wwPDB EM Validation Summary Report (i)

Nov 13, 2023 – 06:16 PM EST

PDB ID	:	8UXI
EMDB ID	:	EMD-42765
Title	:	Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	3.29 Å(reported)
Based on initial model	:	7UA5

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

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

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

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

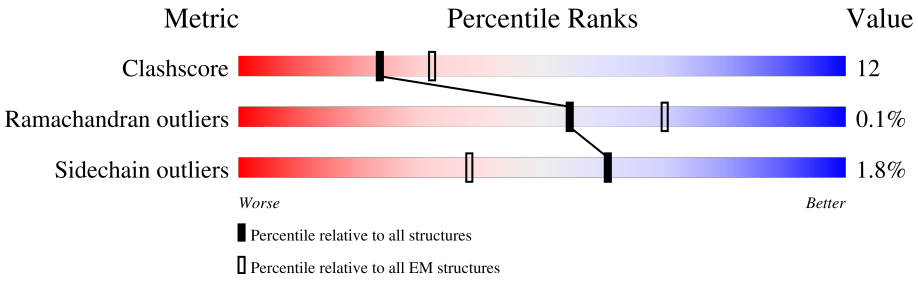
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	4967	11% 58% 22% • 19%
1	B	4967	11% 58% 22% • 19%
1	C	4967	11% 58% 22% • 19%
1	D	4967	11% 58% 22% • 19%
2	E	108	• 78% 19% • •
2	F	108	• 78% 19% • •
2	G	108	• 77% 19% • •
2	H	108	• 79% 18% • •

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 32032	C 20411	N 5451	O 5955	S 215	2	0
1	B	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	C	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	D	4004	Total 32032	C 20411	N 5451	O 5955	S 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

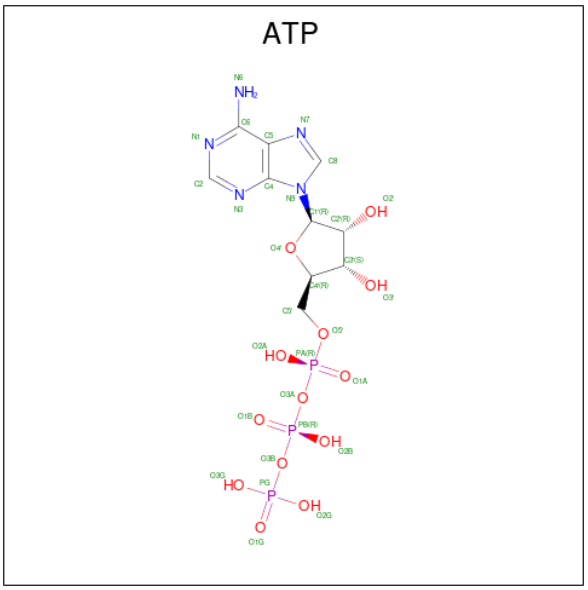
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

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

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

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



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

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

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

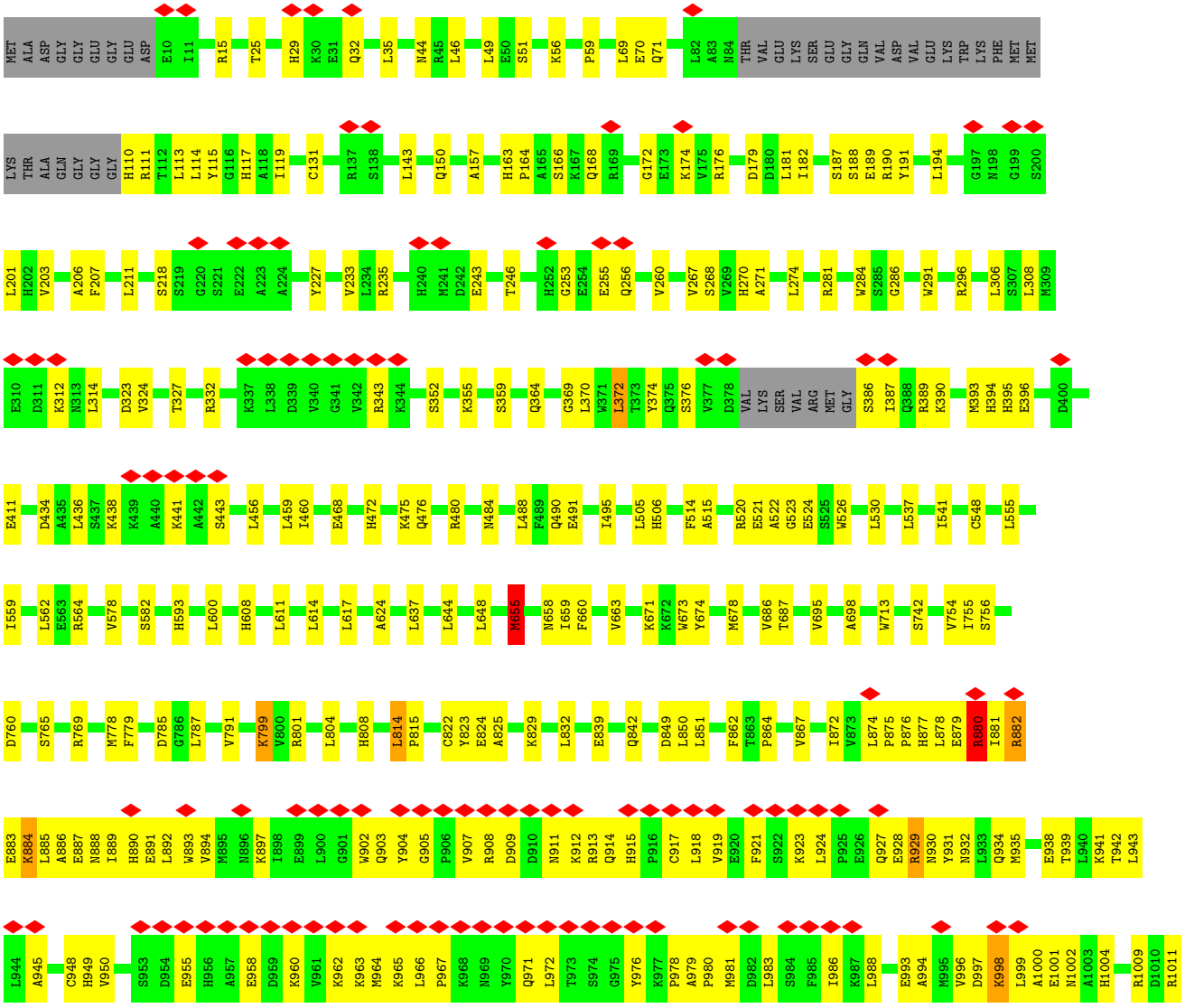
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

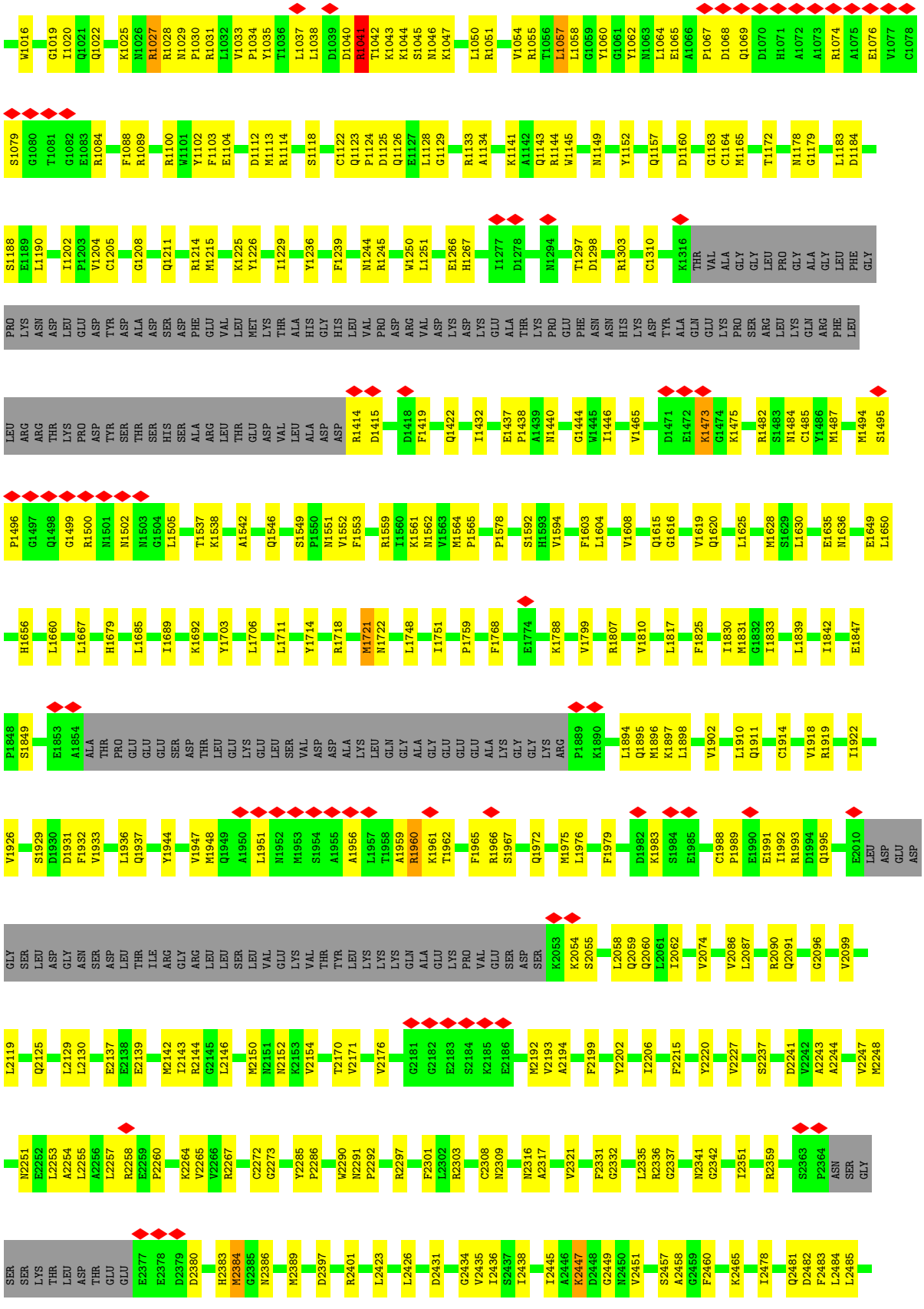
3 Residue-property plots (i)

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:

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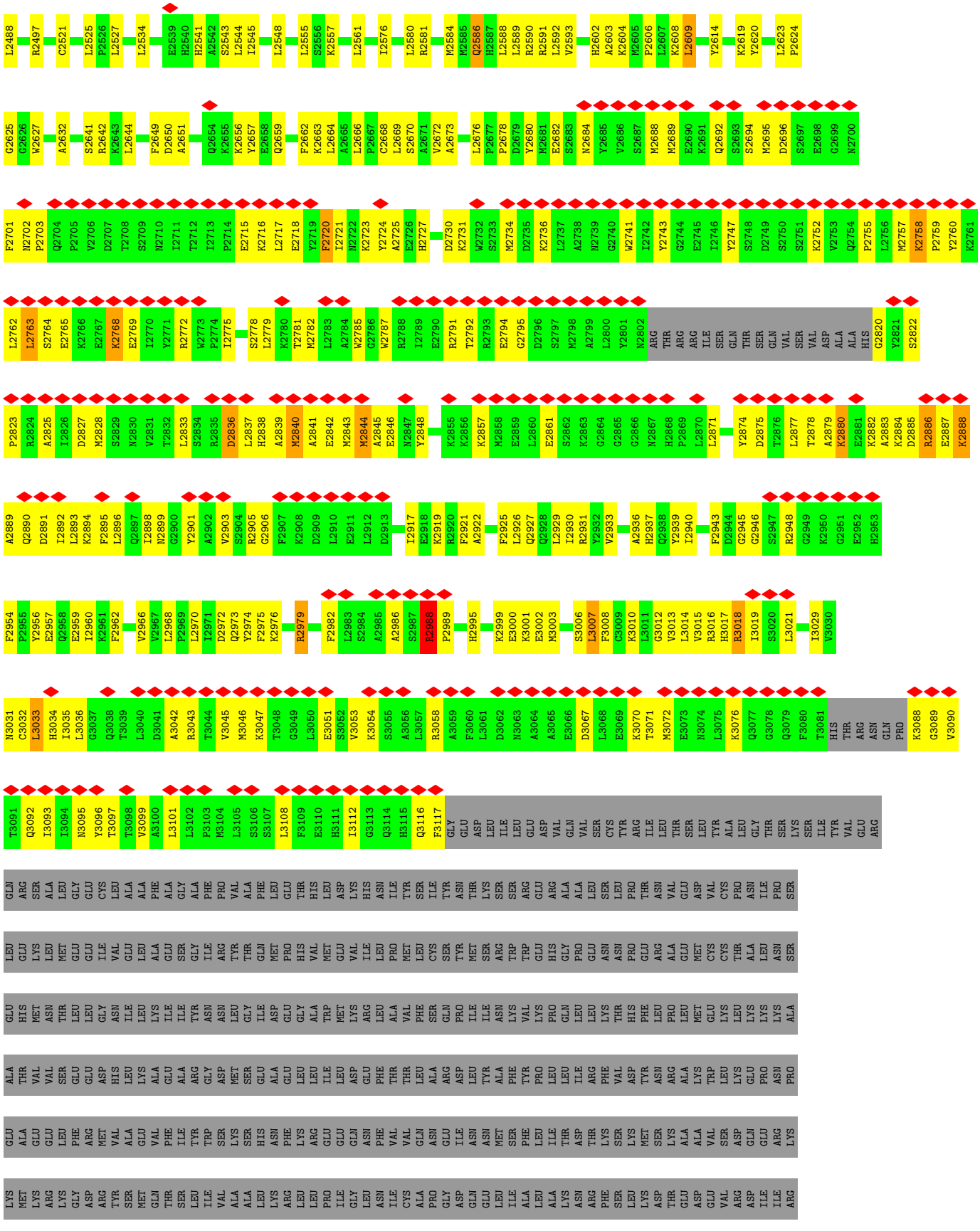
S1079 G1080 T1081 G1082 E1083 R1084 F1088 R1089 R1100 W1101 Y1102 F1103 E1104 D1112 M1113 R1114 S1118 C1122 Q1123 P1124 D1125 Q1126 E1127 L1128 G1129 R1133 A1134 K1141 A1142 Q1143 R1144 W1145 N1149 Y1152 Q1157 D1160 G1163 C1164 M1165 T1172 N1178 G1179 L1183 D1184
S1188 E1189 L1190 I1202 P1203 V1204 C1205 G1208 Q1211 R1214 M1215 K1225 Y1226 I1229 Y1236 F1239 N1244 R1245 W1250 L1251 E1266 H1267 I1277 D1278 N1294 T1297 D1298 R1303 C1310 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY
PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU
LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1418 F1419 Q1422 I1432 E1437 P1438 A1439 N1440 G1444 W1445 I1446 V1465 D1471 E1472 K1473 G1474 K1475 R1482 S1483 N1484 C1485 Y1486 M1487 M1494 S1495
P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 T1537 K1538 A1542 Q1546 S1549 P1550 N1551 V1552 F1553 R1559 I1560 K1561 N1562 V1563 M1564 P1565 P1578 S1592 H1593 V1594 F1603 L1604 V1608 Q1615 G1616 V1619 Q1620 L1625 M1628 S1629 L1630 E1635 N1636 E1649 L1650
H1656 L1660 L1667 H1679 L1685 I1689 K1692 Y1703 L1706 L1711 Y1714 R1718 M1721 N1722 L1748 I1751 P1759 F1768 E1774 K1788 V1799 R1807 V1810 L1817 F1825 I1830 M1831 G1832 I1833 L1839 I1842 E1847
P1848 S1849 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1894 Q1895 M1896 K1897 L1898 V1902 L1910 Q1911 C1914 V1918 R1919 I1922
V1926 S1929 D1930 D1931 F1932 V1933 L1936 Q1937 Y1944 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 Q1972 M1975 L1976 F1979 D1982 K1983 S1984 E1985 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 GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 L2058 Q2059 Q2060 L2061 I2062 V2074 V2086 L2087 R2090 Q2091 G2096 V2099
L2119 Q2125 L2129 L2130 E2137 E2138 E2139 M2142 I2143 R2144 G2145 L2146 M2150 N2151 N2152 K2153 V2154 T2170 V2171 V2176 G2181 G2182 E2183 S2184 K2185 E2186 M2192 V2193 A2194 F2199 Y2202 I2206 F2215 Y2220 V2227 S2237 D2241 V2242 A2243 A2244 V2247 M2248
N2251 E2252 L2253 A2254 L2255 A2256 L2257 R2258 E2259 P2260 K2264 V2265 V2266 R2267 C2272 G2273 Y2285 P2286 W2290 N2291 P2292 R2297 F2301 L2302 R2303 C2308 N2309 N2316 A2317 V2321 F2331 G2332 L2335 R2336 G2337 N2341 G2342 I2351 R2359 S2363 P2364 ASN SER GLY
SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 G2385 N2386 M2389 D2397 R2401 L2423 L2426 D2431 G2434 V2435 I2436 S2437 I2438 I2445 A2446 K2447 D2448 G2449 N2450 V2451 S2457 A2458 G2459 F2460 K2465 I2478 Q2481 D2482 F2483 L2484 L2485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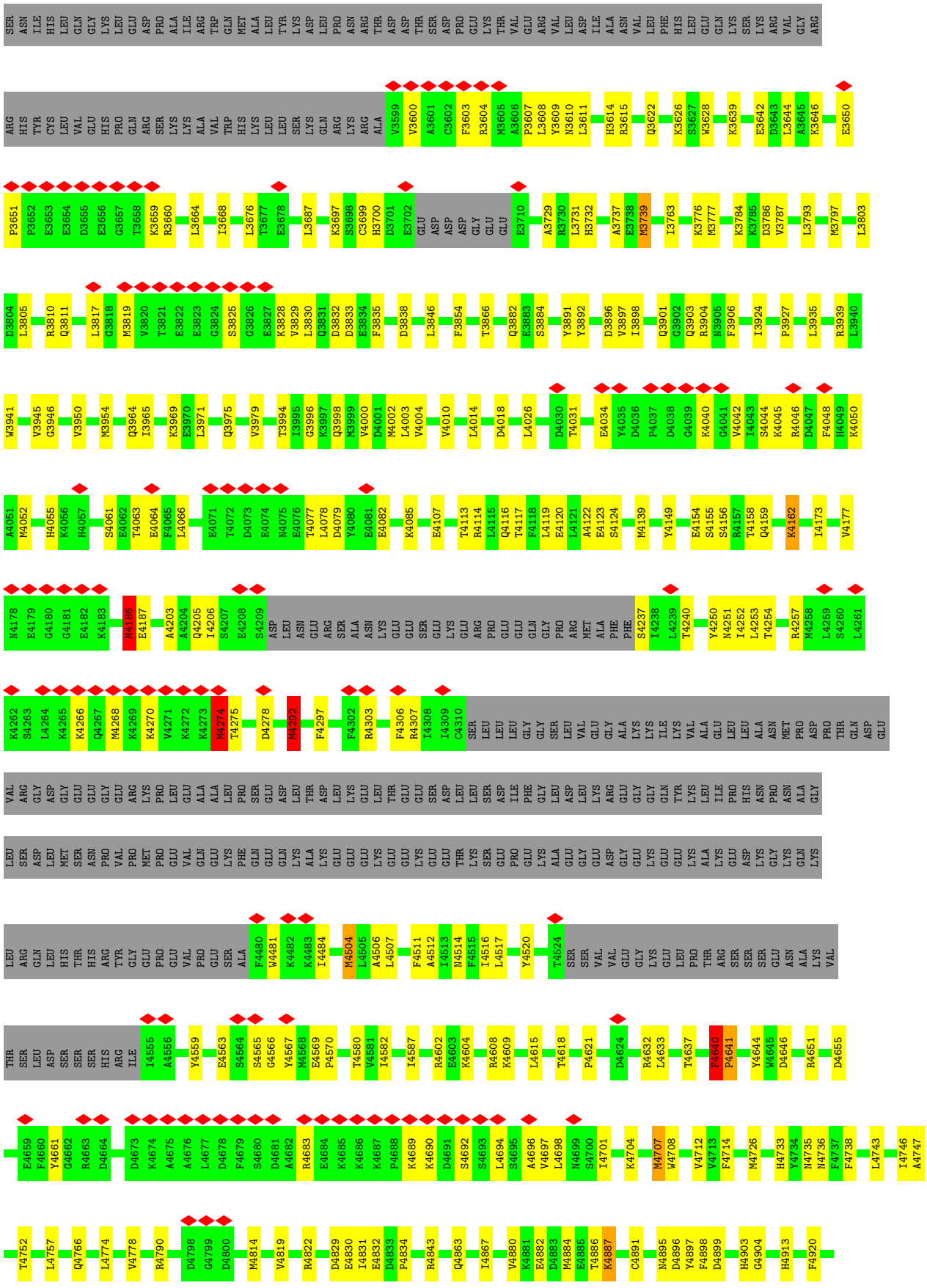
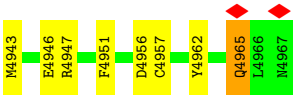
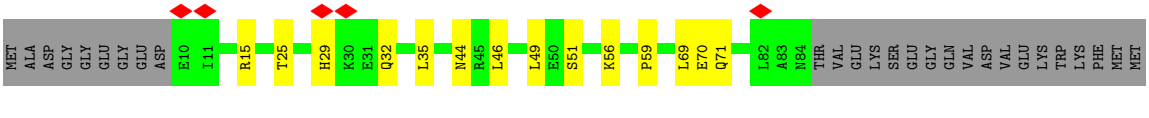
G2625 G2626 W2627 A2632 S2641 R2642 K2643 L2644 F2649 D2650 A2651 Q2654 K2655 K2656 Y2657 E2658 Q2659 F2662 K2663 L2664 A2665 L2666 P2667 C2668 L2669 S2670 A2671 V2672 A2673 L2676 P2677 P2678 D2679 Y2680 M2681 E2682 S2683 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700
F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 P2720 I2721 N2722 K2723 Y2724 A2725 E2726 H2727 D2730 K2731 W2732 S2733 M2734 D2735 K2736 L2737 A2738 W2739 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 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 A2845 E2846 N2847 Y2848 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 Y2874 D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888
A2889 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 V2903 S2904 R2905 G2906 P2907 K2908 D2909 L2910 E2911 L2912 D2913 I2917 E2918 K2919 R2920 F2921 A2922 F2925 L2926 Q2927 Q2928 L2929 I2930 R2931 Y2932 V2933 A2936 H2937 Q2938 Y2939 I2940 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2962 H2953
F2954 P2955 Y2956 E2957 Q2958 E2959 I2960 K2961 F2962 V2966 Y2967 L2968 P2969 L2970 I2971 D2972 Q2973 Y2974 F2975 K2976 R2979 F2982 L2983 S2984 A2985 A2986 S2987 R2988 P2989 H2995 K2999 E3000 K3001 E3002 M3003 S3006 L3007 F3008 C3009 K3010 L3011 G3012 V3013 L3014 V3015 R3016 H3017 R3018 I3019 S3020 L3021 I3029 V3030
N3031 C3032 L3033 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 P3103 M3104 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 VAL GLU ASP SER
GLN ARG SER ALA LEU MET GLY GLU CYS LEU ASP LYS HIS ASN ILE TYR SER ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA LEU SER LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN 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 ASP 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 LYS LYS ALA
ALA THR VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ASP ASP PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU PRO ASN PRO
GLU ALA GLU GLU LEU PHE ARG MET VAL ALA ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU LEU ILE THR ASP THR LYS SER LYS MET SER LYS LYS 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 LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLN GLU ILE ARG
WORLDWIDE PDB PROTEIN DATA BANK

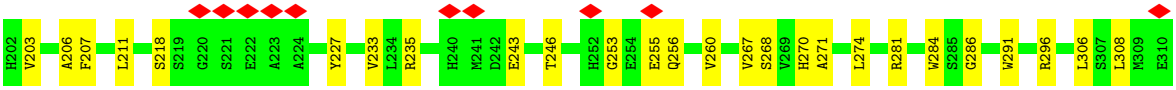


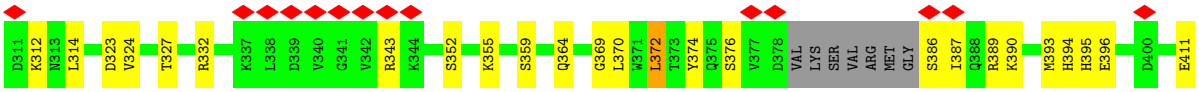


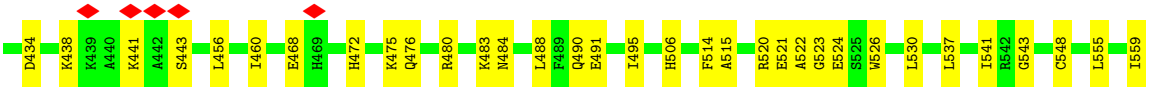
• Molecule 1: Ryanodine receptor 2

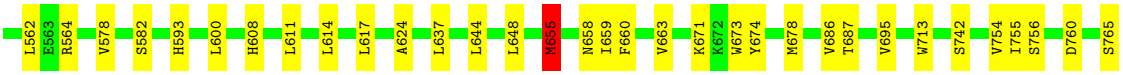
Chain B:

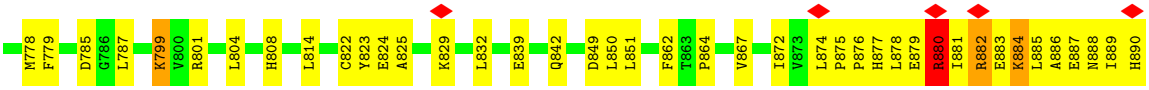


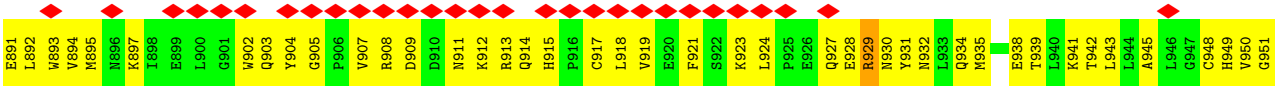


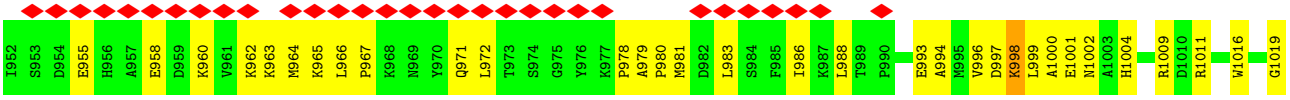


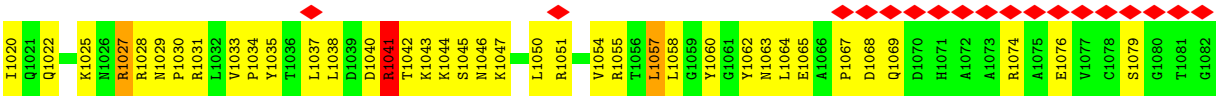


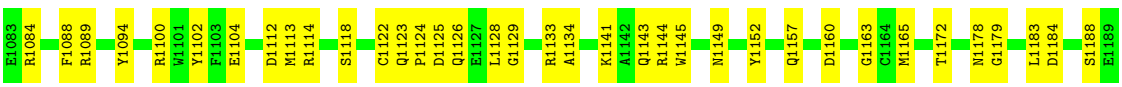


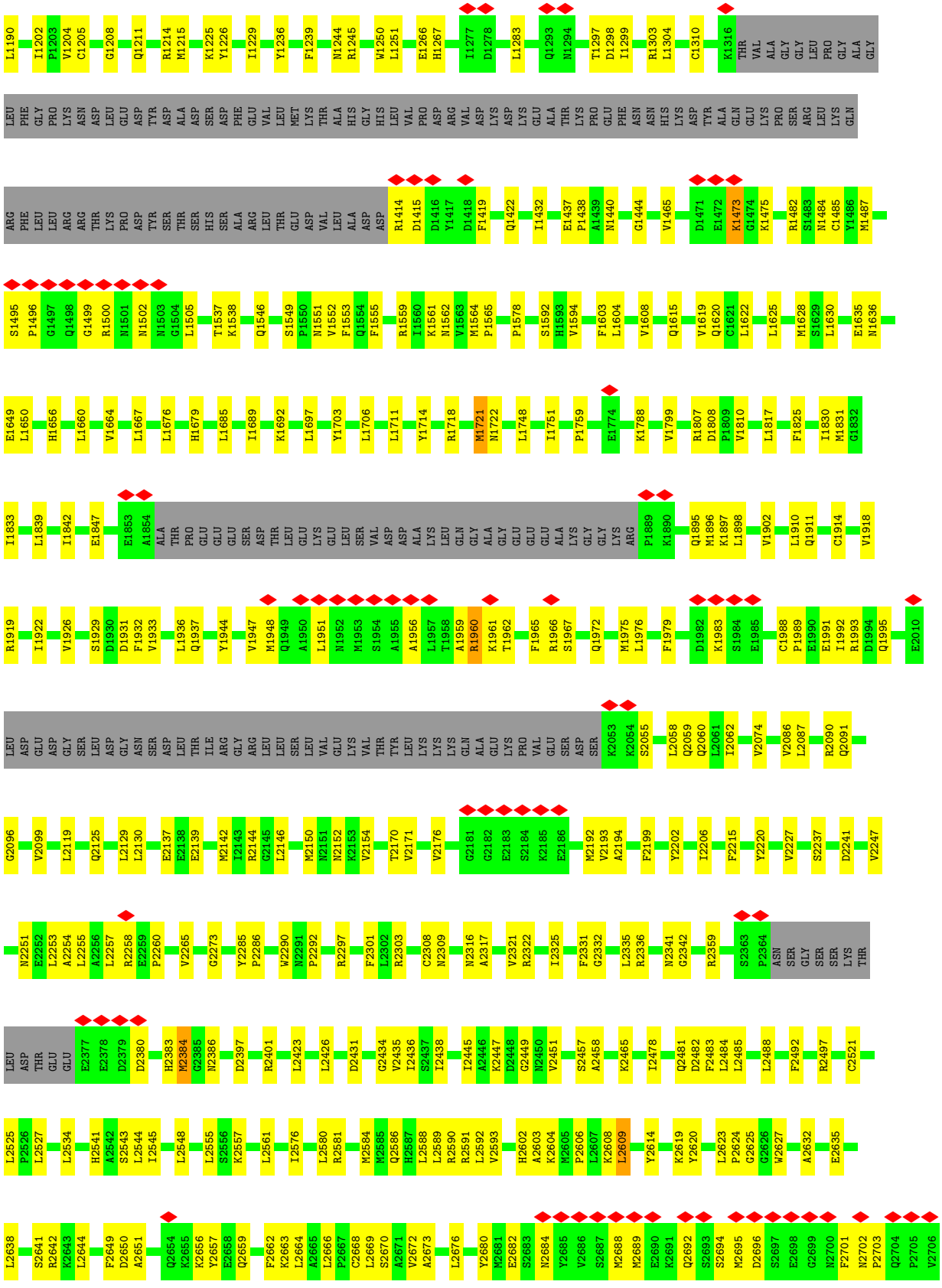








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LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN
ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 Q1422 I1432 E1437 P1438 A1439 N1440 G1444 V1465 D1471 E1472 K1473 G1474 K1475 R1482 S1483 N1484 C1485 V1486 M1487
S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 T1537 K1538 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 F1555 R1559 I1560 K1561 N1562 V1563 M1564 P1565 P1578 S1592 H1593 V1594 F1603 L1604 V1608 Q1615 V1619 Q1620 C1621 L1622 L1625 M1628 S1629 L1630 E1635 N1636
E1649 L1650 H1656 L1660 V1664 L1667 L1676 H1679 L1685 I1689 K1692 L1697 Y1703 L1706 L1711 Y1714 R1718 M1721 N1722 L1748 I1751 P1759 E1774 K1788 V1799 R1807 D1808 P1809 V1810 L1817 F1825 I1830 M1831 G1832
I1833 L1839 I1842 E1847 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 Q1895 M1896 K1897 L1898 V1902 L1910 Q1911 C1914 V1918
R1919 I1922 V1926 S1929 D1930 D1931 F1932 V1933 L1936 Q1937 Y1944 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 Q1972 M1975 L1976 F1979 D1982 K1983 S1984 E1985 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 L2058 Q2059 Q2060 L2061 I2062 V2074 V2086 L2087 R2090 Q2091
G2096 V2099 L2119 Q2125 L2129 L2130 E2137 E2138 E2139 M2142 I2143 R2144 G2145 L2146 M2150 N2151 N2152 K2153 V2154 T2170 V2171 V2176 G2181 G2182 E2183 S2184 K2185 E2186 M2192 V2193 A2194 F2199 Y2202 I2206 F2215 Y2220 V2227 S2237 D2241 V2247
N2251 E2252 L2253 A2254 L2255 A2256 L2257 R2258 E2259 P2260 V2265 G2273 Y2285 P2286 W2290 N2291 P2292 R2297 F2301 L2302 R2303 C2308 N2309 N2316 A2317 V2321 R2322 I2325 F2331 G2332 L2335 R2336 N2341 G2342 R2359 S2363 P2364 ASN SER GLY SER SER LYS THR
LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 G2385 N2386 D2397 R2401 L2423 L2426 D2431 G2434 V2435 I2436 S2437 I2438 I2445 A2446 K2447 D2448 G2449 N2450 V2451 S2457 A2458 K2465 I2478 Q2481 D2482 F2483 L2484 L2485 L2488 F2492 R2497 C2521
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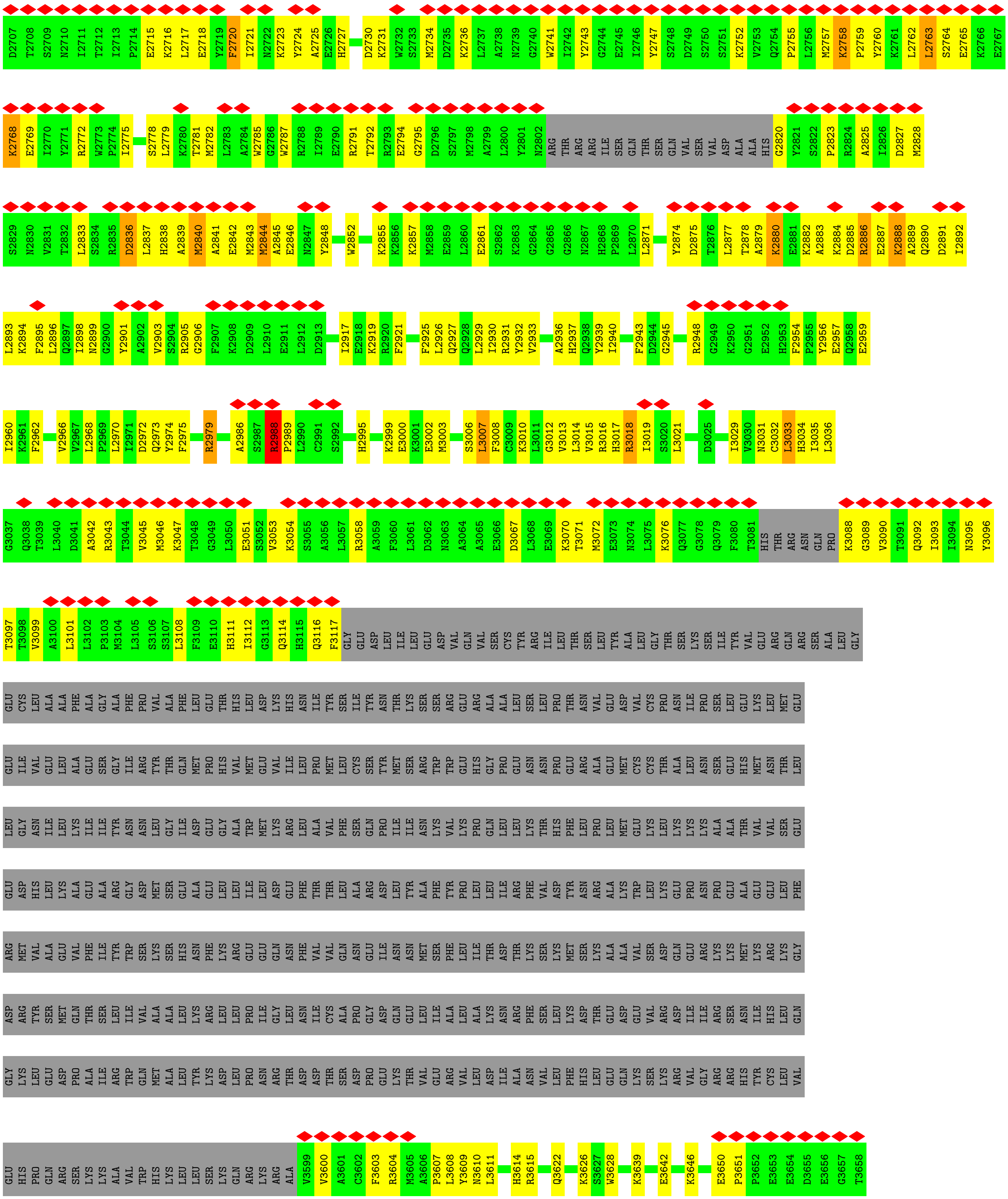
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K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ILE SER GLN THR SER GLN VAL SER VAL ASP 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 A2845 E2846 N2847 Y2848 W2852 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 S2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 Y2874 D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892
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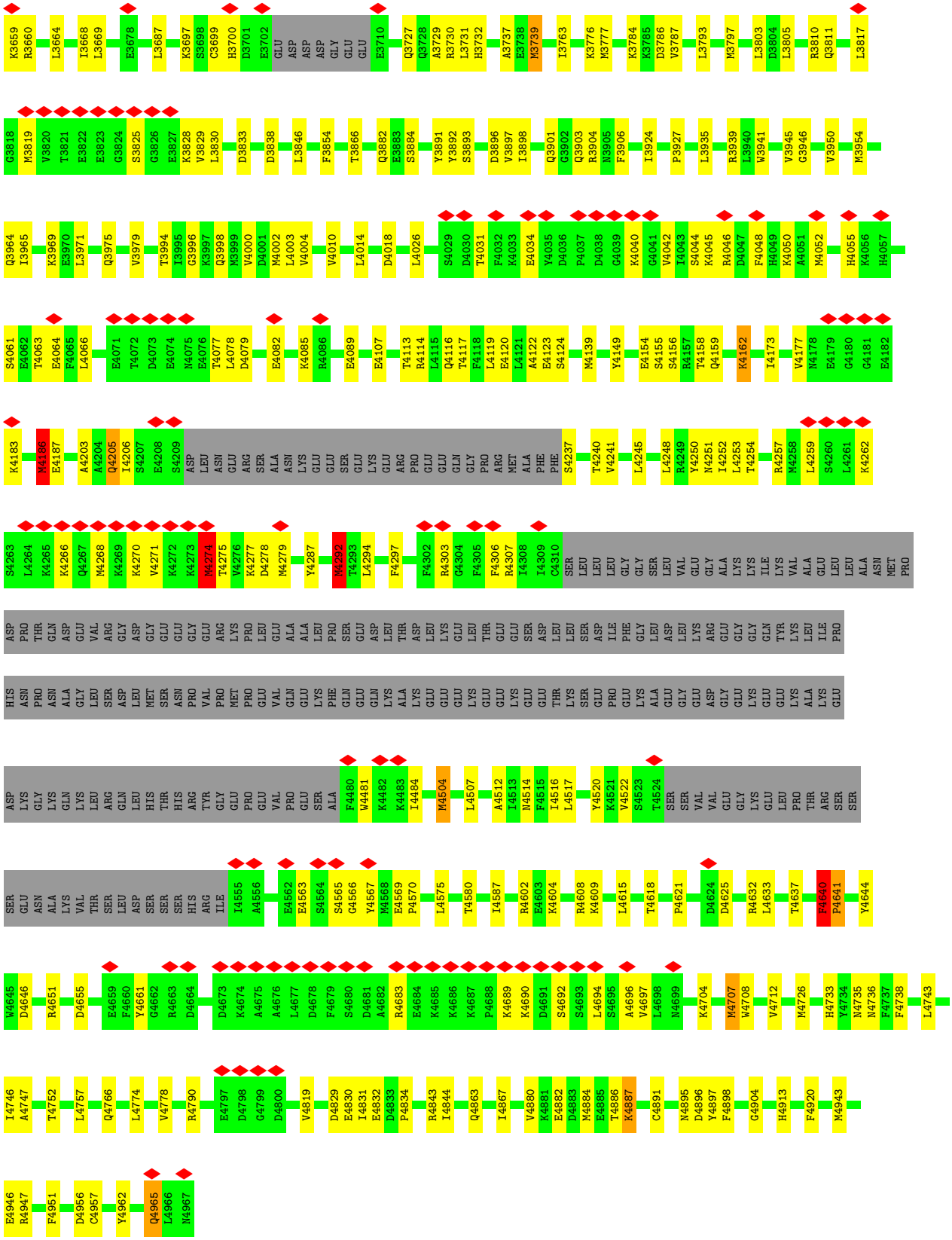
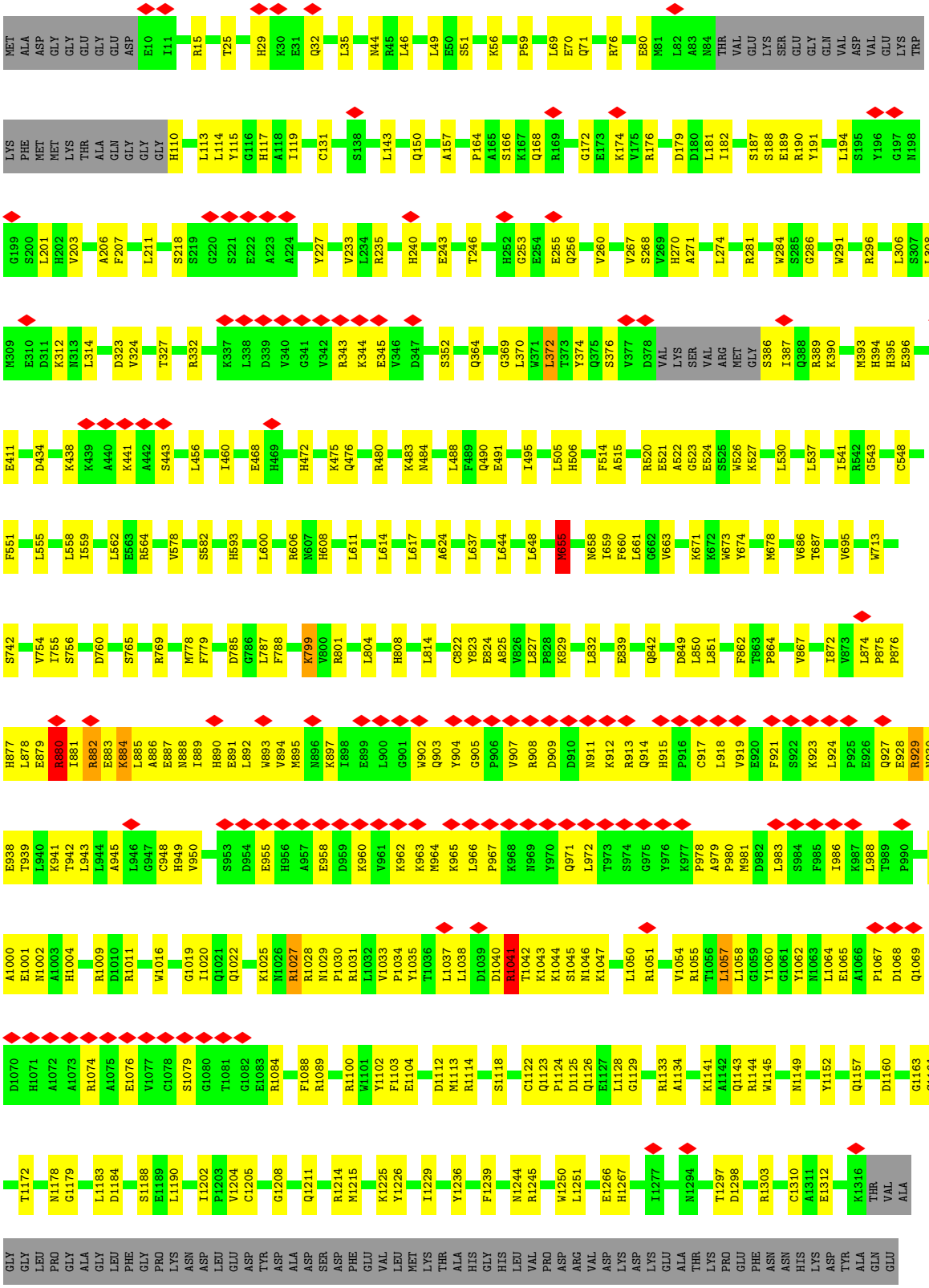
I2960 K2961 F2962 V2966 V2967 L2968 P2969 L2970 I2971 D2972 Q2973 Y2974 F2975 R2979 A2986 S2987 R2988 P2989 L2990 C2991 S2992 H2995 K2999 E3000 K3001 E3002 M3003 S3006 L3007 F3008 C3009 K3010 L3011 G3012 V3013 L3014 V3015 R3016 H3017 R3018 I3019 S3020 L3021 D3025 I3029 V3030 N3031 C3032 L3033 H3034 I3035 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 P3103 M3104 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 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 ASN SER GLU HIS MET ASN THR LEU
LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA THR VAL VAL SER GLU
GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE
ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN 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 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 L3611 H3614 R3615 Q3622 K3626 S3627 W3628 K3639 E3642 K3646 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658



• Molecule 1: Ryanodine receptor 2

Chain C:


11%
58%
22%
19%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LYS PHE MET MET LYS THR ALA GLN GLY GLY GLY H110 L113 L114 Y115 G116 H117 A118 I119 C131 S138 L143 Q150 A157 P164 A165 S166 K167 Q168 R169 G172 E173 K174 V175 R176 D179 D180 L181 I182 S187 S188 E189 R190 Y191 L194 S195 Y196 G197 N198
G199 S200 L201 H202 V203 A206 F207 L211 S218 S219 G220 S221 E222 A223 A224 Y227 V233 L234 R235 H240 E243 T246 H252 G253 E254 E255 Q256 V260 V267 S268 V269 H270 A271 L274 R281 W284 S285 G286 W291 R296 L306 S307 L308
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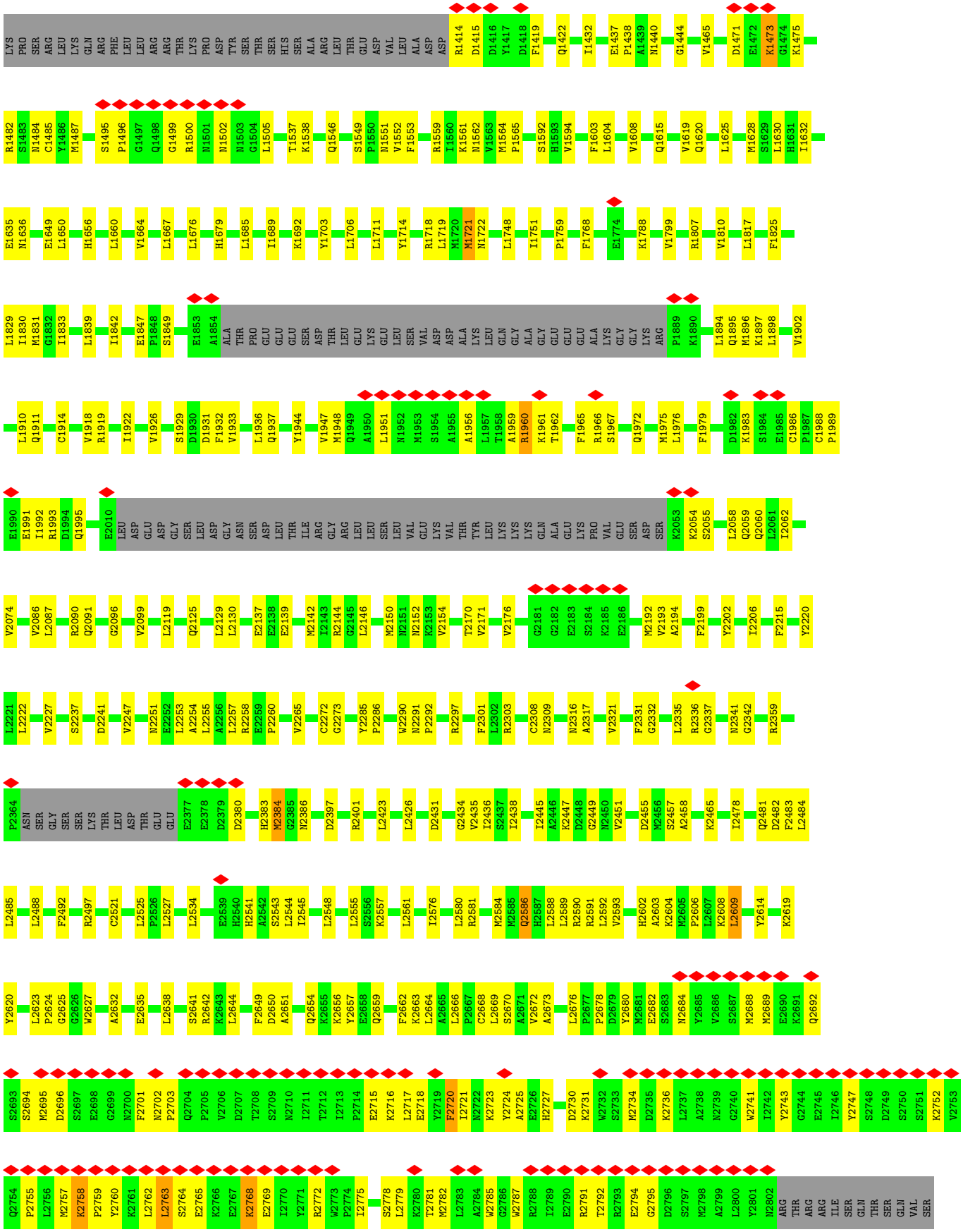
E411 D434 K438 K439 A440 K441 A442 S443 L456 I460 E468 H469 H472 K475 Q476 R480 K483 N484 L488 F489 Q490 E491 I495 L505 H506 F514 A515 R520 E521 A522 G523 E524 S525 W526 K527 L530 L537 I541 R542 G543 C548
F551 L555 L558 I559 L562 E563 R564 V578 S582 H593 L600 R606 N607 H608 L611 L614 L617 A624 L637 L644 L648 M655 N658 I659 F660 L661 G662 V663 K671 K672 W673 Y674 H678 V686 T687 V695 W713
S742 V754 I755 S756 D760 S765 R769 M778 F779 D785 G786 L787 F788 K799 V800 R801 L804 H808 L814 C822 Y823 E824 A825 V826 L827 P828 K829 L832 E839 Q842 D849 L850 L851 P862 T863 P864 V867 I872 V873 L874 P875 P876
H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935
E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 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 I986 K987 L988 T989 P990 E993 A994 M995 V996 D997 K998 L999
A1000 E1001 N1002 A1003 H1004 R1009 D1010 R1011 W1016 G1019 I1020 Q1021 Q1022 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 L1050 R1051 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069
D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 F1088 R1089 R1100 W1101 Y1102 F1103 E1104 D1112 M1113 R1114 S1118 C1122 Q1123 P1124 D1125 Q1126 E1127 L1128 G1129 R1133 A1134 K1141 A1142 Q1143 R1144 W1145 N1149 Y1152 Q1157 D1160 G1163 C1164 M1165
T1172 N1178 G1179 L1183 D1184 S1188 E1189 L1190 I1202 P1203 V1204 C1205 G1208 Q1211 R1214 M1215 K1225 Y1226 I1229 Y1236 F1239 N1244 R1245 W1250 L1251 E1266 H1267 I1277 N1294 T1297 D1298 R1303 C1310 A1311 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 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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E1635 N1636 E1649 L1650 H1656 L1660 V1664 L1667 L1676 H1679 L1685 I1689 K1692 Y1703 L1706 L1711 Y1714 R1718 L1719 M1720 M1721 N1722 L1748 I1751 P1759 F1768 E1774 K1788 V1799 R1807 V1810 L1817 F1825
L1829 I1830 M1831 G1832 I1833 L1839 I1842 E1847 P1848 S1849 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 L1894 Q1895 M1896 K1897 L1898 V1902
L1910 Q1911 C1914 V1918 R1919 I1922 V1926 S1929 D1930 D1931 F1932 V1933 L1936 Q1937 Y1944 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 Q1972 M1975 L1976 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 L2058 Q2059 Q2060 L2061 I2062
V2074 V2086 L2087 R2090 Q2091 G2096 V2099 L2119 Q2125 L2129 L2130 E2137 E2138 E2139 M2142 I2143 R2144 G2145 L2146 M2150 N2151 N2152 K2153 V2154 T2170 V2171 V2176 G2181 G2182 E2183 S2184 K2185 E2186 M2192 V2193 A2194 F2199 Y2202 I2206 F2215 Y2220
L2221 L2222 V2227 S2237 D2241 V2247 N2251 E2252 L2253 A2254 L2255 A2256 L2257 R2258 E2259 P2260 V2265 C2272 G2273 Y2285 P2286 W2290 N2291 P2292 R2297 F2301 L2302 R2303 C2308 N2309 N2316 A2317 V2321 F2331 G2332 L2335 R2336 G2337 N2341 G2342 R2359
P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 G2385 N2386 D2397 R2401 L2423 L2426 D2431 G2434 V2435 I2436 S2437 I2438 I2445 A2446 K2447 D2448 G2449 N2450 V2451 D2455 M2456 S2457 A2458 K2465 I2478 Q2481 F2482 L2484
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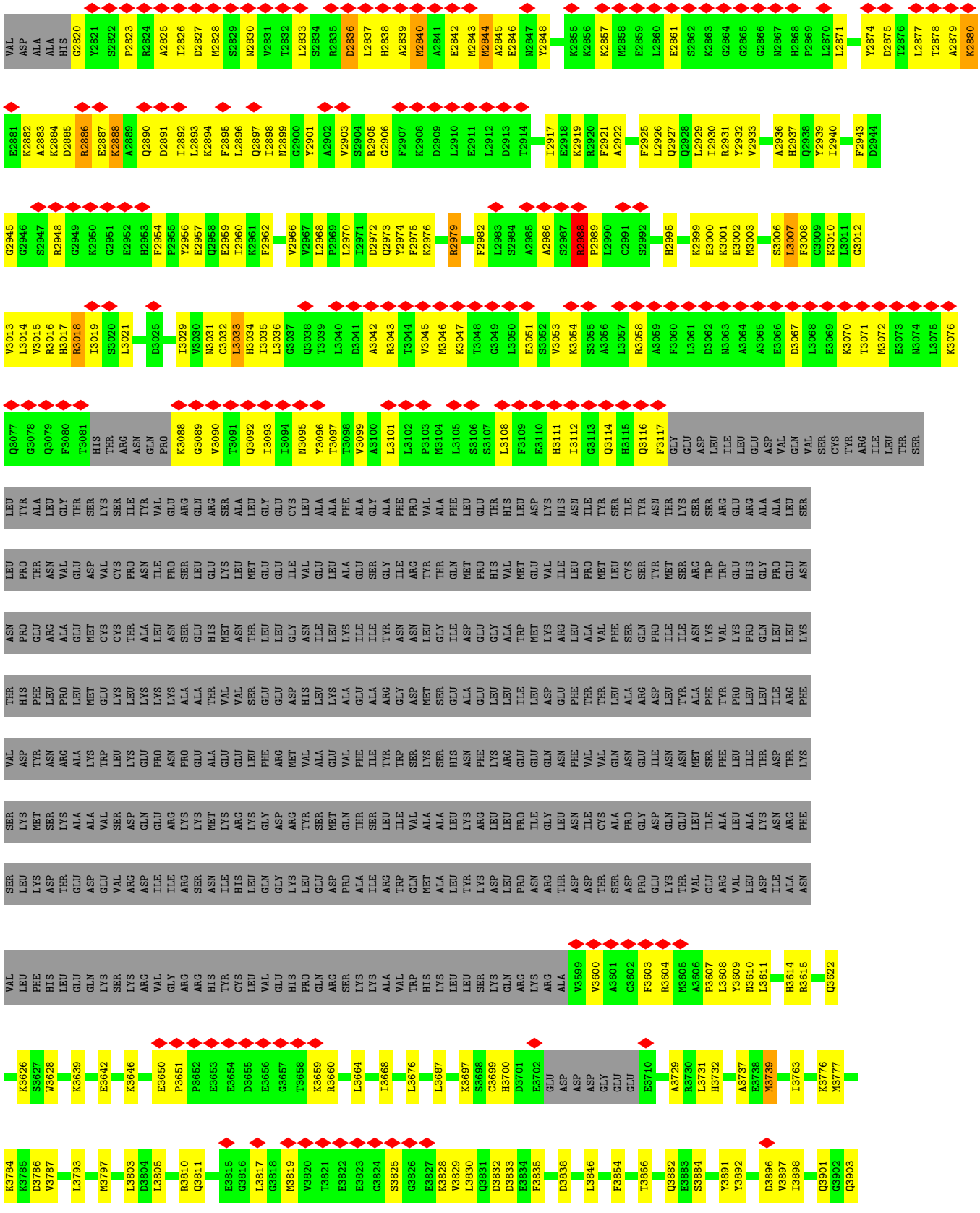
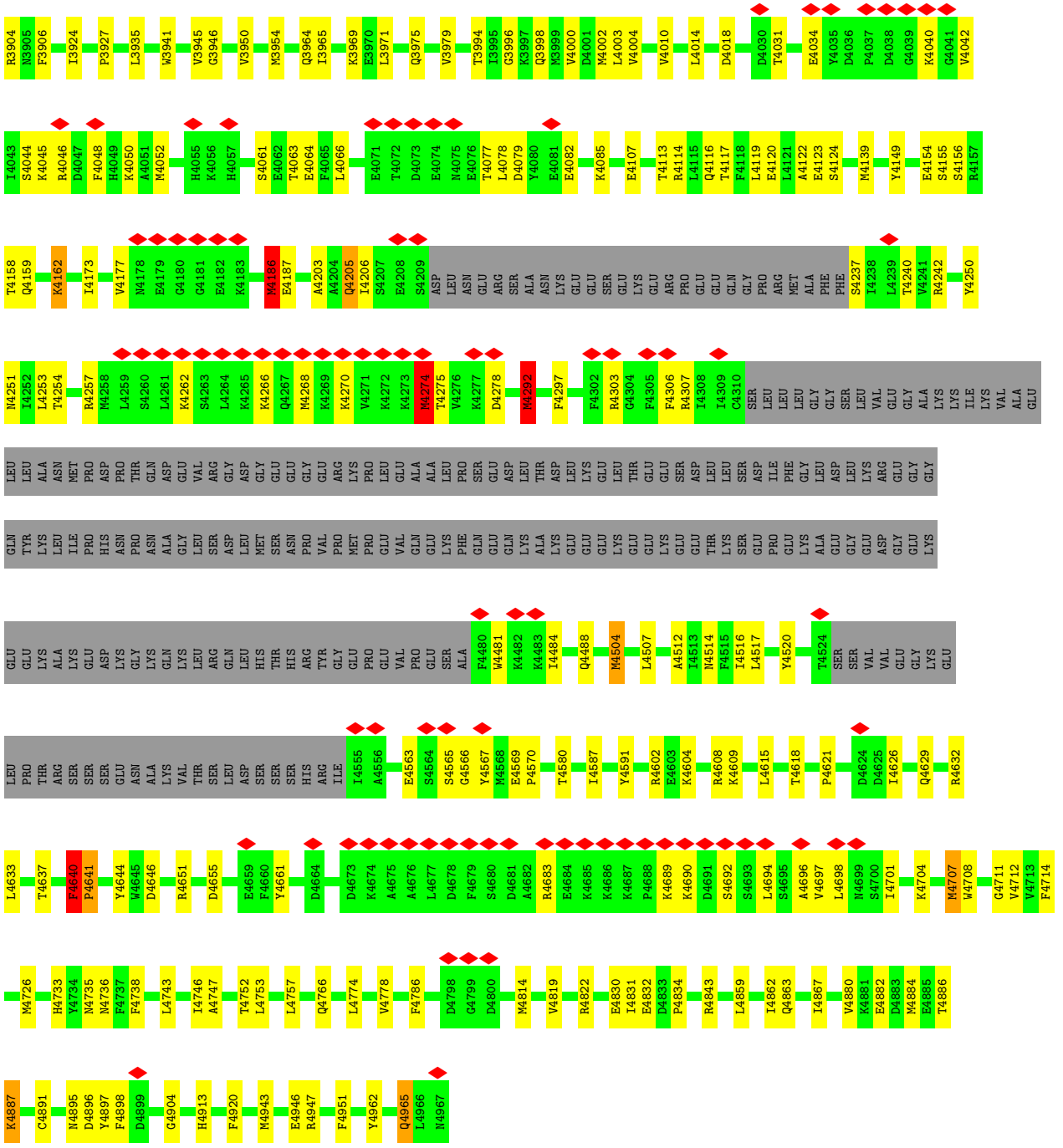
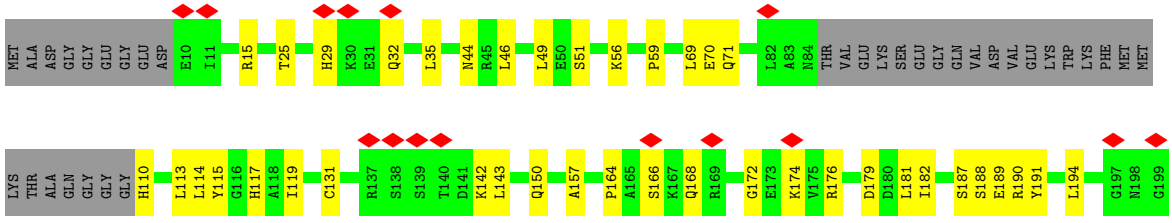
Y2620 L2623 P2624 G2625 G2626 W2627 A2632 E2635 L2638 S2641 R2642 K2643 L2644 F2649 D2650 A2651 Q2654 K2655 K2656 Y2657 E2658 Q2659 F2662 K2663 L2664 A2665 L2666 P2667 C2668 L2669 S2670 A2671 V2672 A2673 L2676 P2677 P2678 D2679 Y2680 M2681 E2682 S2683 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692
S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 P2720 I2721 N2722 K2723 Y2724 A2725 E2726 H2727 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 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

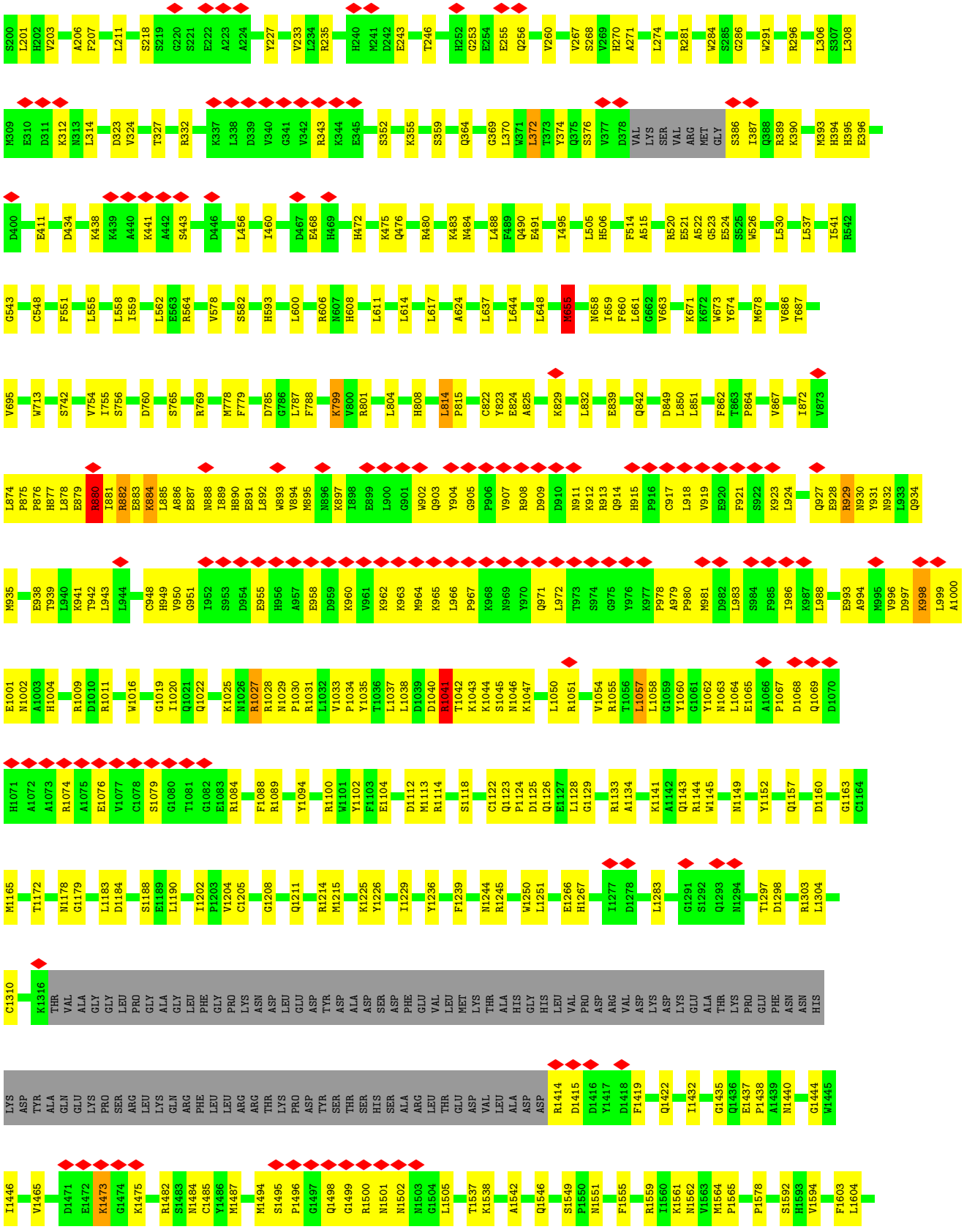




• Molecule 1: Ryanodine receptor 2

Chain D:

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L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 Q927 E928 R929 N930 Y931 N932 L933 Q934
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E1001 N1002 A1003 H1004 R1009 D1010 R1011 W1016 G1019 I1020 Q1021 Q1022 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 L1050 R1051 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070
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M1165 T1172 N1178 G1179 L1183 D1184 S1188 E1189 L1190 I1202 P1203 V1204 C1205 G1208 Q1211 R1214 M1215 K1225 Y1226 I1229 Y1236 F1239 N1244 R1245 W1250 L1251 E1266 H1267 I1277 D1278 L1283 G1291 S1292 Q1293 N1294 T1297 D1298 R1303 L1304
C1310 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU 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 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 Q1422 I1432 G1435 Q1436 E1437 P1438 A1439 N1440 G1444 W1445
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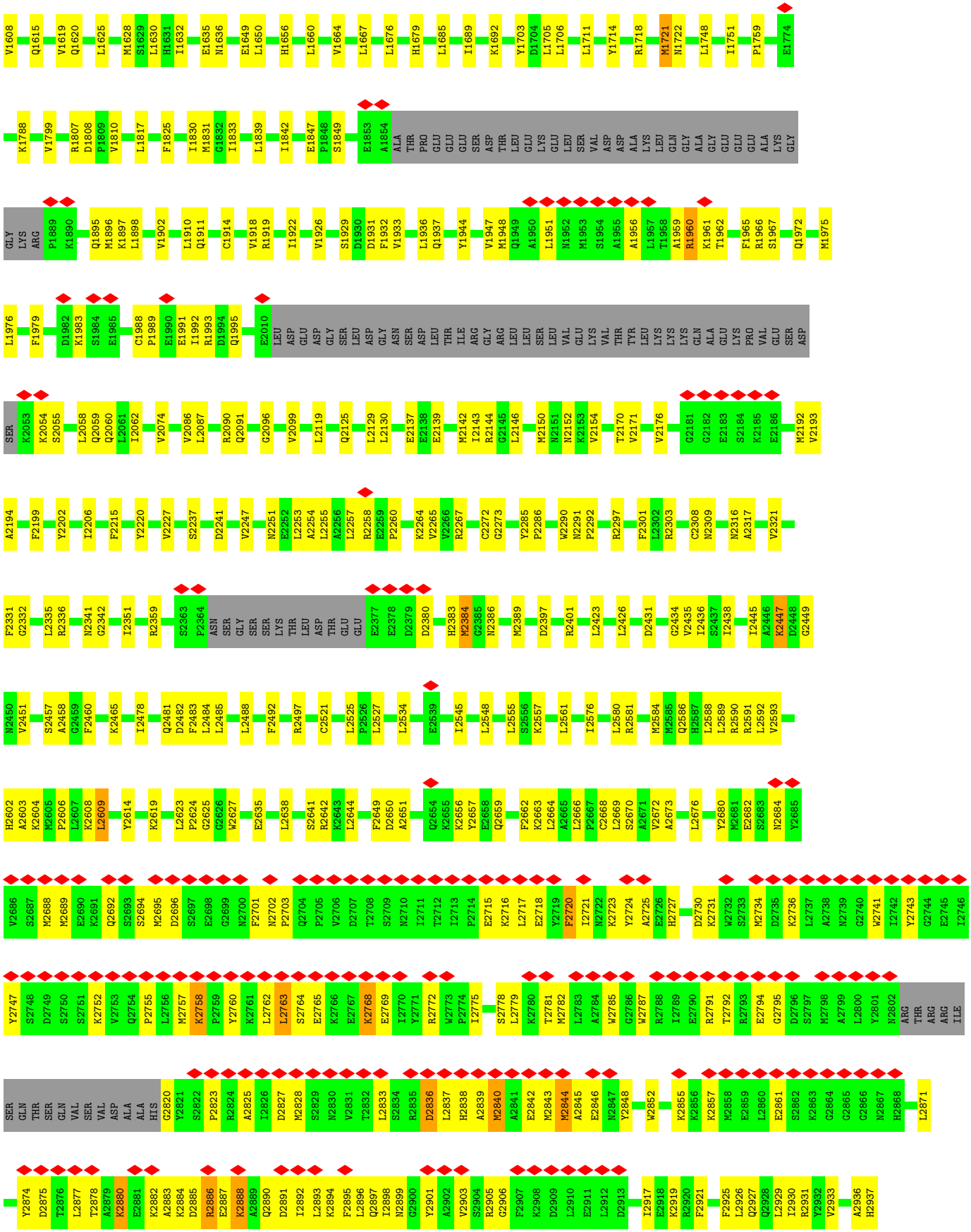
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GLY LYS ARG P1889 K1890 Q1895 M1896 K1897 L1898 V1902 L1910 Q1911 C1914 V1918 R1919 I1922 V1926 S1929 D1930 D1931 F1932 V1933 L1936 Q1937 Y1944 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 Q1972 M1975
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SER K2053 K2054 S2055 L2058 Q2059 Q2060 L2061 I2062 V2074 V2086 L2087 R2090 Q2091 G2096 V2099 L2119 Q2125 L2129 L2130 E2137 E2138 E2139 M2142 I2143 R2144 G2145 L2146 M2150 N2151 N2152 K2153 V2154 T2170 V2171 V2176 G2181 G2182 E2183 S2184 K2185 E2186 M2192 V2193
A2194 F2199 Y2202 I2206 F2215 Y2220 V2227 S2237 D2241 V2247 N2251 E2252 L2253 A2254 L2255 A2256 L2257 R2258 E2259 P2260 K2264 V2265 V2266 R2267 C2272 G2273 Y2285 P2286 W2290 N2291 P2292 R2297 F2301 L2302 R2303 C2308 N2309 N2316 A2317 V2321
F2331 G2332 L2335 R2336 N2341 G2342 I2351 R2359 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 G2385 N2386 M2389 D2397 R2401 L2423 L2426 D2431 G2434 V2435 I2436 S2437 I2438 I2445 A2446 K2447 D2448 G2449
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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 P3103 M3104 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 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 ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE 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 ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG

PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU 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 ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA

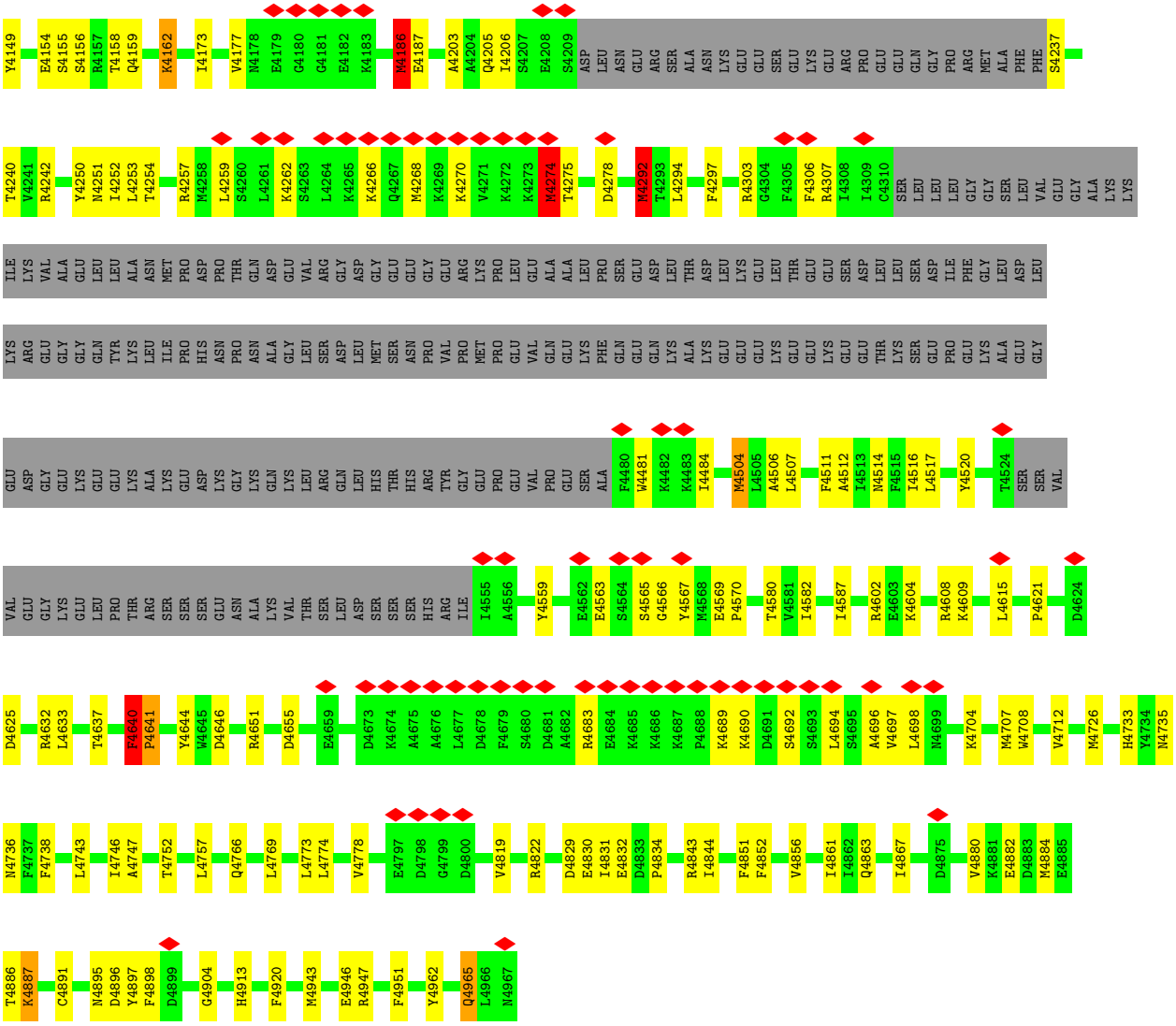
ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609 N3610 L3611 H3614 R3615

Q3622 K3626 S3627 W3628 K3639 E3642 K3646 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3664 I3668 L3676 L3687 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 A3729 R3730 L3731 H3732 A3737 E3738 M3739 K3776 M3777 K3784

K3785 D3786 V3787 L3793 M3797 L3803 D3804 L3805 R3810 Q3811 E3815 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 K3828 V3829 L3830 Q3831 D3832 D3833 E3834 F3835 L3846 F3854 T3866 Q3882 E3883 S3884 Y3891 Y3892 D3896 V3897 I3898 Q3901 G3902 Q3903 R3904 N3905 F3906

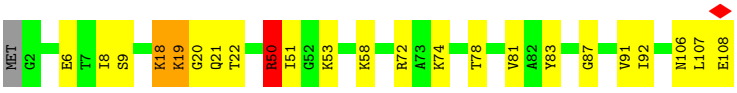
I3924 P3927 L3935 R3939 L3940 W3941 V3945 G3946 V3950 M3954 Q3964 I3965 K3969 E3970 L3971 Q3975 V3979 T3994 I3995 G3996 K3997 Q3998 M3999 V4000 D4001 M4002 L4003 V4004 V4010 L4014 D4018 K4022 L4026 D4030 T4031 F4032 K4033 E4034 Y4035 D4036 P4037 D4038

G4039 K4040 G4041 V4042 I4043 S4044 K4045 R4046 D4047 F4048 H4049 K4050 A4051 M4052 H4055 K4056 H4057 S4061 E4062 T4063 E4064 F4065 L4066 E4071 T4072 D4073 E4074 N4075 E4076 T4077 L4078 D4079 Y4080 E4081 E4082 K4085 L4105 S4106 E4107 T4113 R4114 L4115 Q4116 T4117 F4118 L4119 E4120 L4121 A4122 E4123 S4124 M4139



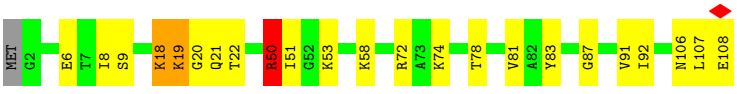
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



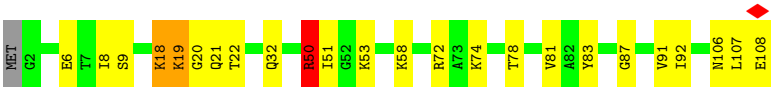
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



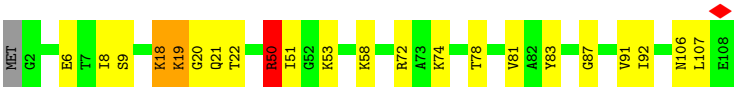
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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	149448	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	0.599	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.007	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, ATP, CA

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	0/32738	0.53	16/44213 (0.0%)
1	B	0.26	0/32738	0.53	16/44213 (0.0%)
1	C	0.26	0/32738	0.53	16/44213 (0.0%)
1	D	0.26	0/32738	0.53	16/44213 (0.0%)
2	E	0.30	0/834	0.61	2/1123 (0.2%)
2	F	0.30	0/834	0.61	2/1123 (0.2%)
2	G	0.30	0/834	0.61	2/1123 (0.2%)
2	H	0.30	0/834	0.61	2/1123 (0.2%)
All	All	0.26	0/134288	0.53	72/181344 (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	4
1	B	0	4
1	C	0	4
1	D	0	4
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	24

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4274	MET	CB-CG-SD	7.23	134.10	112.40
1	B	4274	MET	CB-CG-SD	7.23	134.10	112.40
1	C	4274	MET	CB-CG-SD	7.23	134.09	112.40
1	D	4274	MET	CB-CG-SD	7.23	134.09	112.40
2	F	50	ARG	CA-CB-CG	6.99	128.78	113.40

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2827	ASP	Peptide
1	A	4640	PHE	Peptide
1	A	880	ARG	Sidechain,Peptide
2	E	50	ARG	Sidechain,Peptide
2	F	50	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	32032	0	31689	797	0
1	B	32032	0	31689	795	0
1	C	32032	0	31689	816	0
1	D	32032	0	31689	797	0
2	E	818	0	821	19	0
2	F	818	0	821	17	0
2	G	818	0	821	18	0
2	H	818	0	821	15	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	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	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	3207	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 3207 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4237:SER:N	1:B:4240:THR:HG1	1.59	1.01
1:D:4237:SER:N	1:D:4240:THR:HG1	1.59	0.99
1:C:4814:MET:HE1	1:D:4844:ILE:HG21	1.44	0.97
1:A:4237:SER:N	1:A:4240:THR:HG1	1.63	0.96
1:C:4237:SER:N	1:C:4240:THR:HG1	1.61	0.95

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%)	3852 (97%)	123 (3%)	3 (0%)	51	81
1	B	3978/4967 (80%)	3852 (97%)	123 (3%)	3 (0%)	51	81
1	C	3978/4967 (80%)	3851 (97%)	124 (3%)	3 (0%)	51	81
1	D	3978/4967 (80%)	3850 (97%)	125 (3%)	3 (0%)	51	81
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	16332/20300 (80%)	15805 (97%)	515 (3%)	12 (0%)	54 81

5 of 12 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%)	3452 (98%)	61 (2%)	60 78
1	B	3513/4358 (81%)	3452 (98%)	61 (2%)	60 78
1	C	3513/4358 (81%)	3452 (98%)	61 (2%)	60 78
1	D	3513/4358 (81%)	3452 (98%)	61 (2%)	60 78
2	E	88/89 (99%)	85 (97%)	3 (3%)	37 65
2	F	88/89 (99%)	85 (97%)	3 (3%)	37 65
2	G	88/89 (99%)	85 (97%)	3 (3%)	37 65
2	H	88/89 (99%)	85 (97%)	3 (3%)	37 65
All	All	14404/17788 (81%)	14148 (98%)	256 (2%)	61 78

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2886	ARG
1	D	3033	LEU
1	B	2656	LYS
1	B	2447	LYS
1	D	4066	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3811	GLN
1	D	1452	GLN
1	C	888	ASN
1	D	1046	ASN
1	D	3903	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	A	5004	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	D	5002	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
4	ATP	A	5002	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
4	ATP	B	5004	-	26,33,33	0.61	0	31,52,52	0.73	2 (6%)
4	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
4	ATP	C	5004	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	D	5004	-	26,33,33	0.58	0	31,52,52	0.73	2 (6%)
4	ATP	B	5002	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)

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	A	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	B	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	D	5004	-	-	6/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5004	ATP	C5-C6-N6	2.33	123.90	120.35
4	A	5004	ATP	C5-C6-N6	2.31	123.86	120.35
4	D	5002	ATP	C5-C6-N6	2.30	123.85	120.35
4	B	5004	ATP	C5-C6-N6	2.30	123.85	120.35
4	B	5002	ATP	C5-C6-N6	2.30	123.84	120.35

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	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C3'-C4'-C5'-O5'
4	A	5004	ATP	C5'-O5'-PA-O3A

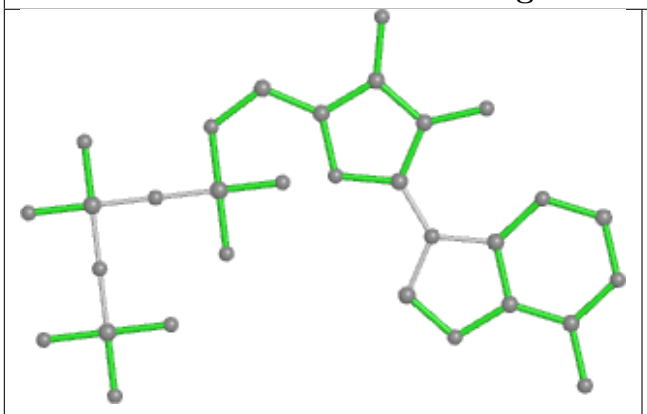
There are no ring outliers.

4 monomers are involved in 8 short contacts:

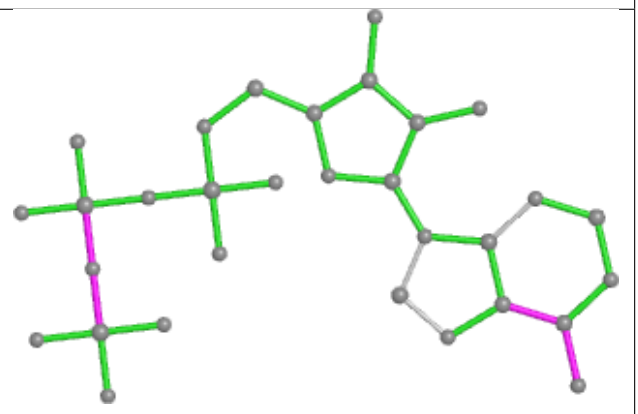
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5004	ATP	2	0
4	B	5004	ATP	2	0
4	C	5004	ATP	2	0
4	D	5004	ATP	2	0

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

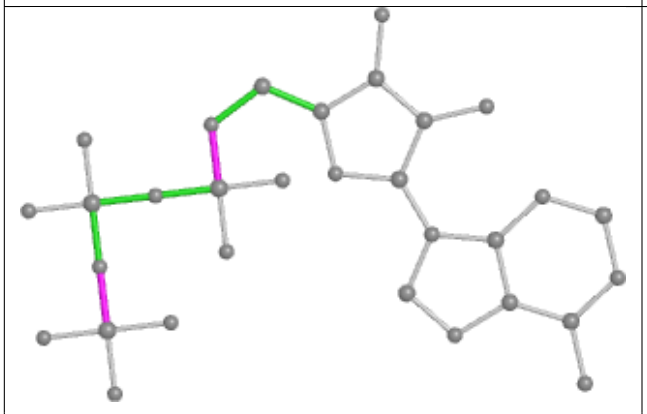
Ligand ATP A 5004



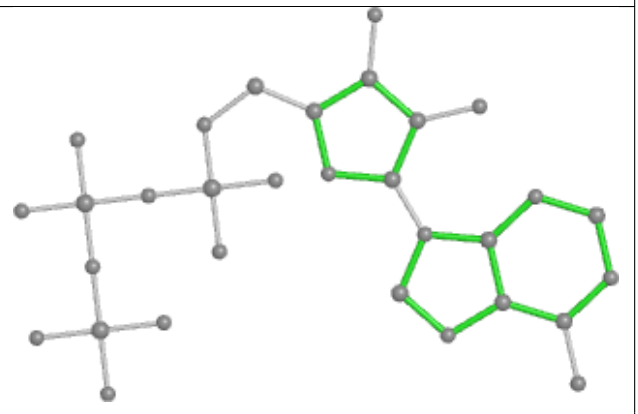
Bond lengths



Bond angles

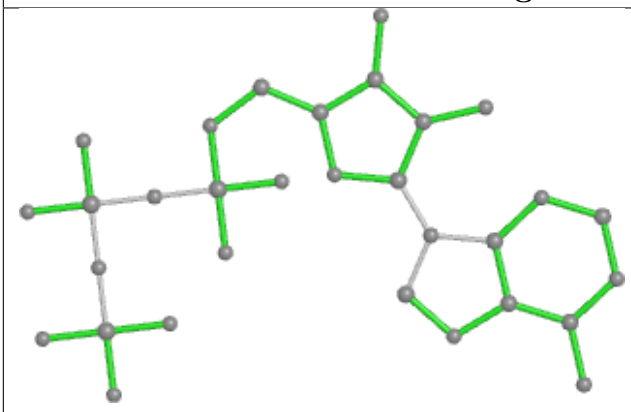


Torsions

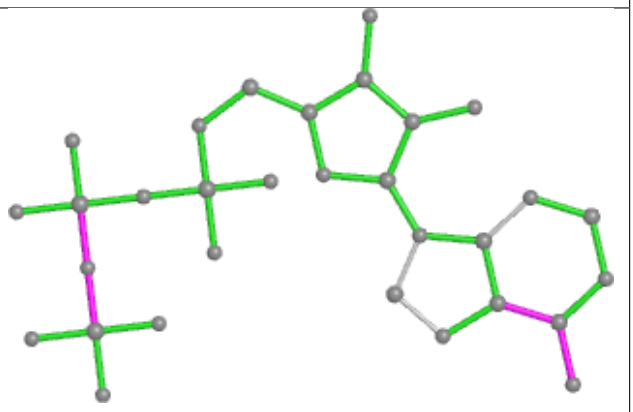


Rings

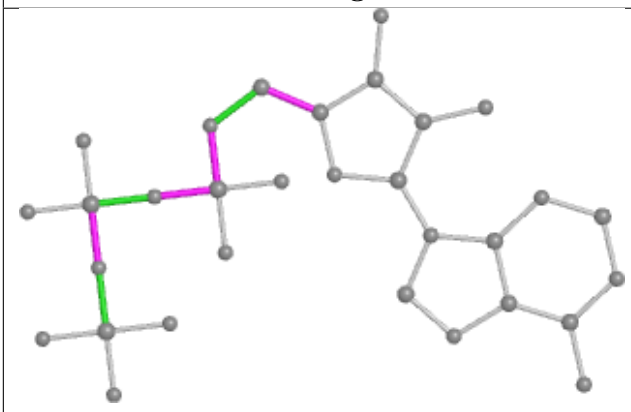
Ligand ATP D 5002



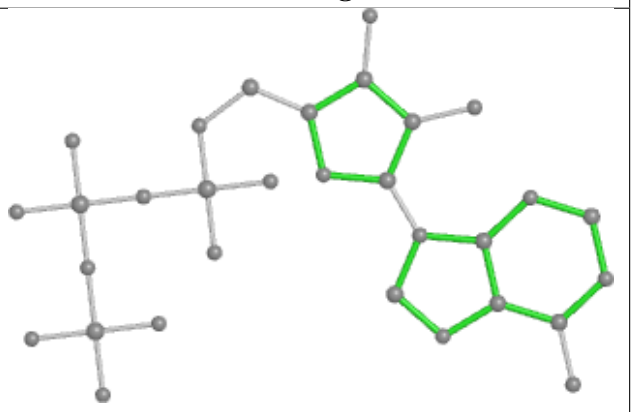
Bond lengths



Bond angles

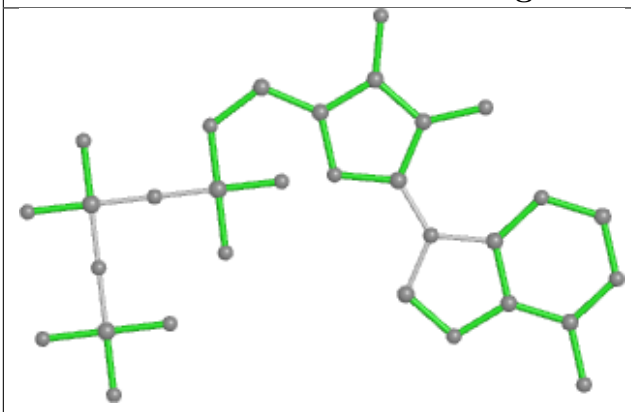


Torsions

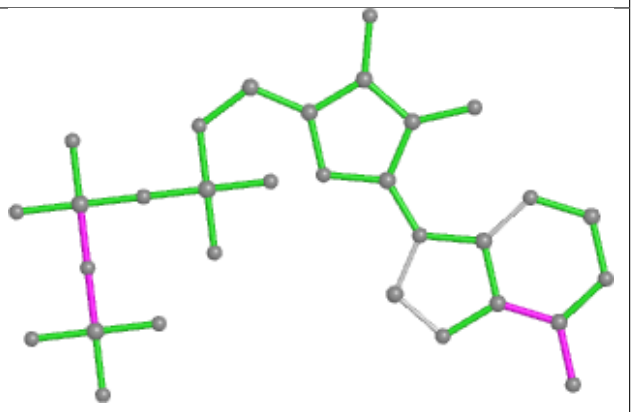


Rings

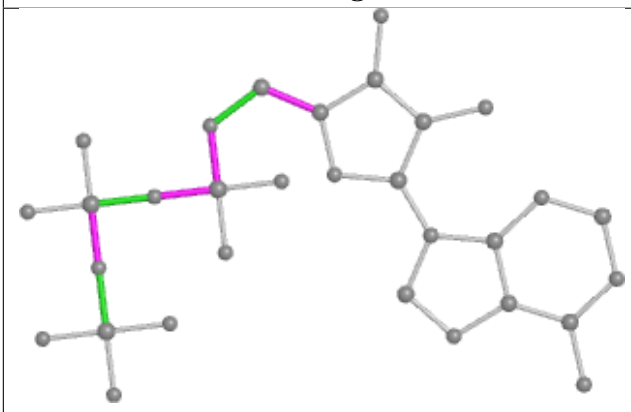
Ligand ATP A 5002



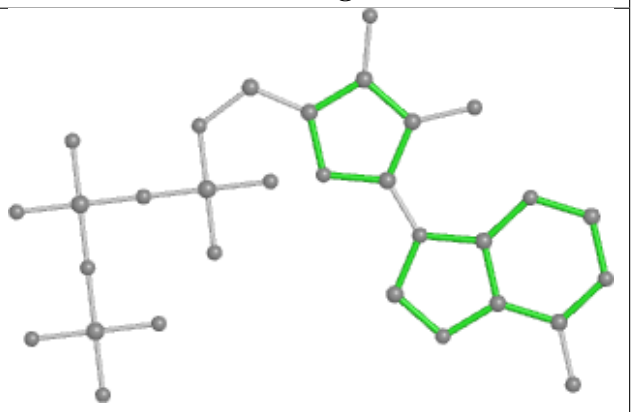
Bond lengths



Bond angles

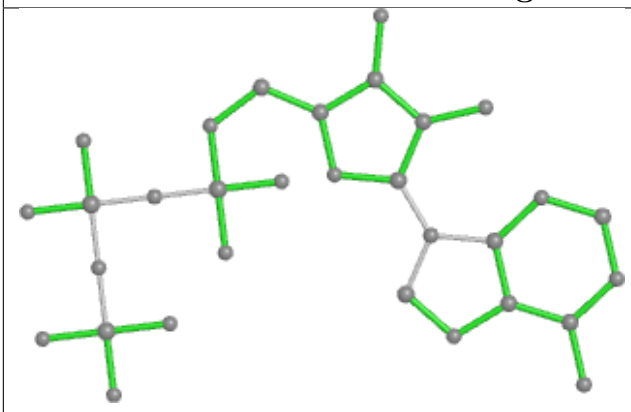


Torsions

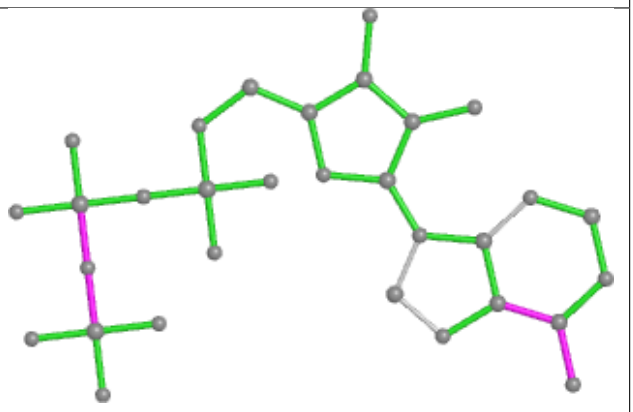


Rings

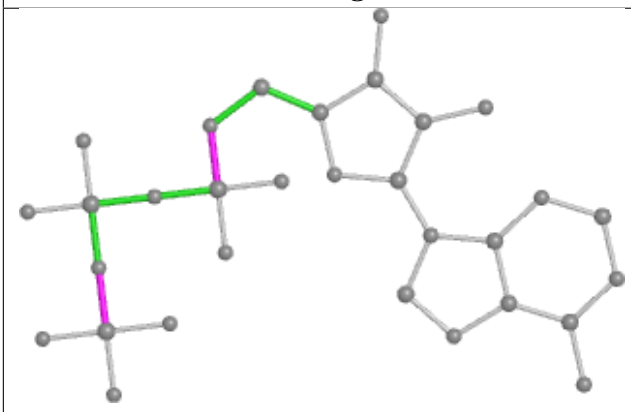
Ligand ATP B 5004



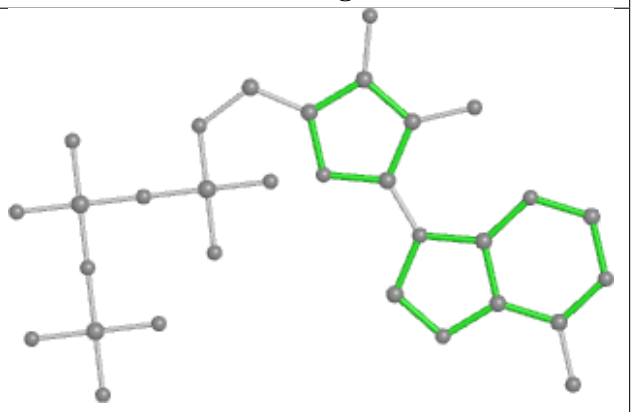
Bond lengths



Bond angles

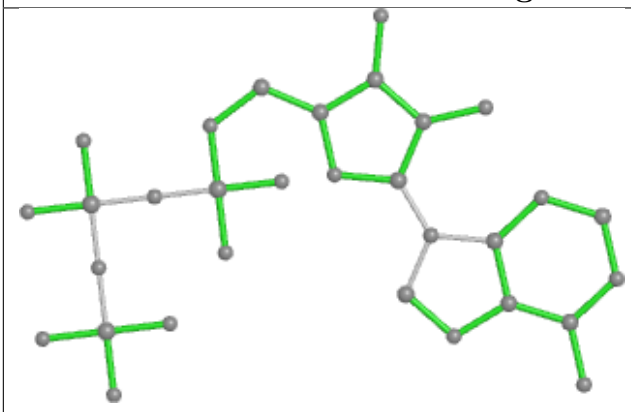


Torsions

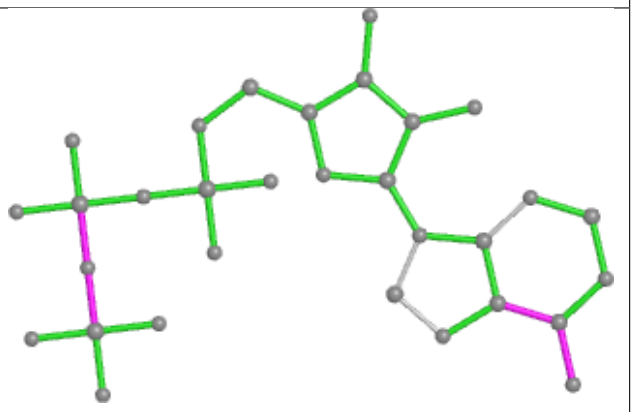


Rings

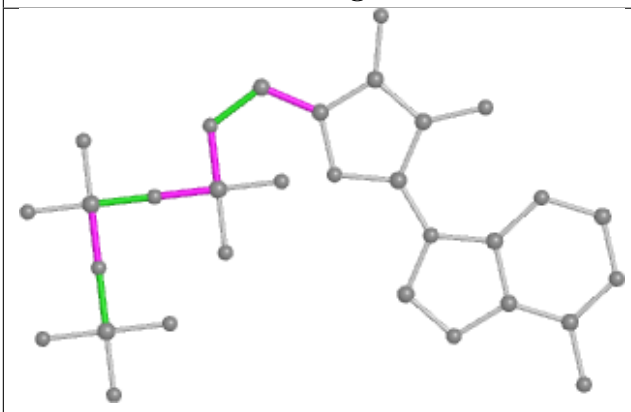
Ligand ATP C 5002



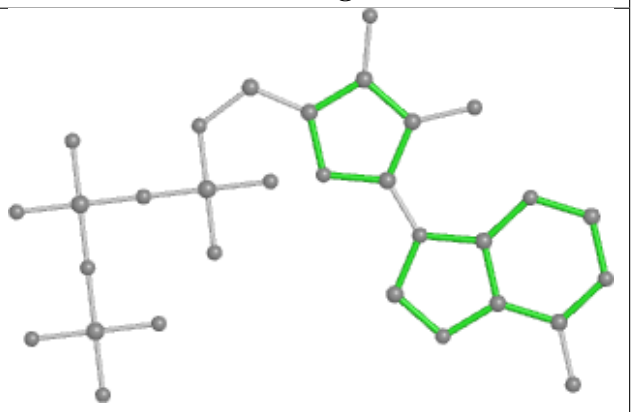
Bond lengths



Bond angles

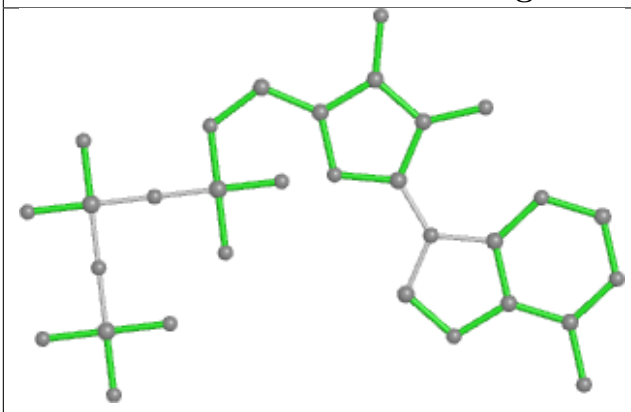


Torsions

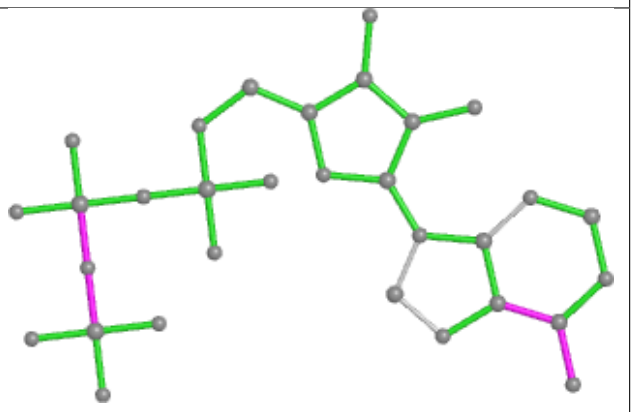


Rings

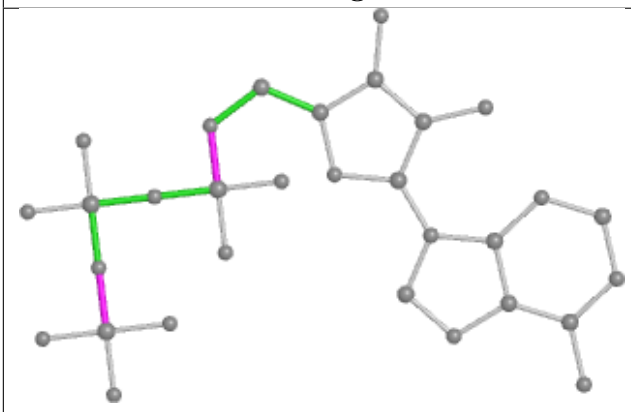
Ligand ATP C 5004



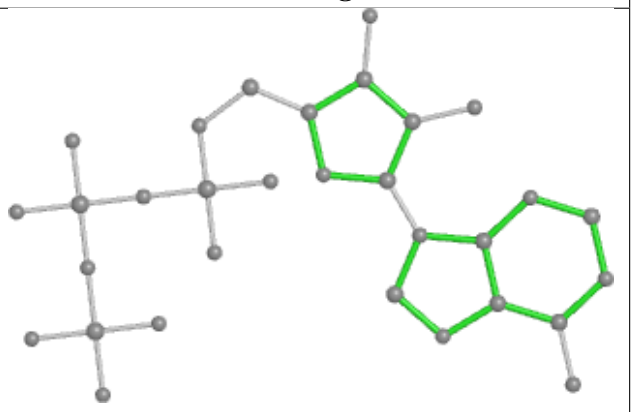
Bond lengths



Bond angles

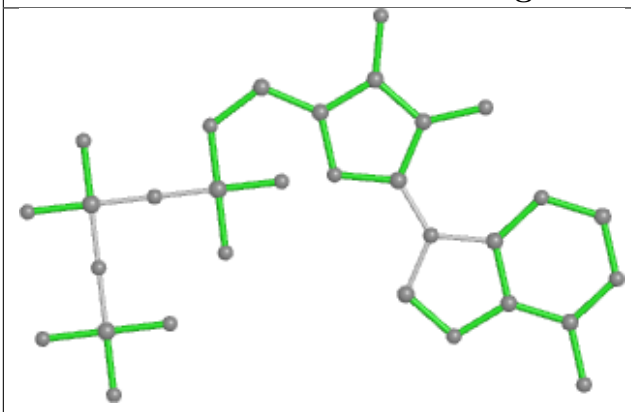


Torsions

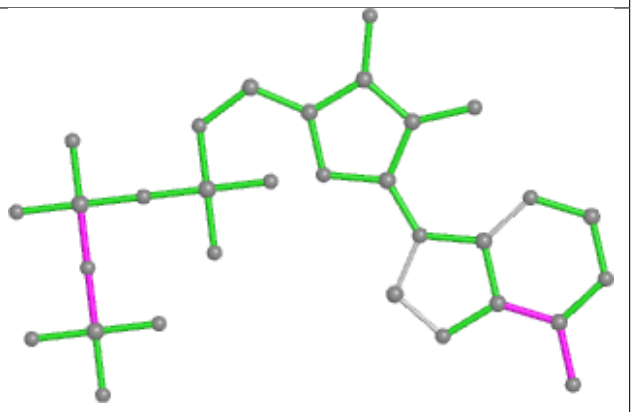


Rings

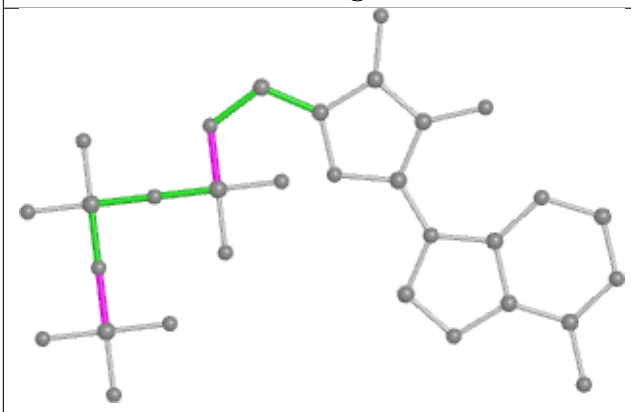
Ligand ATP D 5004



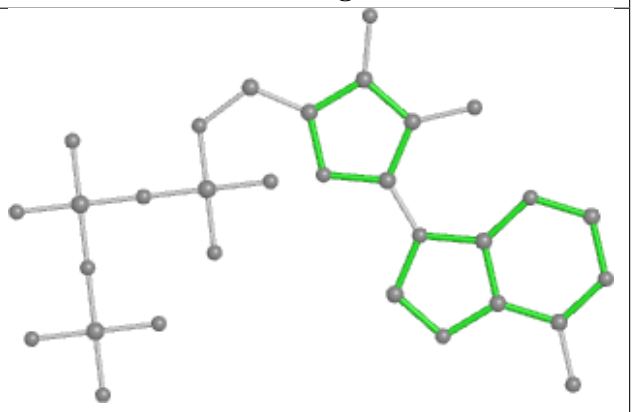
Bond lengths



Bond angles

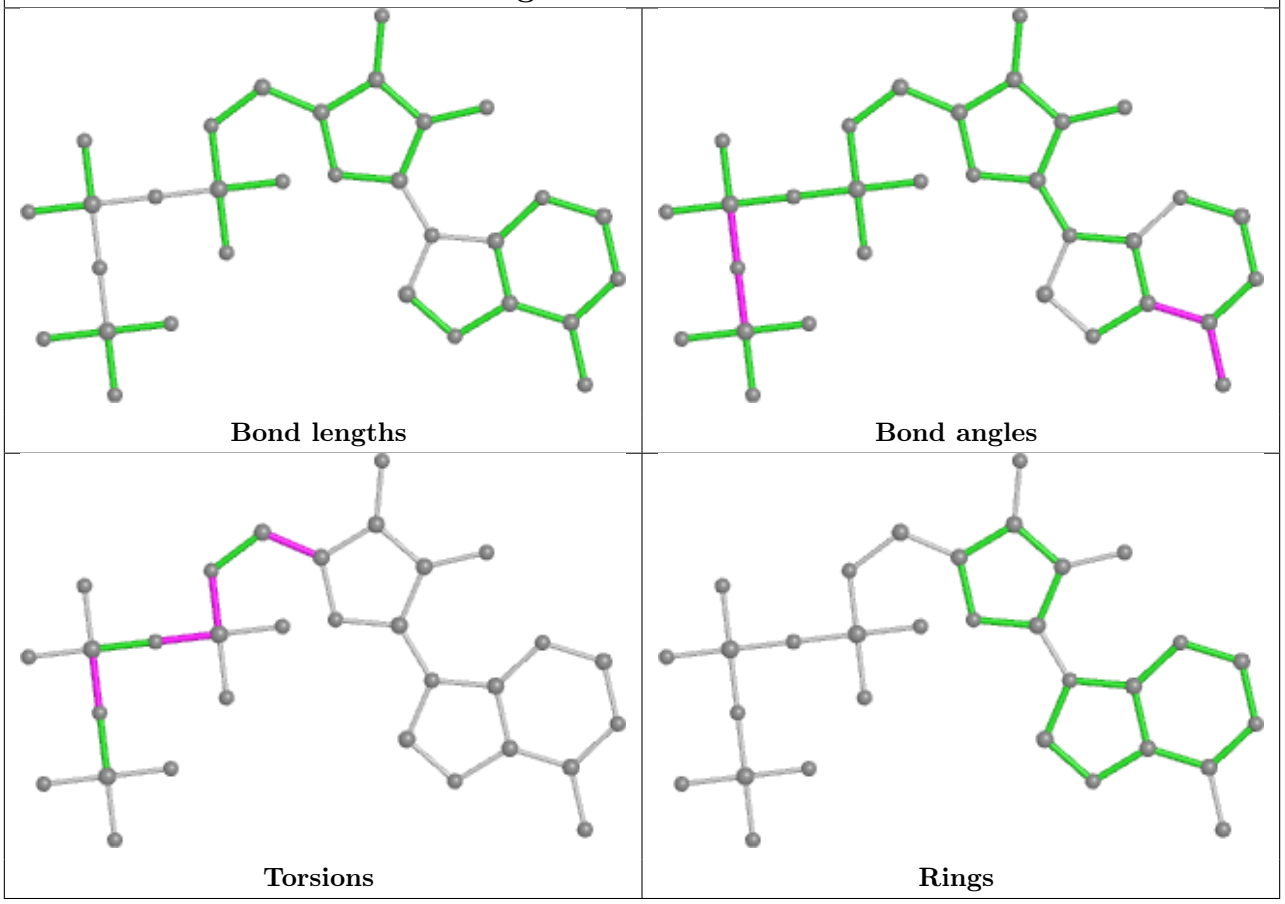


Torsions



Rings

Ligand ATP B 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.

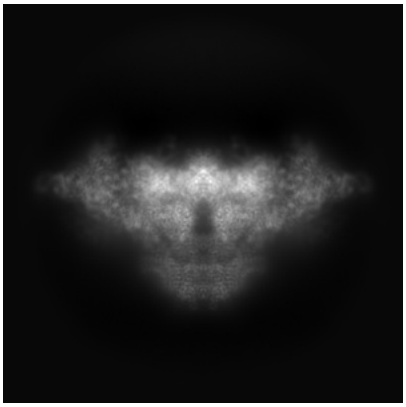
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42765. These allow visual inspection of the internal detail of the map and identification of artifacts.

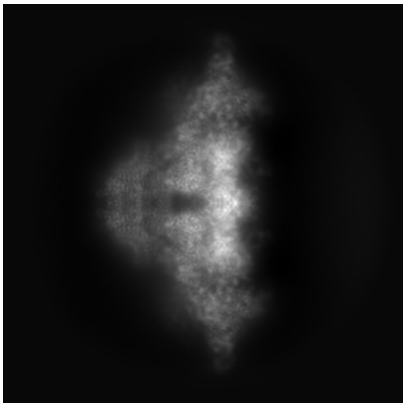
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

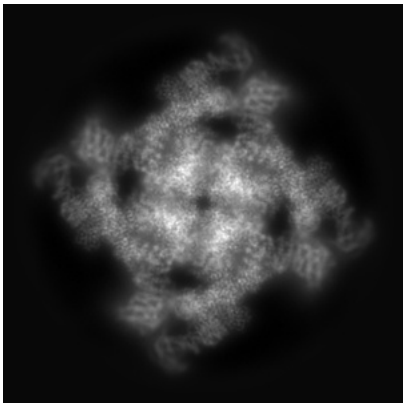
6.1.1 Primary map



X



Y



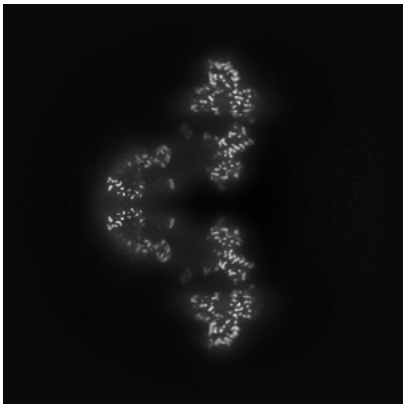
Z

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

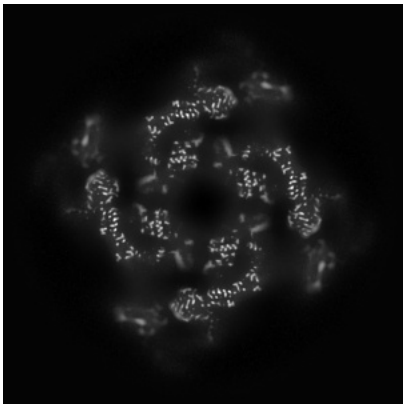
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

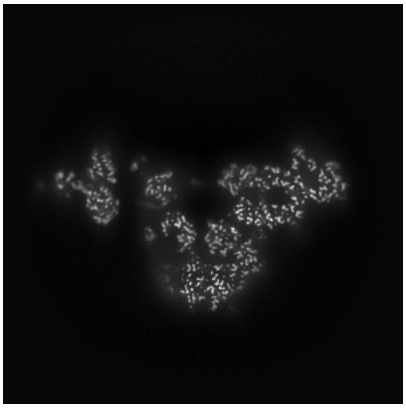


Z Index: 256

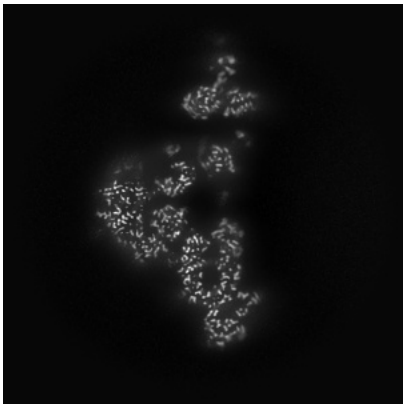
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

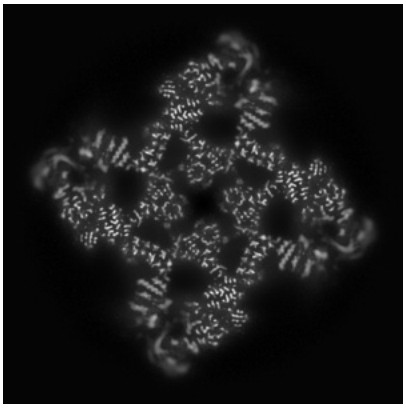
6.3.1 Primary map



X Index: 239



Y Index: 239



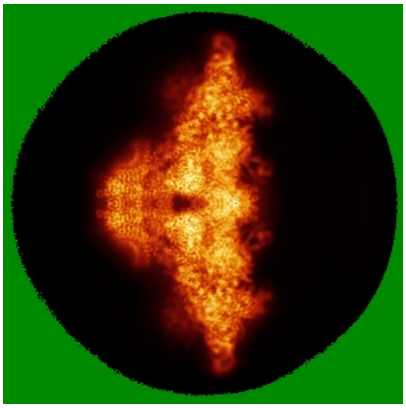
Z Index: 277

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

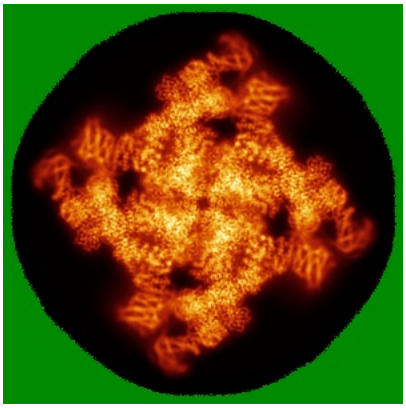
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

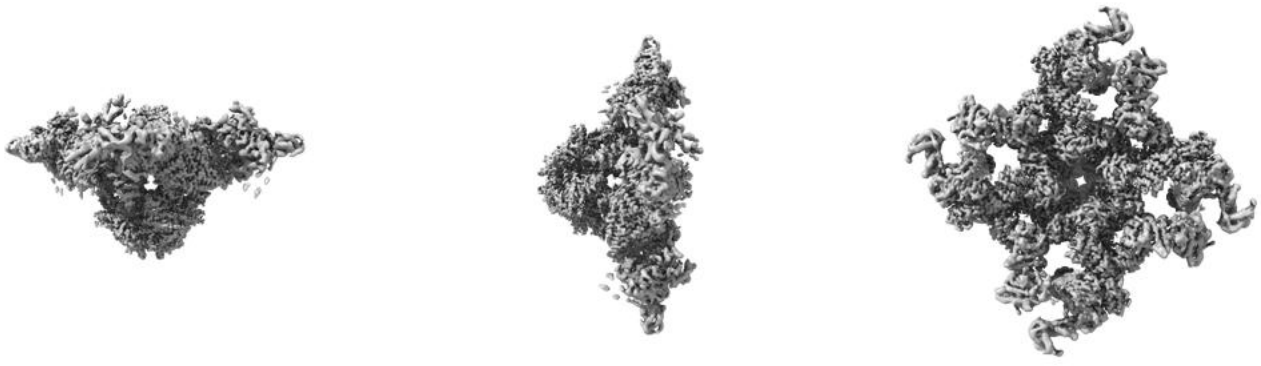


Z

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.

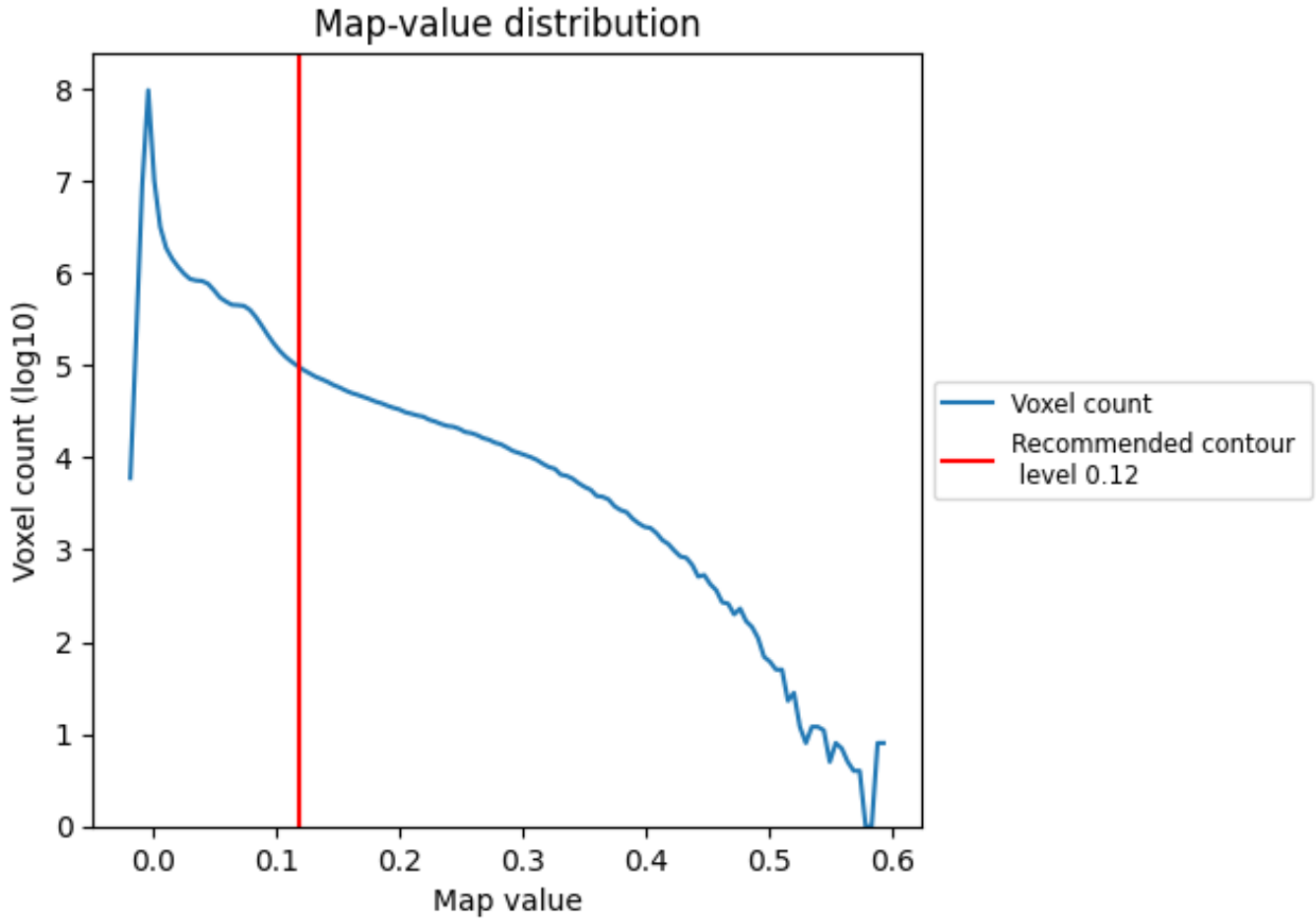
6.6 Mask visualisation (i)

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

7 Map analysis

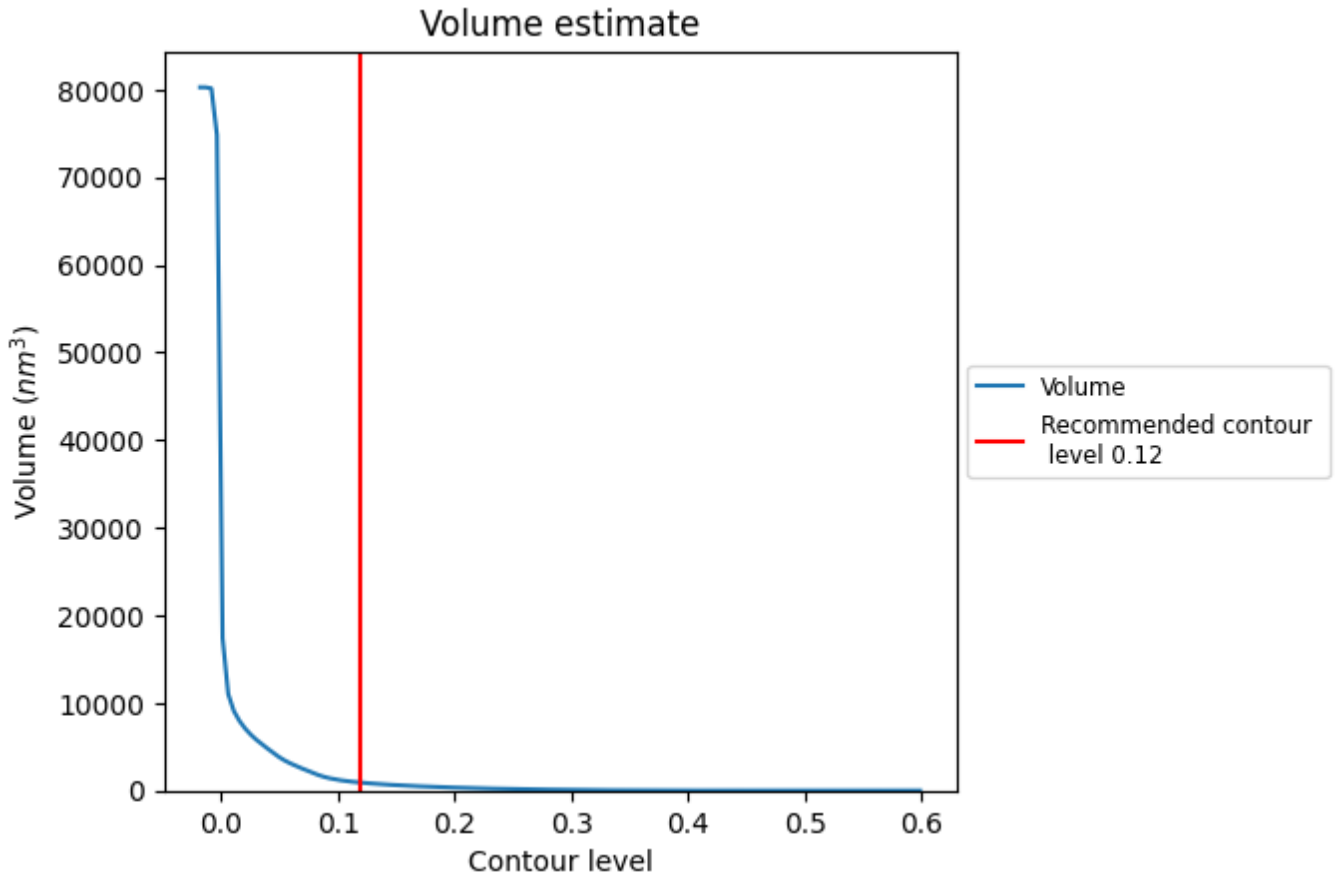
This section contains the results of statistical analysis of the map.

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.

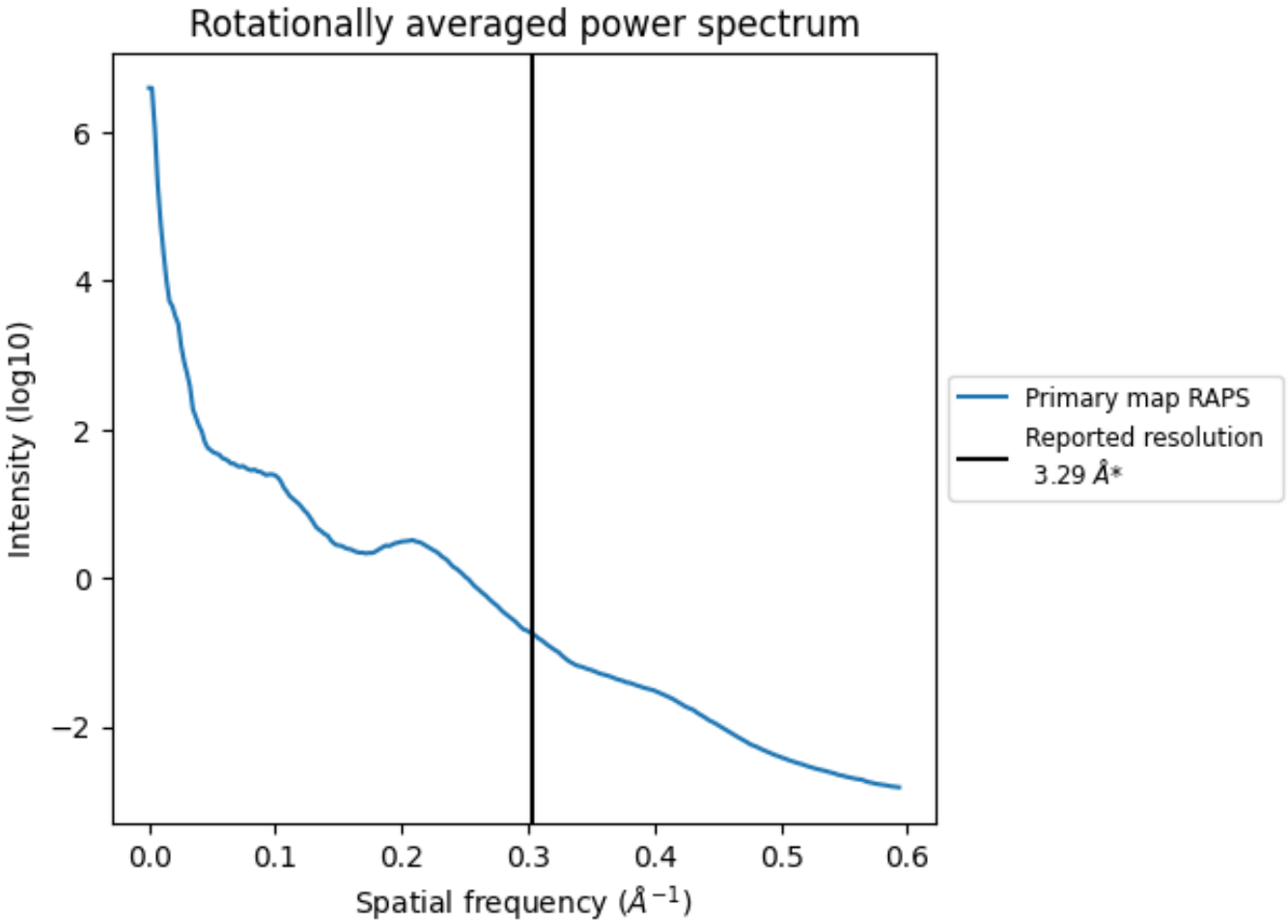
7.2 Volume estimate (i)



The volume at the recommended contour level is 906 nm^3; this corresponds to an approximate mass of 818 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 0.304 Å^{-1}

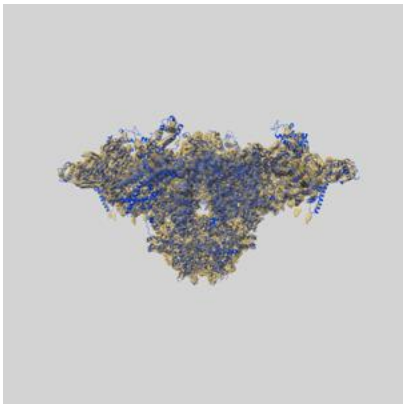
8 Fourier-Shell correlation (i)

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

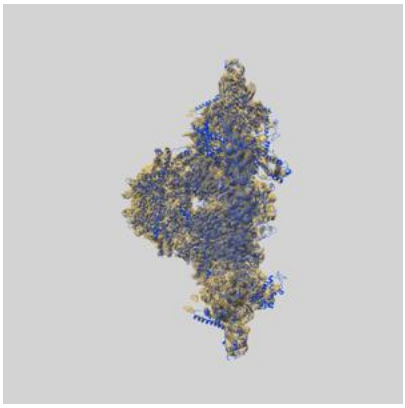
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42765 and PDB model 8UXI. Per-residue inclusion information can be found in section 3 on page 6.

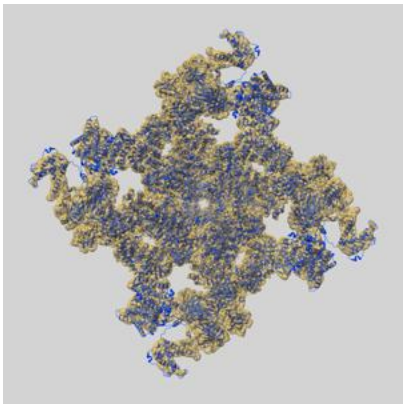
9.1 Map-model overlay



X



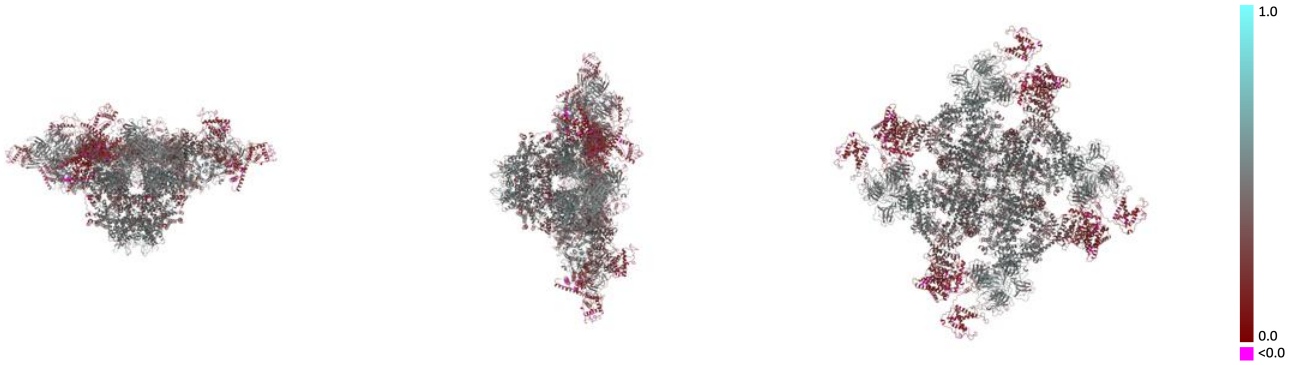
Y



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.

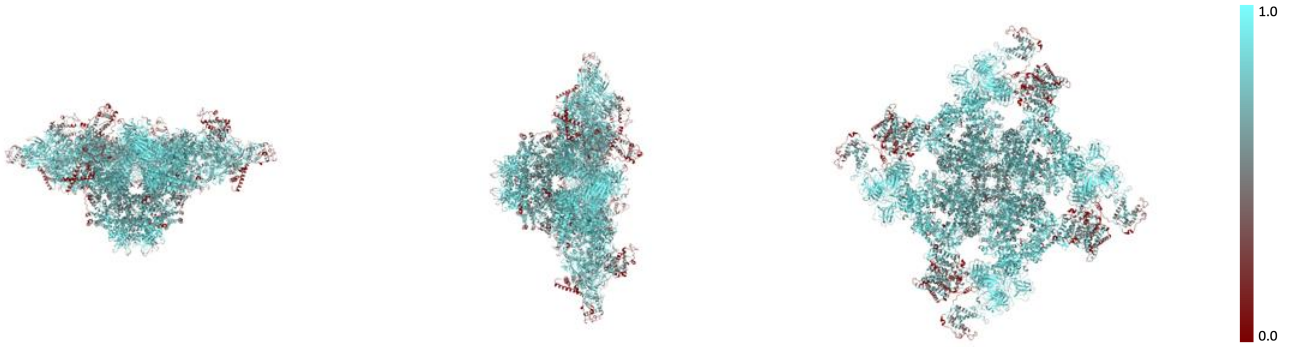
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

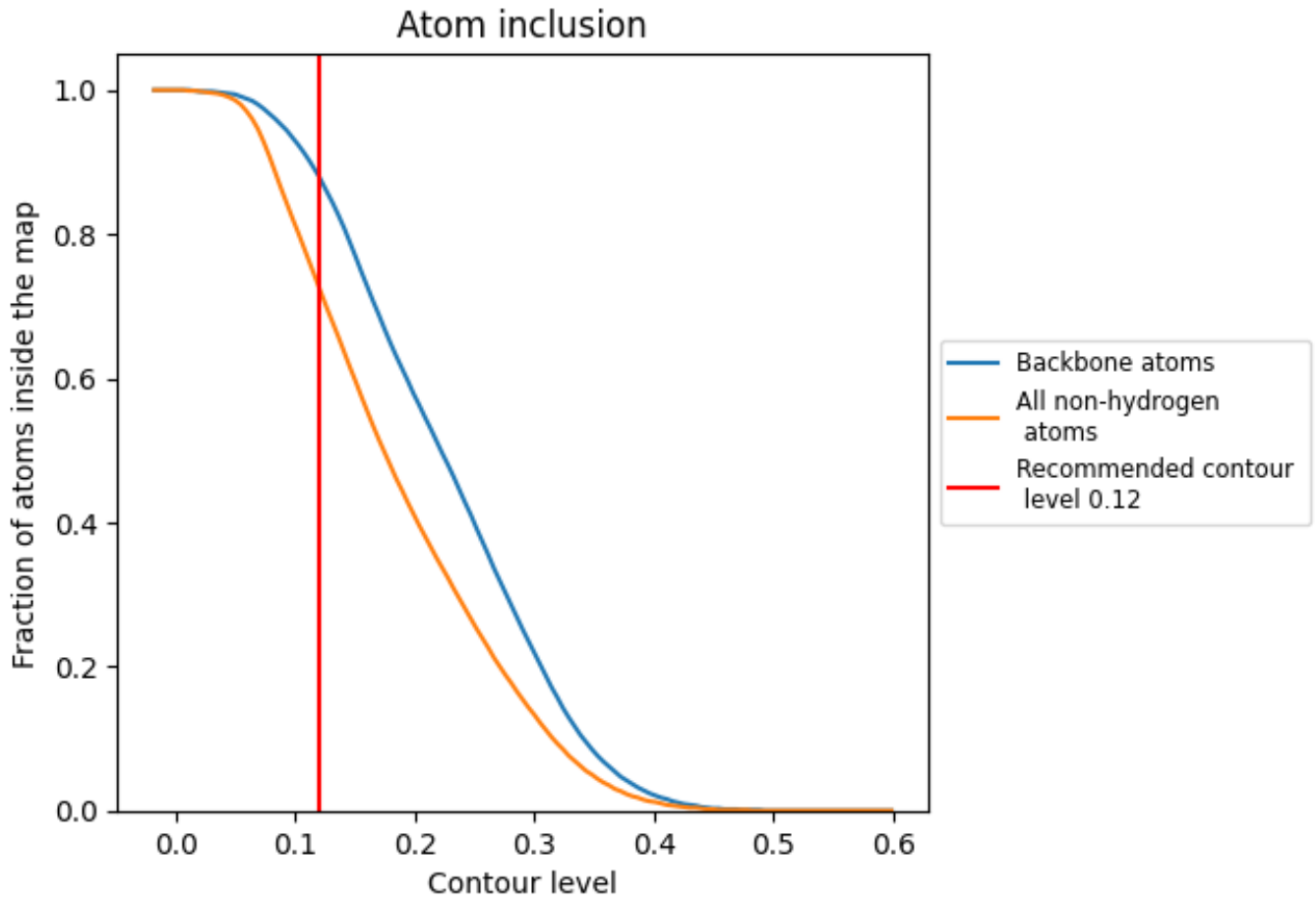
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.3900
A	0.7250	0.3900
B	0.7210	0.3840
C	0.7290	0.3950
D	0.7170	0.3790
E	0.8420	0.4870
F	0.8340	0.4830
G	0.8420	0.4880
H	0.8510	0.4860