wwPDB EM Validation Summary Report

Oct 13, 2024 – 09:35 PM EDT

PDB ID	:	7UA5
EMDB ID	:	EMD-26415
Title	:	Structure of dephosphorylated human RyR2 in the closed state
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	2.83 Å(reported)
Based on initial model	:	7U9Q

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

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

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

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

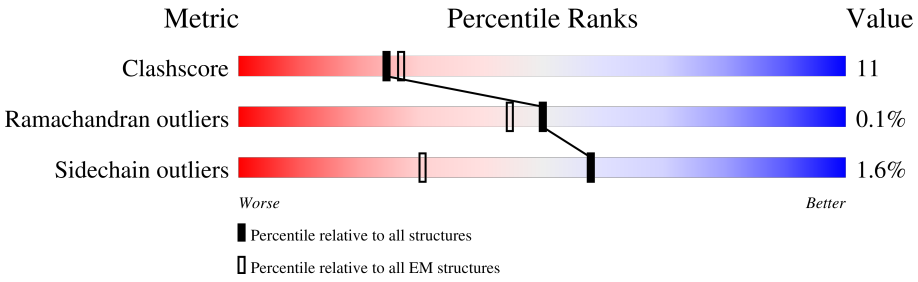
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.83 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% 64% 20% • 15%
1	B	4967	10% 64% 20% • 15%
1	C	4967	10% 64% 20% • 15%
1	D	4967	10% 64% 20% • 15%
2	E	108	• 84% 15% •
2	F	108	• 84% 15% •
2	G	108	• 85% 14% •
2	H	108	• 83% 16% •

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

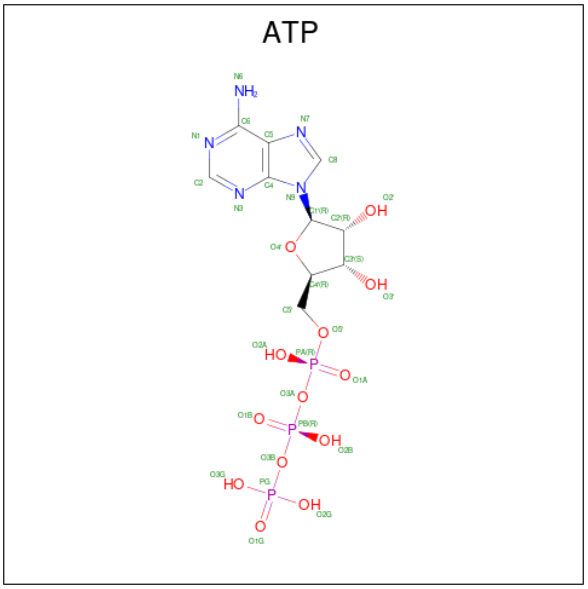
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 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).

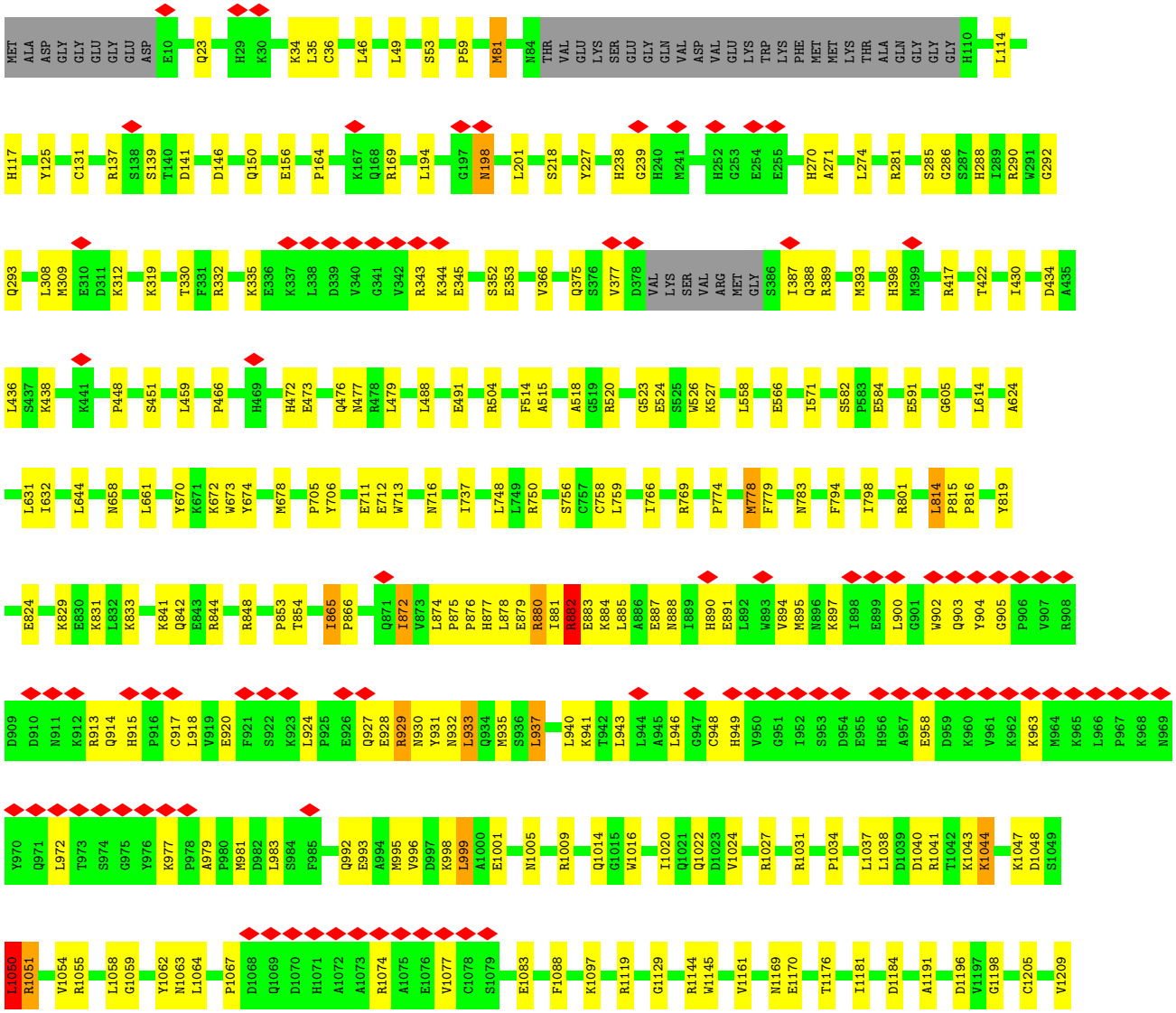


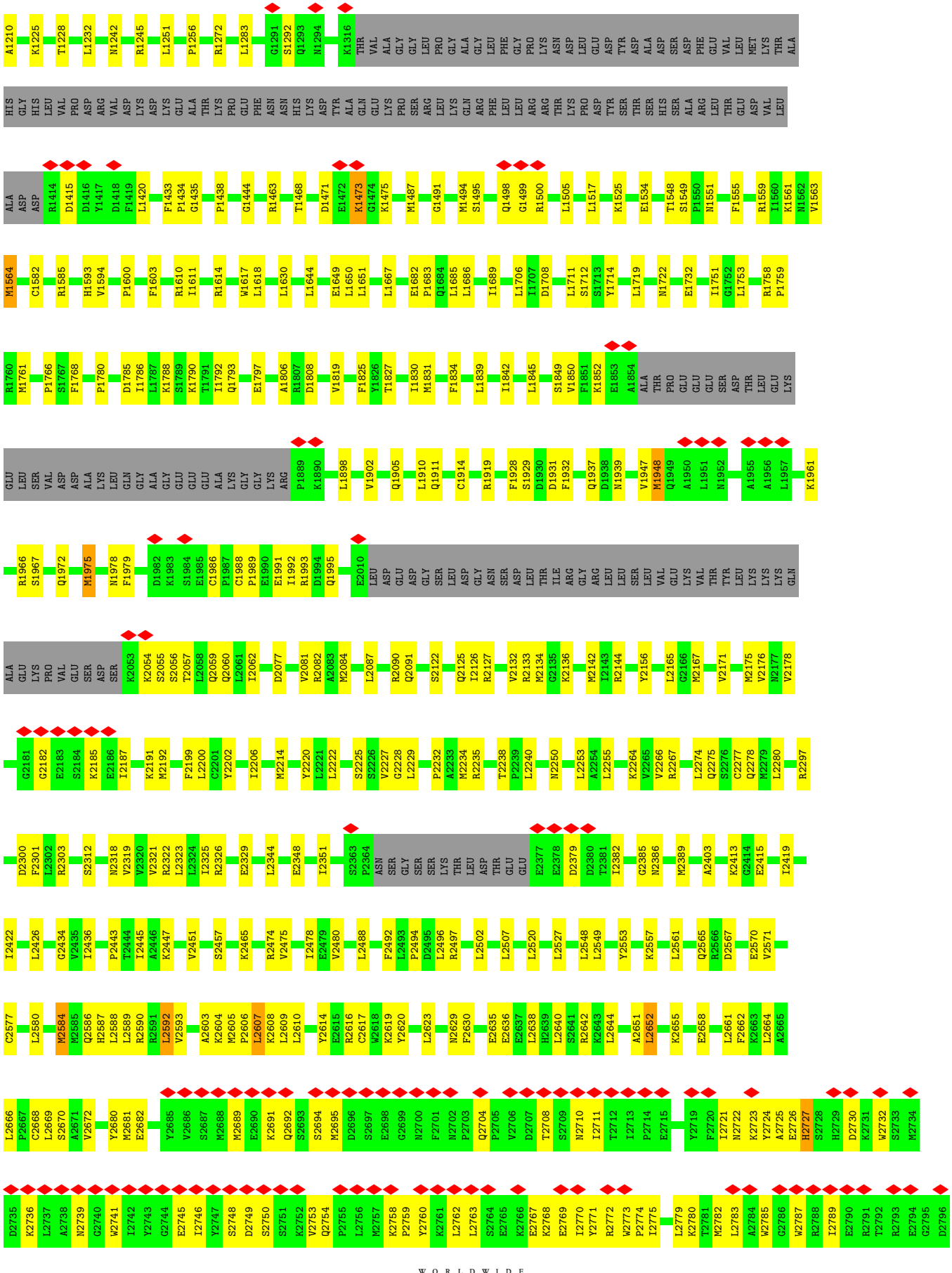
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

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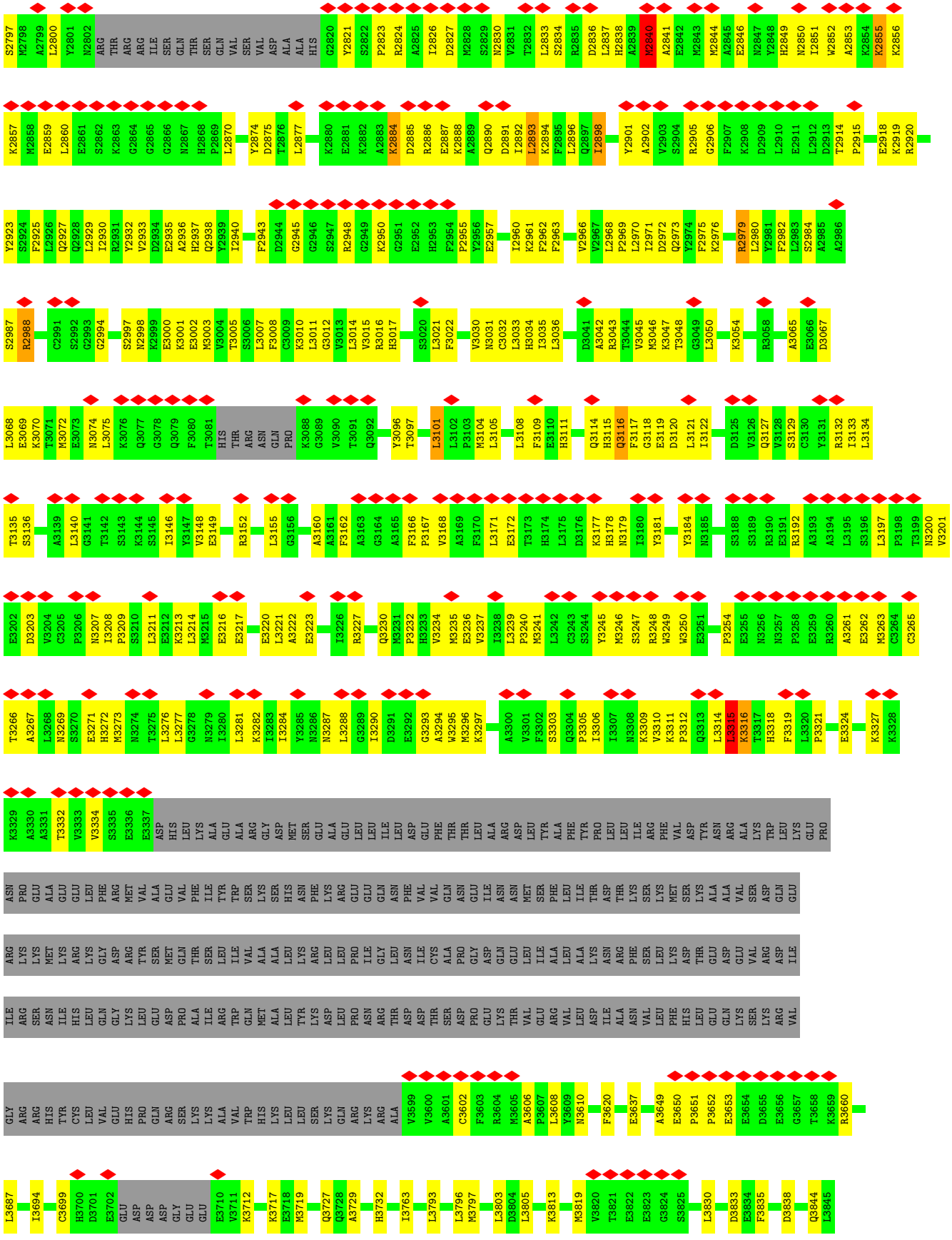
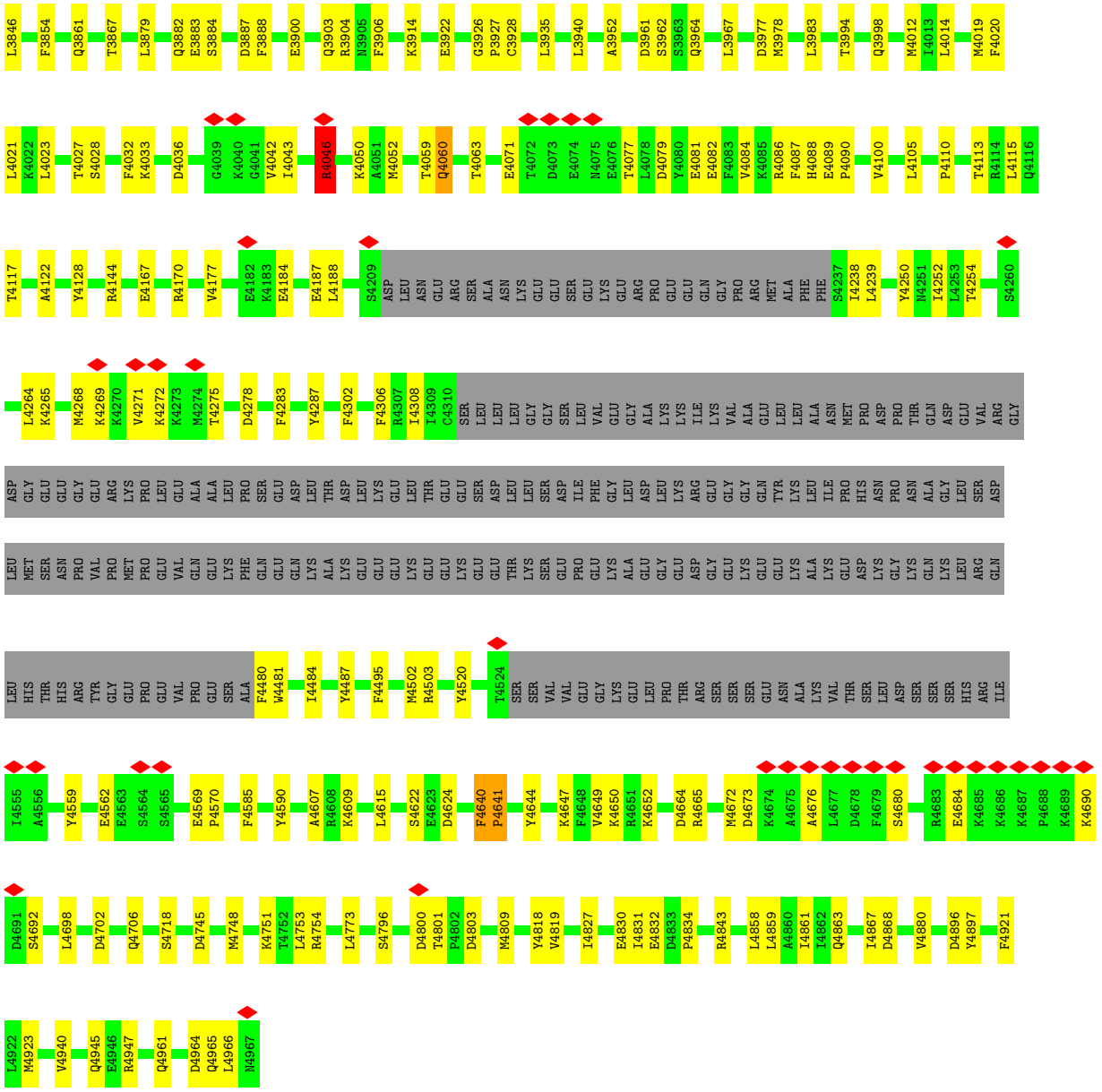
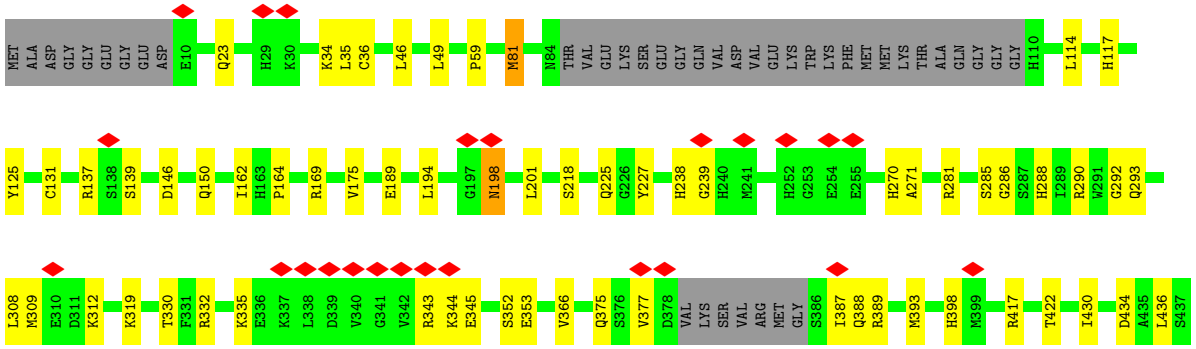
HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO LYS ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU
ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 L1420 F1433 P1434 G1435 P1438 G1444 R1463 T1468 D1471 E1472 K1473 G1474 K1475 M1487 G1491 M1494 S1495 Q1498 G1499 R1500 L1505 L1517 K1525 E1534 T1548 S1549 P1550 N1551 F1555 R1559 I1560 K1561 N1562 V1563
M1564 C1582 R1585 H1593 V1594 P1600 F1603 R1610 I1611 R1614 W1617 L1618 L1630 L1644 E1649 L1650 L1651 L1667 E1682 P1683 Q1684 L1685 L1686 I1689 L1706 I1707 D1708 L1711 S1712 S1713 Y1714 L1719 N1722 E1732 T1751 G1752 L1753 R1758 P1759
R1760 M1761 P1766 S1767 F1768 P1780 D1785 I1786 L1787 K1788 S1789 K1790 T1791 I1792 Q1793 E1797 A1806 R1807 D1808 V1819 F1825 Y1826 T1827 I1830 M1831 F1834 L1839 I1842 L1845 S1849 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 GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1898 V1902 Q1905 L1910 Q1911 C1914 R1919 F1928 S1929 D1930 D1931 F1932 Q1937 D1938 N1939 V1947 M1948 Q1949 A1950 L1951 N1952 A1955 A1956 L1957 K1961
R1966 S1967 Q1972 M1975 N1978 F1979 D1982 K1983 S1984 E1985 C1986 P1987 C1988 P1989 E1990 E1991 I1992 R1993 D1994 Q1995 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 Q2059 Q2060 L2061 I2062 D2077 V2081 R2082 A2083 M2084 L2087 R2090 Q2091 S2122 Q2125 I2126 R2127 V2132 R2133 M2134 G2135 K2136 M2142 I2143 R2144 Y2156 L2165 G2166 M2167 V2171 M2175 V2176 N2177 V2178
G2181 G2182 E2183 S2184 K2185 E2186 I2187 K2191 M2192 F2199 L2200 C2201 Y2202 I2206 M2214 Y2220 L2221 L2222 S2225 S2226 Y2227 G2228 L2229 P2232 A2233 M2234 R2235 T2238 P2239 L2240 N2250 L2253 A2254 L2255 K2264 Y2265 Y2266 R2267 L2274 Q2275 S2276 C2277 Q2278 M2279 L2280 R2297
D2300 F2301 L2302 R2303 S2312 N2318 V2319 V2320 V2321 R2322 L2323 L2324 I2325 R2326 E2329 L2344 E2348 I2351 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 G2385 N2386 M2389 A2403 K2413 G2414 E2415 I2419
I2422 L2426 G2434 V2435 I2436 P2443 T2444 I2445 A2446 K2447 V2451 S2457 K2465 R2474 V2475 I2478 E2479 V2480 L2488 F2492 L2493 P2494 D2495 L2496 R2497 L2502 L2507 L2520 L2527 L2548 L2549 Y2553 K2557 L2561 Q2565 R2566 D2567 E2570 V2571
C2577 L2580 M2584 M2585 Q2586 H2587 L2588 L2589 R2590 R2591 L2592 V2593 A2603 K2604 M2605 P2606 K2607 K2608 L2609 L2610 Y2614 E2615 R2616 C2617 W2618 K2619 Y2620 L2623 N2629 F2630 E2635 E2636 E2637 L2638 H2639 L2640 S2641 R2642 K2643 L2644 A2651 L2652 K2655 E2658 L2661 F2662 K2663 L2664 A2665
L2666 P2667 C2668 L2669 S2670 A2671 V2672 Y2680 M2681 E2682 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 Y2719 F2720 I2721 N2722 K2723 Y2724 A2725 E2726 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 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796

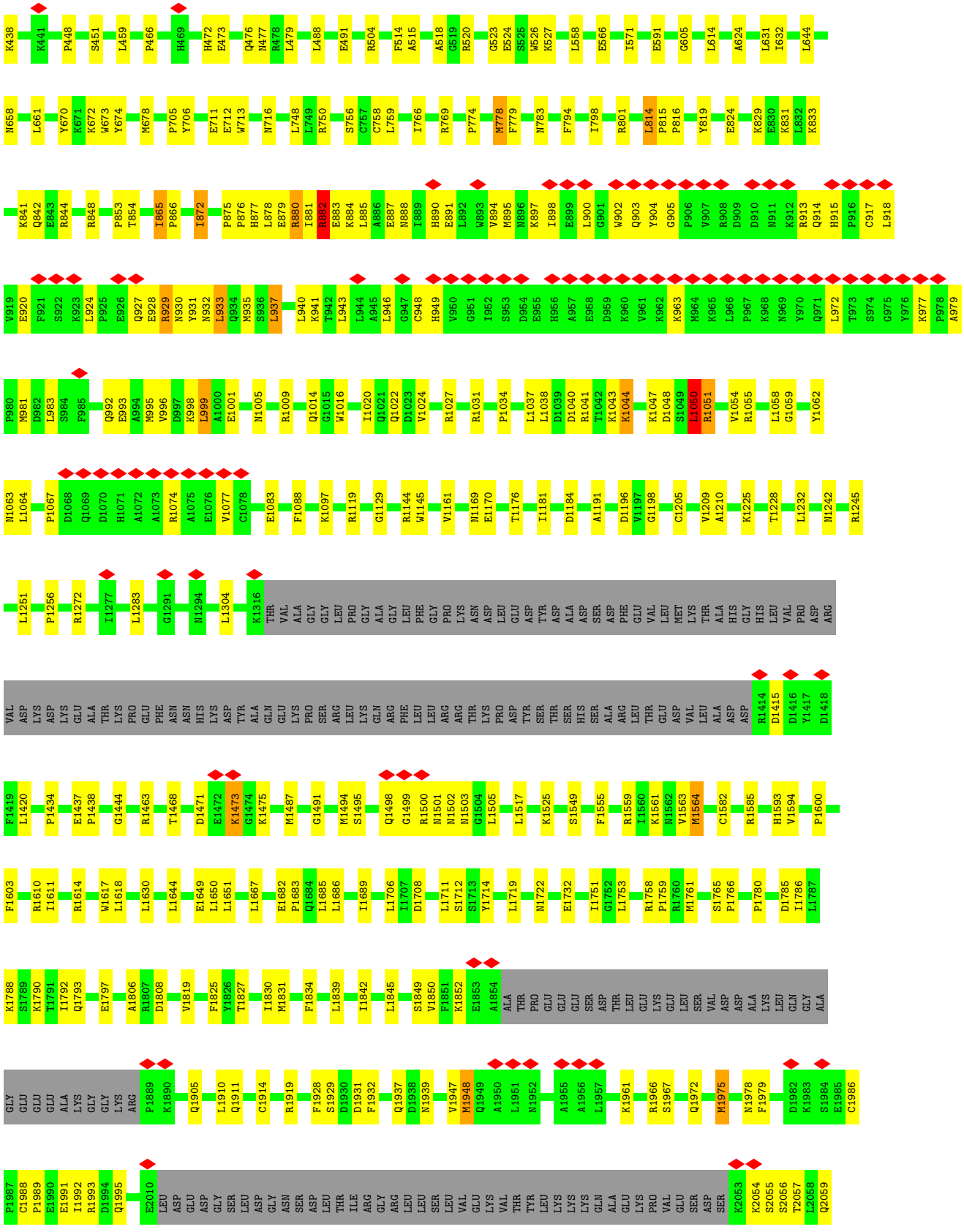




• Molecule 1: Ryanodine receptor 2

Chain B:

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N658 L661 Y670 K671 K672 W673 Y674 M678 P705 Y706 E711 E712 W713 N716 L748 L749 R750 S756 C757 C758 L759 I766 R769 P774 M778 F779 N783 F794 I798 R801 L814 P815 P816 Y819 E824 K829 E830 K831 L832 K833
K841 Q842 E843 R844 R848 P853 T854 I865 P866 I872 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918
V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979
P980 M981 D982 L983 S984 F985 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1005 R1009 Q1014 G1015 W1016 I1020 Q1021 Q1022 D1023 V1024 R1027 R1031 P1034 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 K1047 D1048 S1049 L1050 R1051 V1054 R1055 L1058 G1059 Y1062
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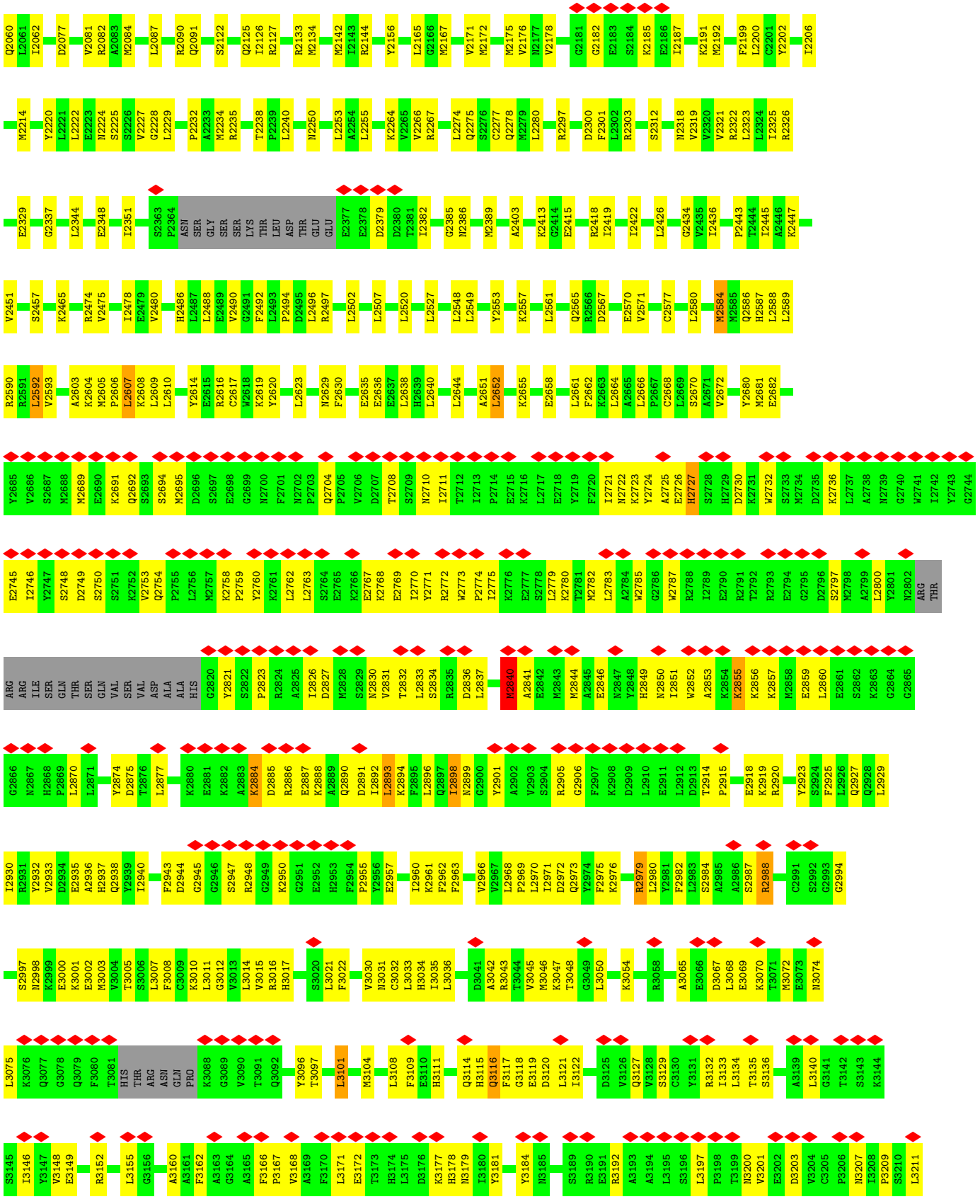
L1251 P1256 R1272 I1277 L1283 G1291 N1294 L1304 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG
VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU GLU LYS PRO SER ARG LEU LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418
F1419 L1420 P1434 E1437 P1438 G1444 R1463 T1468 D1471 E1472 K1473 G1474 K1475 M1487 G1491 M1494 S1495 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 L1517 K1525 S1549 F1555 R1559 T1560 K1561 N1562 V1563 M1564 C1582 R1585 H1593 V1594 P1600
F1603 R1610 I1611 R1614 W1617 L1618 L1630 L1644 E1649 L1650 L1651 L1667 E1682 P1683 Q1684 L1685 L1686 I1689 L1706 I1707 D1708 L1711 S1712 S1713 Y1714 L1719 N1722 E1732 I1751 G1752 L1753 R1758 P1759 R1760 M1761 S1765 P1766 P1780 D1785 I1786 L1787
K1788 S1789 K1790 T1791 I1792 Q1793 E1797 A1806 R1807 D1808 V1819 F1825 Y1826 T1827 I1830 M1831 F1834 L1839 I1842 L1845 S1849 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 ALA LYS GLY GLY LYS ARG P1889 K1890 Q1905 L1910 Q1911 C1914 R1919 F1928 S1929 D1930 D1931 F1932 Q1937 D1938 N1939 V1947 M1948 Q1949 A1950 L1951 N1952 A1955 A1956 L1957 K1961 R1966 S1967 Q1972 M1975 N1978 F1979 D1982 K1983 S1984 E1985 C1986
P1987 C1988 P1989 E1990 E1991 I1992 R1993 D1994 Q1995 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 Q2059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E2329 G2337 L2344 E2348 I2351 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 G2385 N2386 M2389 A2403 K2413 G2414 E2415 R2418 I2419 I2422 L2426 G2434 V2435 I2436 P2443 T2444 I2445 A2446 K2447
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R2590 R2591 L2592 V2593 A2603 K2604 M2605 P2606 L2607 K2608 L2609 L2610 Y2614 E2615 R2616 C2617 W2618 K2619 Y2620 L2623 N2629 F2630 E2635 E2636 E2637 L2638 H2639 L2640 L2644 A2651 L2652 K2655 E2658 L2661 F2662 K2663 L2664 A2665 L2666 P2667 C2668 L2669 S2670 A2671 V2672 Y2680 M2681 E2682
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 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744
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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 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 Y2874 D2875 T2876 L2877 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 E2918 K2919 R2920 Y2923 S2924 F2925 L2926 Q2927 Q2928 L2929
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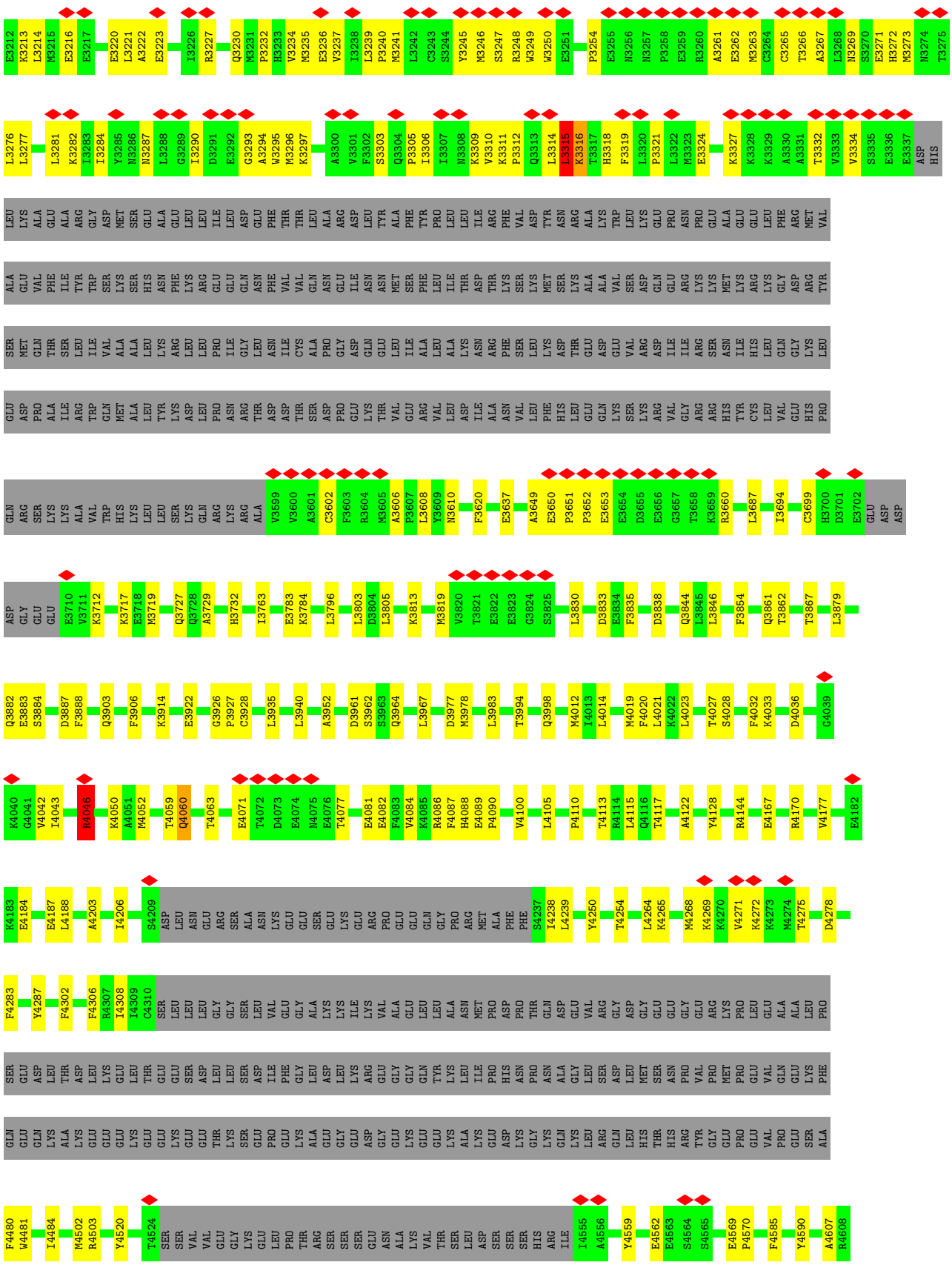
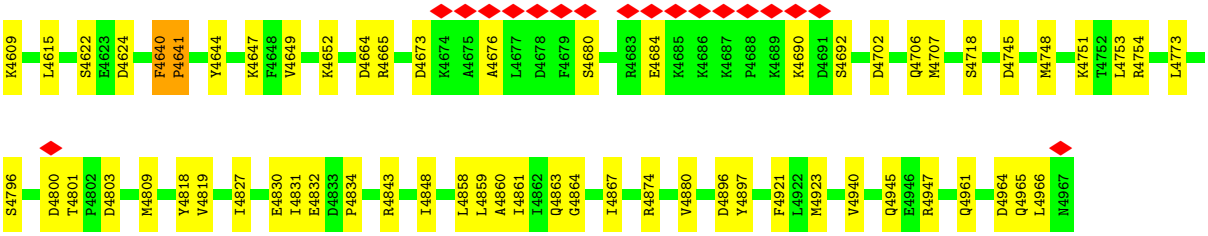
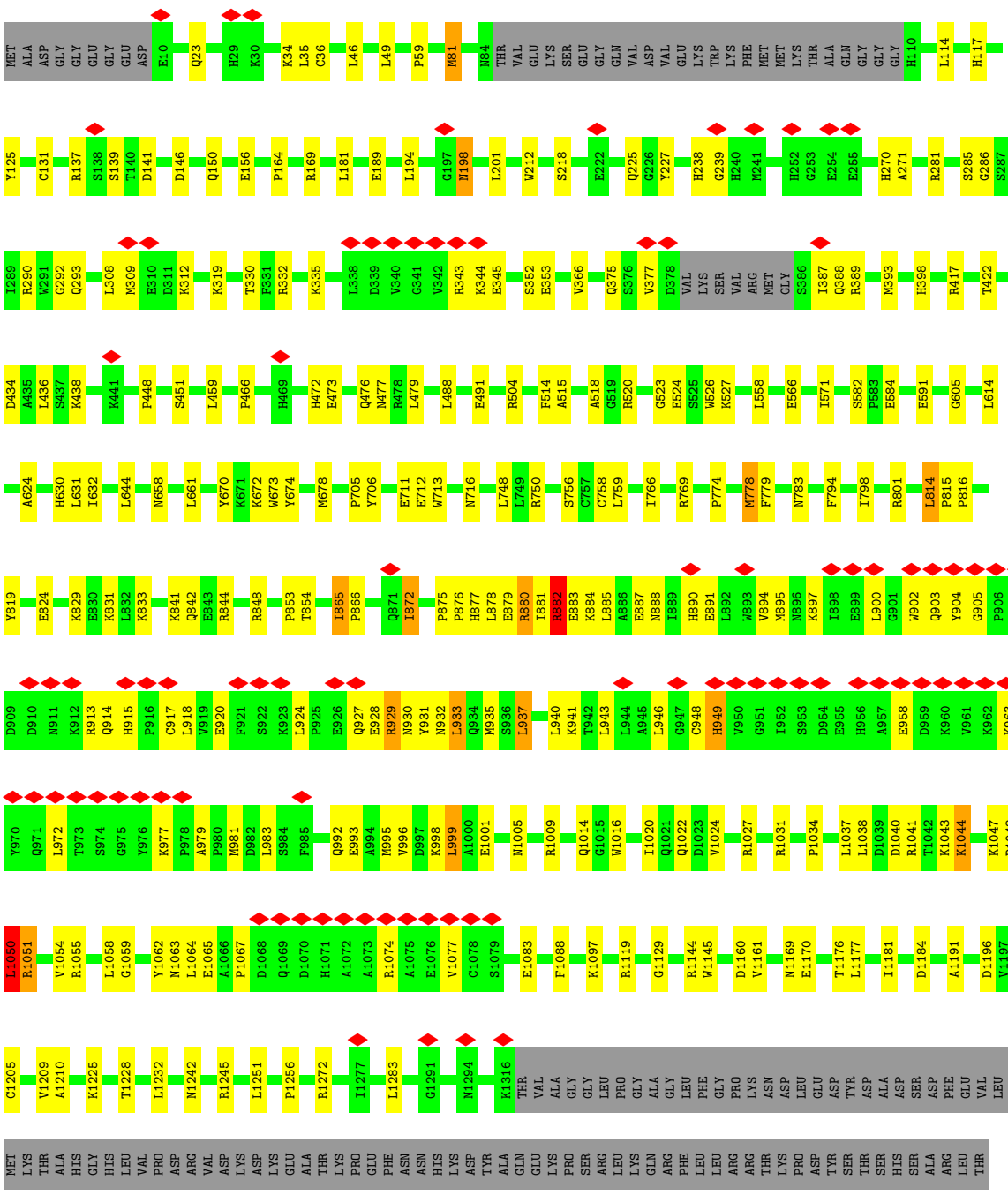
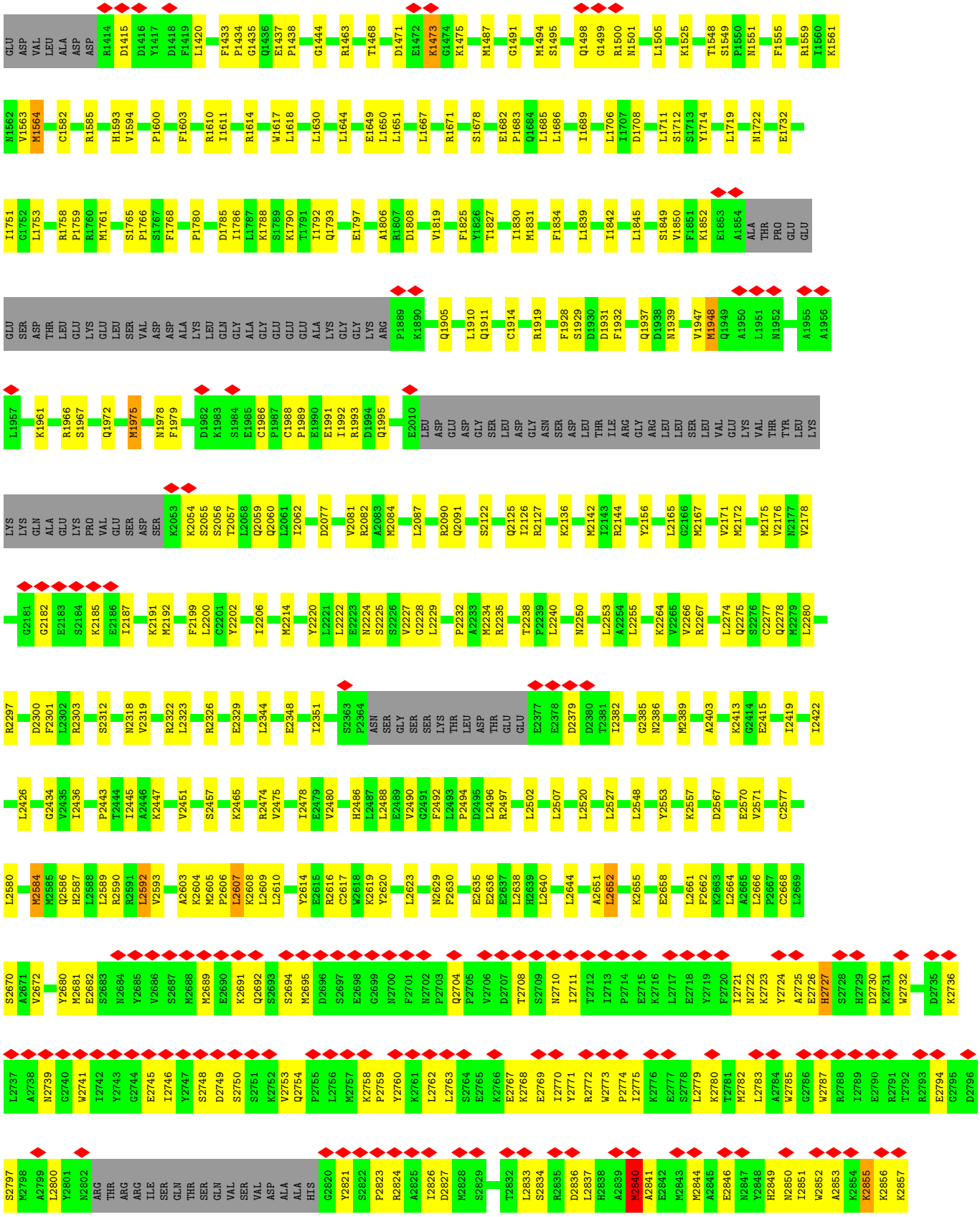




• Molecule 1: Ryanodine receptor 2

Chain C:

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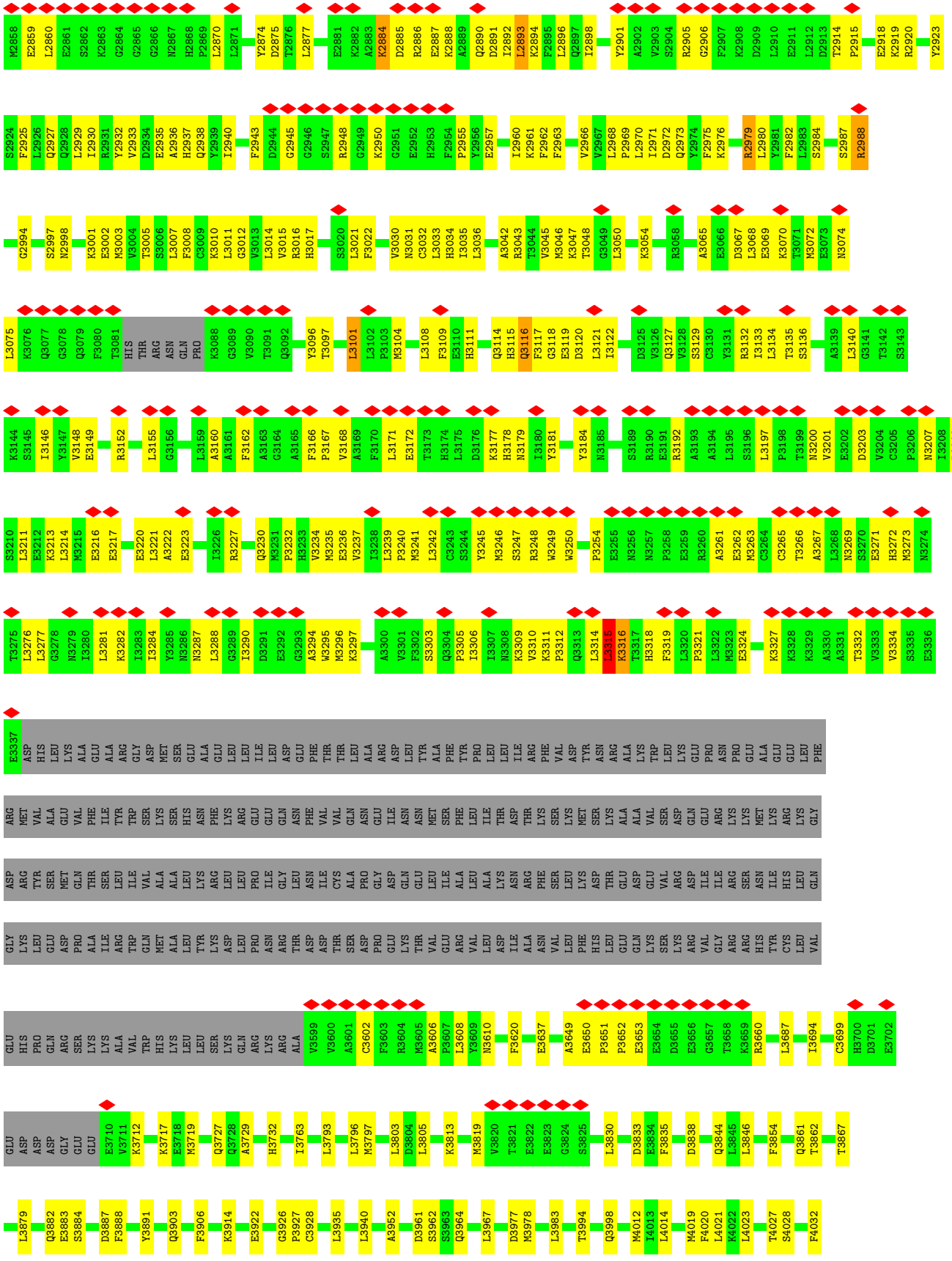
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ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN GLN ASN ASP PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY
ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLU GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE 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 ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER 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 ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609 N3610 F3620 E3637 A3649 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3687 I3694 C3699 H3700 D3701 E3702
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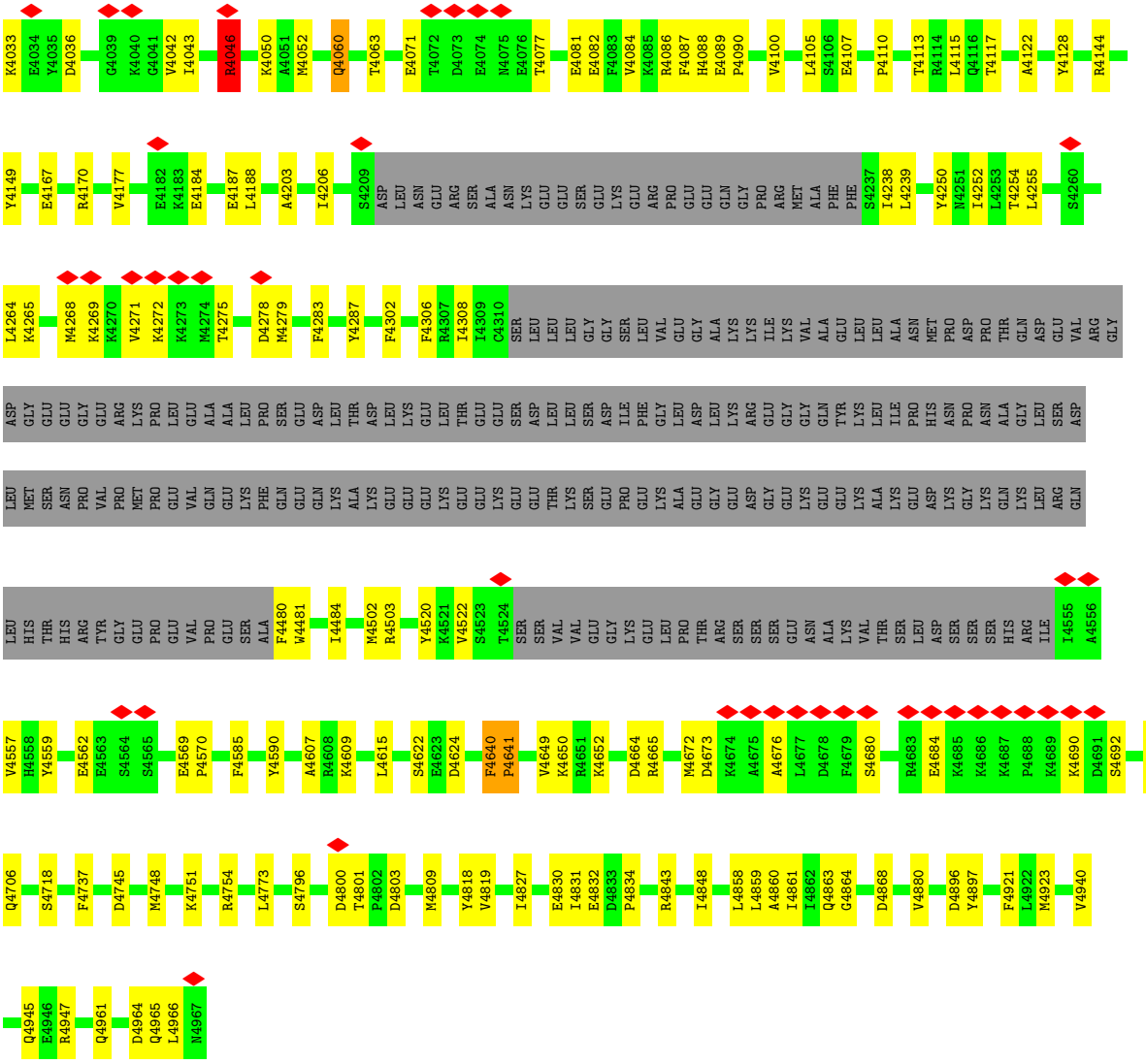
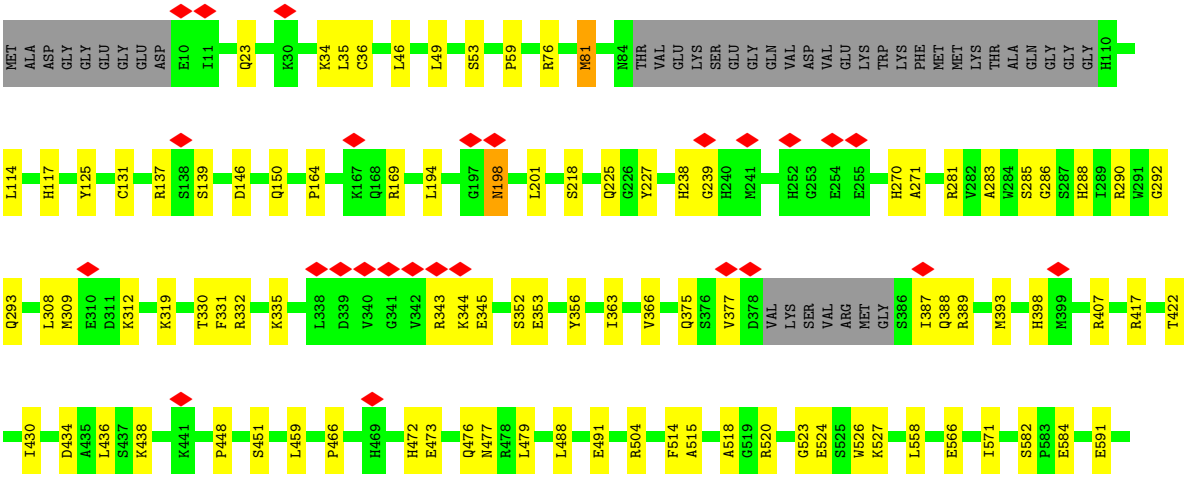
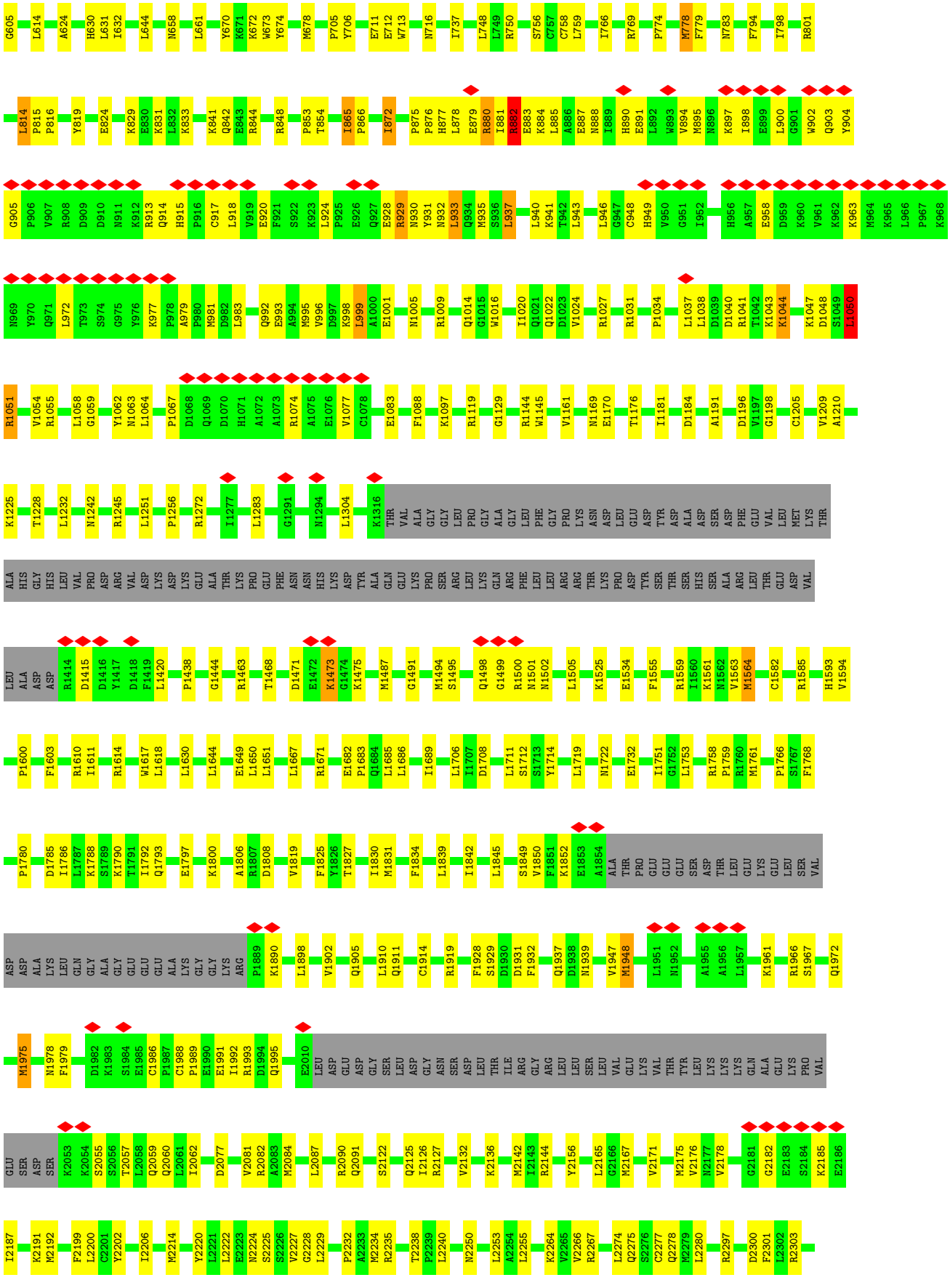


• Molecule 1: Ryanodine receptor 2

Chain D:

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K1225 T1228 L1232 N1242 R1245 L1251 P1256 R1272 I1277 L1283 G1291 N1294 L1304 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 F1419 L1420 P1438 G1444 R1463 T1468 D1471 E1472 K1473 G1474 K1475 M1487 G1491 M1494 S1495 Q1498 G1499 R1500 N1501 N1502 L1505 K1525 E1534 F1555 R1559 I1560 K1561 N1562 V1563 M1564 C1582 R1585 H1593 V1594
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P1780 D1785 I1786 L1787 K1788 S1789 K1790 T1791 I1792 Q1793 E1797 K1800 A1806 R1807 D1808 V1819 F1825 Y1826 T1827 I1830 M1831 F1834 L1839 I1842 L1845 S1849 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 ALA LYS GLY GLY LYS ARG P1889 K1890 L1898 V1902 Q1905 L1910 Q1911 C1914 R1919 F1928 S1929 D1930 D1931 F1932 Q1937 D1938 N1939 V1947 M1948 L1951 N1952 A1955 A1956 L1957 K1961 R1966 S1967 Q1972
M1975 N1978 F1979 D1982 K1983 S1984 E1985 C1986 P1987 C1988 P1989 E1990 E1991 I1992 R1993 D1994 Q1995 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
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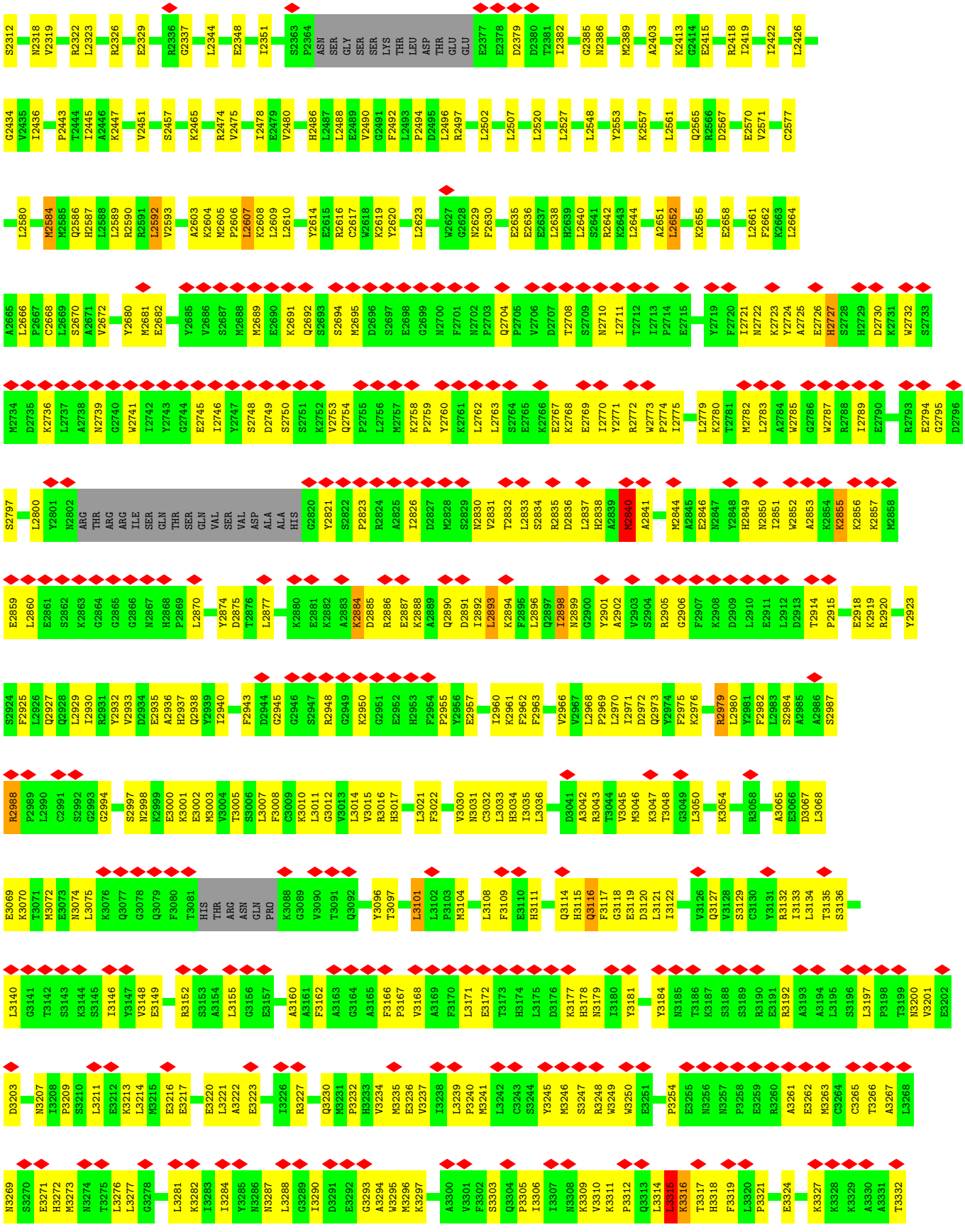

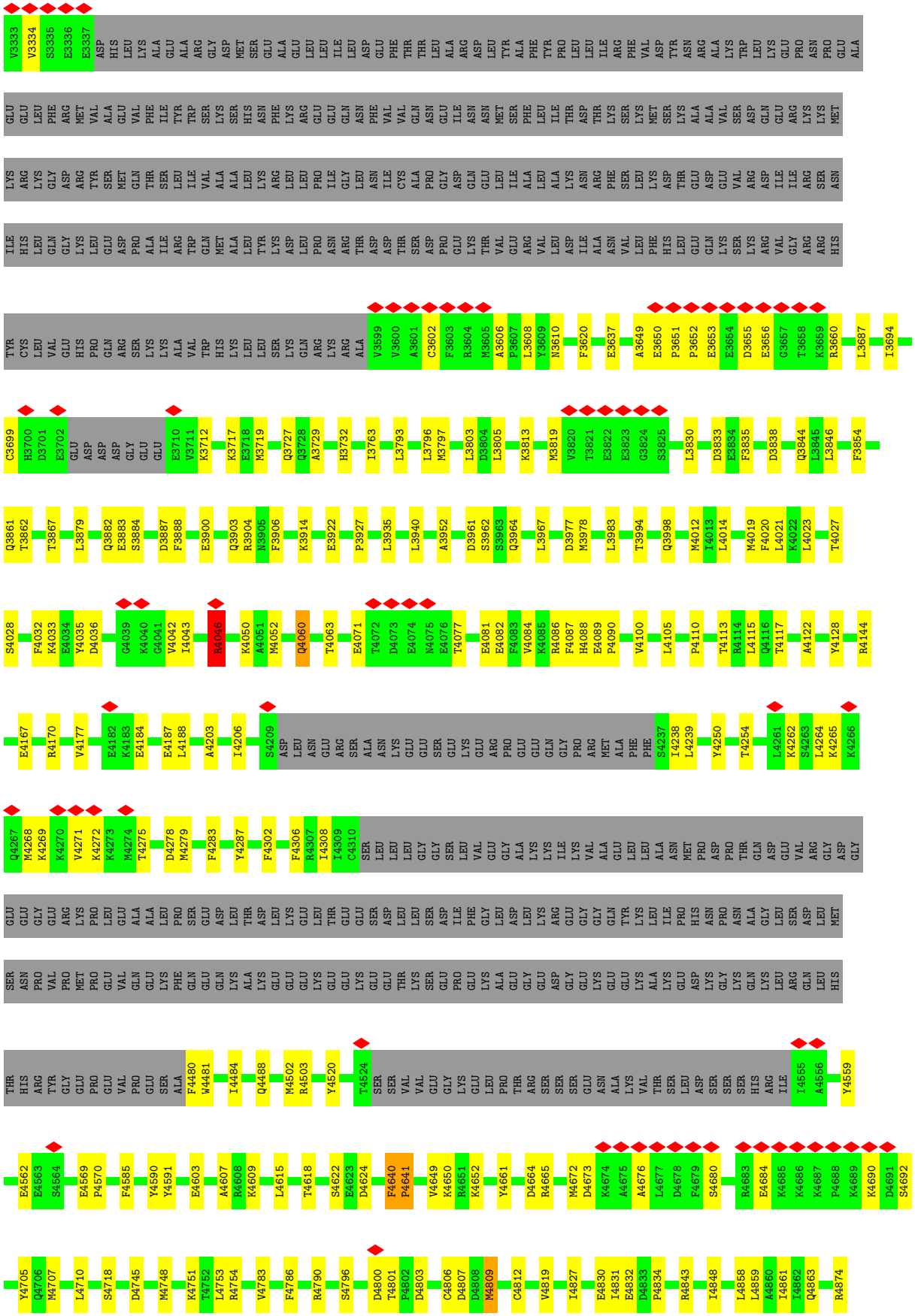
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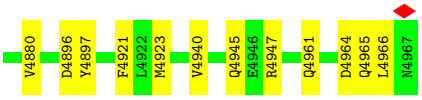
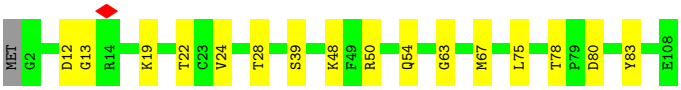
GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU GLU ARG LYS LYS MET
LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL 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 GLU ASP GLY 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 ALA LEU TYR LYS ASP LEU PRO PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ALA LEU ASP ILE ALA ASN VAL 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 ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609 N3610 F3620 E3637 A3649 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3687 I3694
C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 K3712 K3717 E3718 M3719 Q3727 Q3728 A3729 H3732 I3763 L3793 L3796 M3797 L3803 D3804 L3805 K3813 M3819 V3820 T3821 E3822 E3823 G3824 S3825 L3830 D3833 E3834 F3835 D3838 Q3844 L3845 L3846 F3854
Q3861 T3862 T3867 L3879 Q3882 E3883 S3884 D3887 F3888 E3900 Q3903 R3904 N3905 F3906 K3914 E3922 P3927 L3935 L3940 A3952 D3961 S3962 S3963 Q3964 L3967 D3977 M3978 L3983 T3994 Q3998 M4012 I4013 L4014 M4019 F4020 L4021 K4022 L4023 T4027
S4028 F4032 K4033 E4034 Y4035 D4036 G4039 K4040 G4041 V4042 I4043 R4046 K4050 A4051 M4052 Q4060 T4063 E4071 T4072 D4073 E4074 N4075 E4076 T4077 E4081 E4082 F4083 V4084 K4085 R4086 F4087 H4088 E4089 P4090 V4100 L4105 P4110 T4113 R4114 L4115 Q4116 T4117 A4122 Y4128 R4144
E4167 R4170 V4177 E4182 K4183 E4184 E4187 L4188 A4203 I4206 S4209 ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLY PRO ARG MET ALA PHE PHE S4237 I4238 L4239 Y4250 T4254 L4261 K4262 S4263 L4264 K4265 K4266
Q4267 M4268 K4269 K4270 V4271 K4272 K4273 M4274 T4275 D4278 M4279 F4283 Y4287 F4302 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY 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 LEU LYS GLU LEU THR ASP LEU LYS GLU GLU SER ASP LEU 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 GLU GLU LYS GLU GLU LYS GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU GLU ASP GLY GLU LYS GLU VAL GLU GLY LYS LEU GLN LYS LEU ARG LEU HIS
THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA F4480 W4481 I4484 Q4488 M4502 R4503 Y4520 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 SER HIS ARG ILE I4555 A4556 Y4559
E4562 E4563 S4564 E4569 P4570 F4585 Y4590 Y4591 E4603 A4607 R4608 K4609 L4615 T4618 S4622 E4623 D4624 F4640 P4641 V4649 K4650 R4651 K4652 Y4661 D4664 R4665 M4672 D4673 K4674 A4675 A4676 L4677 D4678 F4679 S4680 R4683 E4684 K4685 K4686 K4687 P4688 K4689 K4690 D4691 S4692
V4705 Q4706 M4707 L4710 S4718 D4745 M4748 K4751 T4752 L4753 R4754 V4783 F4786 R4790 S4796 D4800 T4801 P4802 D4803 C4806 D4807 D4808 M4809 C4812 V4819 I4827 E4830 I4831 E4832 D4833 P4834 R4843 I4848 L4858 L4859 A4860 I4861 I4862 Q4863 R4874



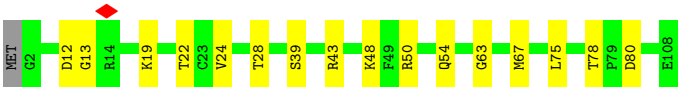
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



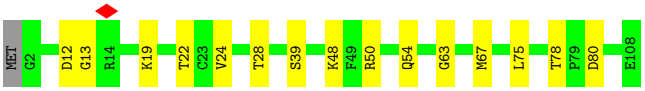
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



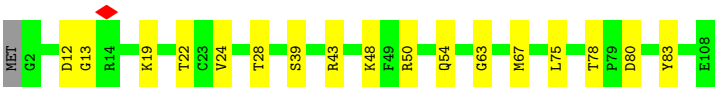
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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	90375	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	0.667	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.26	0/34511	0.52	11/46614 (0.0%)
1	B	0.26	0/34511	0.52	11/46614 (0.0%)
1	C	0.26	0/34511	0.52	11/46614 (0.0%)
1	D	0.26	0/34511	0.52	11/46614 (0.0%)
2	E	0.29	0/834	0.55	0/1123
2	F	0.28	0/834	0.55	0/1123
2	G	0.28	0/834	0.55	0/1123
2	H	0.28	0/834	0.55	0/1123
All	All	0.26	0/141380	0.52	44/190948 (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 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3315	LEU	CA-CB-CG	11.88	142.62	115.30
1	B	3315	LEU	CA-CB-CG	11.88	142.61	115.30
1	A	3315	LEU	CA-CB-CG	11.87	142.60	115.30
1	D	3315	LEU	CA-CB-CG	11.86	142.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	937	LEU	CA-CB-CG	8.36	134.52	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	ARG	Sidechain
1	A	4640	PHE	Peptide
1	A	882	ARG	Sidechain
1	B	1051	ARG	Sidechain
1	B	882	ARG	Sidechain

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	738	0
1	B	33771	0	33455	732	0
1	C	33771	0	33455	732	0
1	D	33771	0	33455	744	0
2	E	818	0	821	10	0
2	F	818	0	821	11	0
2	G	818	0	821	10	0
2	H	818	0	821	11	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
All	All	138608	0	137200	2898	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 11.

The worst 5 of 2898 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:1498:GLN:NE2	1:D:2899:ASN:O	1.91	1.04
1:A:4060:GLN:HE21	1:A:4060:GLN:HA	1.21	1.04
1:A:882:ARG:NH2	1:A:933:LEU:O	1.92	1.03
1:B:4060:GLN:HA	1:B:4060:GLN:HE21	1.21	1.02
1:C:4060:GLN:HA	1:C:4060:GLN:HE21	1.21	1.01

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%)	4067 (97%)	127 (3%)	4 (0%)	48	69
1	B	4198/4967 (84%)	4065 (97%)	129 (3%)	4 (0%)	48	69
1	C	4198/4967 (84%)	4064 (97%)	130 (3%)	4 (0%)	48	69
1	D	4198/4967 (84%)	4063 (97%)	131 (3%)	4 (0%)	48	69
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%)	16667 (97%)	529 (3%)	16 (0%)	50	69

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

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Mol	Chain	Res	Type
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	3708/4358 (85%)	3649 (98%)	59 (2%)	58	79
1	B	3708/4358 (85%)	3649 (98%)	59 (2%)	58	79
1	C	3708/4358 (85%)	3649 (98%)	59 (2%)	58	79
1	D	3708/4358 (85%)	3647 (98%)	61 (2%)	58	79
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%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	15184/17788 (85%)	14946 (98%)	238 (2%)	58	79

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4269	LYS
1	D	3101	LEU
1	C	2303	ARG
1	D	3007	LEU
1	D	4809	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2850	ASN
1	C	3127	GLN
1	D	3178	HIS
1	C	3114	GLN

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Mol	Chain	Res	Type
1	C	3178	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 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	D	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	A	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	D	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
4	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
4	ATP	C	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	B	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	B	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
4	ATP	C	5002	-	28,33,33	0.62	0	34,52,52	0.60	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	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	4/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	4/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	4/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	4/18/38/38	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	5003	ATP	C5-C6-N6	2.33	123.86	120.31
4	B	5003	ATP	C5-C6-N6	2.33	123.85	120.31
4	D	5002	ATP	C5-C6-N6	2.33	123.85	120.31
4	D	5003	ATP	C5-C6-N6	2.32	123.85	120.31
4	B	5002	ATP	C5-C6-N6	2.30	123.82	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-O3A-PA-O5'
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	PB-O3A-PA-O5'

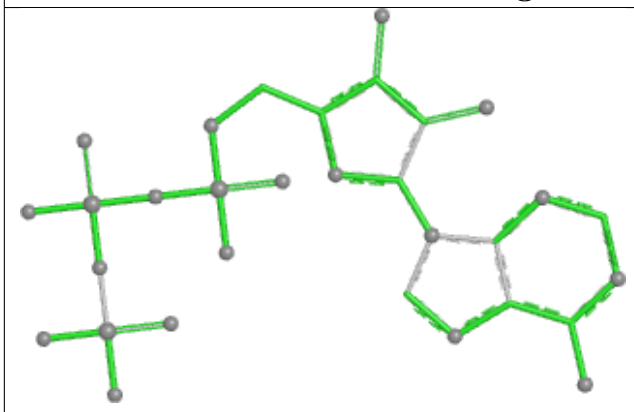
There are no ring outliers.

No monomer is involved in short contacts.

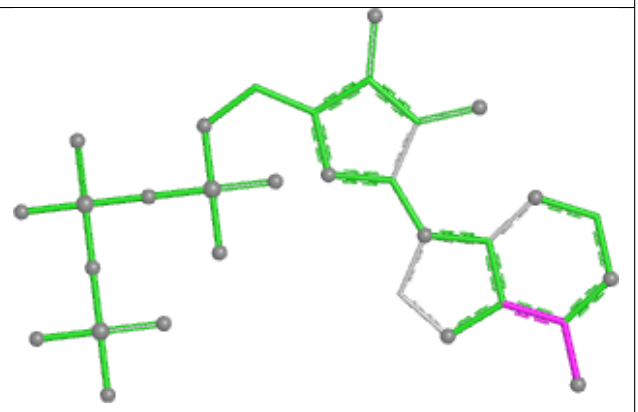
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

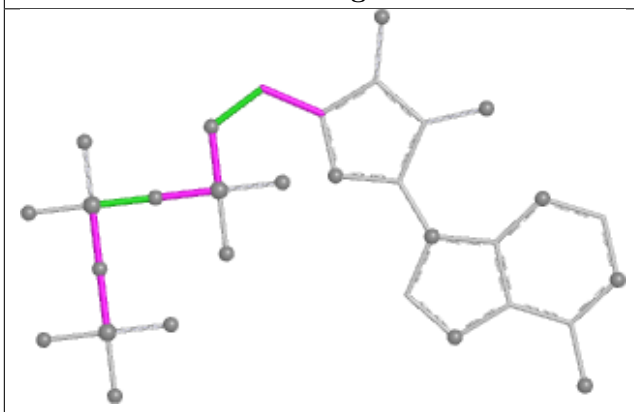
Ligand ATP D 5003



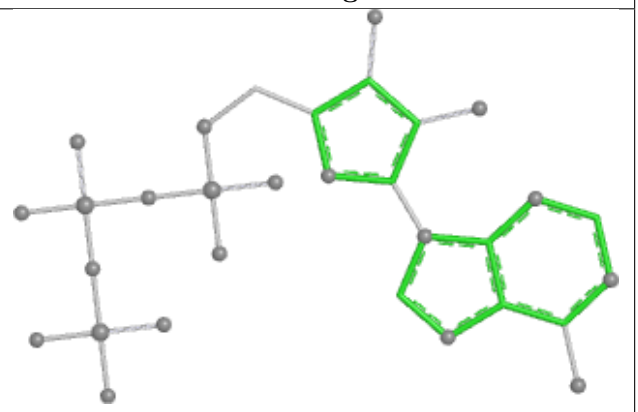
Bond lengths



Bond angles

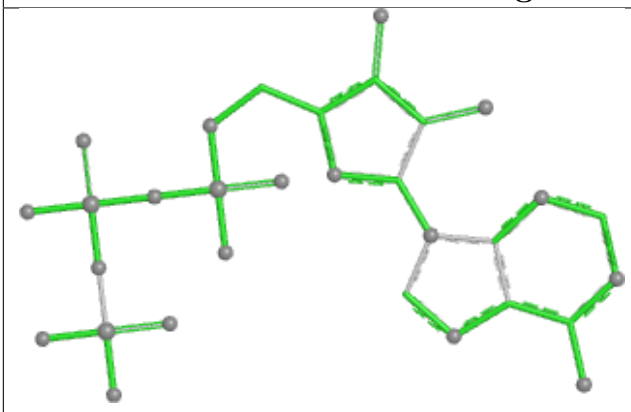


Torsions

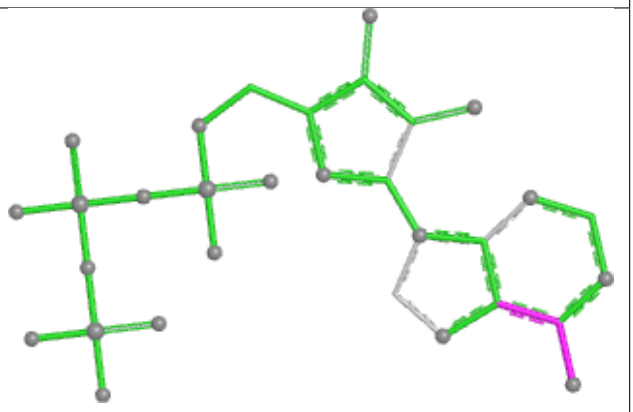


Rings

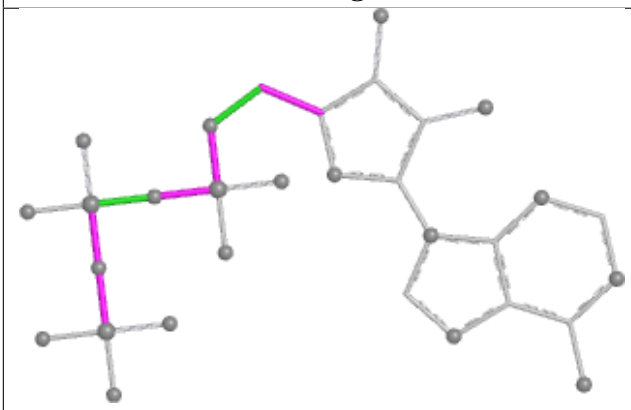
Ligand ATP A 5003



Bond lengths



Bond angles



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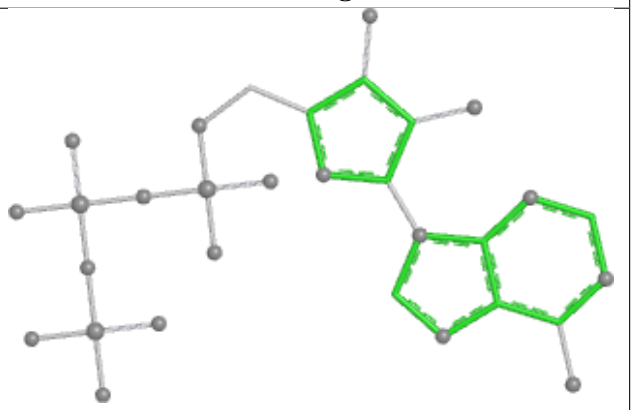
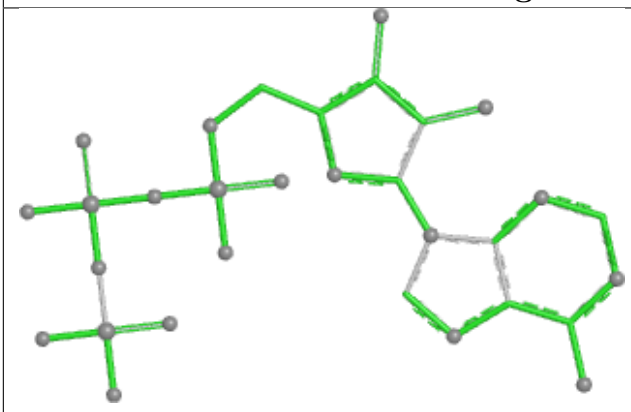


Rings

Ligand ATP D 5002



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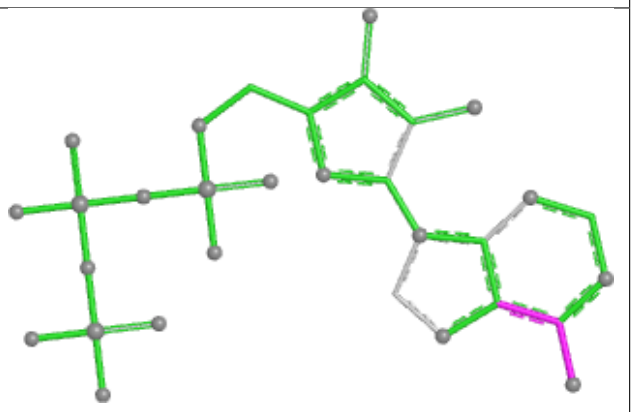
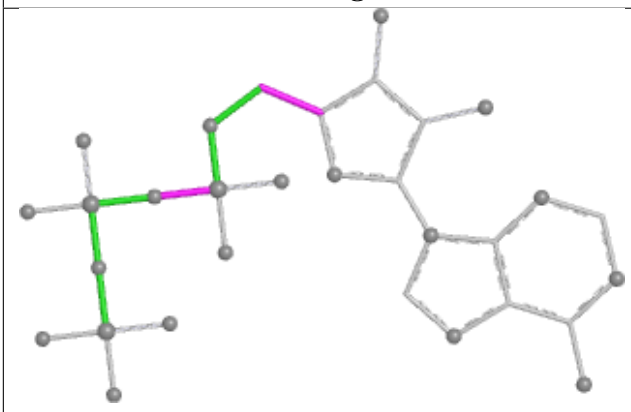
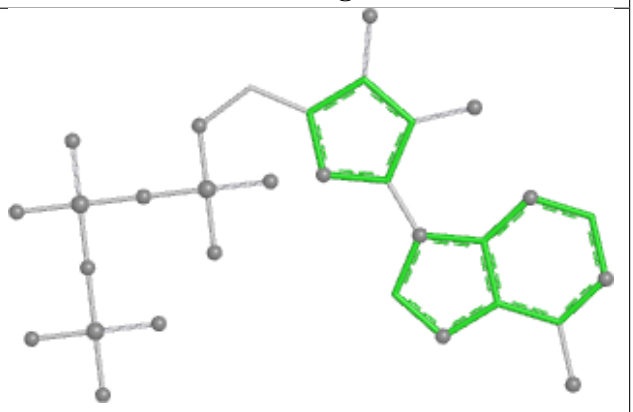


Bond angles

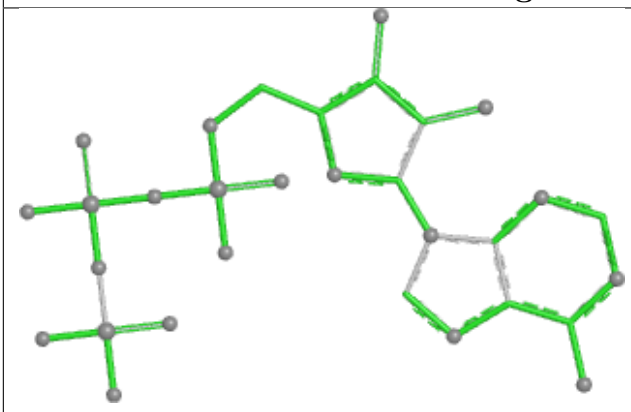


Torsions

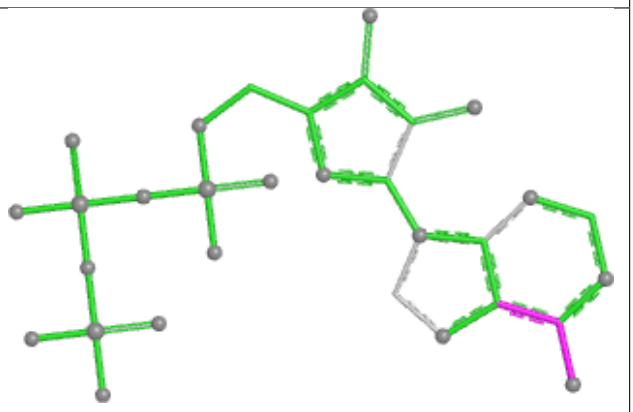


Rings

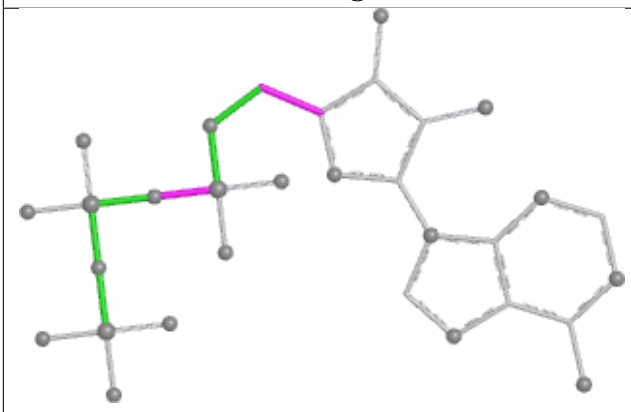
Ligand ATP A 5002



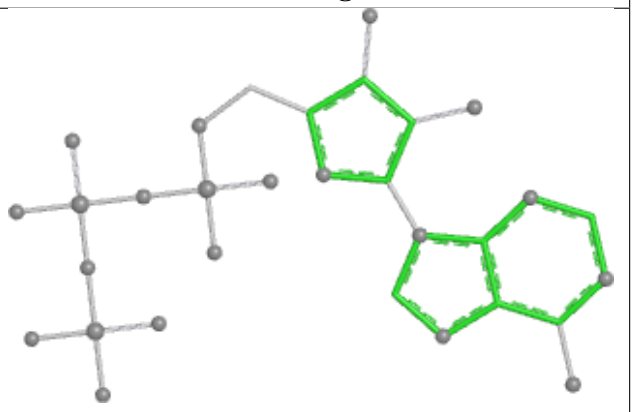
Bond lengths



Bond angles

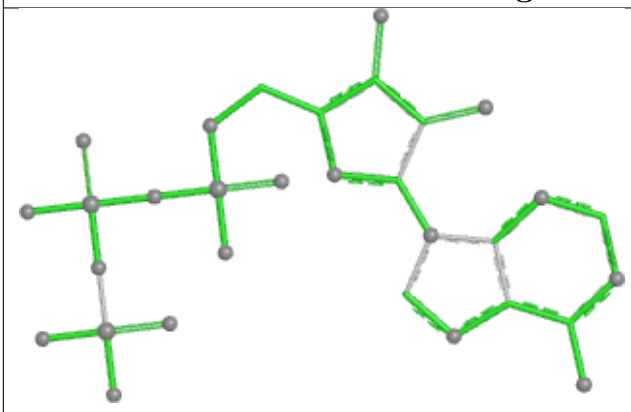


Torsions

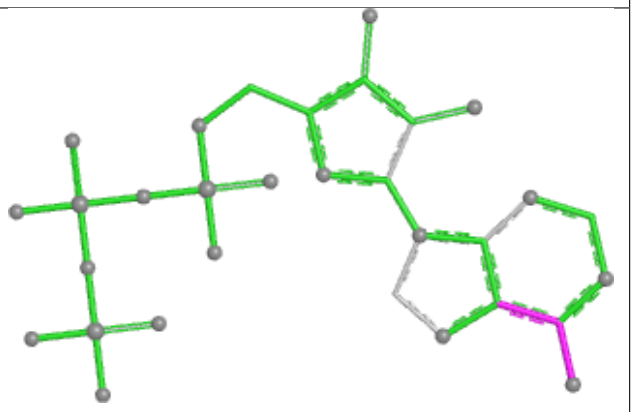


Rings

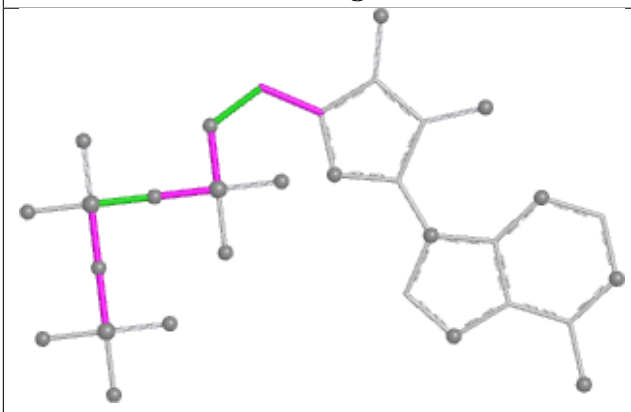
Ligand ATP C 5003



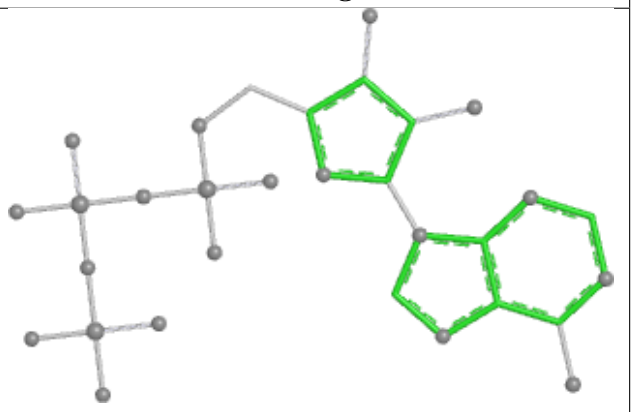
Bond lengths



Bond angles

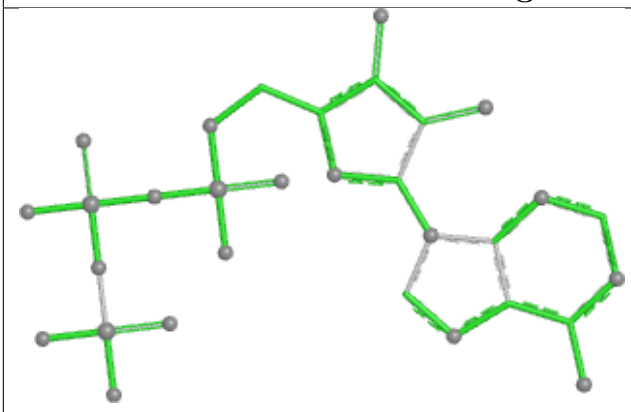


Torsions

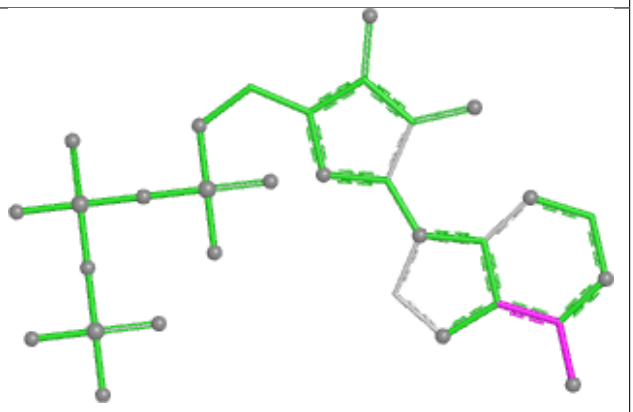


Rings

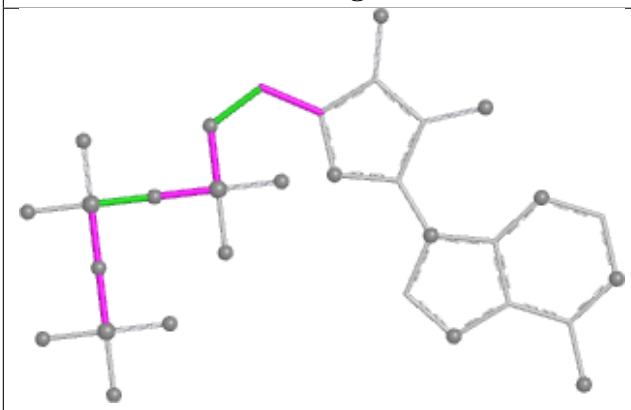
Ligand ATP B 5003



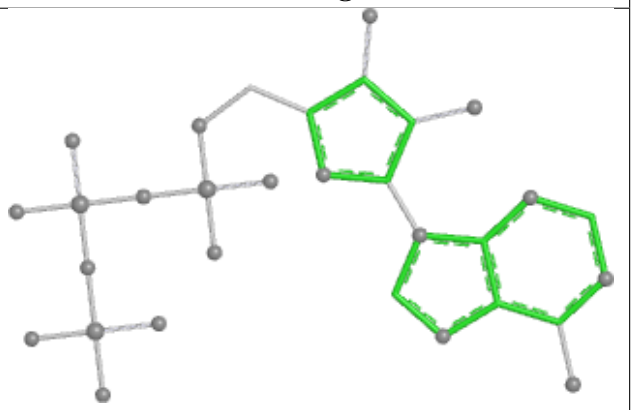
Bond lengths



Bond angles

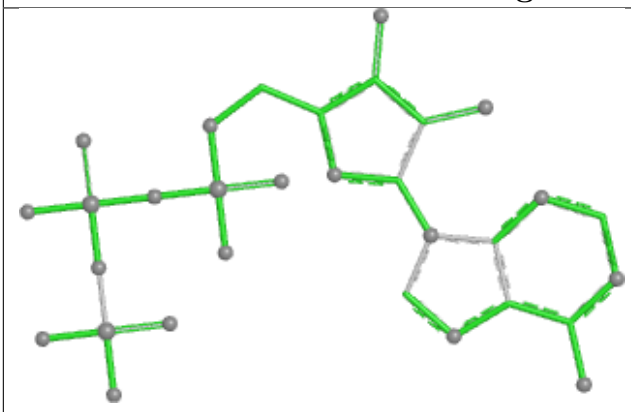


Torsions

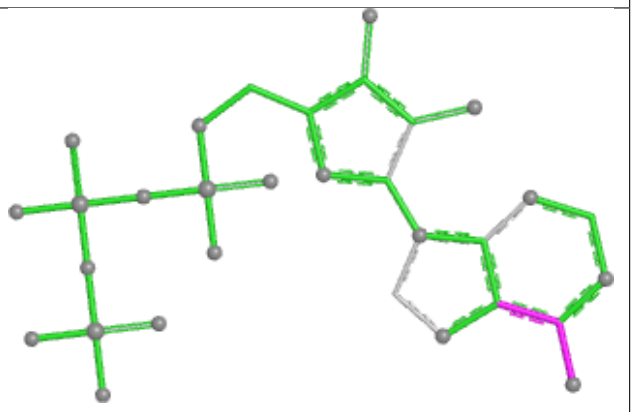


Rings

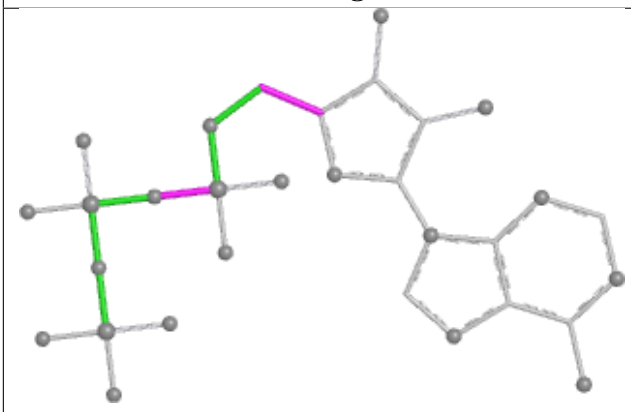
Ligand ATP B 5002



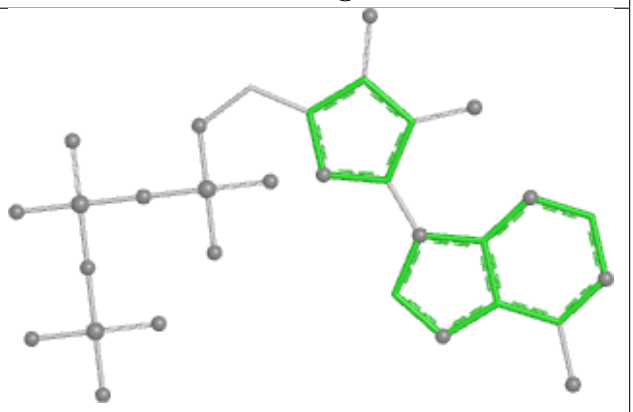
Bond lengths



Bond angles

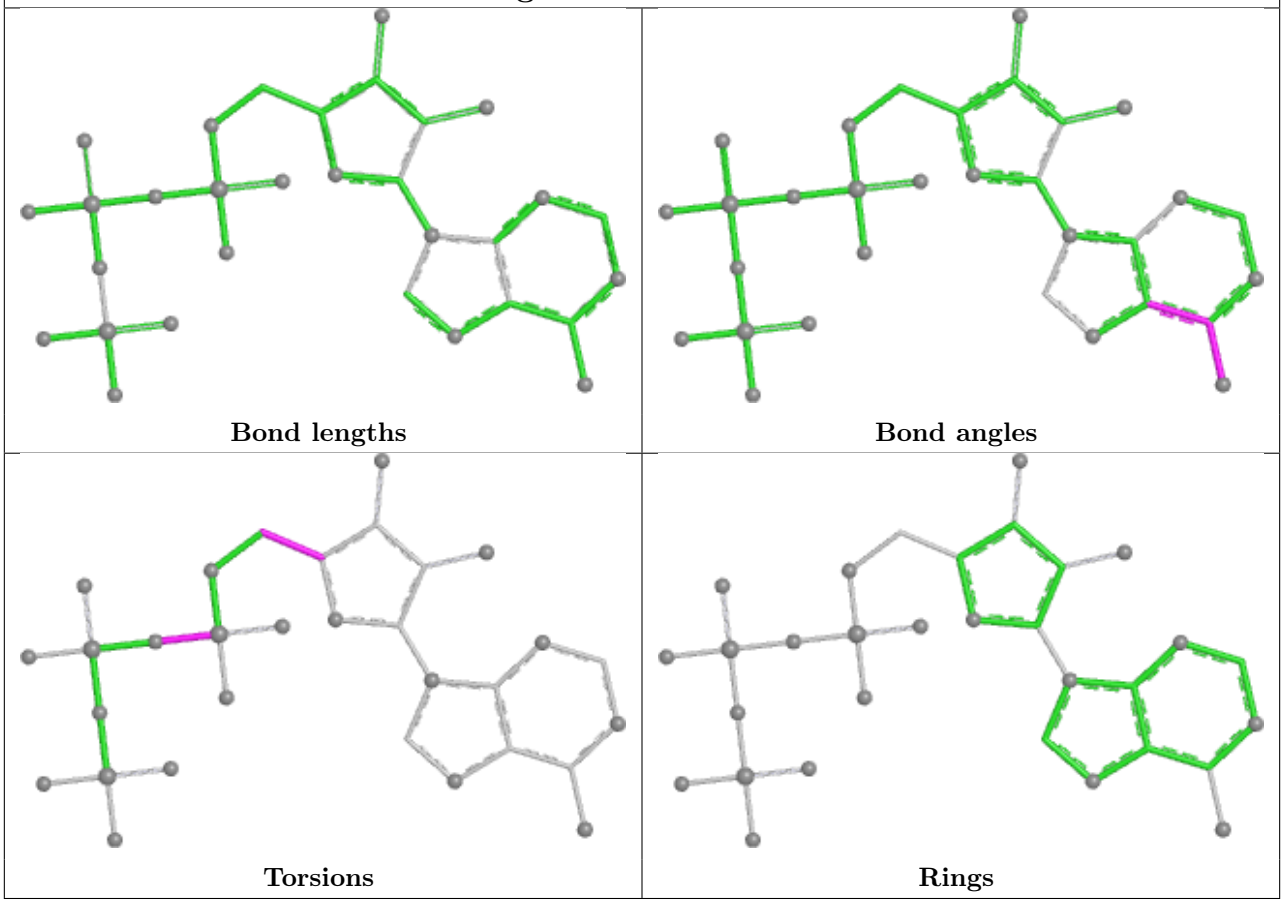


Torsions



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.

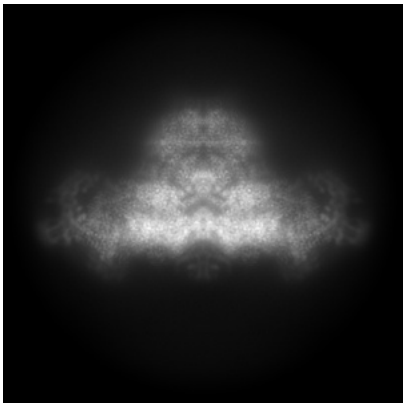
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26415. These allow visual inspection of the internal detail of the map and identification of artifacts.

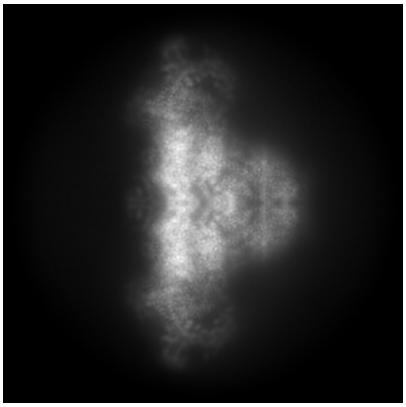
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

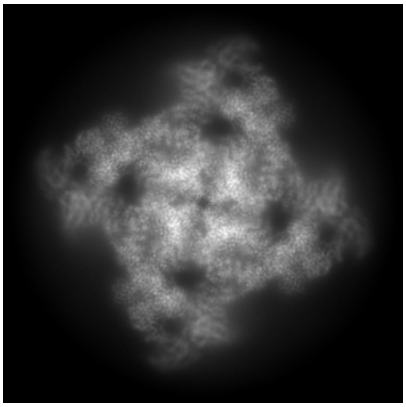
6.1.1 Primary map



X



Y

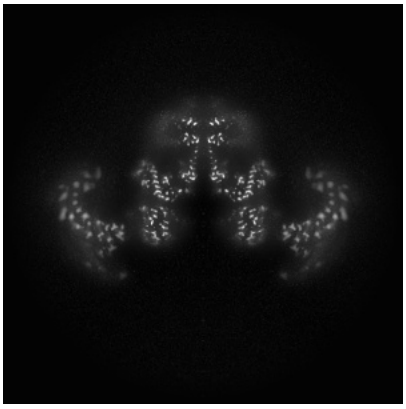


Z

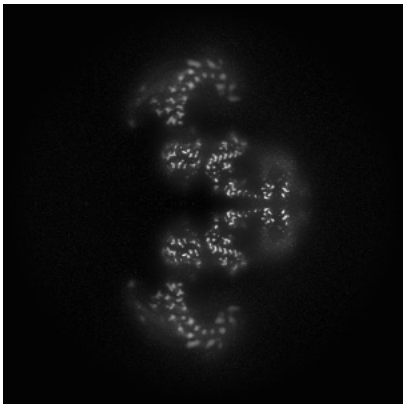
The images above show the map projected in three orthogonal directions.

6.2 Central slices

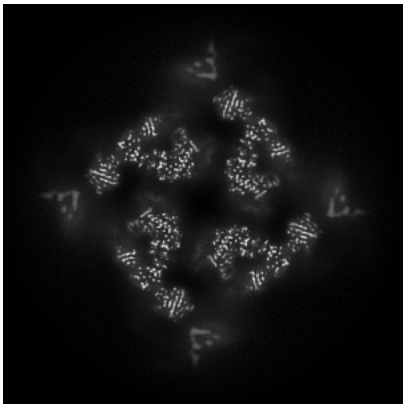
6.2.1 Primary map



X Index: 256



Y Index: 256

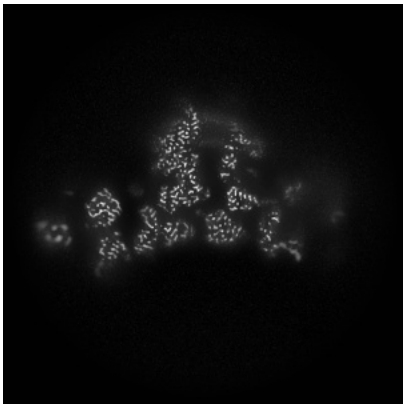


Z Index: 256

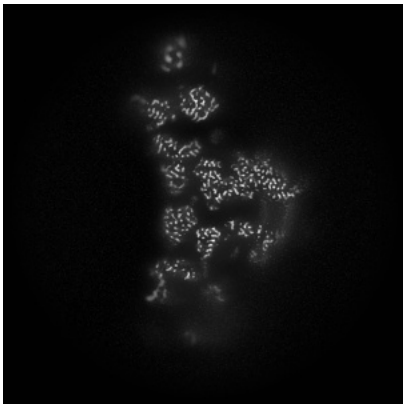
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

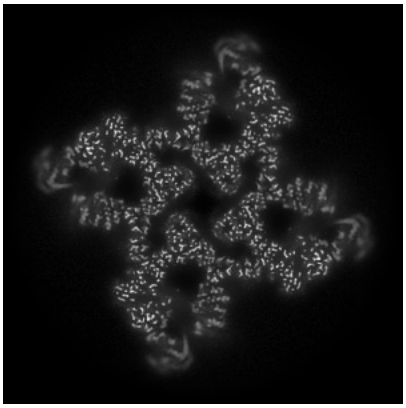
6.3.1 Primary map



X Index: 219



Y Index: 219

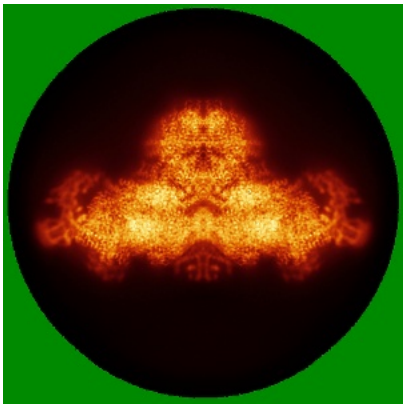


Z Index: 223

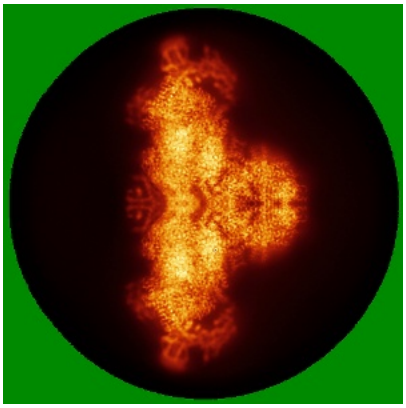
The images above show the largest variance slices of the map in three orthogonal directions.

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

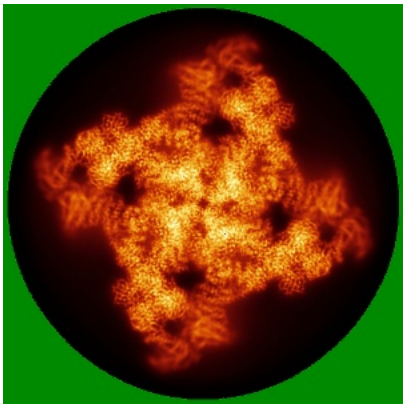
6.4.1 Primary map



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

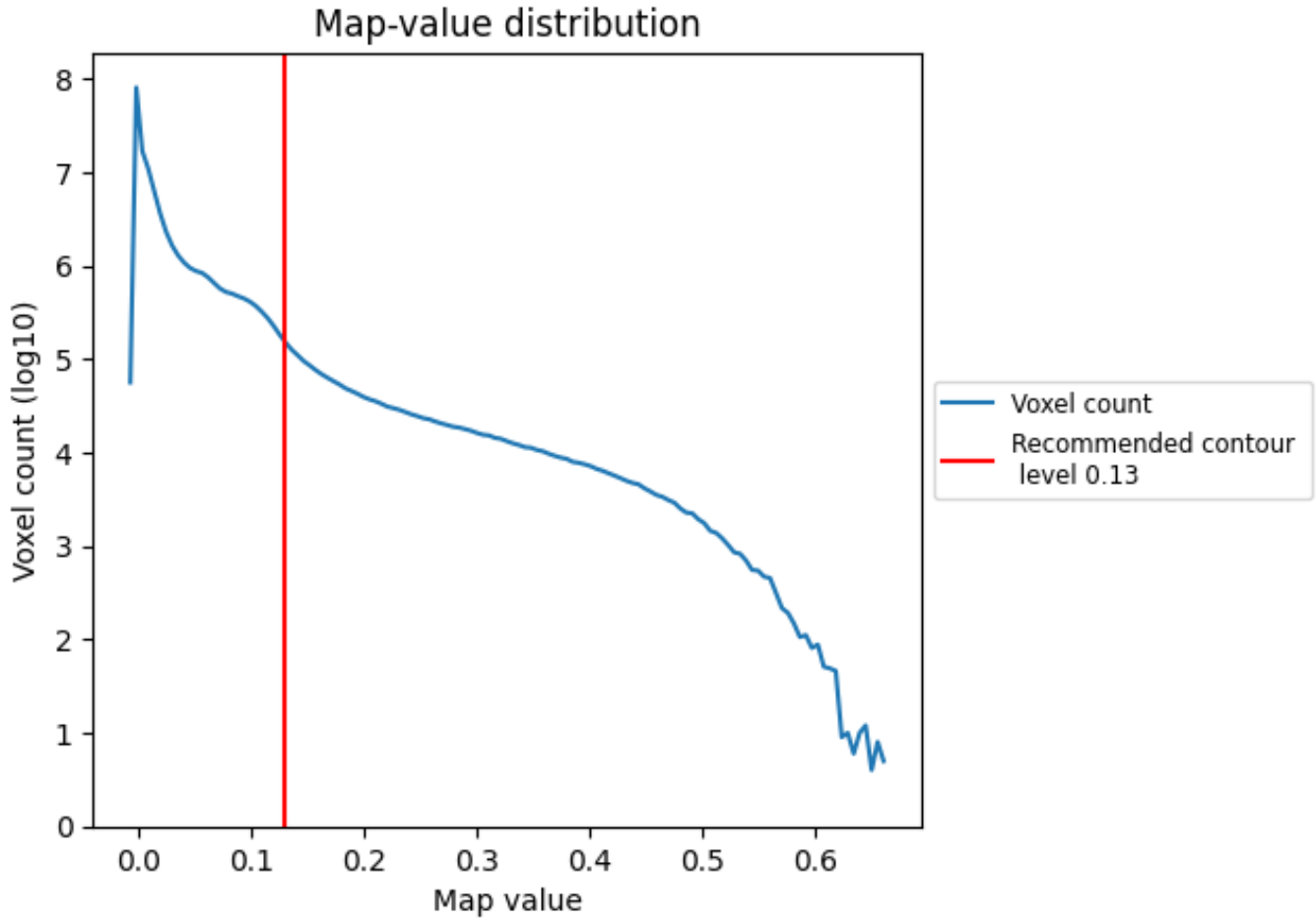
6.6 Mask visualisation (i)

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

7 Map analysis

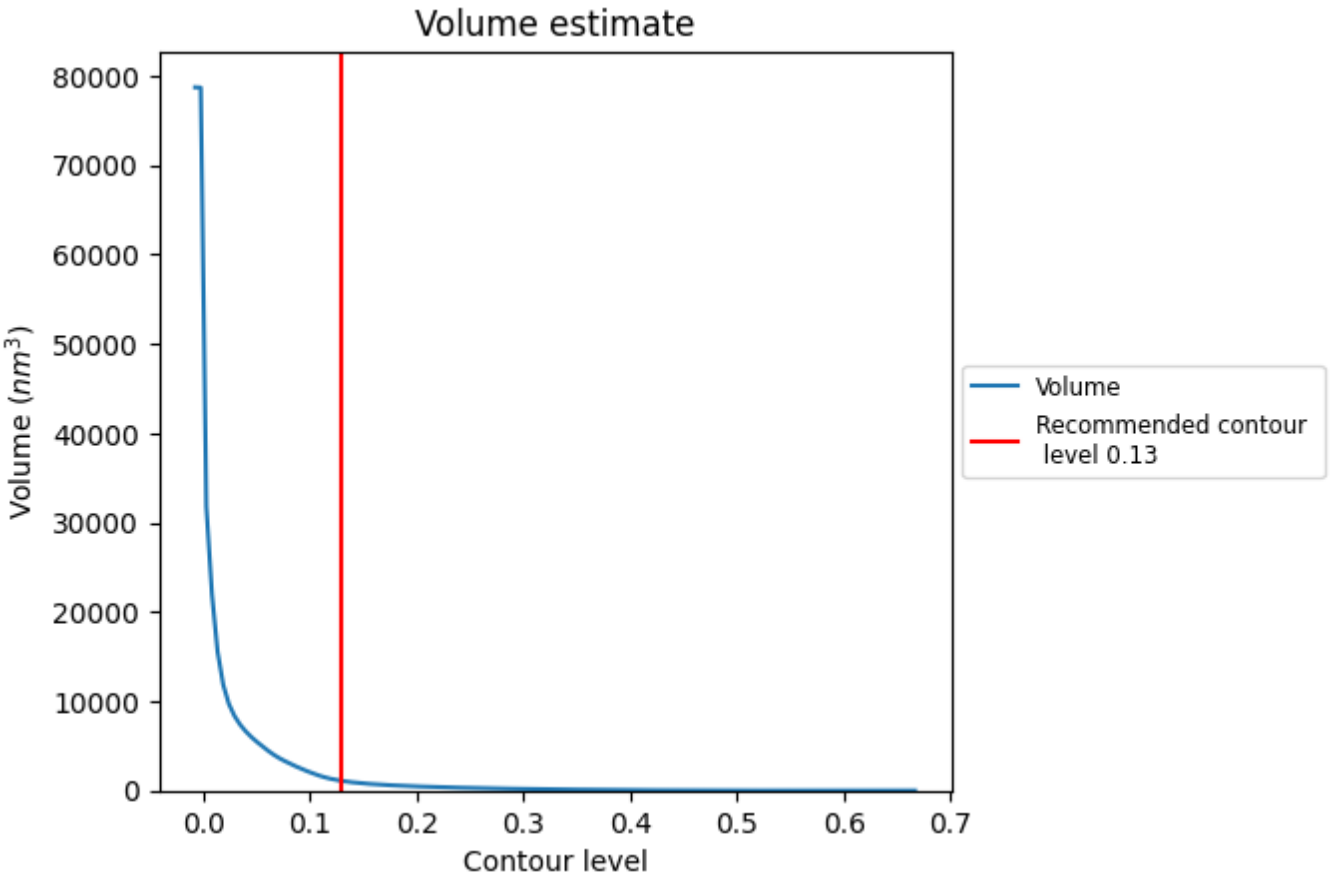
This section contains the results of statistical analysis of the map.

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.

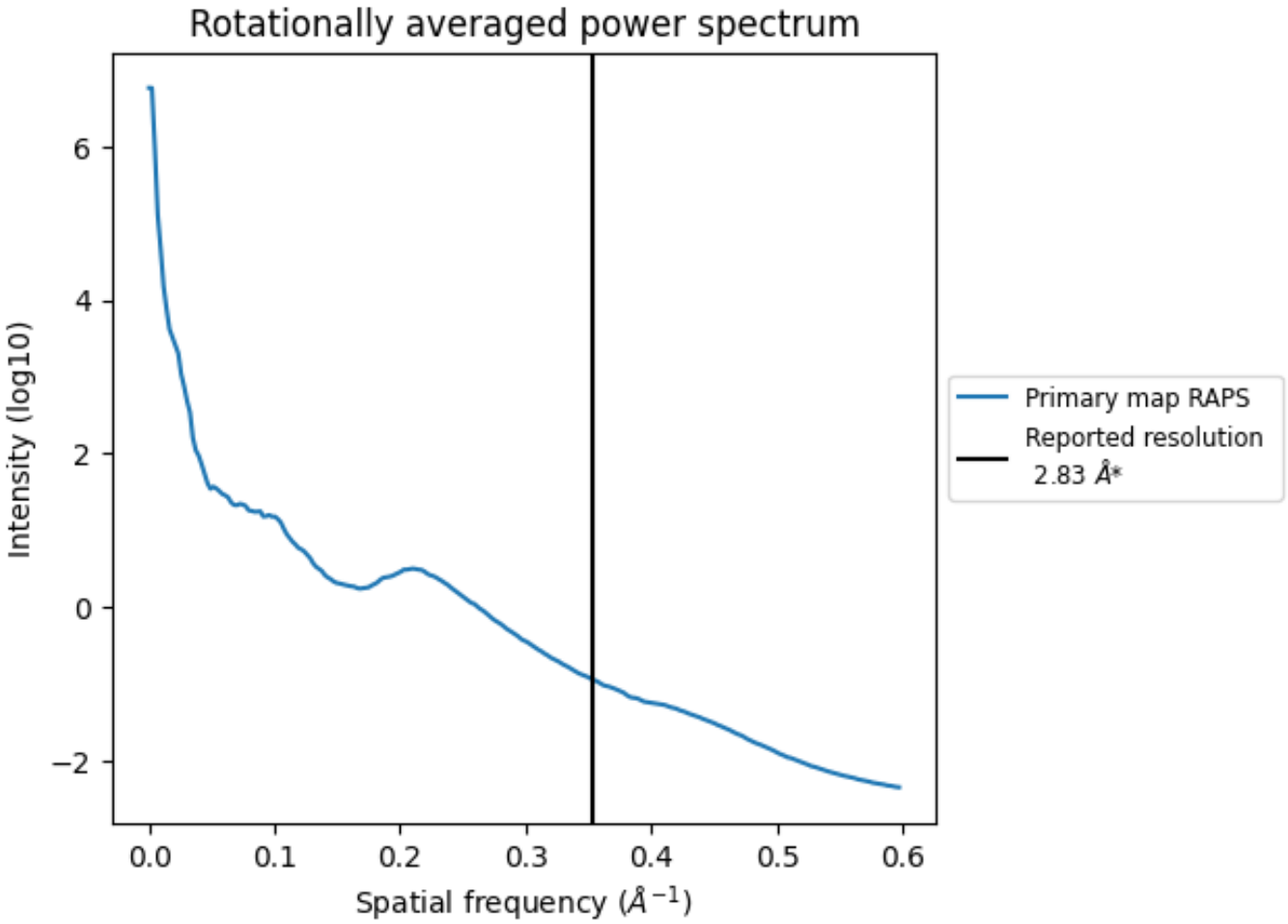
7.2 Volume estimate (i)



The volume at the recommended contour level is 1083 nm^3; this corresponds to an approximate mass of 978 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 0.353 Å^{-1}

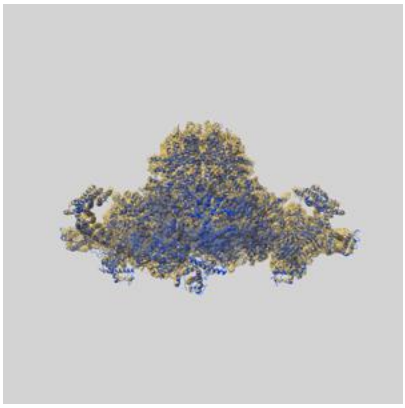
8 Fourier-Shell correlation

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

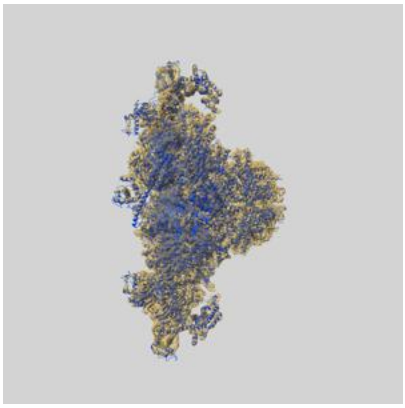
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26415 and PDB model 7UA5. Per-residue inclusion information can be found in section 3 on page 5.

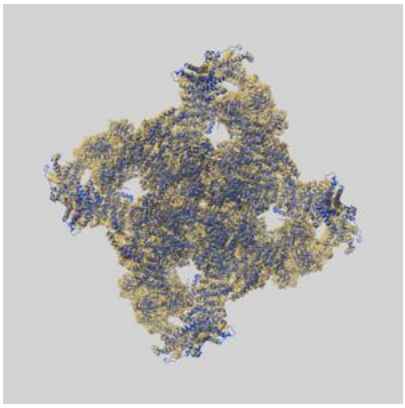
9.1 Map-model overlay



X



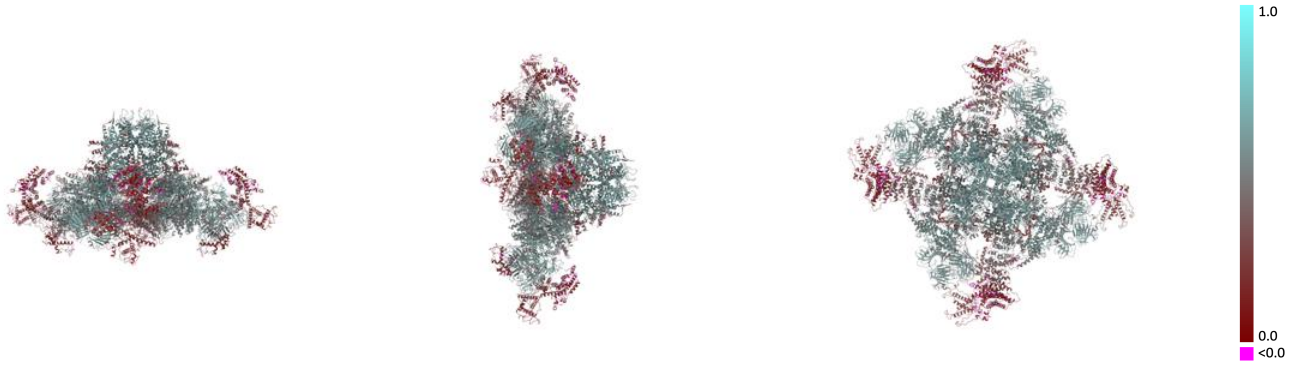
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

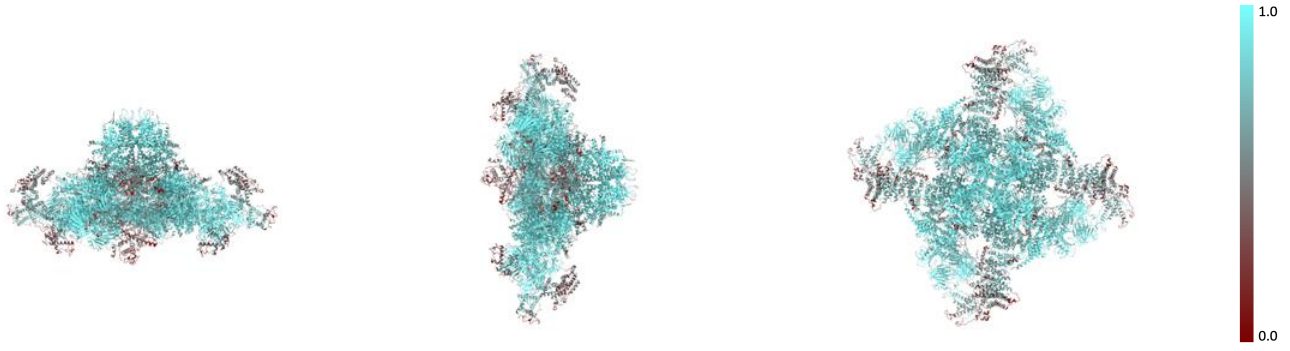
9.2 Q-score mapped to coordinate model



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.

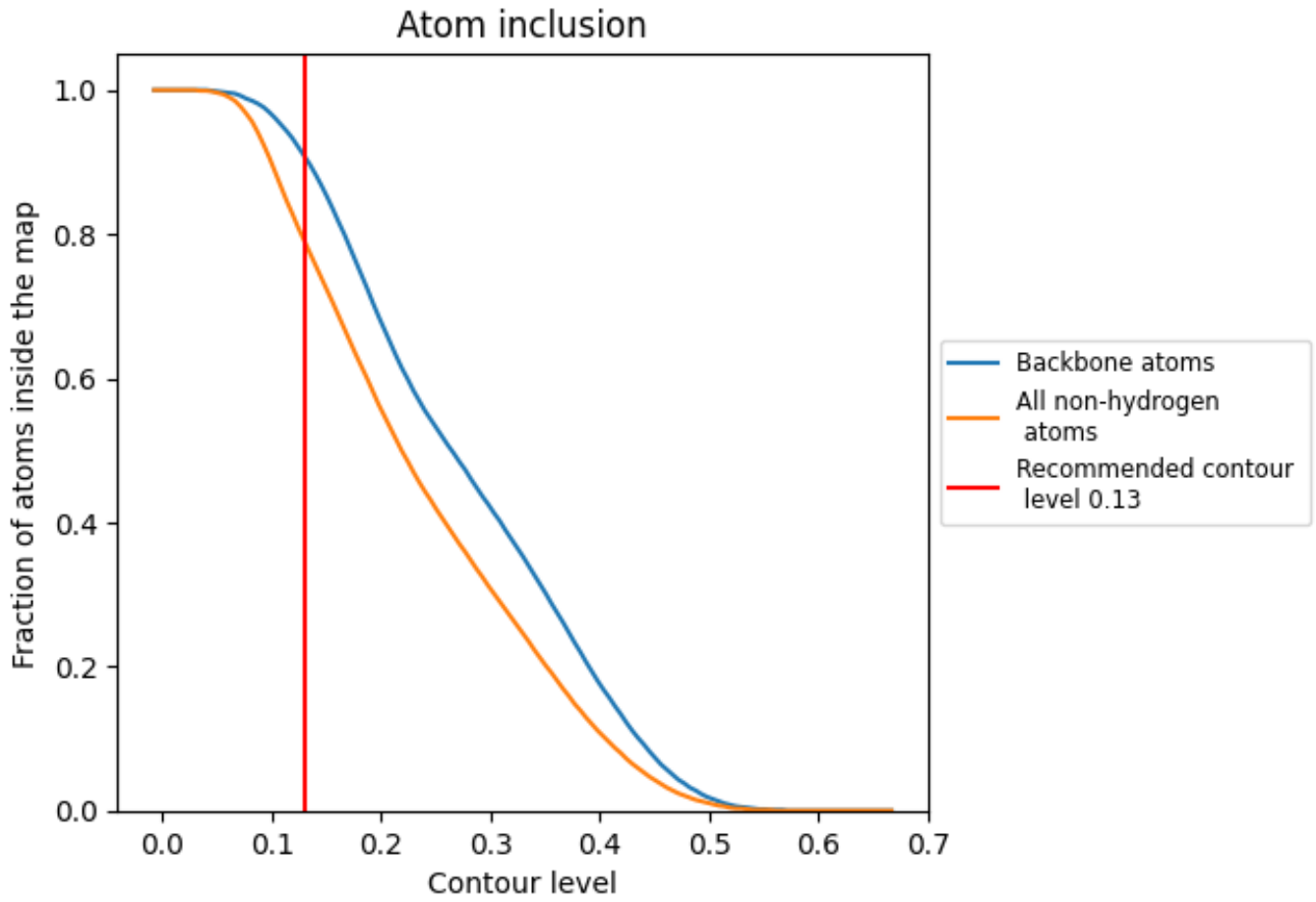
9.3 Atom inclusion mapped to coordinate model



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 79% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.4480
A	0.7880	0.4490
B	0.7880	0.4480
C	0.7880	0.4470
D	0.7850	0.4380
E	0.9220	0.5670
F	0.9260	0.5600
G	0.9220	0.5650
H	0.9230	0.5640