 W1101 Y1102 E1106 T1107 V1108 M1113 R1114 S1118 C1122 Q1123 P1124 E1127 L1128 G1129 R1133 R1144 W1145 Y1152 W1156 V1161 M1165 V1166 M1173 M1174 L1177 E1180 I1181 D1184 E1189 L1190 A1191 F1192
K1193 G1198 V1204 C1205 S1206 V1212 G1213 R1214 D1220 V1221 S1222 Y1226 E1234 E1237 T1243 N1244 M1249 W1250 L1251 S1252 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 H1265 I1277 L1283 K1284 K1288 G1291 S1292 Q1293 N1294 D1298 I1299 M1300 R1303 P1307
E1312 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 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 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 Y1426 Y1427 Y1428 S1429 V1430 R1431 I1432 F1433 P1434 N1440 I1446 H1451
V1467 T1468 D1471 E1472 K1473 H1477 E1478 S1479 R1482 S1483 Y1486 C1489 A1490 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 E1506 L1518 N1523 G1524 K1525 Y1531 E1534 F1540 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 I1560
V1563 M1564 P1565 L1566 L1570 P1578 Q1589 F1590 L1595 W1596 M1599 F1603 L1604 K1605 V1606 R1610 I1611 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 D1623 M1628 S1629 L1630 D1640 I1641 L1642 E1643 L1644 T1645 E1646 E1649 L1650 L1651 K1652 F1653 H1656 L1667 H1670
H1674 L1685 L1686 Y1687 A1688 I1689 E1690 N1691 P1695 Y1703 L1706 L1711 E1724 Y1725 I1726 V1727 E1732 I1736 L1748 P1749 L1757 D1785 I1786 L1787 K1788 S1789 K1790 T1791 I1792 Q1793 M1794 L1795 T1796 E1797 E1801 D1808 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 I1842 L1843
Q1844 F1851 K1852 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 ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 M1896 K1897 L1898 Y1902 L1910 Q1911 Y1912 L1913 C1914 V1918 R1919 V1926
S1929 D1930 D1931 F1932 N1939 Q1940 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 E1964 F1965 R1966 L1977 N1978 F1979 K1980 D1981 D1982 K1983 S1984 P1989 E1990 E1991 I1992 R1993 L1996 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 LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 S2056 T2057 L2058 I2062 M2066 V2074 M2084 R2090 Q2091 Y2092 G2096 V2099 R2127 S2128 L2129 L2130 S2131
V2132 R2133 M2134 G2135 E2138 E2139 M2142 I2143 L2146 M2150 V2154 Q2157 H2158 P2159 N2160 L2161 M2162 R2163 A2164 L2165 T2170 V2171 M2172 M2175 V2176 N2177 V2178 G2181 G2182 E2183 S2184 K2185 E2186 I2187 M2192 N2195 R2198 Y2202 F2203 C2204 R2205 I2206 Q2209 K2212 A2213
M2214 Y2220 V2227 G2228 L2229 R2235 P2260 D2261 L2262 E2263 V2266 L2274 M2279 W2290 L2299 R2303 F2307 N2318 V2321 R2322 E2329 C2330 F2331 G2332 P2333 A2334 L2335 R2336 G2337 M2347 E2348 E2349 A2350 I2351 K2352 I2353 R2359 D2360 P2364 ASN SER GLY SER


SER LYS THR LEU ASP THR GLU GLU
E2377 E2378 D2379 D2380 H2383 M2384 I2388 L2395 I2396 D2397 R2401 E2415 R2418 I2419 R2420 S2421 I2422 I2427 L2432 I2436 F2440 Q2441 M2442 D2455 A2458 G2459 F2460 K2465 F2471 V2475 V2480 Q2481 D2482 F2483 L2488
F2492 L2493 P2494 D2495 L2496 R2497 L2502 D2503 T2504 S2508 A2513 L2516 N2517 R2518 C2521 T2522 L2525 P2526 T2529 R2530 E2539 V2552 Y2553 R2554 K2557 D2567 S2568 I2569 E2570 V2571 G2572 L2573 I2576 L2580 R2581 P2582 S2583 M2584 M2585 L2589 R2590 R2591 L2592 V2593
M2605 P2606 L2610 R2616 K2619 L2623 G2626 W2627 G2628 N2629 F2630 E2635 E2636 E2637 L2644 I2648 A2651 L2652 K2655 Q2659 K2663 L2666 P2678 D2679 Y2680 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 Y2724 H2727 S2728 H2729 D2730 K2731 W2732 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 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 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER 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 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 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 L2929 I2930 V2933 H2937 I2940 F2943 D2944 S2947 R2948 G2949 K2950 G2951 E2952 H2953 Y2956 E2957 Q2958 E2959 I2960 K2961 F2962 F2963 A2964
K2965 V2966 Y2967 L2968 P2969 L2970 Q2973 K2976 R2979 L2980 Y2981 F2982 L2983 S2984 A2985 A2986 S2987 R2988 P2989 L2990 G2993 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007 F3008 C3009 K3010 V3013 H3016 H3017 R3018 I3019 S3020 L3021 F3022 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039
L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3054 S3055 A3056 L3057 R3058 A3059 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099
A3100 L3101 L3102 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE ILE PRO ASN LEU ASP VAL GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLU GLU ILE VAL GLU
ALA PHE ALA GLY ALA PHE PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU SER LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL GLU
LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU GLU ASN ASN PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU LEU GLU GLU ILE VAL GLY
LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS TRP LEU LYS GLU PRO ASN ALA THR VAL VAL SER LEU LEU GLU ASP HIS LEU
LYS ALA GLU LEU ALA ARG GLY GLU ASP MET SER GLU ALA GLU LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU LEU GLU GLU LEU PHE ARG MET VAL ALA
GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN ASN GLU ILE ASN ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER



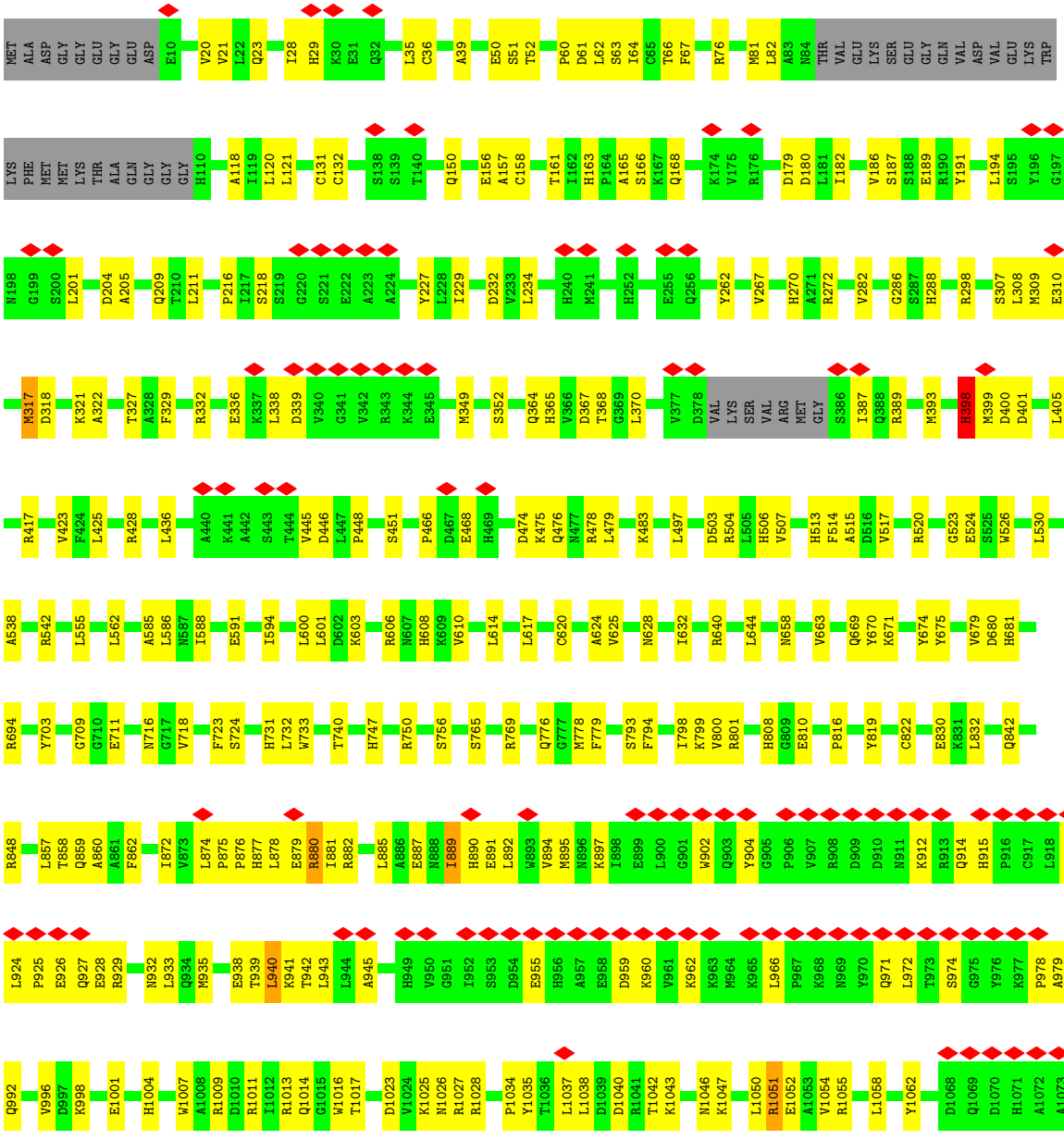


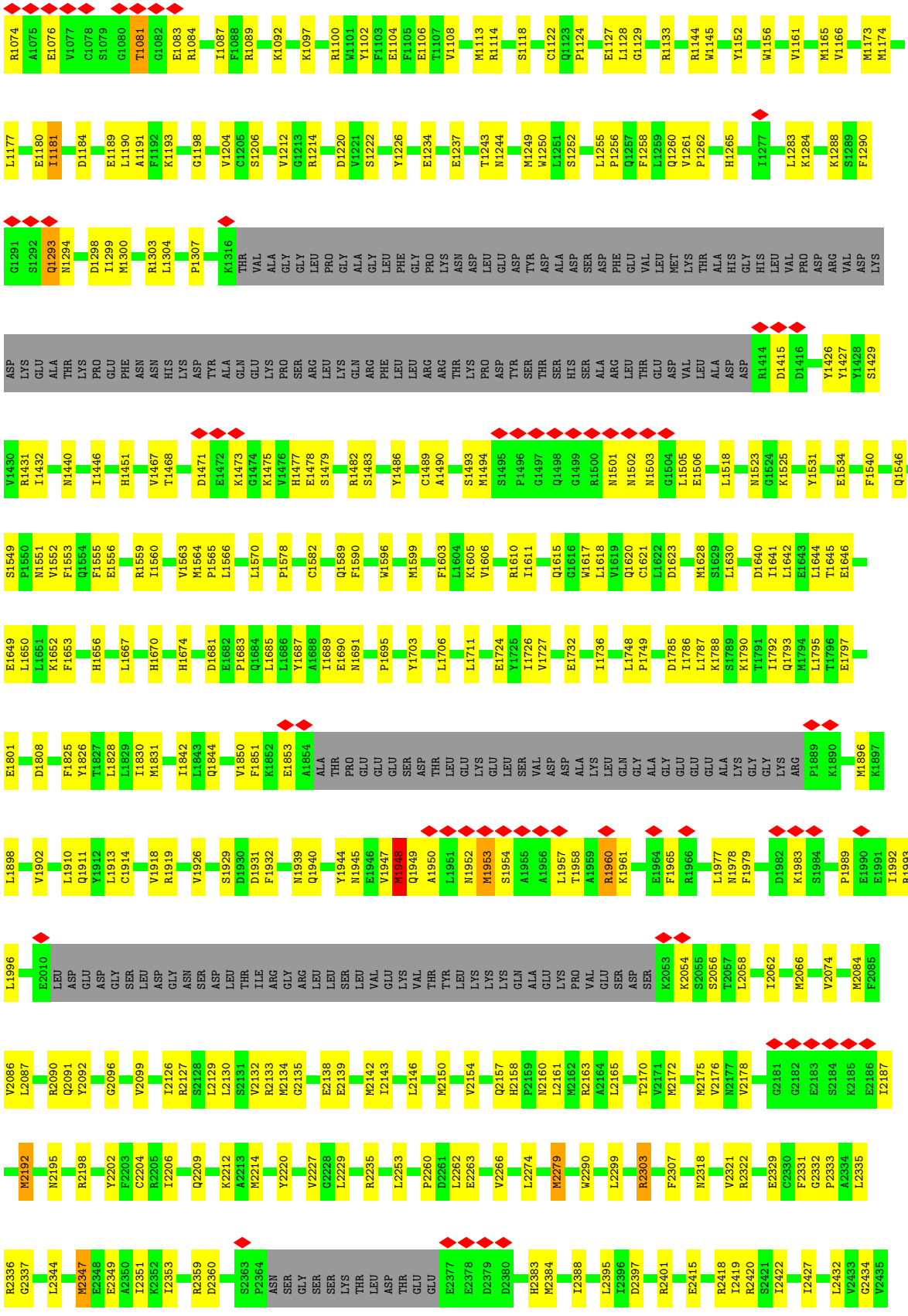




• Molecule 1: Ryanodine receptor 2

Chain B:


R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 I1087 F1088 R1089 K1092 K1097 R1100 W1101 Y1102 F1103 E1104 F1105 E1106 T1107 V1108 M1113 R1114 S1118 C1122 Q1123 P1124 E1127 L1128 G1129 R1133 R1144 W1145 Y1152 W1156 V1161 M1165 V1166 M1173 M1174
L1177 E1180 I1181 D1184 E1189 L1190 A1191 F1192 K1193 G1198 V1204 C1205 S1206 V1212 G1213 R1214 D1220 V1221 S1222 Y1226 E1234 E1237 T1243 N1244 M1249 W1250 L1251 S1252 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 H1265 I1277 L1283 K1284 K1288 S1289 F1290
G1291 S1292 Q1293 N1294 D1298 I1299 M1300 R1303 L1304 P1307 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 LEU LYS GLN ARG ARG THR THR LYS PRO ASP ASP TYR SER THR SER HIS SER ASP ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1426 Y1427 Y1428 S1429
V1430 R1431 I1432 N1440 I1446 H1451 V1467 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 R1482 S1483 Y1486 C1489 A1490 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 E1506 L1518 N1523 G1524 K1525 Y1531 E1534 F1540 Q1546
S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 I1560 V1563 M1564 P1565 L1566 L1570 P1578 C1582 Q1589 F1590 W1596 M1599 F1603 L1604 K1605 V1606 R1610 I1611 Q1615 G1616 W1617 L1618 V1619 Q1620 C1621 L1622 D1623 M1628 S1629 L1630 D1640 I1641 L1642 E1643 L1644 T1645 E1646
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E1801 D1808 F1825 Y1826 T1827 L1828 L1829 I1830 M1831 I1842 L1843 Q1844 V1850 F1851 K1852 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 P1889 K1890 M1896 K1897
L1898 V1902 L1910 Q1911 Y1912 L1913 C1914 V1918 R1919 V1926 S1929 D1930 D1931 F1932 N1939 Q1940 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 E1964 F1965 R1966 L1977 N1978 F1979 D1982 K1983 S1984 P1989 E1990 E1991 I1992 R1993
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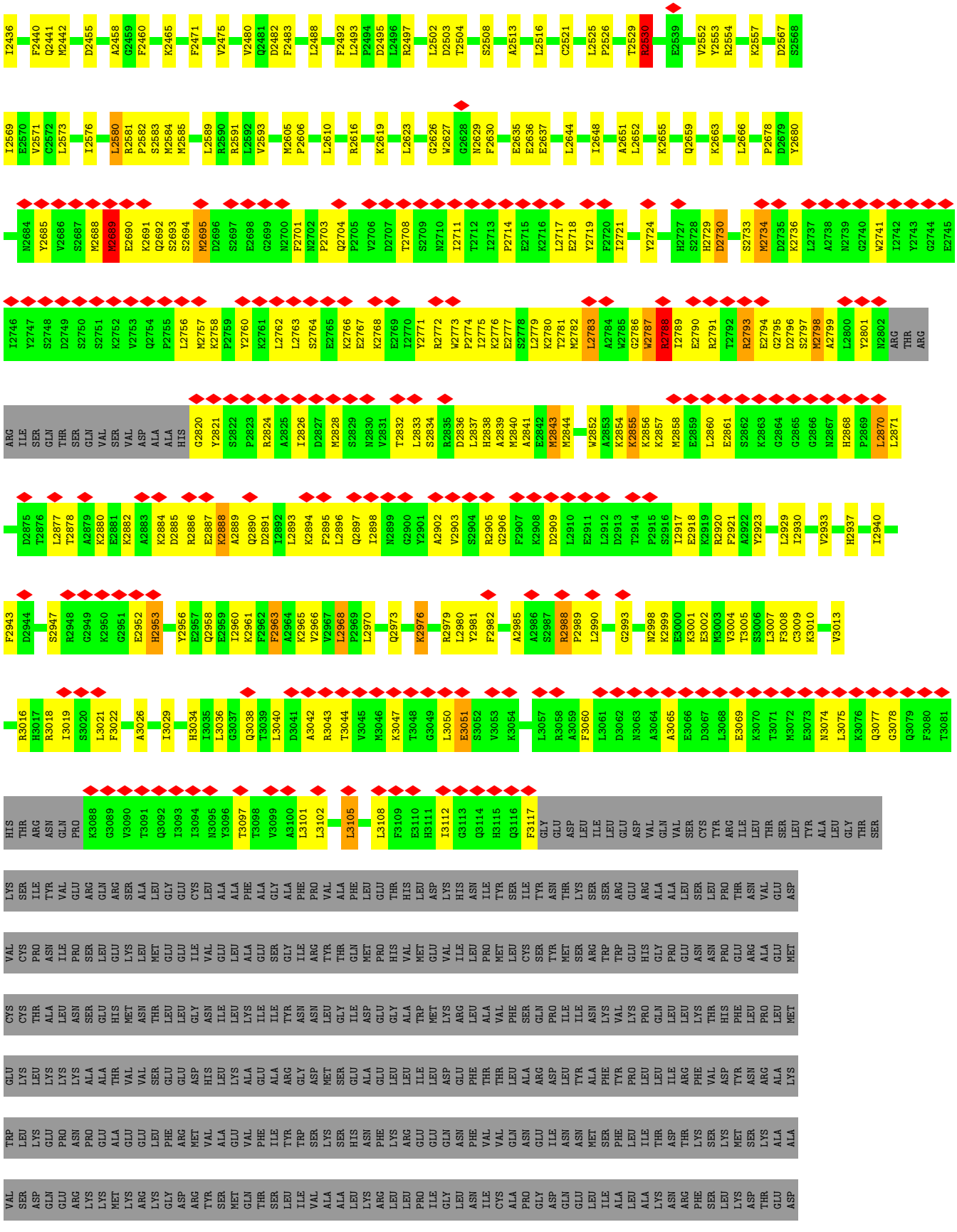
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I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG
ARG ILE SER 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 W2852 A2853 K2854 W2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871
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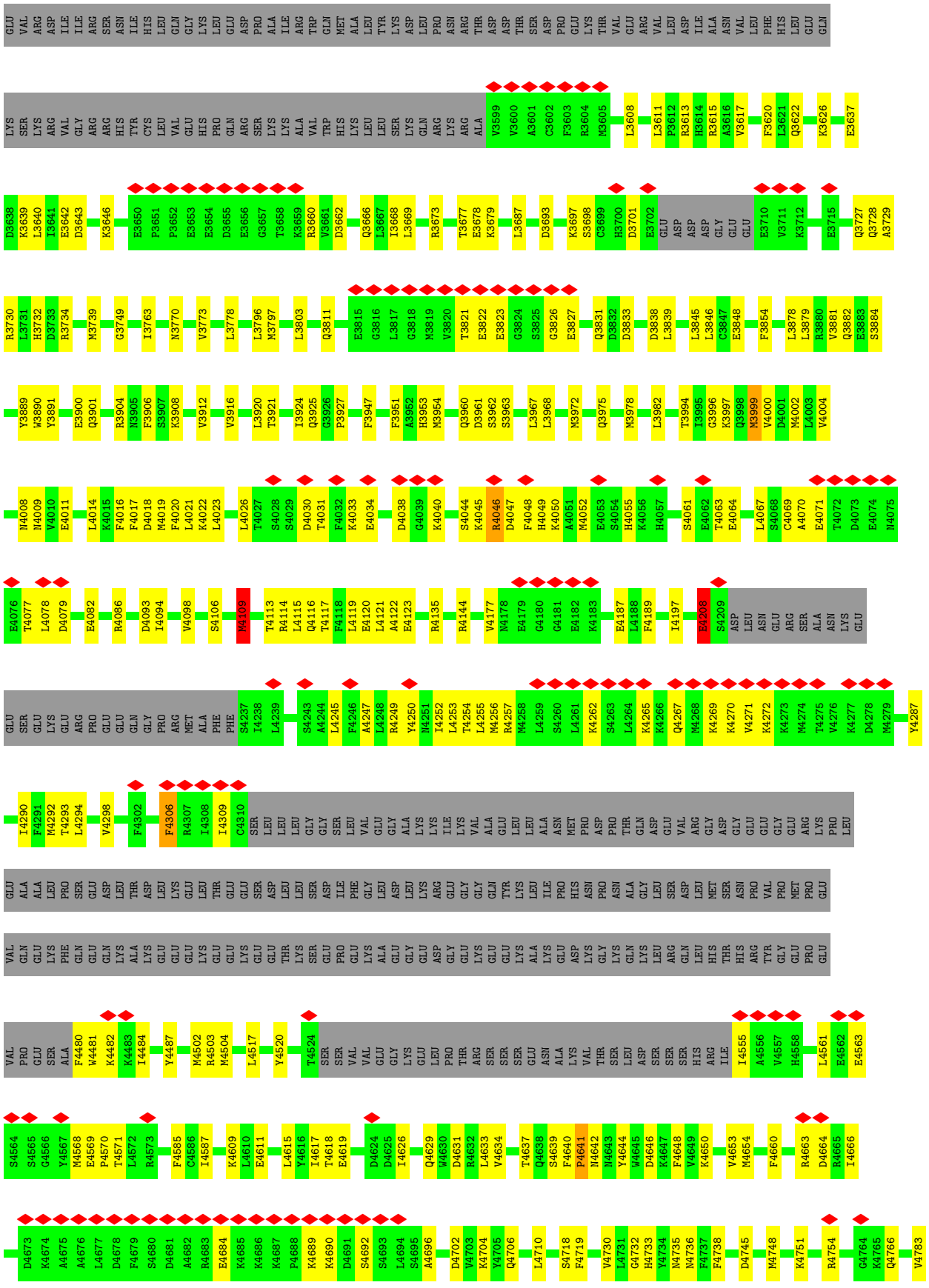
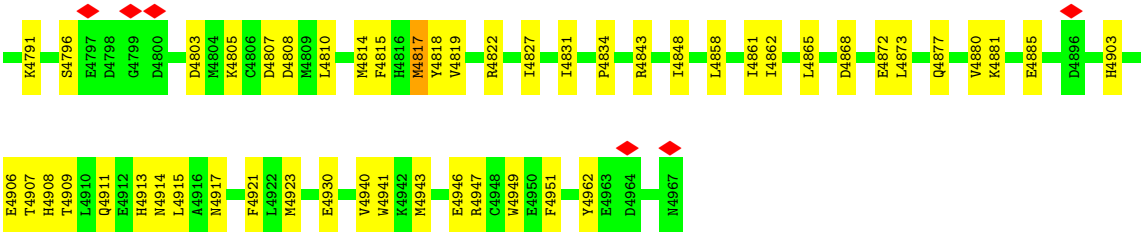
HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 L3105 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER
LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU SER SER LEU PRO THR ASN VAL ASP
VAL CYS PRO ASN ILE PRO SER LEU GLU GLU LYS LEU MET GLU GLU ILE VAL GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLU ARG ALA GLU MET
CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP PRO GLY GLY ALA THR MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET
GLU LYS LEU LYS LYS ALA ALA THR VAL VAL SER GLU LEU LYS ALA GLU ASP HIS LEU LEU LEU ILE LEU ASP GLU GLU LEU LEU ILE LEU ARG GLY ASP ALA ARG GLY ASP MET SER GLU ALA GLU GLU LEU ILE LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA LYS
TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA
VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP

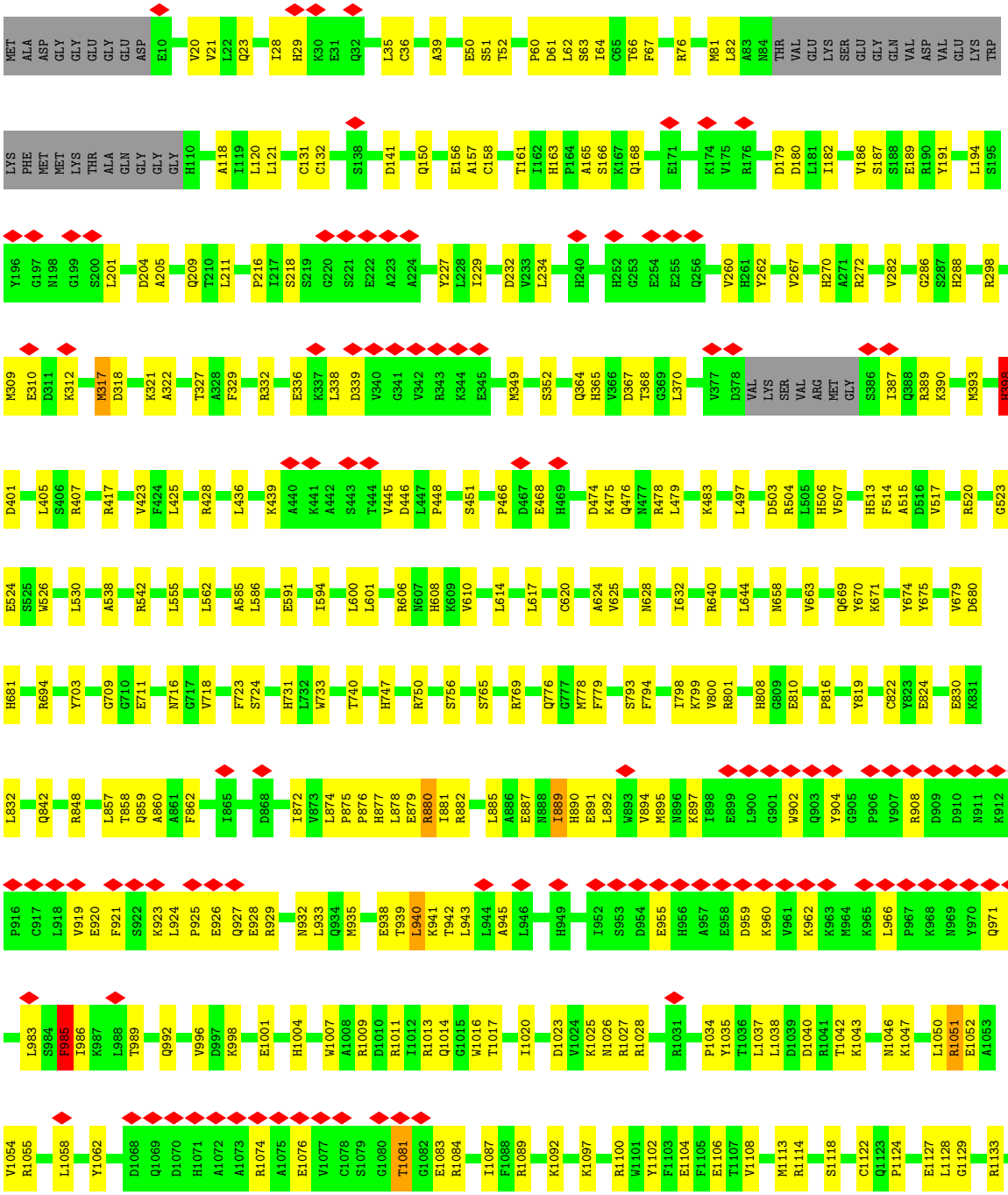


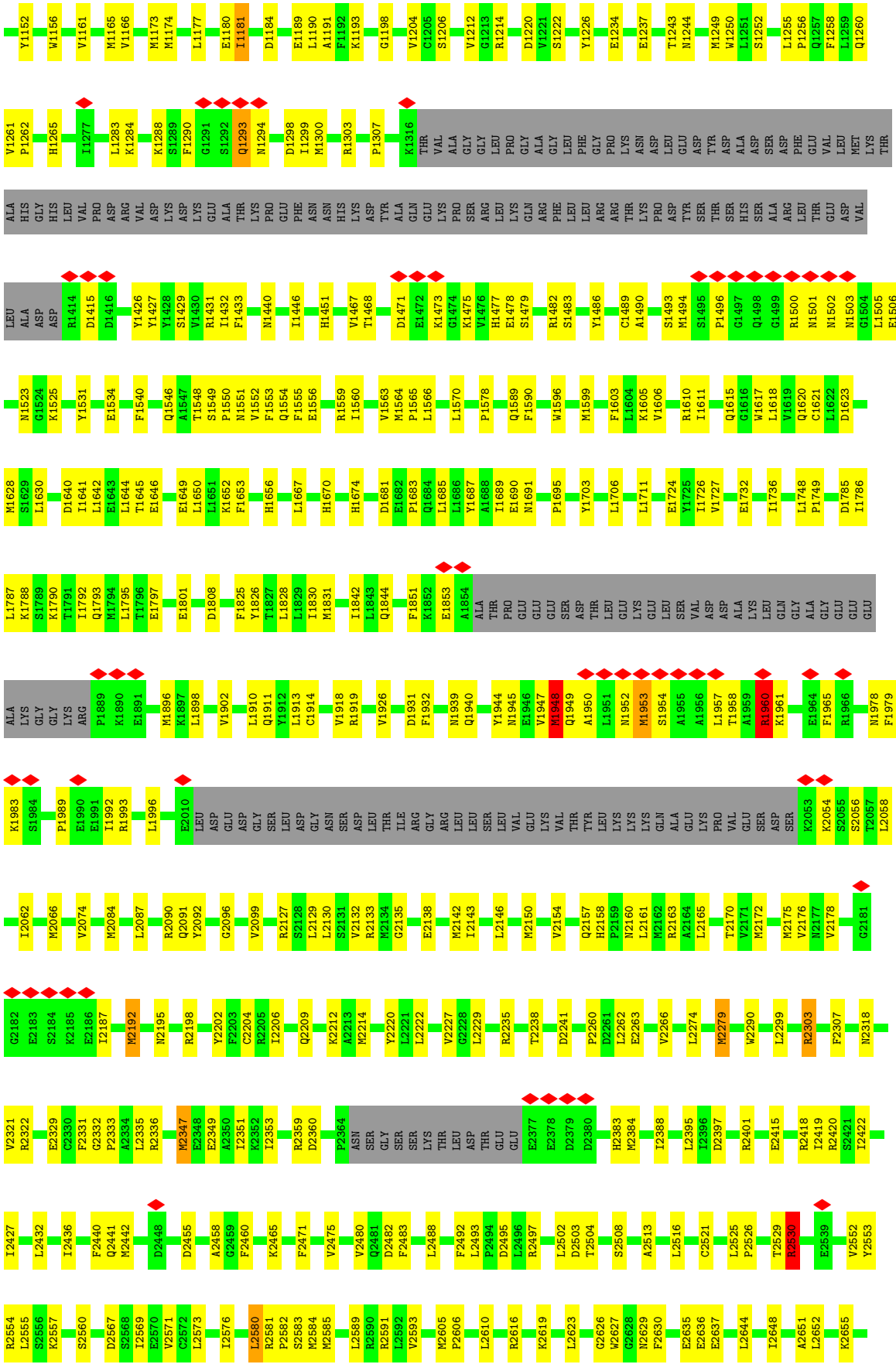


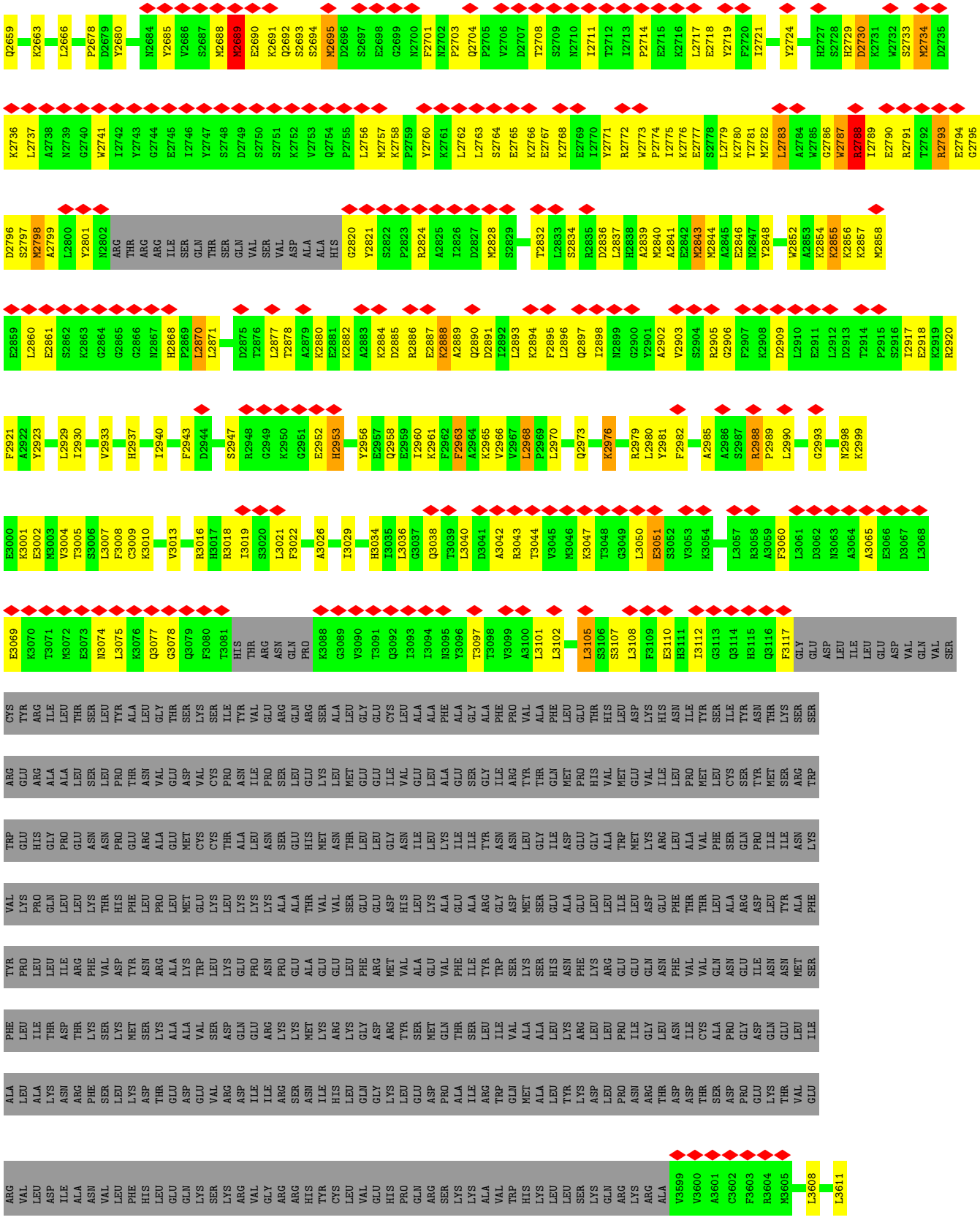


• Molecule 1: Ryanodine receptor 2

Chain C:

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D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 W2852 A2853 K2854 K2855 K2856 K2857 M2858
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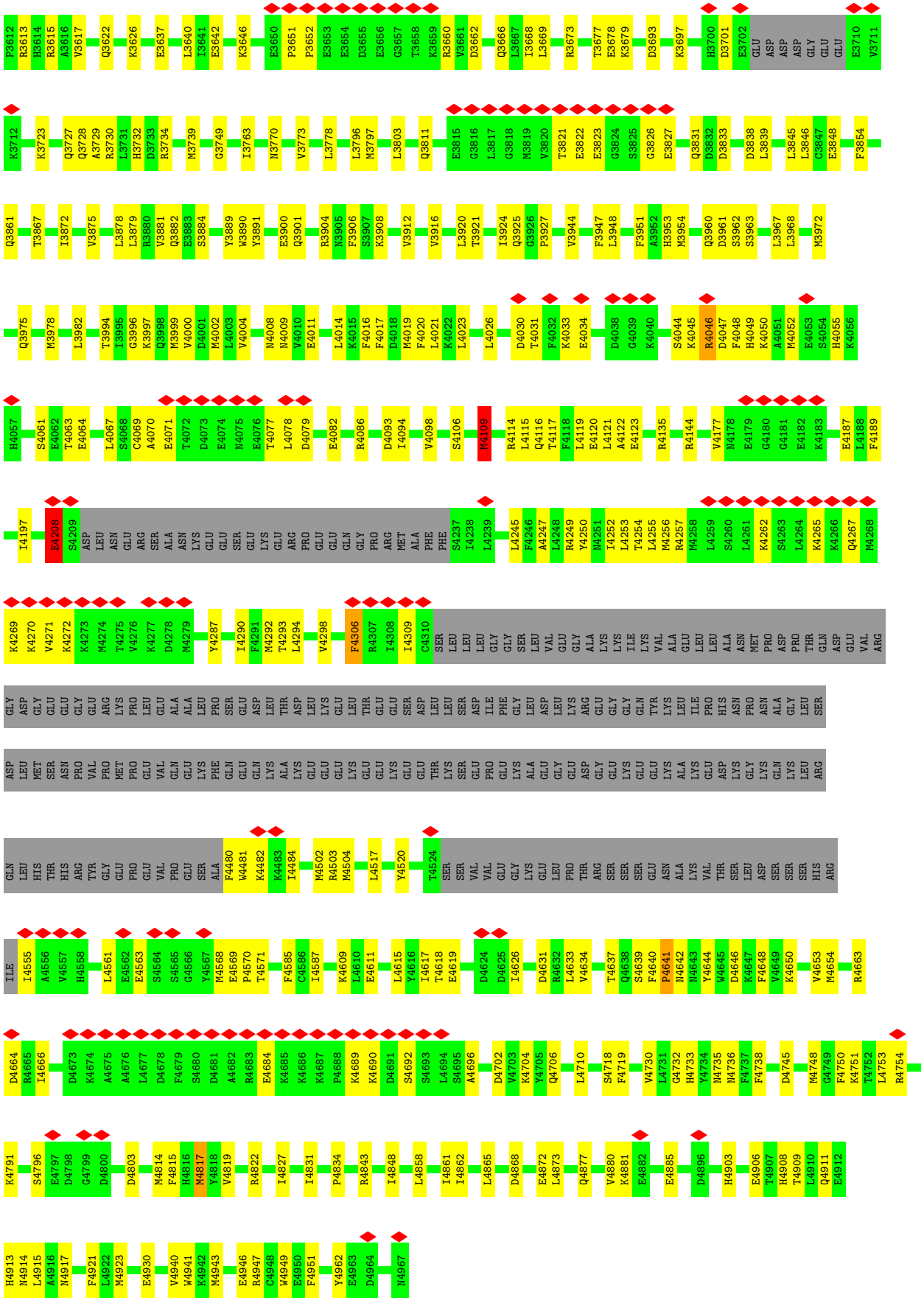
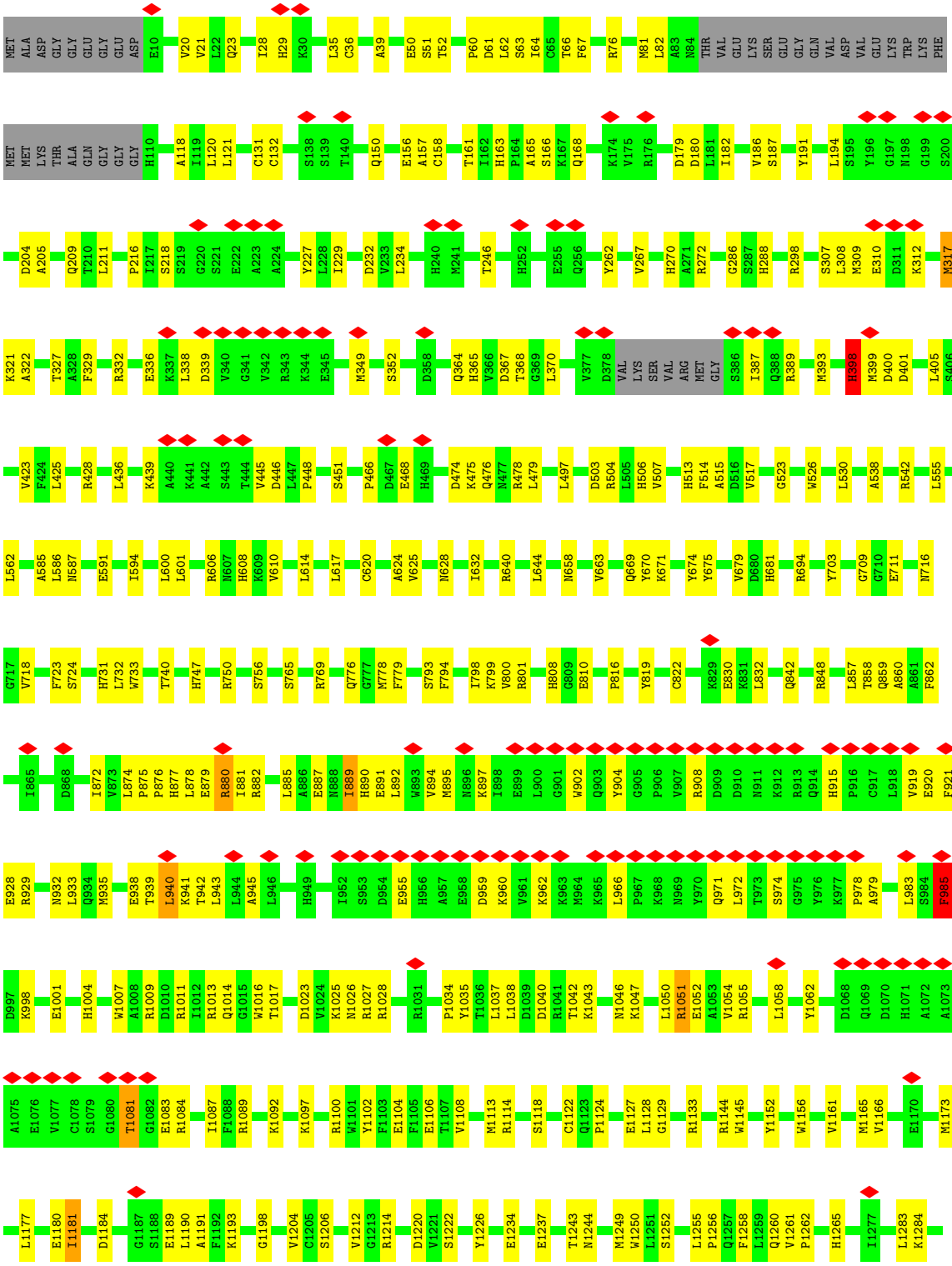
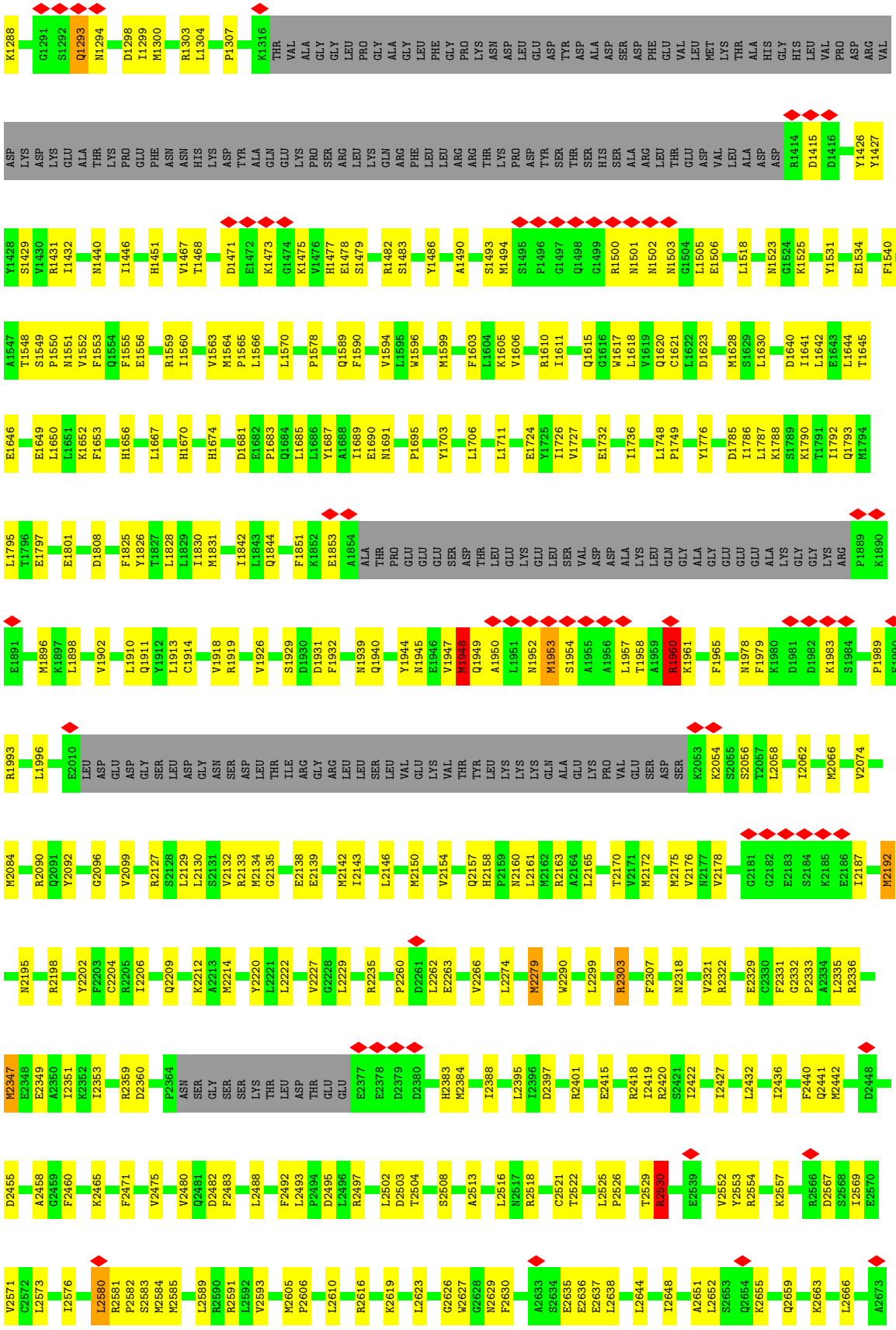
E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER
CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER
ARG GLU ARG ALA ALA LEU SER LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU GLU LYS LEU MET GLU GLU ILE VAL GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET ARG TRP
TRP GLU HIS GLY PRO GLU ASN ASN PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS
VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS ALA ALA THR VAL VAL SER GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU LEU ALA ARG ASP LEU TYR ALA PHE
TYR PRO LEU LEU ILE ARG PHE VAL TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER
PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE
ALA LEU ALA LYS ASN ARG PHE SER LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU
ARG VAL LEU ASP ILE ALA ASN VAL LEU LEU PHE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 L3608 L3611

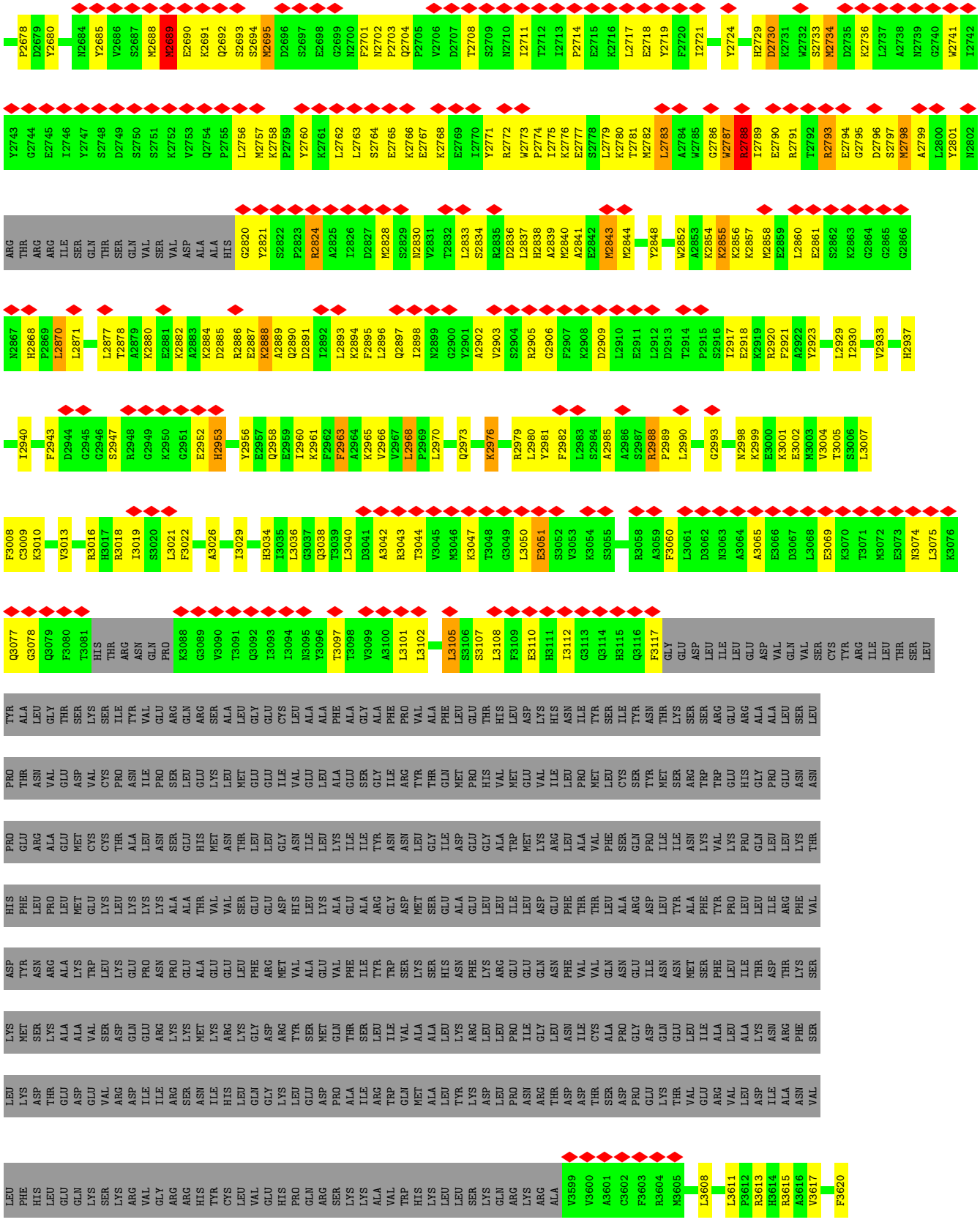


• Molecule 1: Ryanodine receptor 2

Chain D:

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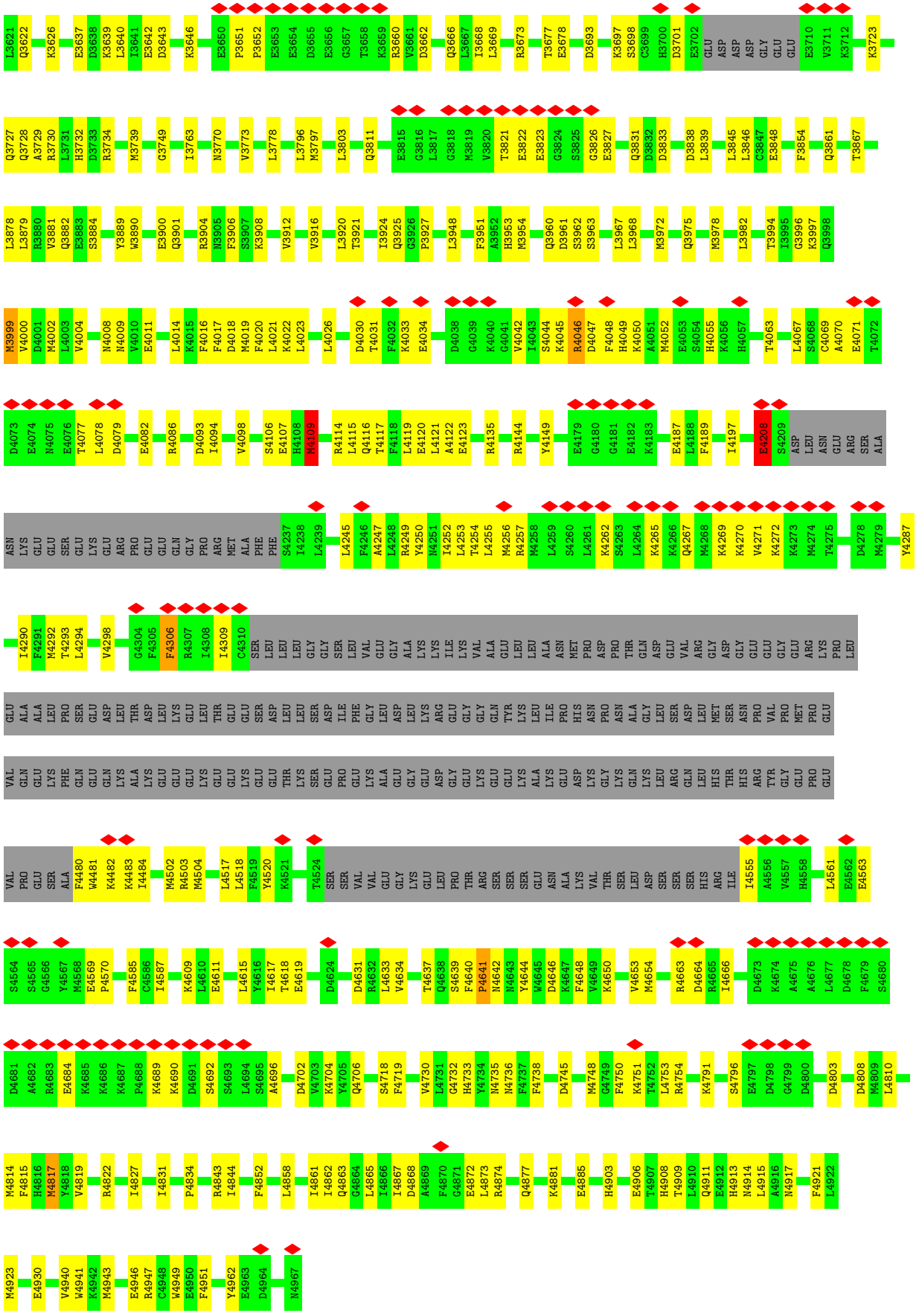
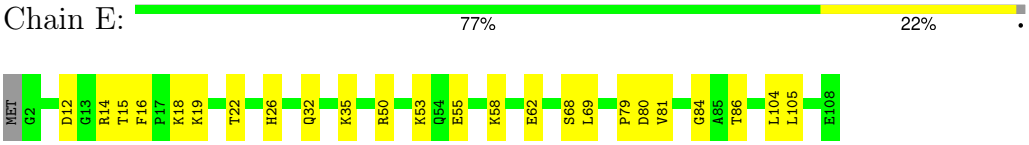
Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU
TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO VAL ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU SER LEU
PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL ILE LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN
PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR
HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS ALA ALA THR VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA ILE LEU ARG PHE VAL
ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA ALA GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER
LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER
LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP LYS ILE ALA ASN VAL
LEU PHE HIS LEU GLU GLN LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ALA ARG V3599 V3600 A3601 C3602 F3603 R3604 M3605 L3608 L3611 P3612 R3613 H3614 R3615 A3616 V3617 F3620


L3621 Q3622 K3626 E3637 D3638 K3639 L3640 I3641 E3642 D3643 K3646 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 V3661 D3662 Q3666 L3667 I3668 L3669 R3673 T3677 E3678 D3693 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 K3712 K3723
Q3727 Q3728 A3729 R3730 L3731 H3732 D3733 R3734 M3739 G3749 I3763 N3770 V3773 L3778 L3796 M3797 L3803 Q3811 E3815 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 Q3831 D3832 D3833 D3838 L3839 L3845 L3846 C3847 E3848 F3854 Q3861 T3867
L3878 L3879 R3880 V3881 Q3882 E3883 S3884 Y3889 W3890 E3900 Q3901 R3904 N3905 F3906 S3907 K3908 V3912 V3916 L3920 T3921 I3924 Q3925 G3926 P3927 L3948 F3951 A3952 H3953 M3954 Q3960 D3961 S3962 S3963 L3967 L3968 M3972 Q3975 M3978 L3982 T3994 I3995 G3996 K3997 Q3998
M3999 V4000 D4001 M4002 L4003 V4004 N4008 N4009 V4010 E4011 L4014 K4015 F4016 F4017 D4018 M4019 F4020 L4021 K4022 L4023 L4026 D4030 T4031 F4032 K4033 E4034 D4038 G4039 K4040 G4041 V4042 I4043 S4044 K4045 R4046 D4047 F4048 H4049 K4050 A4051 M4052 E4053 S4054 H4055 K4056 H4057 T4063 L4067 S4068 C4069 A4070 E4071 T4072
D4073 E4074 N4075 E4076 T4077 L4078 D4079 E4082 R4086 D4093 I4094 V4098 S4106 E4107 H4108 M4109 R4114 L4115 Q4116 T4117 F4118 L4119 E4120 L4121 A4122 E4123 R4135 R4144 Y4149 E4179 G4180 G4181 E4182 K4183 E4187 L4188 F4189 I4197 E4208 S4209 ASP LEU ASN GLU ARG SER ALA
ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN GLY PRO ARG MET ALA PHE PHE S4237 I4238 L4239 L4245 F4246 A4247 L4248 R4249 Y4250 N4251 I4252 L4253 T4254 L4255 M4256 R4257 M4258 L4259 S4260 L4261 K4262 S4263 L4264 K4265 K4266 Q4267 M4268 K4269 K4270 V4271 K4272 K4273 M4274 T4275 D4278 M4279 Y4287
I4290 F4291 M4292 T4293 L4294 V4298 G4304 F4305 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLU GLY GLU ARG LYS PRO LEU
GLU ALA ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER ASN PRO VAL PRO MET PRO GLU
VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU ASP GLY GLU GLY ASP GLY GLU LYS GLU GLU LYS ALA LYS GLU ASP LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU
VAL PRO GLU SER ALA F4480 W4481 K4482 K4483 I4484 M4502 R4503 M4504 L4517 L4518 F4519 Y4520 K4521 T4524 SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG SER SER SER GLU ASN ALA LYS VAL THR SER LEU ASP SER SER HIS ARG ILE I4455 A4556 V4557 H4558 L4561 E4562 E4563
S4564 S4565 G4566 Y4567 M4568 E4569 P4570 F4585 C4586 I4587 K4609 L4610 E4611 L4615 Y4616 T4617 T4618 E4619 D4624 D4631 R4632 L4633 V4634 T4637 Q4638 S4639 F4640 P4641 N4642 N4643 Y4644 W4645 D4646 K4647 F4648 V4649 K4650 V4653 M4654 R4663 D4664 R4665 I4666 D4673 K4674 A4675 A4676 L4677 D4678 F4679 S4680
D4681 A4682 R4683 E4684 K4685 K4686 K4687 P4688 K4689 K4690 D4691 S4692 S4693 L4694 S4695 A4696 D4702 V4703 K4704 Y4705 Q4706 S4718 F4719 V4730 L4731 G4732 H4733 Y4734 N4735 N4736 F4737 F4738 D4745 M4748 G4749 F4750 K4751 T4752 L4753 R4754 K4791 S4796 E4797 D4798 G4799 D4800 D4803 D4808 M4809 L4810
M4814 F4815 H4816 M4817 Y4818 V4819 R4822 I4827 I4831 P4834 R4843 I4844 F4852 L4858 I4861 I4862 Q4863 G4864 L4865 I4866 I4867 D4868 A4869 F4870 G4871 E4872 L4873 R4874 Q4877 K4881 E4885 H4903 E4906 T4907 H4908 T4909 L4910 Q4911 E4912 H4913 N4914 L4915 A4916 N4917 F4921 L4922
M4923 E4930 V4940 W4941 K4942 M4943 E4946 R4947 C4948 W4949 E4950 F4951 Y4962 E4963 D4964 N4967

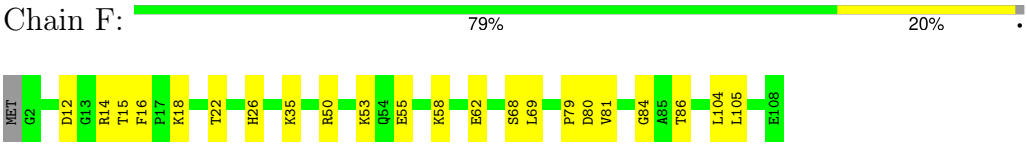
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



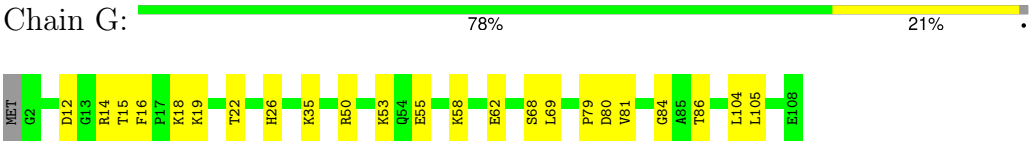

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



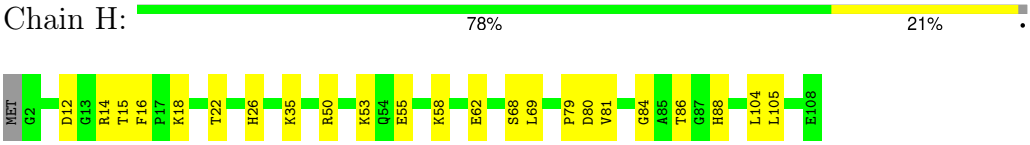

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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, Not provided | |
| Number of particles used | 55886 | 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 | 0.564 | Depositor |
| Minimum map value | -0.016 | Depositor |
| Average map value | 0.008 | Depositor |
| Map value standard deviation | 0.027 | Depositor |
| Recommended contour level | 0.12 | Depositor |
| Map size (Å) | 431.36, 431.36, 431.36 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8425, 0.8425, 0.8425 | 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, CA, 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 | 1/32738 (0.0%) | 0.55 | 17/44213 (0.0%) |
| 1 | B | 0.27 | 1/32738 (0.0%) | 0.55 | 17/44213 (0.0%) |
| 1 | C | 0.27 | 1/32738 (0.0%) | 0.54 | 17/44213 (0.0%) |
| 1 | D | 0.27 | 1/32738 (0.0%) | 0.55 | 17/44213 (0.0%) |
| 2 | E | 0.27 | 0/834 | 0.53 | 0/1123 |
| 2 | F | 0.27 | 0/834 | 0.53 | 0/1123 |
| 2 | G | 0.27 | 0/834 | 0.53 | 0/1123 |
| 2 | H | 0.27 | 0/834 | 0.53 | 0/1123 |
| All | All | 0.27 | 4/134288 (0.0%) | 0.54 | 68/181344 (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 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 2787 | TRP | CB-CG | -6.00 | 1.39 | 1.50 |
| 1 | D | 2787 | TRP | CB-CG | -6.00 | 1.39 | 1.50 |
| 1 | A | 2787 | TRP | CB-CG | -5.99 | 1.39 | 1.50 |
| 1 | C | 2787 | TRP | CB-CG | -5.98 | 1.39 | 1.50 |

The worst 5 of 68 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 2279 | MET | CB-CG-SD | 10.74 | 144.62 | 112.40 |
| 1 | C | 2279 | MET | CB-CG-SD | 10.74 | 144.61 | 112.40 |
| 1 | B | 2279 | MET | CB-CG-SD | 10.73 | 144.60 | 112.40 |
| 1 | D | 2279 | MET | CB-CG-SD | 10.73 | 144.58 | 112.40 |
| 1 | D | 2279 | MET | CA-CB-CG | 10.43 | 131.03 | 113.30 |

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 2530 | ARG | Sidechain |
| 1 | A | 2788 | ARG | Sidechain |
| 1 | A | 398 | HIS | Peptide |
| 1 | B | 2530 | ARG | Sidechain |
| 1 | B | 398 | HIS | 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 | 32032 | 0 | 31689 | 830 | 0 |
| 1 | B | 32032 | 0 | 31689 | 827 | 0 |
| 1 | C | 32032 | 0 | 31689 | 812 | 0 |
| 1 | D | 32032 | 0 | 31689 | 815 | 0 |
| 2 | E | 818 | 0 | 821 | 14 | 0 |
| 2 | F | 818 | 0 | 821 | 12 | 0 |
| 2 | G | 818 | 0 | 821 | 13 | 0 |
| 2 | H | 818 | 0 | 821 | 13 | 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 | 0 | 0 |
| 4 | B | 62 | 0 | 24 | 0 | 0 |
| 4 | C | 62 | 0 | 24 | 0 | 0 |
| 4 | D | 62 | 0 | 24 | 0 | 0 |
| 5 | A | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | C | 1 | 0 | 0 | 0 | 0 |
| 5 | D | 1 | 0 | 0 | 0 | 0 |
| All | All | 131656 | 0 | 130136 | 3262 | 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 12.

The worst 5 of 3262 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:A:4279:MET:HE2 | 1:B:4487:TYR:HD1 | 1.30 | 0.93 |
| 1:D:2857:LYS:HE3 | 1:D:2871:LEU:HD23 | 1.52 | 0.92 |
| 1:A:2857:LYS:HE3 | 1:A:2871:LEU:HD23 | 1.52 | 0.92 |
| 1:C:2857:LYS:HE3 | 1:C:2871:LEU:HD23 | 1.52 | 0.91 |
| 1:B:2857:LYS:HE3 | 1:B:2871:LEU:HD23 | 1.52 | 0.90 |

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 | 3978/4967 (80%) | 3861 (97%) | 113 (3%) | 4 (0%) | 48 | 79 |
| 1 | B | 3978/4967 (80%) | 3862 (97%) | 112 (3%) | 4 (0%) | 48 | 79 |
| 1 | C | 3978/4967 (80%) | 3861 (97%) | 113 (3%) | 4 (0%) | 48 | 79 |
| 1 | D | 3978/4967 (80%) | 3862 (97%) | 112 (3%) | 4 (0%) | 48 | 79 |
| 2 | E | 105/108 (97%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | F | 105/108 (97%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | G | 105/108 (97%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | H | 105/108 (97%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 16332/20300 (80%) | 15850 (97%) | 466 (3%) | 16 (0%) | 50 79 |

5 of 16 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2988 | ARG |
| 1 | A | 3927 | PRO |
| 1 | A | 4641 | PRO |
| 1 | B | 2988 | ARG |
| 1 | B | 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 | 3513/4358 (81%) | 3447 (98%) | 66 (2%) | 52 73 |
| 1 | B | 3513/4358 (81%) | 3447 (98%) | 66 (2%) | 52 73 |
| 1 | C | 3513/4358 (81%) | 3447 (98%) | 66 (2%) | 52 73 |
| 1 | D | 3513/4358 (81%) | 3447 (98%) | 66 (2%) | 52 73 |
| 2 | E | 88/89 (99%) | 85 (97%) | 3 (3%) | 32 60 |
| 2 | F | 88/89 (99%) | 85 (97%) | 3 (3%) | 32 60 |
| 2 | G | 88/89 (99%) | 85 (97%) | 3 (3%) | 32 60 |
| 2 | H | 88/89 (99%) | 85 (97%) | 3 (3%) | 32 60 |
| All | All | 14404/17788 (81%) | 14128 (98%) | 276 (2%) | 52 73 |

5 of 276 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 2192 | MET |
| 1 | D | 2530 | ARG |
| 1 | D | 3051 | GLU |
| 1 | B | 1957 | LEU |
| 1 | B | 1939 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 3975 | GLN |
| 1 | D | 2868 | HIS |
| 1 | C | 1046 | ASN |
| 1 | D | 2704 | GLN |
| 1 | D | 4049 | HIS |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 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 | $\#\|Z\| > 2$ |
| 4 | ATP | D | 5002 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 4 | ATP | C | 5004 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 4 | ATP | C | 5002 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 4 | ATP | B | 5002 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 4 | ATP | A | 5004 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 4 | ATP | D | 5004 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 4 | ATP | A | 5002 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 4 | ATP | B | 5004 | - | 28,33,33 | 0.63 | 0 | 34,52,52 | 0.59 | 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 | D | 5002 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | C | 5004 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | C | 5002 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | B | 5002 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | A | 5004 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | D | 5004 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | A | 5002 | - | - | 9/18/38/38 | 0/3/3/3 |
| 4 | ATP | B | 5004 | - | - | 9/18/38/38 | 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 | C | 5002 | ATP | C5-C6-N6 | 2.33 | 123.86 | 120.31 |
| 4 | A | 5004 | ATP | C5-C6-N6 | 2.33 | 123.85 | 120.31 |
| 4 | B | 5004 | ATP | C5-C6-N6 | 2.32 | 123.85 | 120.31 |
| 4 | A | 5002 | ATP | C5-C6-N6 | 2.32 | 123.85 | 120.31 |
| 4 | C | 5004 | ATP | C5-C6-N6 | 2.32 | 123.85 | 120.31 |

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

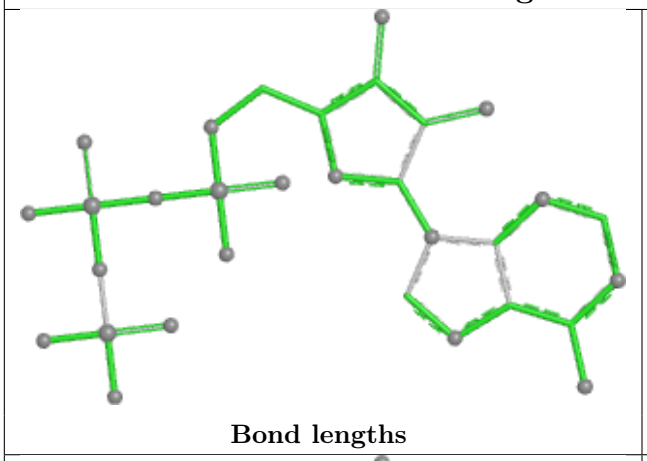
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 5002 | ATP | PB-O3B-PG-O3G |
| 4 | A | 5002 | ATP | C5'-O5'-PA-O1A |
| 4 | A | 5002 | ATP | C5'-O5'-PA-O2A |
| 4 | A | 5002 | ATP | C5'-O5'-PA-O3A |
| 4 | A | 5004 | ATP | C5'-O5'-PA-O2A |

There are no ring outliers.

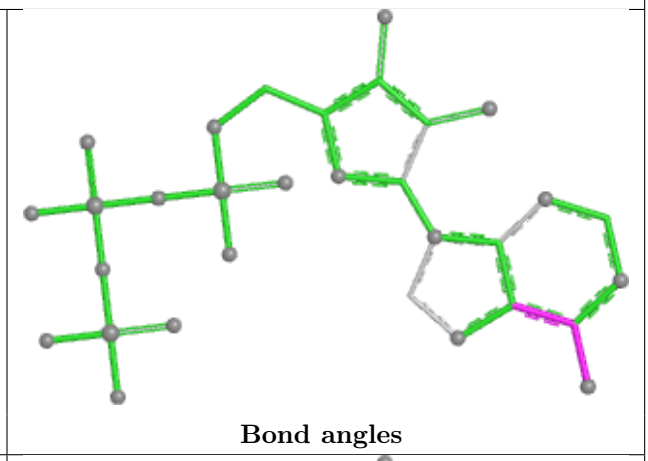
No monomer is involved in short contacts.

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.

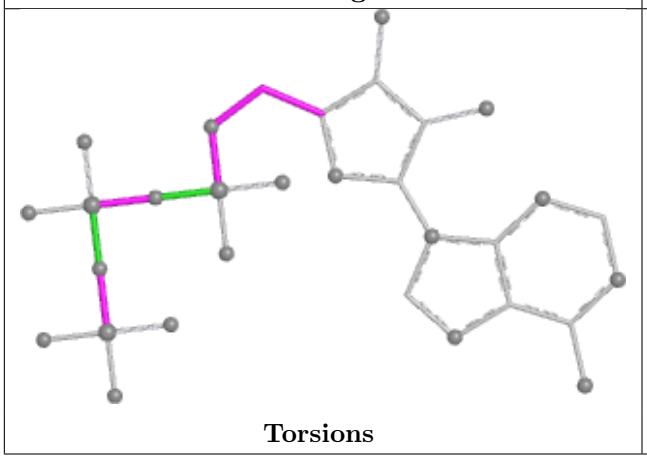
**Ligand ATP D 5002**



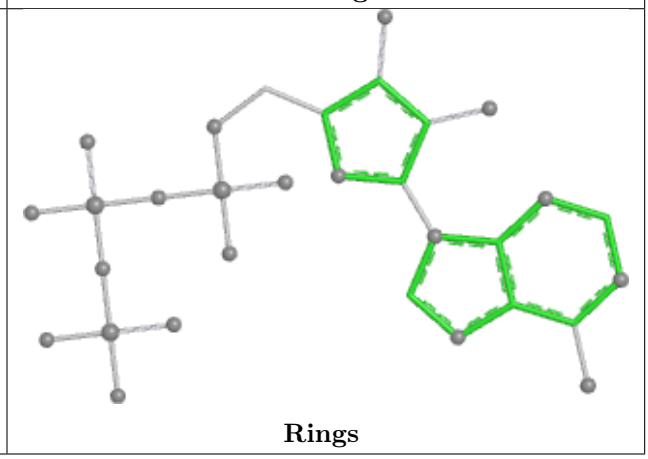
**Bond lengths**



**Bond angles**

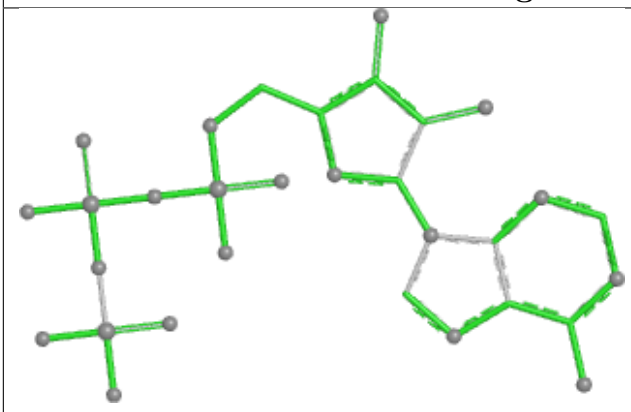


**Torsions**

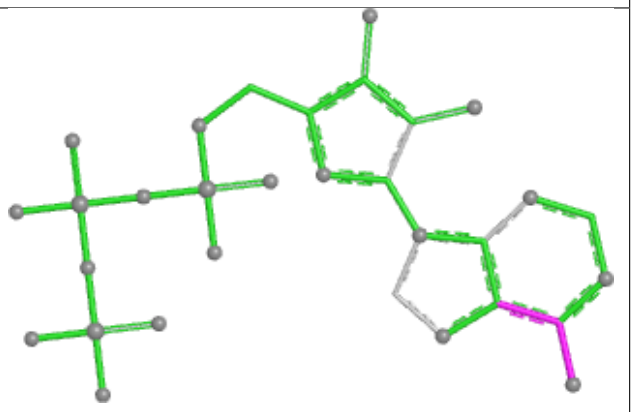


**Rings**

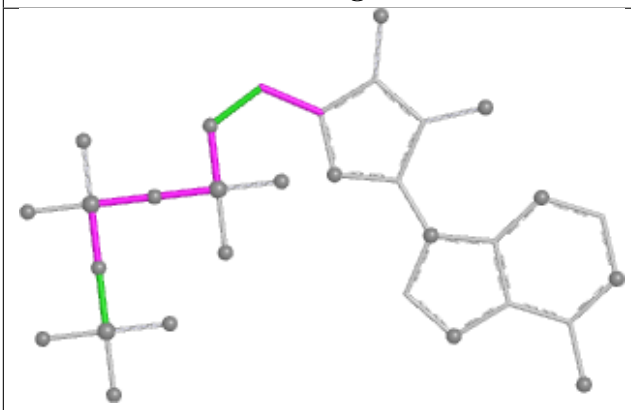
**Ligand ATP C 5004**



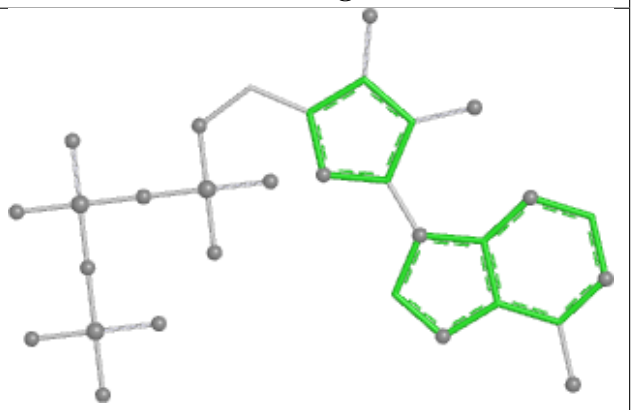
**Bond lengths**



**Bond angles**

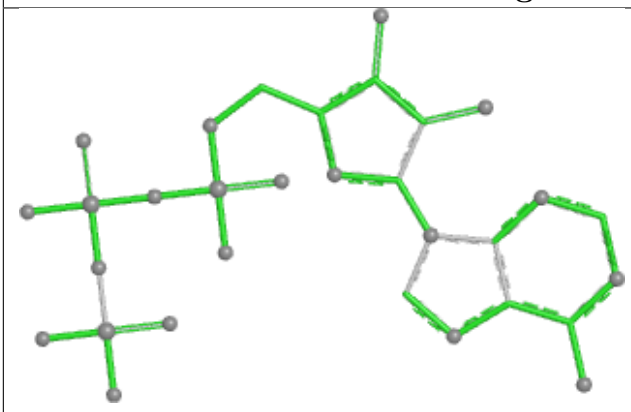


**Torsions**

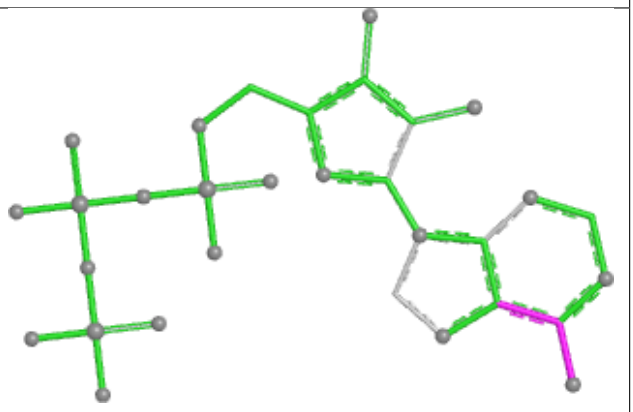


**Rings**

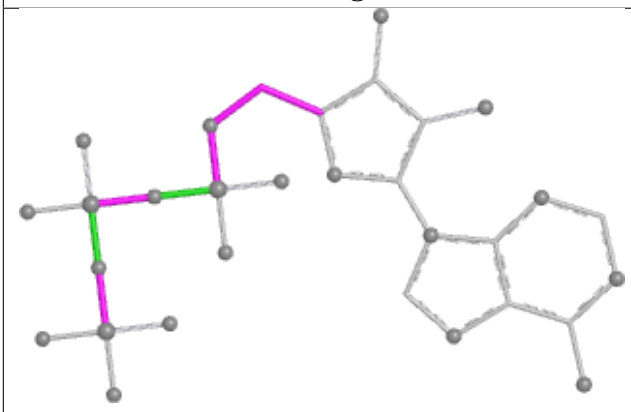
**Ligand ATP C 5002**



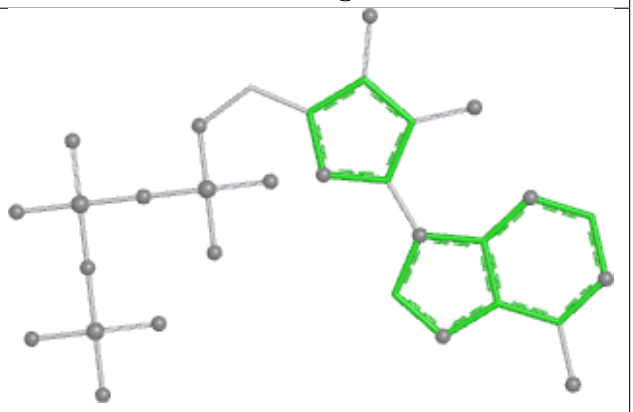
**Bond lengths**



**Bond angles**

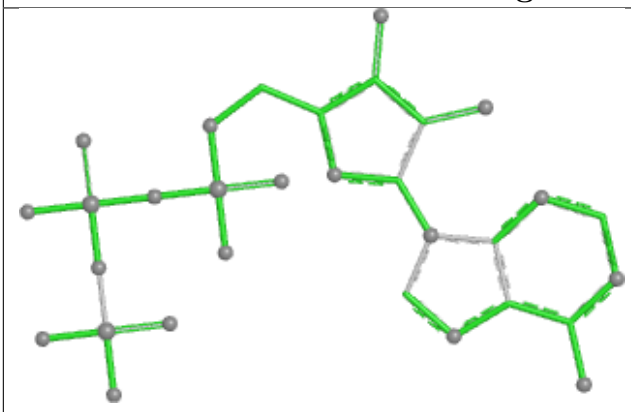


**Torsions**

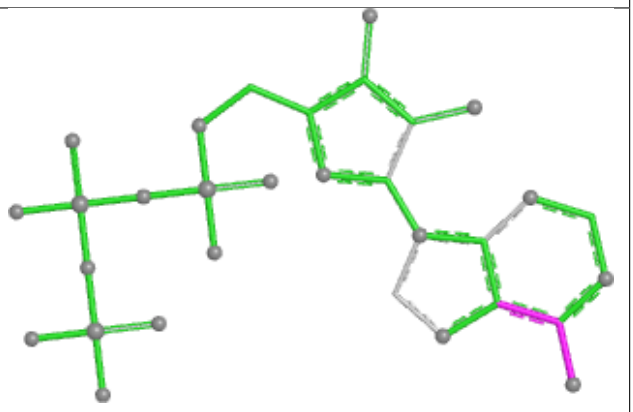


**Rings**

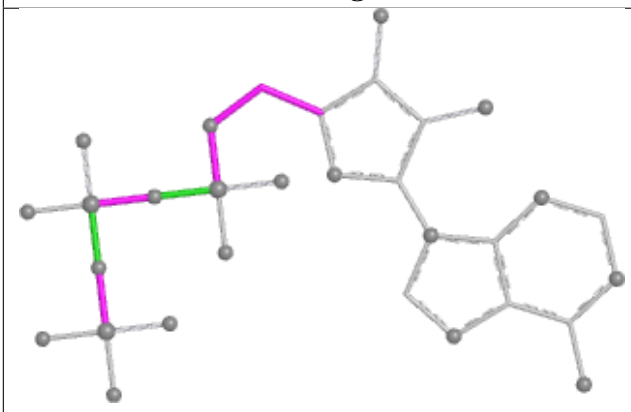
**Ligand ATP B 5002**



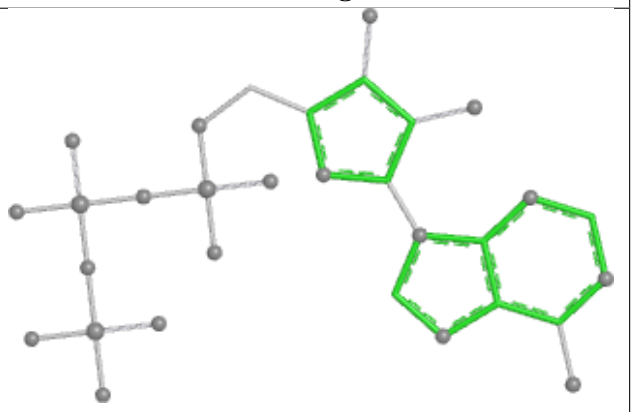
**Bond lengths**



**Bond angles**

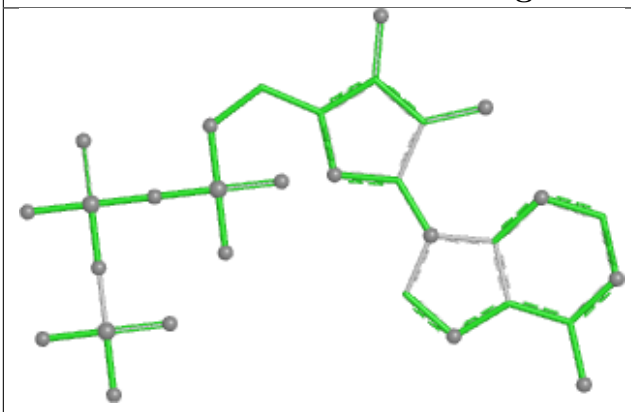


**Torsions**

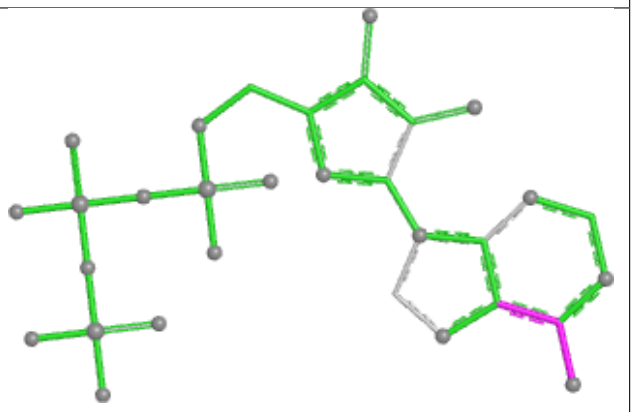


**Rings**

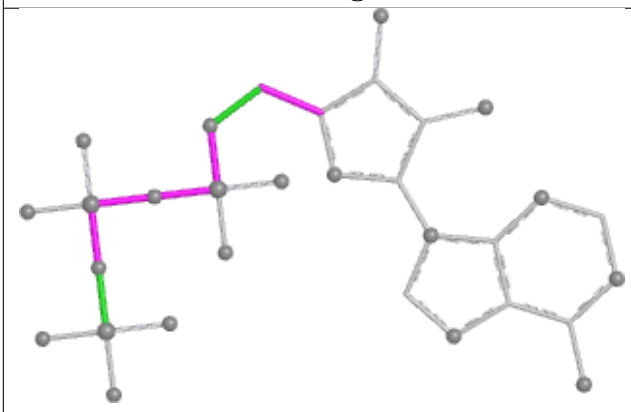
**Ligand ATP A 5004**



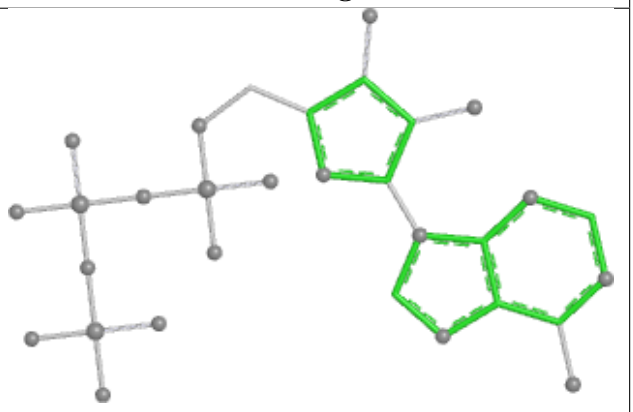
**Bond lengths**



**Bond angles**

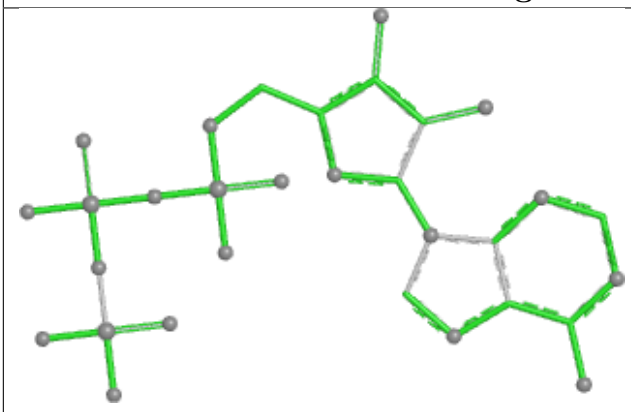


**Torsions**

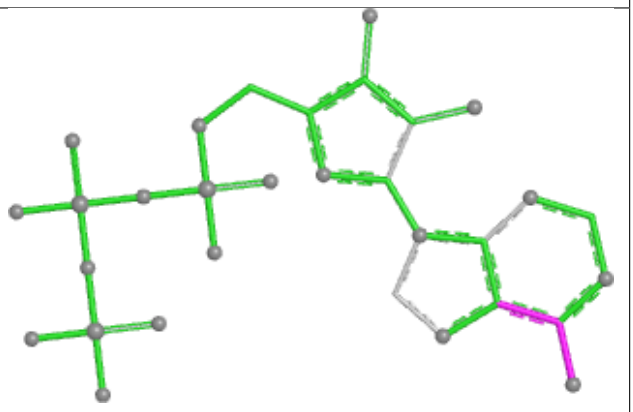


**Rings**

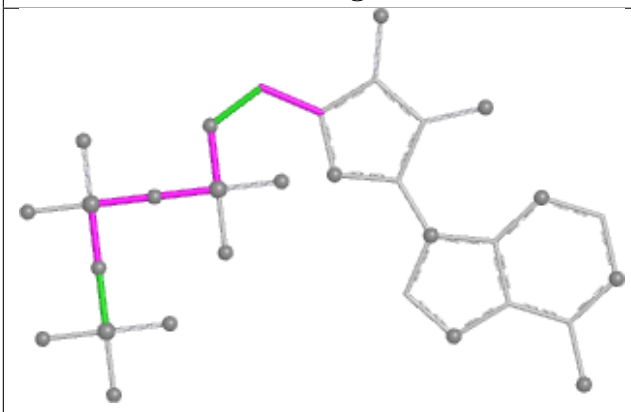
**Ligand ATP D 5004**



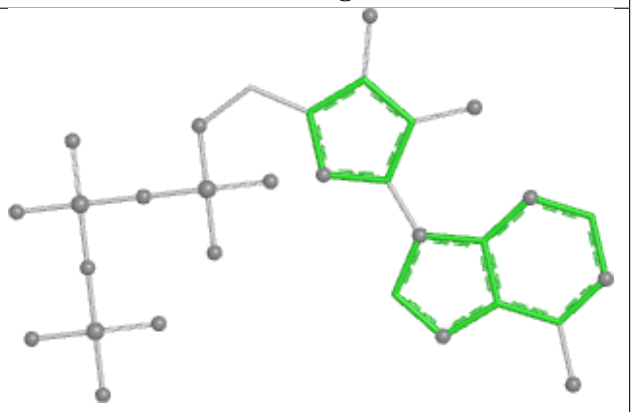
**Bond lengths**



**Bond angles**

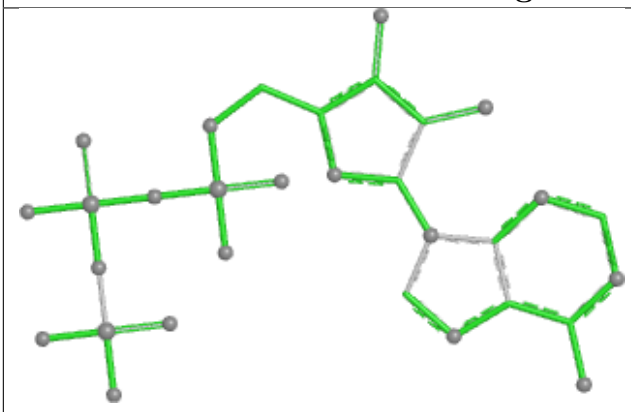


**Torsions**

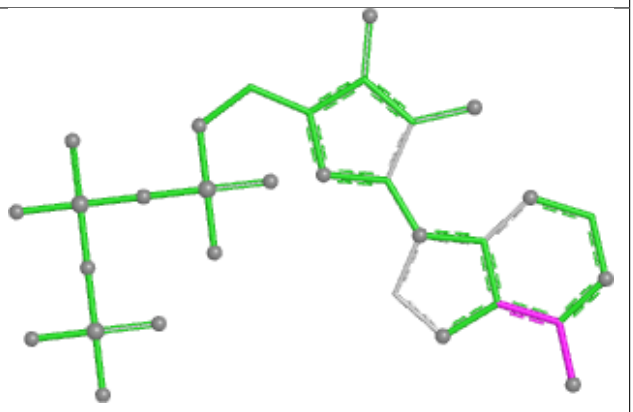


**Rings**

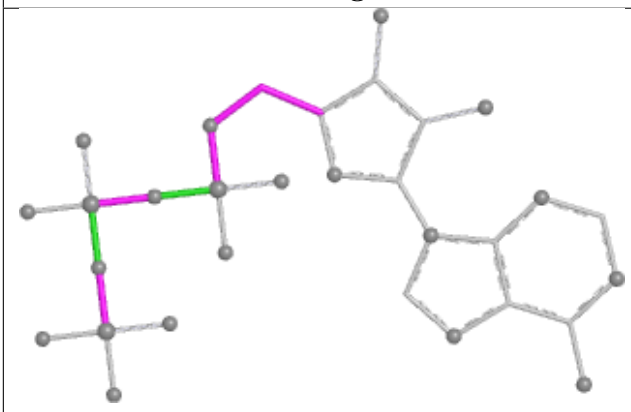
**Ligand ATP A 5002**



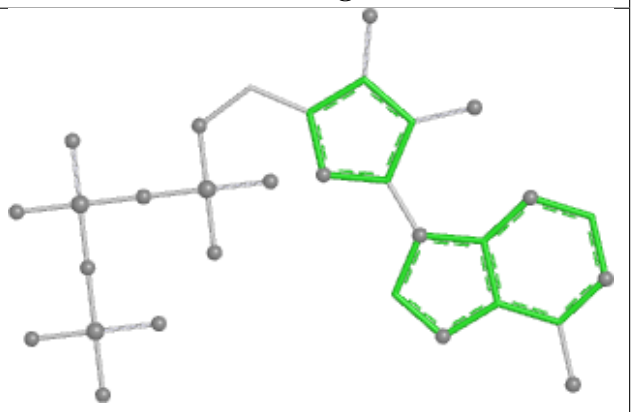
**Bond lengths**



**Bond angles**

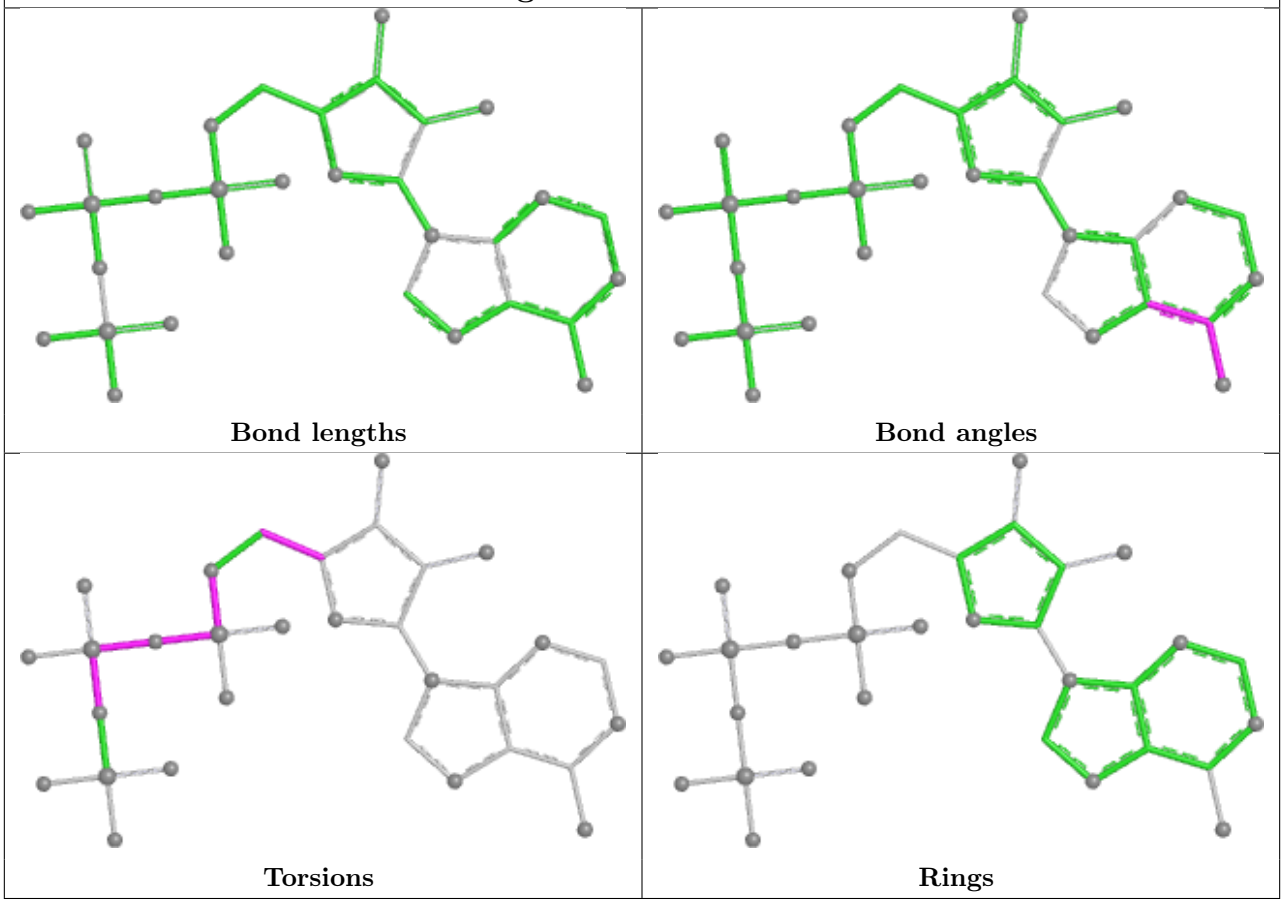


**Torsions**



**Rings**

**Ligand ATP B 5004**




## 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.

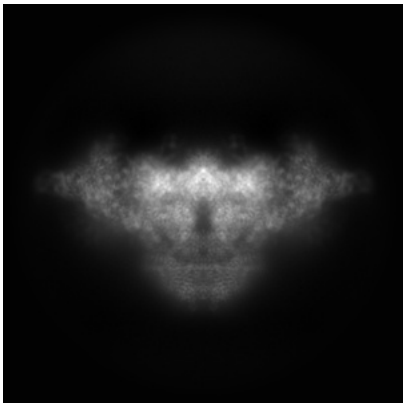
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42764. These allow visual inspection of the internal detail of the map and identification of artifacts.

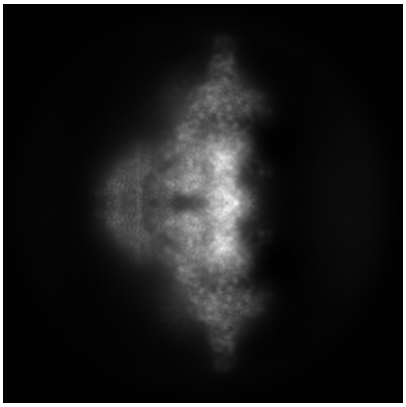
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

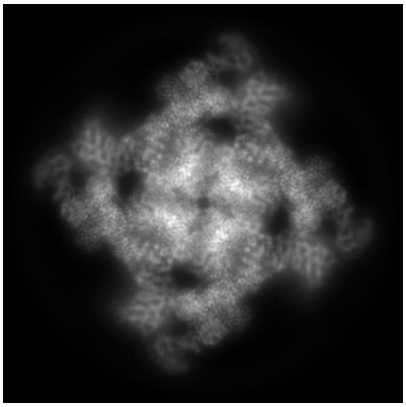
### 6.1.1 Primary map



X



Y

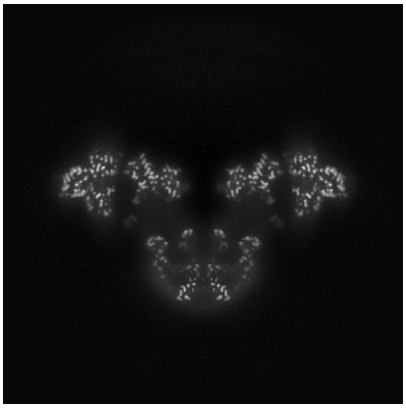


Z

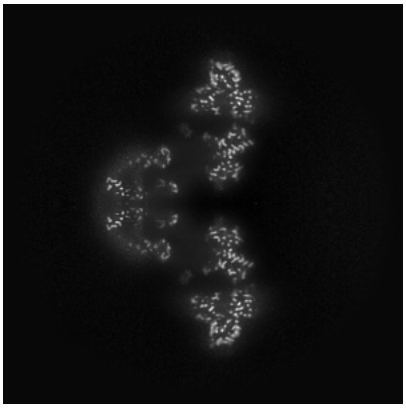
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

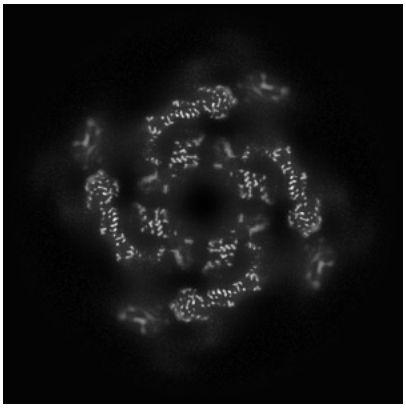
### 6.2.1 Primary map



X Index: 256



Y Index: 256

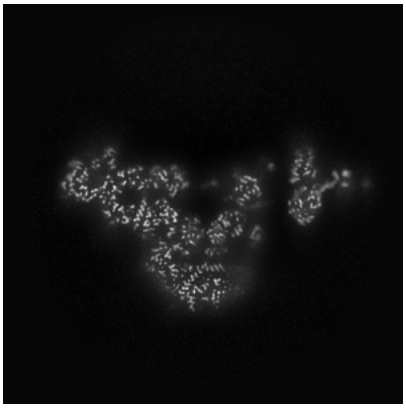


Z Index: 256

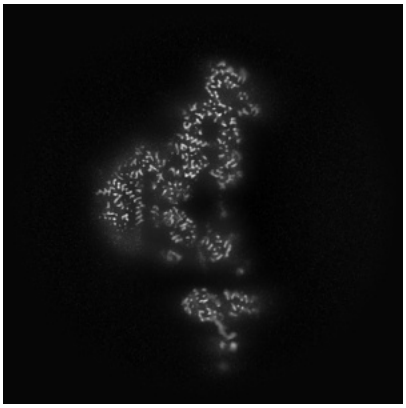
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

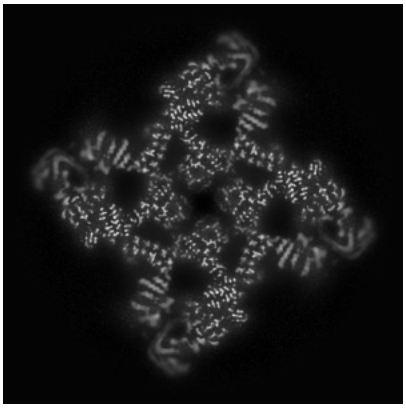
### 6.3.1 Primary map



X Index: 274



Y Index: 274



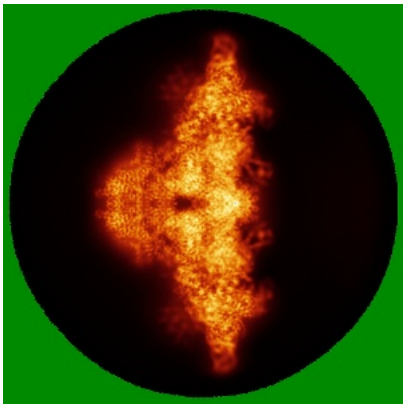
Z Index: 277

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

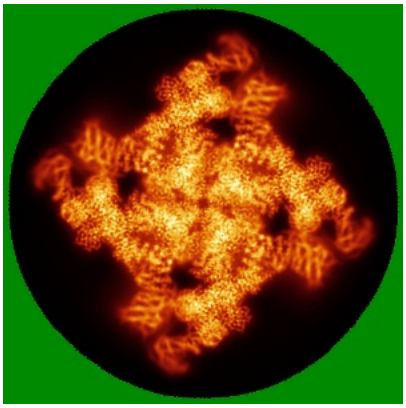
## 6.4 Orthogonal standard-deviation projections (False-color) (i)

### 6.4.1 Primary map

X



Y

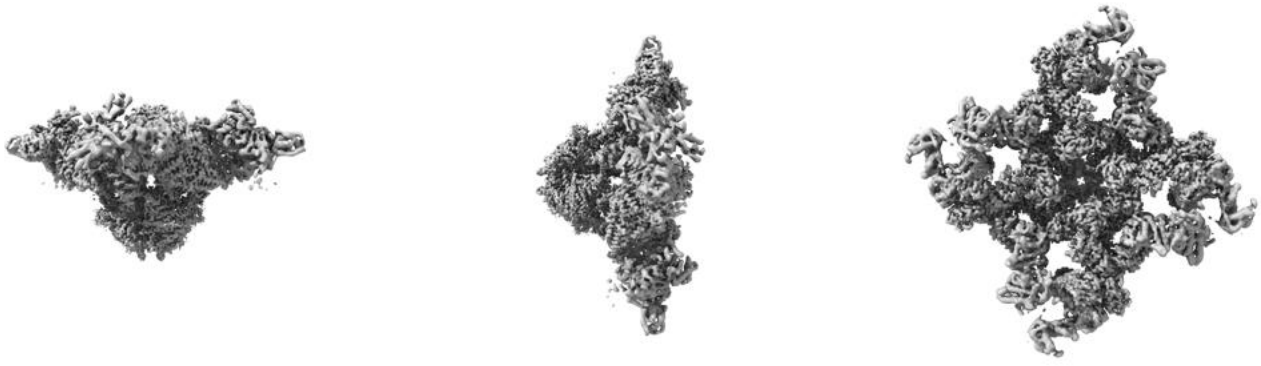


Z

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.

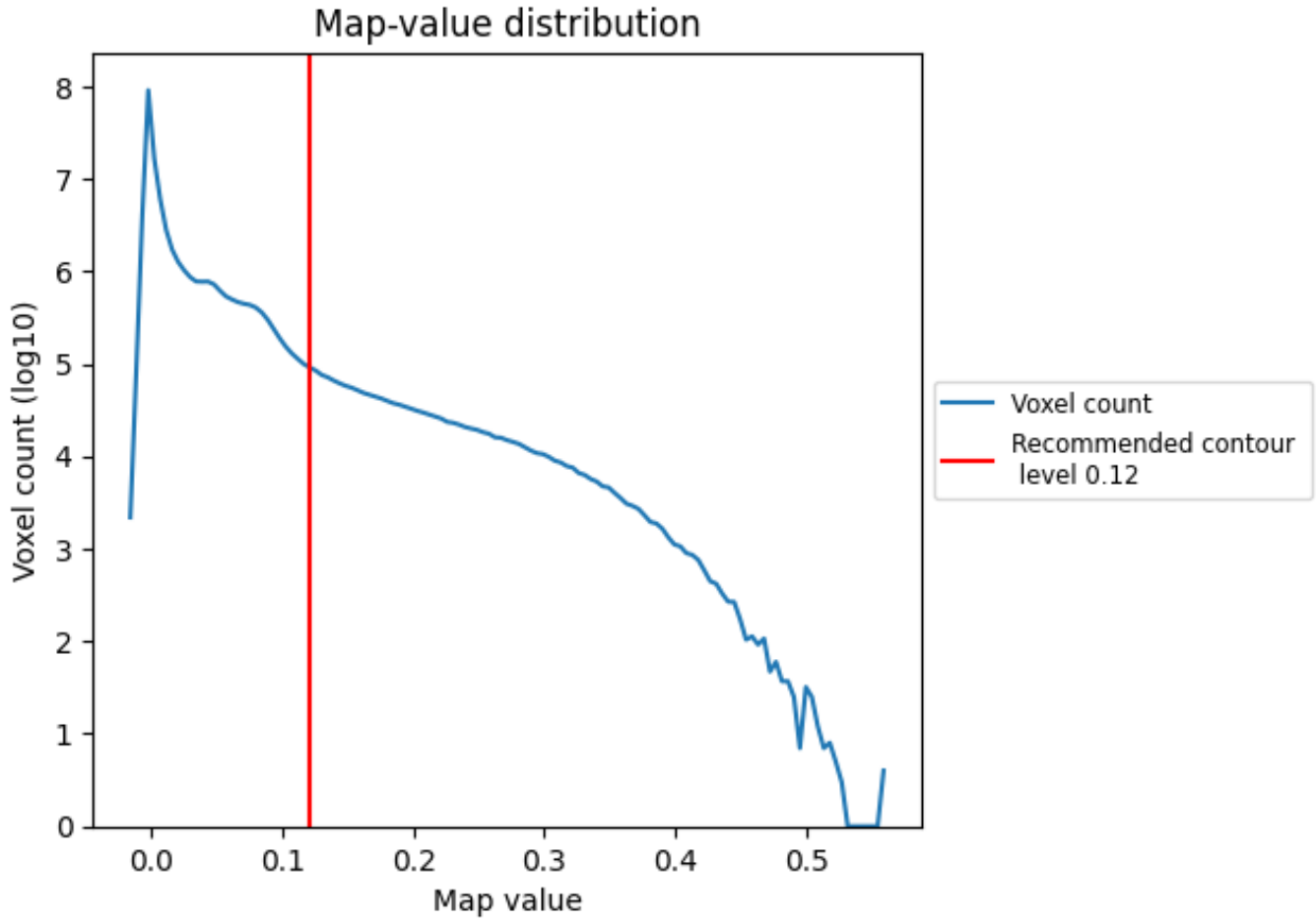
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

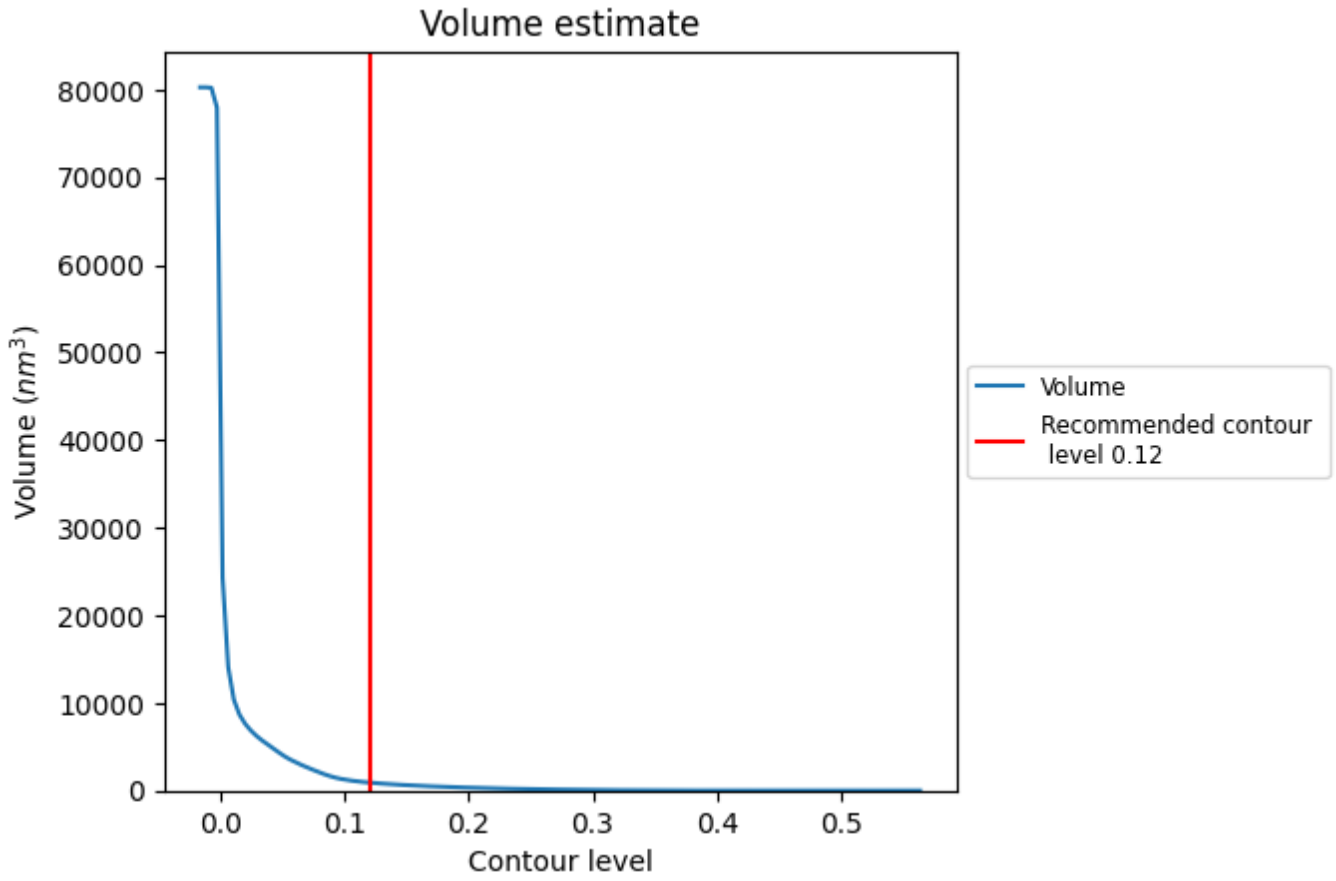
This section contains the results of statistical analysis of the map.

## 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.

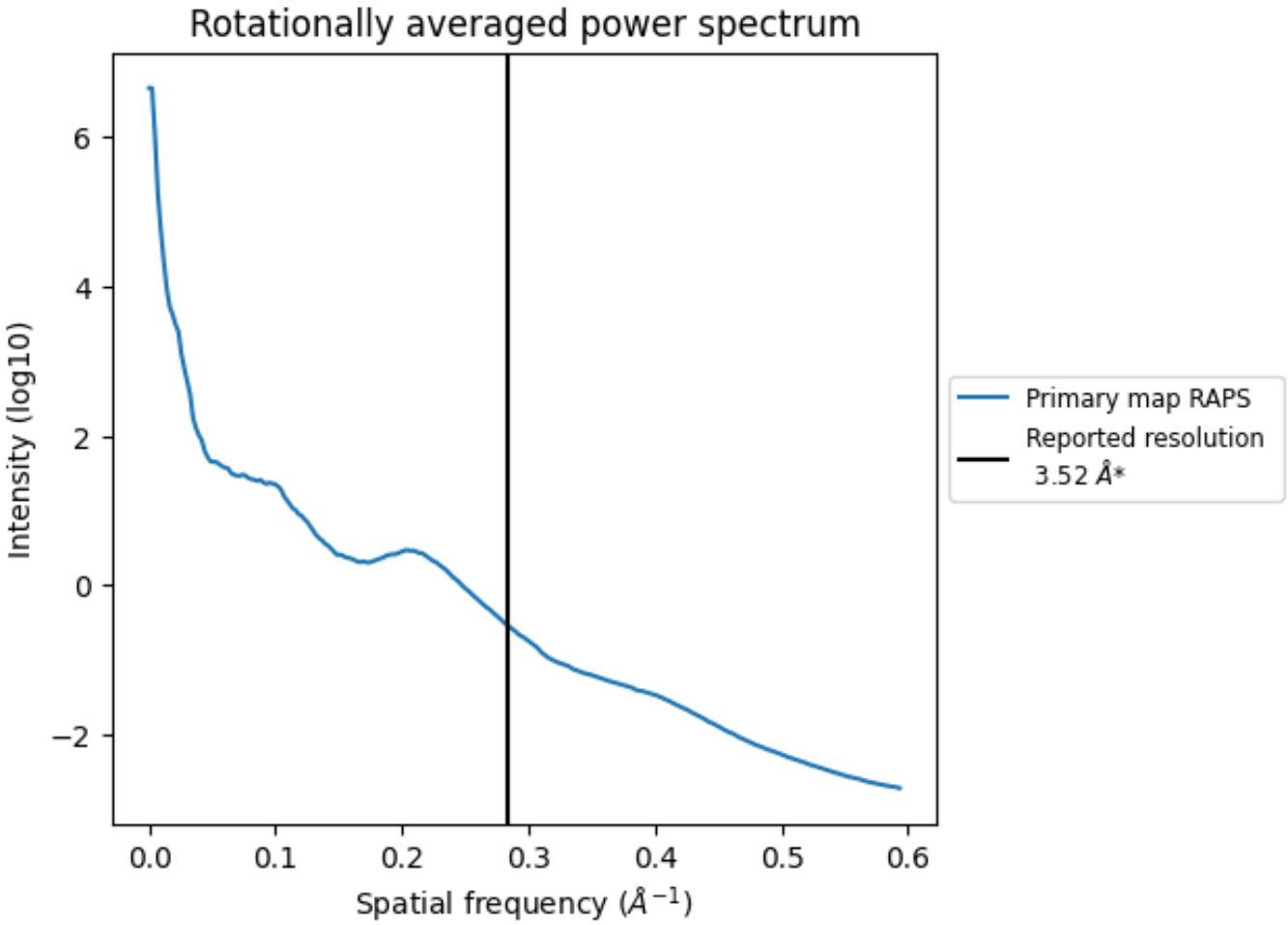
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 911 $nm^3$; this corresponds to an approximate mass of 823 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 0.284 $Å^{-1}$

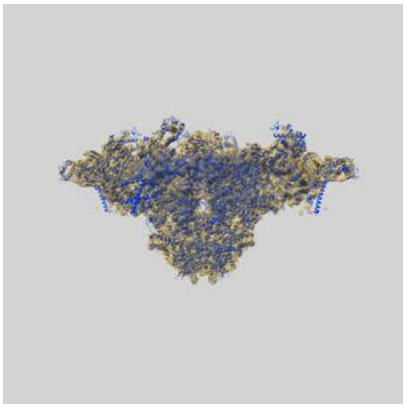
# 8 Fourier-Shell correlation (i)

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

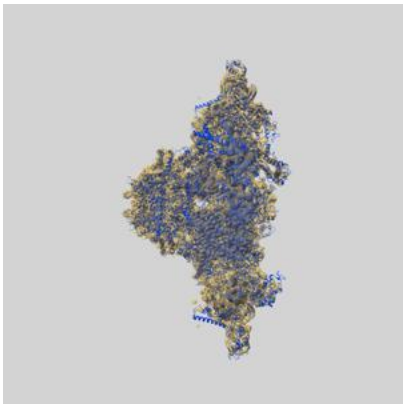
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42764 and PDB model 8UXH. Per-residue inclusion information can be found in section 3 on page 6.

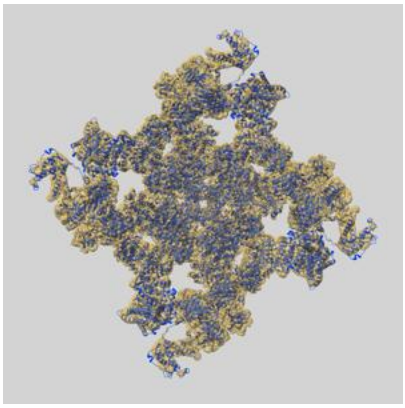
## 9.1 Map-model overlay



X



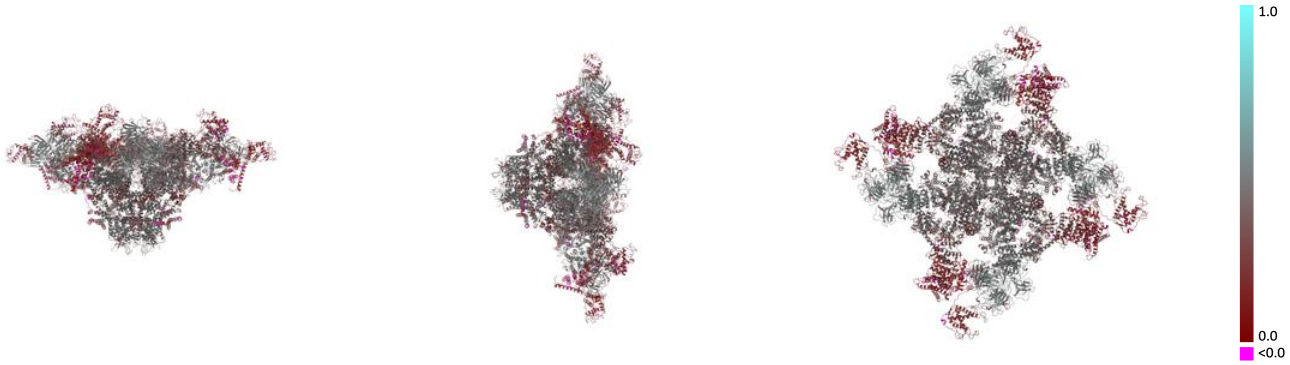
Y



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.

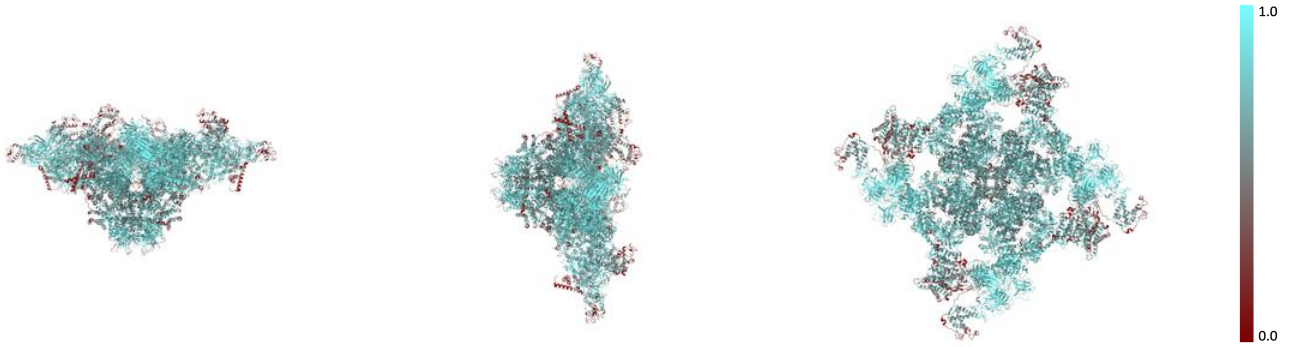
## 9.2 Q-score mapped to coordinate model




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.

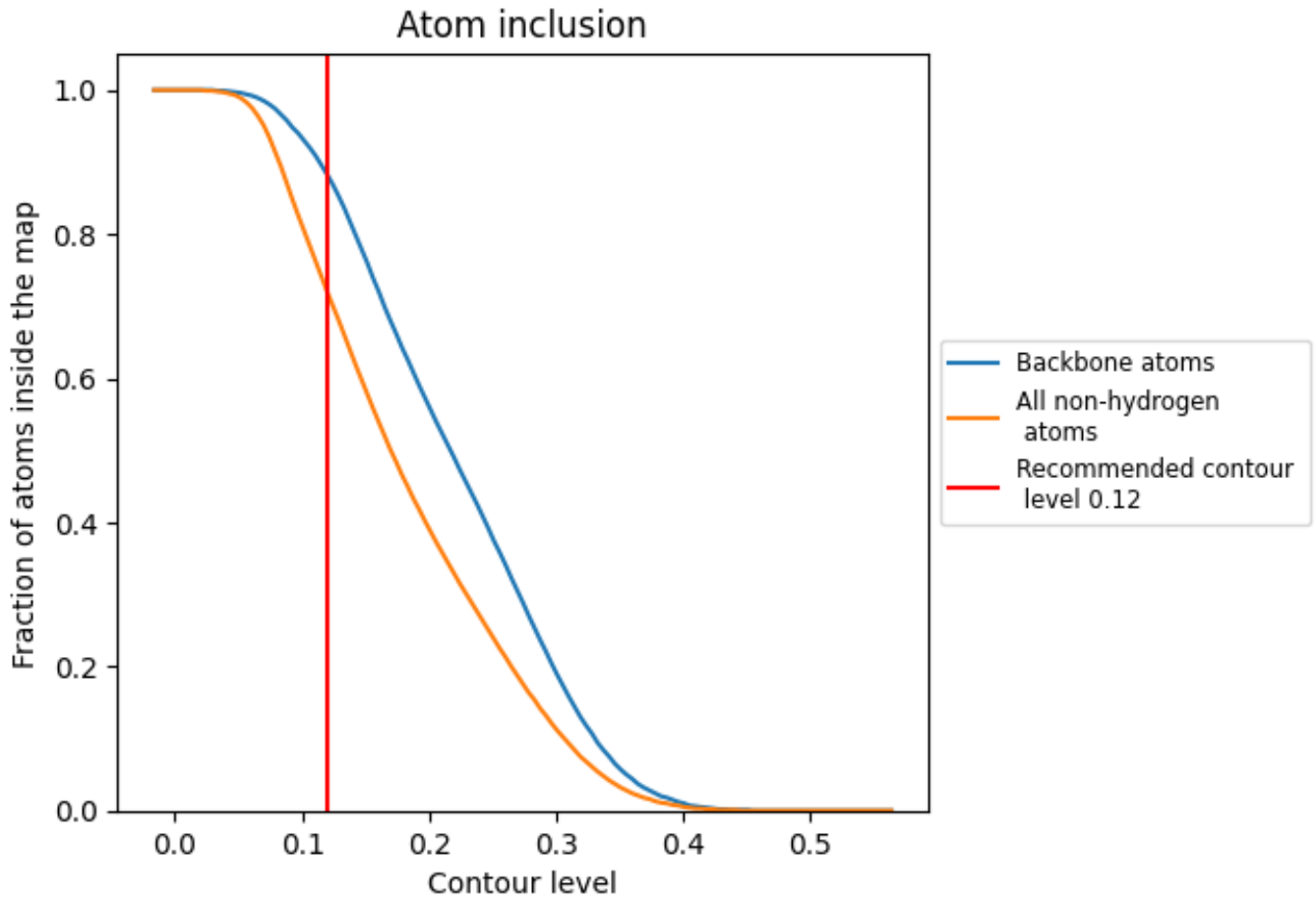
## 9.3 Atom inclusion mapped to coordinate model




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, 88% of all backbone atoms, 72% 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 | 0.7190 | 0.3660 |
| A | 0.7170 | 0.3650 |
| B | 0.7160 | 0.3640 |
| C | 0.7180 | 0.3660 |
| D | 0.7120 | 0.3560 |
| E | 0.8560 | 0.5050 |
| F | 0.8510 | 0.5030 |
| G | 0.8590 | 0.5060 |
| H | 0.8570 | 0.5040 |