wwPDB EM Validation Summary Report

Nov 14, 2023 – 03:27 PM EST

PDB ID	:	8UXC
EMDB ID	:	EMD-42759
Title	:	Structure of PKA phosphorylated human RyR2-R420Q in the primed state
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	2.86 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 ⓘ 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:

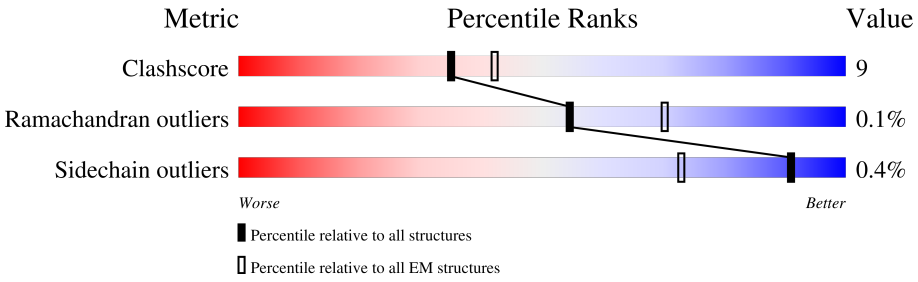
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.86 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	12% 67% 18% 15%
1	B	4967	12% 67% 18% 15%
1	C	4967	12% 67% 18% 15%
1	D	4967	12% 67% 18% 15%
2	E	108	82% 17%
2	F	108	85% 14%
2	G	108	84% 15%
2	H	108	82% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 138600 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 33769	C 21515	N 5743	O 6281	S 230	2	0
1	B	4224	Total 33769	C 21515	N 5743	O 6281	S 230	2	0
1	C	4224	Total 33769	C 21515	N 5743	O 6281	S 230	2	0
1	D	4224	Total 33769	C 21515	N 5743	O 6281	S 230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	engineered mutation	UNP Q92736
B	420	GLN	ARG	engineered mutation	UNP Q92736
C	420	GLN	ARG	engineered mutation	UNP Q92736
D	420	GLN	ARG	engineered mutation	UNP Q92736

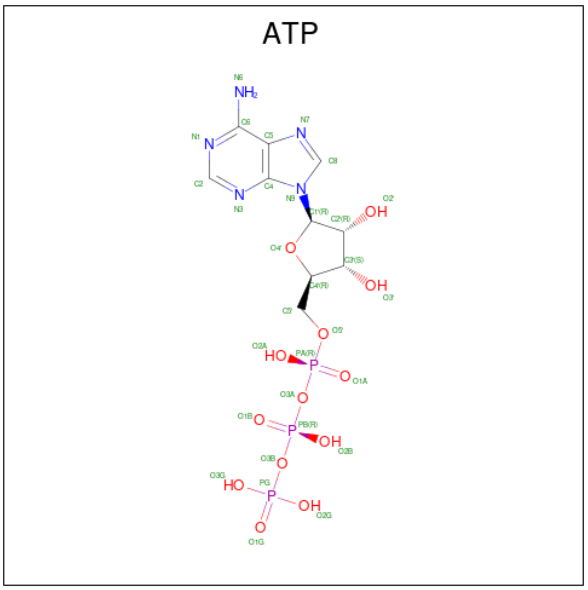
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

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

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

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



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

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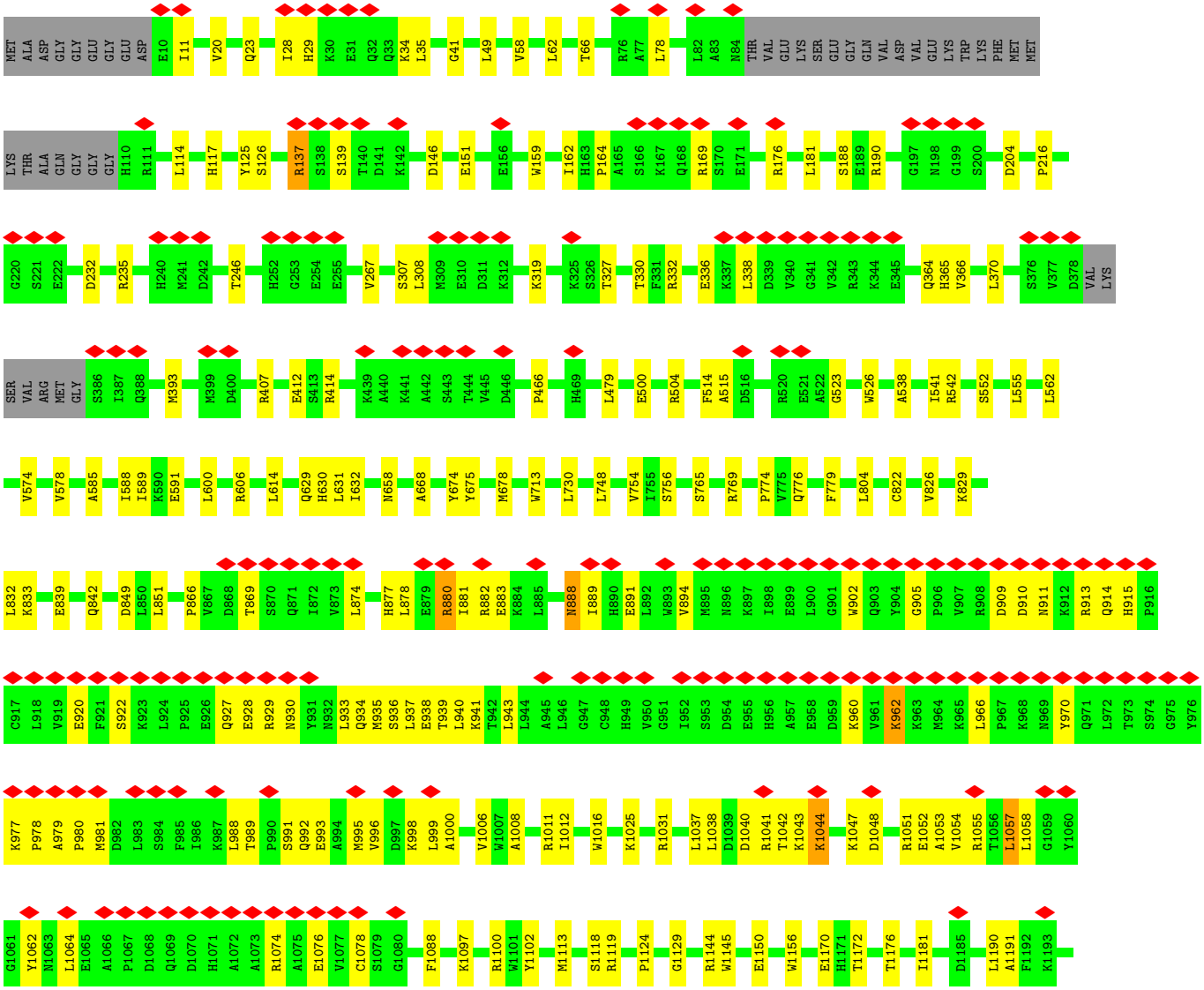
Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

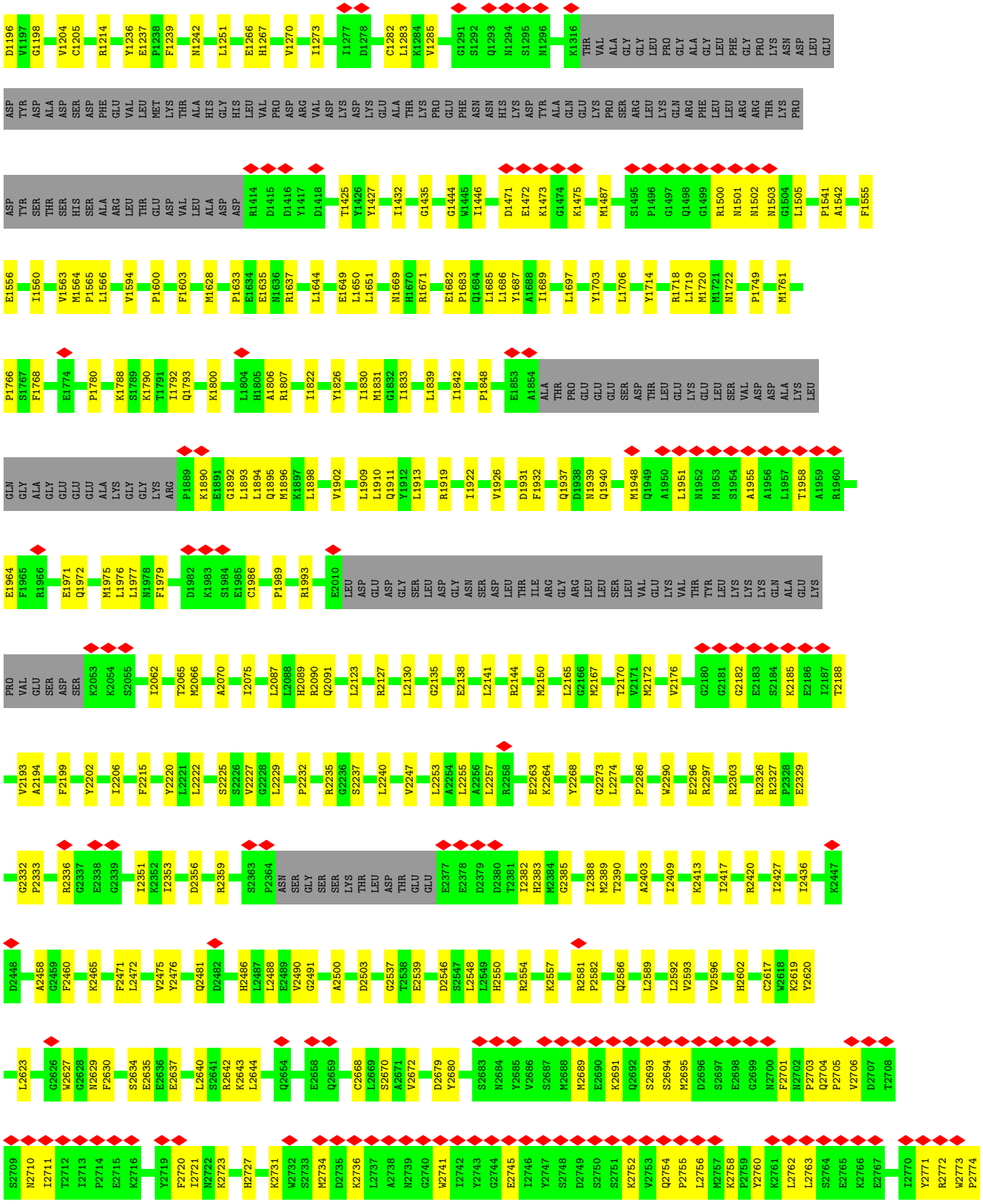
3 Residue-property plots (i)

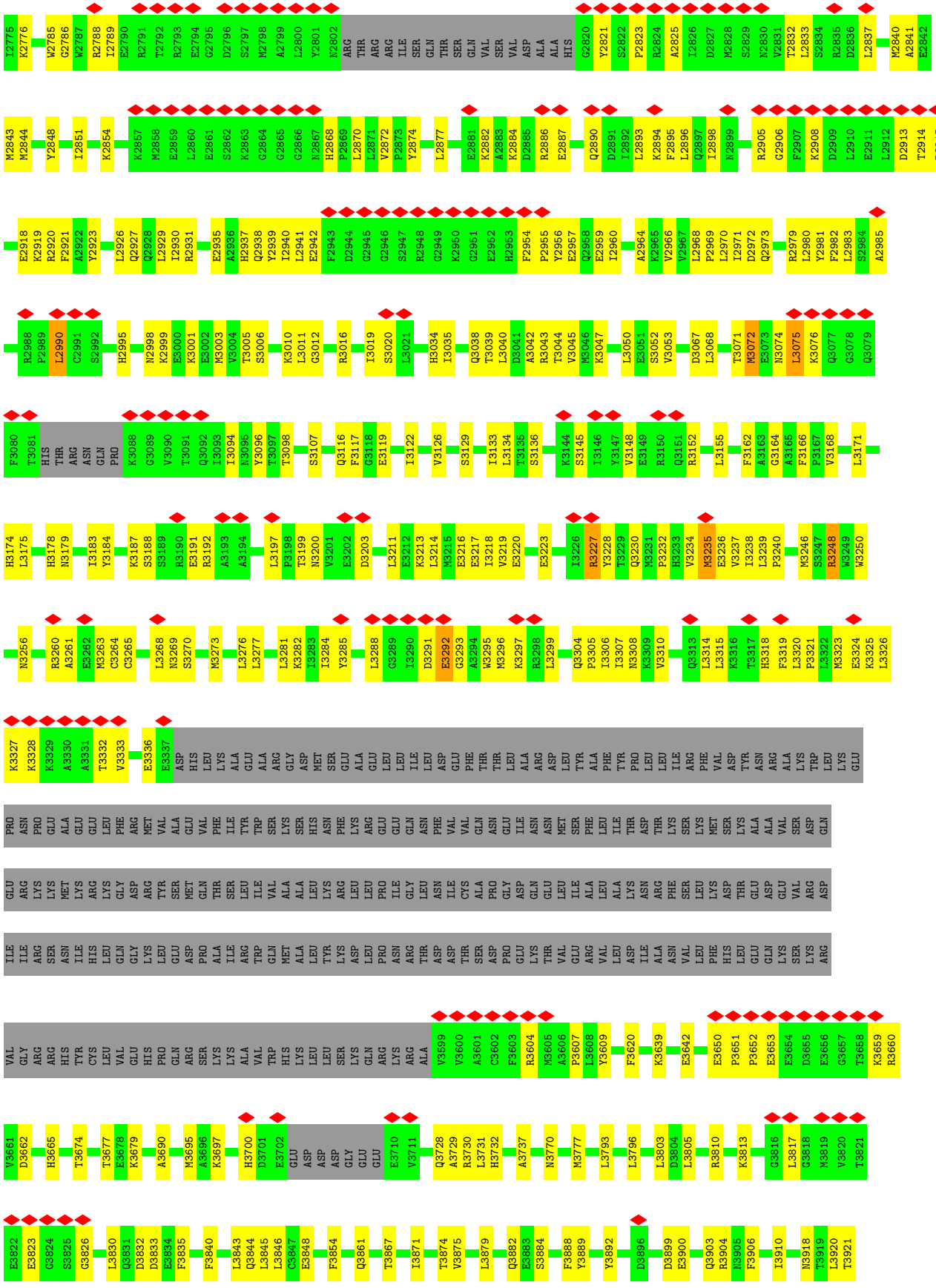
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

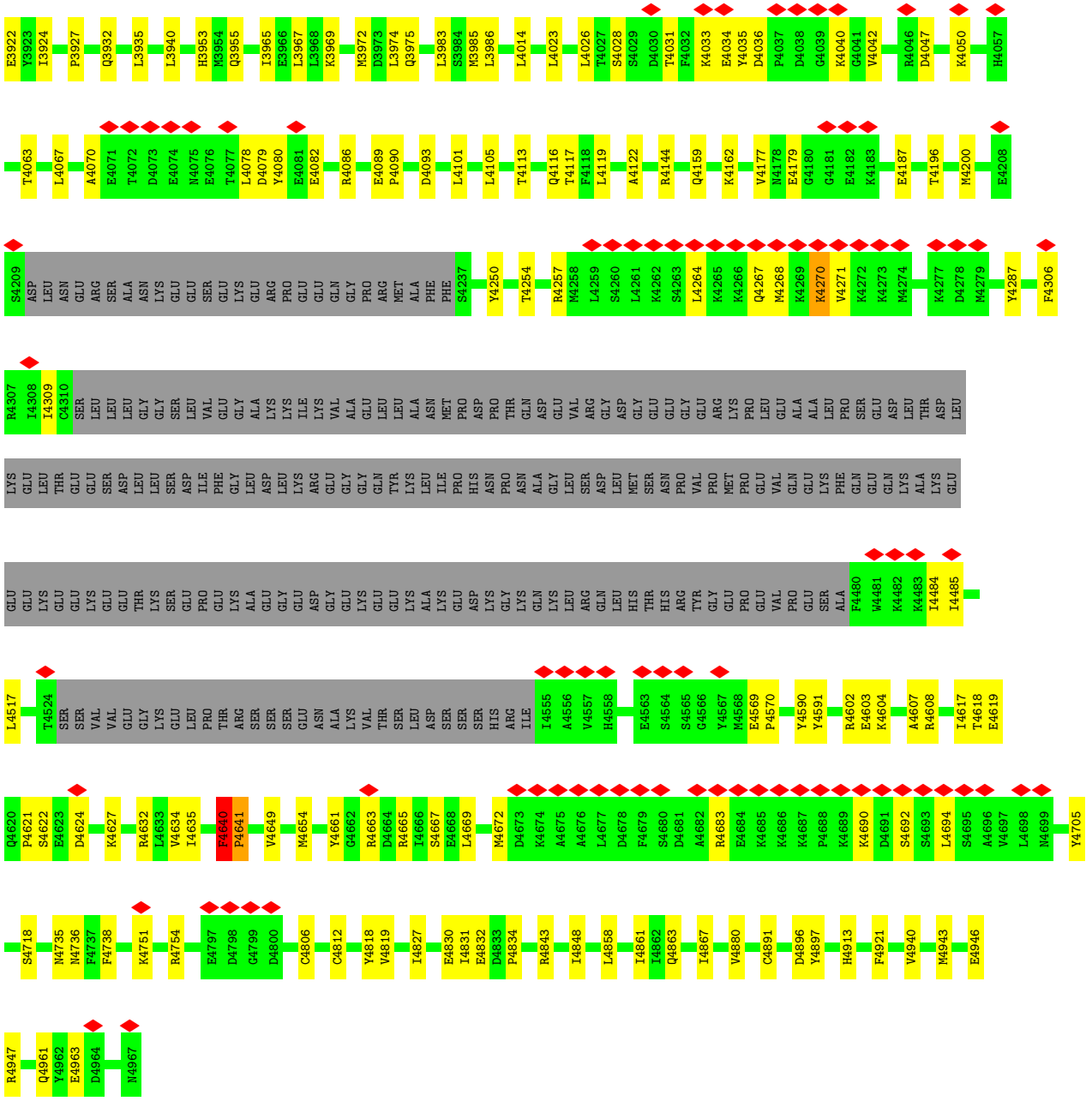
- Molecule 1: Ryanodine receptor 2

Chain A:



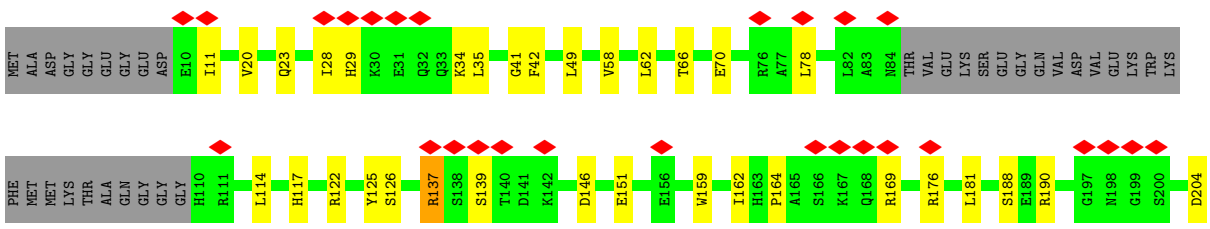

D1196 V1197 G1198 V1204 C1205 R1214 Y1236 E1237 P1238 F1239 N1242 L1251 E1266 H1267 V1270 I1273 I1277 D1278 C1282 L1283 K1284 V1285 G1291 S1292 Q1293 N1294 S1295 N1296 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU
ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS 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 T1425 Y1426 Y1427 I1432 G1435 G1444 W1445 I1446 D1471 E1472 K1473 G1474 K1475 M1487 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 P1541 A1542 F1555
E1556 I1560 V1563 M1564 P1565 L1566 V1594 P1600 F1603 M1628 P1633 E1634 E1635 N1636 R1637 L1644 E1649 L1650 L1651 N1669 H1670 R1671 E1682 P1683 Q1684 L1685 L1686 Y1687 A1688 I1689 L1697 Y1703 L1706 Y1714 R1718 L1719 M1720 M1721 N1722 P1749 M1761
P1766 S1767 F1768 E1774 P1780 K1788 S1789 K1790 T1791 I1792 Q1793 K1800 L1804 H1805 A1806 R1807 I1822 Y1826 I1830 M1831 G1832 I1833 L1839 I1842 P1848 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU
GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 G1892 L1893 L1894 Q1895 M1896 K1897 L1898 V1902 L1909 L1910 Q1911 Y1912 L1913 R1919 I1922 V1926 D1931 F1932 Q1937 D1938 N1939 Q1940 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960
E1964 F1965 R1966 E1971 Q1972 M1975 L1976 L1977 N1978 F1979 D1982 K1983 S1984 E1985 C1986 P1989 R1993 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 I2062 T2065 M2066 A2070 I2075 L2087 I2088 H2089 R2090 Q2091 L2123 R2127 L2130 G2135 E2138 L2141 R2144 M2150 L2165 G2166 M2167 T2170 V2171 M2172 V2176 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 T2188
V2193 A2194 F2199 Y2202 I2206 F2215 Y2220 L2221 L2222 S2225 S2226 V2227 G2228 L2229 P2232 R2235 G2236 S2237 L2240 V2247 L2253 A2254 L2255 A2256 L2257 R2258 E2263 K2264 Y2268 G2273 L2274 P2286 W2290 E2296 R2297 R2303 R2326 R2327 P2328 E2329
G2332 P2333 R2336 G2337 E2338 G2339 I2351 K2352 I2353 D2356 R2359 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 H2383 M2384 G2385 I2388 M2389 T2390 A2403 I2409 K2413 I2417 R2420 I2427 I2436 K2447
D2448 A2458 G2459 F2460 K2465 F2471 L2472 V2475 Y2476 Q2481 D2482 H2486 L2487 L2488 E2489 V2490 G2491 A2500 D2503 G2537 T2538 E2539 D2546 S2547 L2548 L2549 H2550 R2554 K2557 R2581 P2582 Q2586 L2589 L2592 V2593 V2596 H2602 C2617 W2618 K2619 Y2620
L2623 G2626 W2627 G2628 N2629 F2630 S2634 E2635 E2636 E2637 L2640 S2641 R2642 K2643 L2644 Q2654 E2658 Q2659 C2668 L2669 S2670 A2671 V2672 D2679 Y2680 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 Y2719 F2720 I2721 N2722 K2723 H2727 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 I2770 Y2771 R2772 W2773 P2774

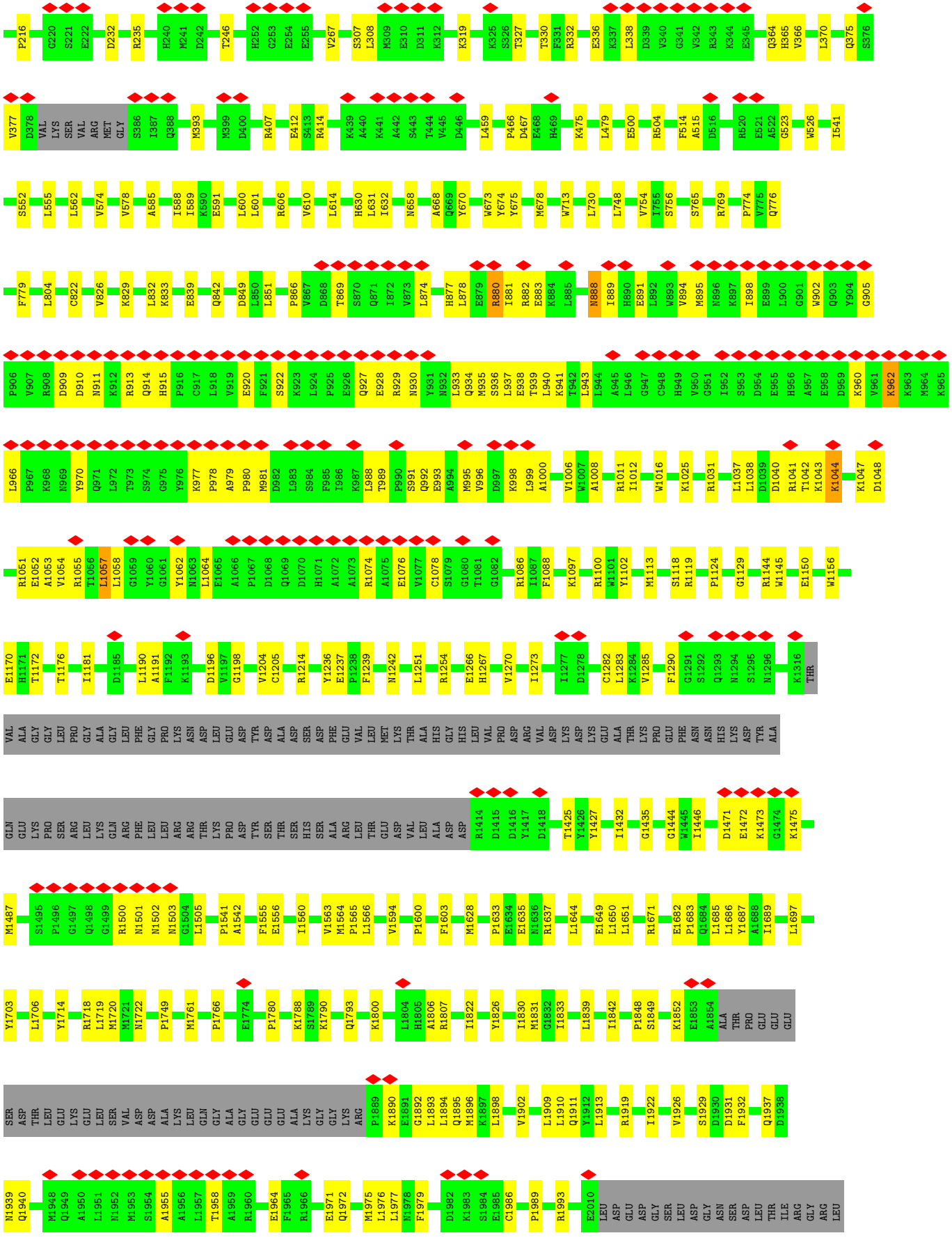


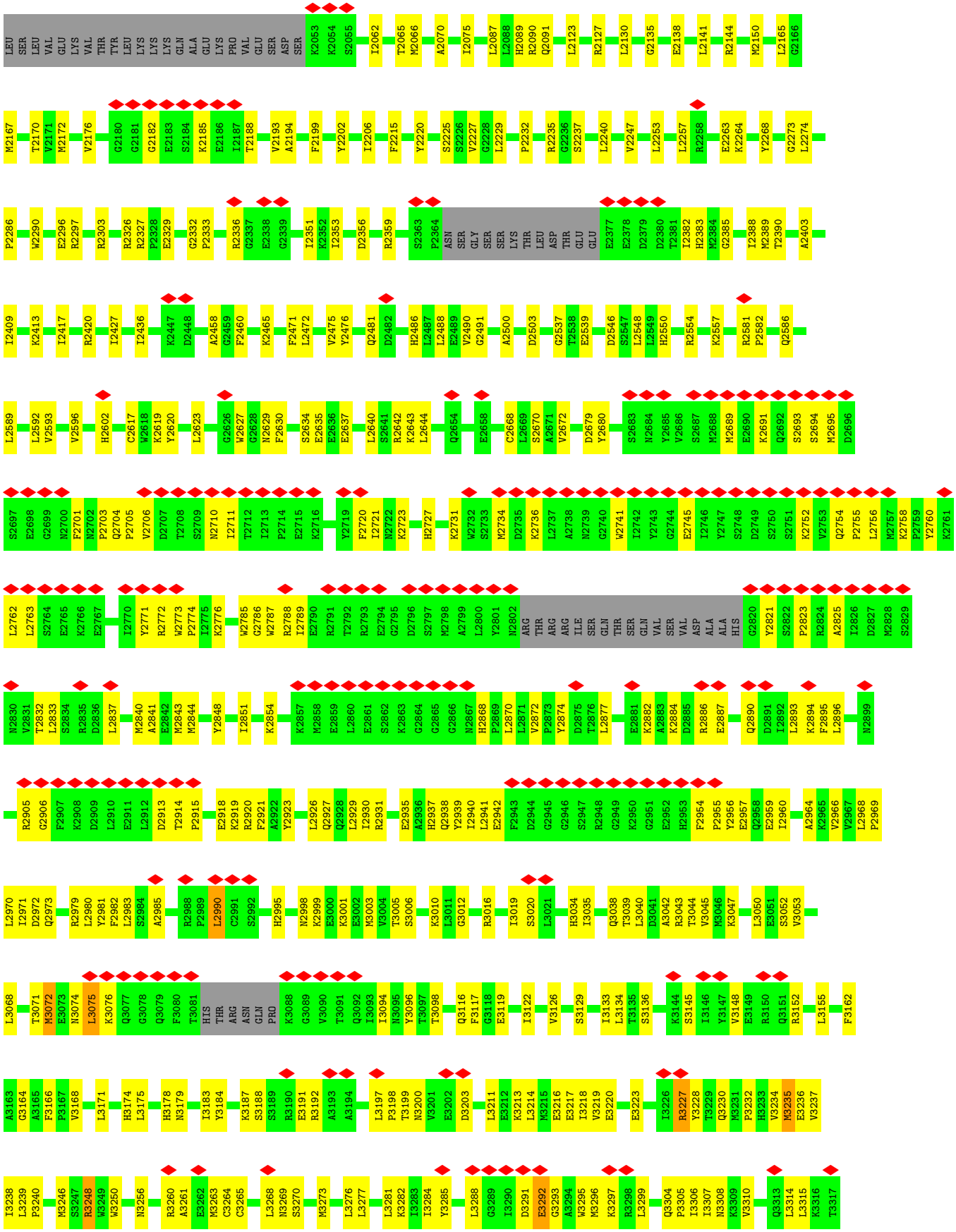


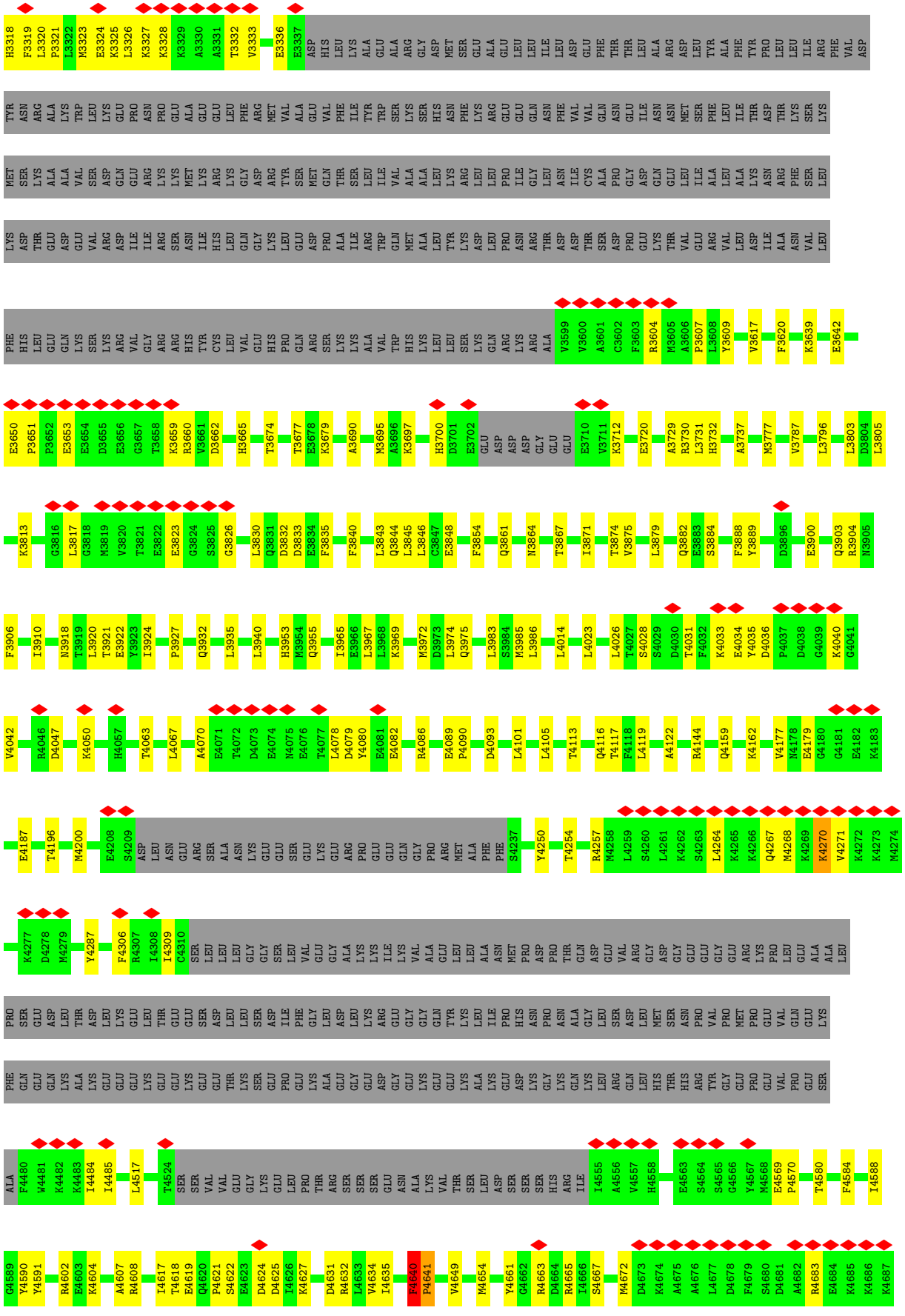
• Molecule 1: Ryanodine receptor 2

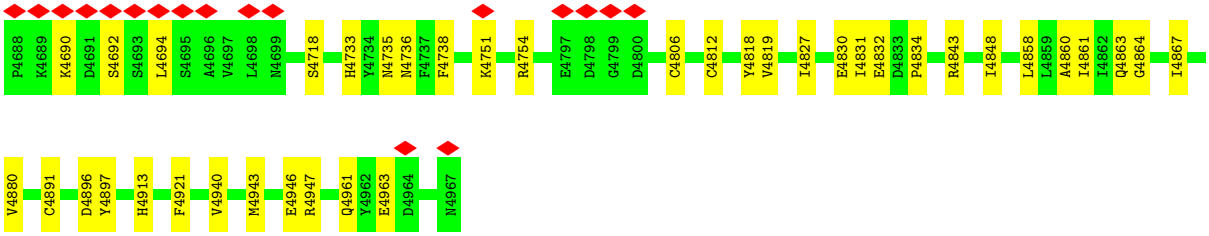
Chain B:




P216 G220 S221 E222 D232 R235 H240 M241 D242 T246 H252 G253 E254 E255 V267 S307 L308 M309 E310 D311 K312 K319 K325 S326 T327 T330 F331 R332 E336 K337 L338 D339 V340 G341 V342 R343 K344 E345 Q364 H365 V366 L370 Q375 S376
V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 M393 M399 D400 R407 E412 S413 R414 K439 A440 K441 A442 S443 T444 V445 D446 L459 P466 D467 E468 H469 K475 L479 E500 R504 F514 A515 D516 R520 E521 A522 G523 W526 I541
S552 L555 L562 V574 V578 A585 I588 T589 K590 E591 L600 L601 R606 V610 L614 H630 L631 I632 N658 A668 Q669 Y670 W673 Y674 Y675 M678 W713 L730 L748 V754 L755 S756 S765 R769 P774 V775 Q776
F779 L804 C822 V826 K829 L832 K833 E839 Q842 D849 L850 L851 P866 V867 D868 T869 S870 Q871 I872 V873 L874 H877 L878 E879 R880 I881 R882 E883 K884 L885 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 E938 T939 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 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 V1006 W1007 A1008 R1011 I1012 W1016 K1025 R1031 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 K1047 D1048
R1051 E1052 A1053 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 R1086 I1087 F1088 K1097 R1100 W1101 Y1102 M1113 S1118 R1119 P1124 G1129 R1144 W1145 E1150 W1156
E1170 H1171 T1172 T1176 I1181 D1185 L1190 A1191 F1192 K1193 D1196 V1197 G1198 V1204 C1205 R1214 Y1236 E1237 P1238 F1239 N1242 L1251 R1254 E1266 H1267 V1270 I1273 I1277 D1278 C1282 L1283 K1284 V1285 F1290 G1291 S1292 Q1293 N1294 S1295 N1296 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 T1425 Y1426 Y1427 I1432 G1435 G1444 W1445 I1446 D1471 E1472 K1473 G1474 K1475
M1487 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 P1541 A1542 F1555 E1556 I1560 V1563 M1564 P1565 L1566 V1594 P1600 F1603 M1628 P1633 E1634 E1635 N1636 R1637 L1644 E1649 L1650 L1651 R1671 E1682 P1683 Q1684 L1685 L1686 Y1687 A1688 I1689 L1697
Y1703 L1706 Y1714 R1718 L1719 M1720 M1721 N1722 P1749 M1761 P1766 E1774 P1780 K1788 S1789 K1790 Q1793 K1800 L1804 H1805 A1806 R1807 I1822 Y1826 I1830 M1831 G1832 I1833 L1839 I1842 P1848 S1849 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU
SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 G1892 L1893 L1894 Q1895 M1896 K1897 L1898 V1902 L1909 L1910 Q1911 Y1912 L1913 R1919 I1922 V1926 S1929 D1930 D1931 F1932 Q1937 D1938
N1939 Q1940 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 E1964 F1965 R1966 E1971 Q1972 M1975 L1976 L1977 N1978 F1979 D1982 K1983 S1984 E1985 C1986 P1989 R1993 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU

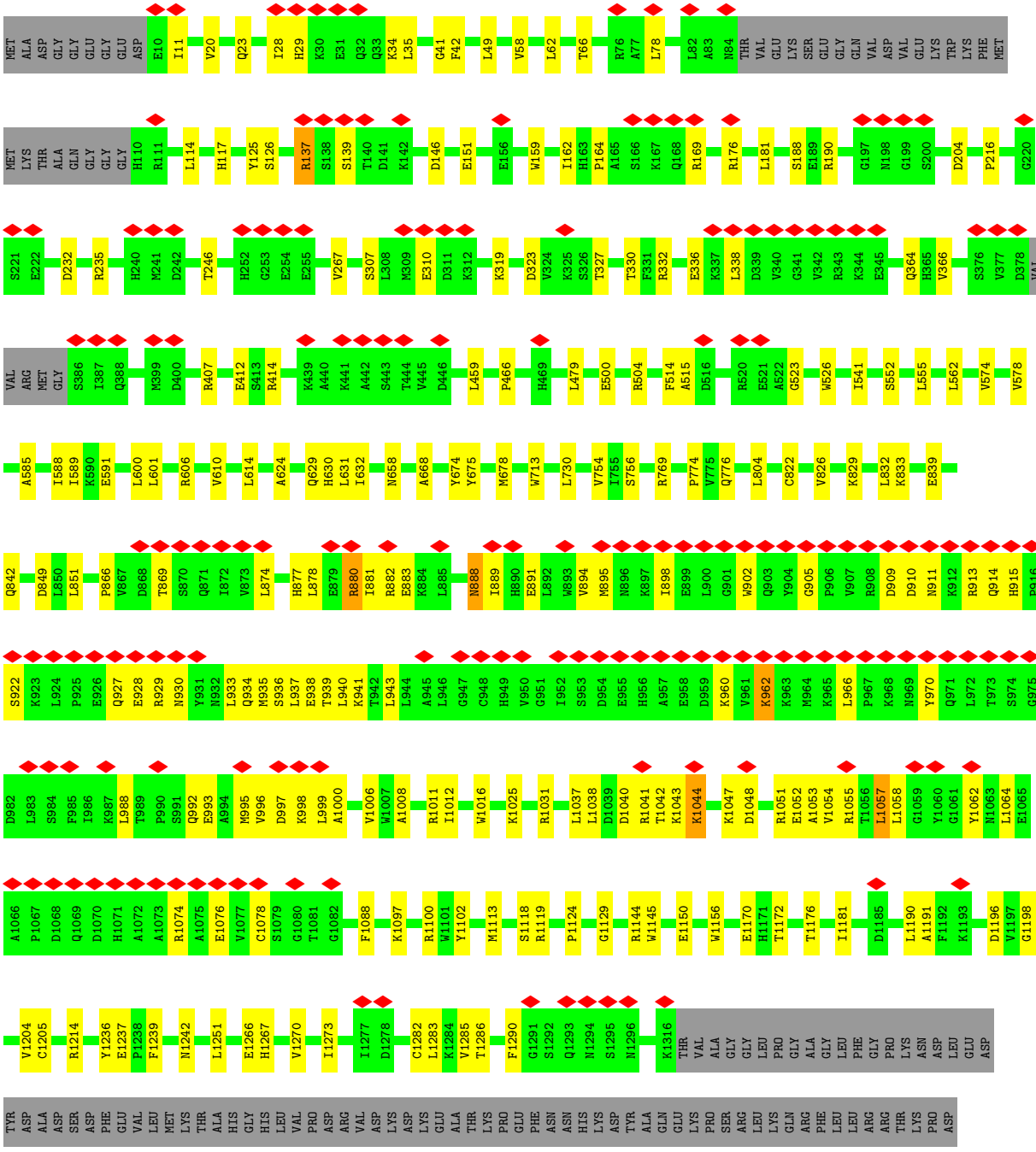

LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 I2062 T2065 M2066 A2070 I2075 L2087 L2088 H2089 R2090 Q2091 L2123 R2127 L2130 G2135 E2138 L2141 R2144 M2150 L2165 G2166
M2167 T2170 V2171 M2172 V2176 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 T2188 V2193 A2194 F2199 Y2202 I2206 F2215 Y2220 S2225 S2226 V2227 G2228 L2229 P2232 R2235 G2236 S2237 L2240 V2247 L2253 L2257 R2258 E2263 K2264 Y2268 G2273 L2274
P2286 W2290 E2296 R2297 R2303 R2326 R2327 P2328 E2329 G2332 P2333 R2336 G2337 E2338 G2339 I2351 K2352 I2353 D2356 R2359 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 H2383 M2384 G2385 I2388 M2389 T2390 A2403
I2409 K2413 I2417 R2420 I2427 I2436 K2447 D2448 A2458 G2459 F2460 K2465 F2471 L2472 V2475 Y2476 Q2481 D2482 H2486 L2487 L2488 E2489 V2490 G2491 A2500 D2503 G2537 T2538 E2539 D2546 S2547 L2548 L2549 H2550 R2554 K2557 R2581 P2582 Q2586
L2589 L2592 V2593 V2596 H2602 C2617 W2618 K2619 Y2620 L2623 G2626 W2627 G2628 N2629 F2630 S2634 E2635 E2636 E2637 L2640 S2641 R2642 K2643 L2644 Q2654 E2658 C2668 L2669 S2670 A2671 V2672 D2679 Y2680 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 Y2719 F2720 I2721 N2722 K2723 H2727 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 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 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 Y2831 T2832 L2833 S2834 R2835 D2836 L2837 M2840 A2841 E2842 M2843 M2844 Y2848 I2851 K2854 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 V2872 P2873 Y2874 D2875 T2876 L2877 E2881 K2882 A2883 K2884 D2885 R2886 E2887 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 N2899
R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 E2918 K2919 R2920 F2921 A2922 Y2923 L2926 Q2927 Q2928 L2929 I2930 R2931 E2935 A2936 H2937 Q2938 Y2939 I2940 L2941 E2942 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 Y2956 E2957 Q2958 E2959 I2960 A2964 K2965 V2966 V2967 L2968 P2969
L2970 I2971 D2972 Q2973 R2979 L2980 Y2981 F2982 L2983 S2984 A2985 R2988 P2989 L2990 C2991 S2992 H2995 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 K3010 L3011 G3012 R3016 I3019 S3020 L3021 H3034 I3035 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 L3060 E3061 S3052 V3053
L3068 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 Q3116 F3117 G3118 E3119 I3122 V3126 S3129 I3133 L3134 T3135 S3136 K3144 S3145 I3146 Y3147 V3148 E3149 R3150 Q3151 R3152 L3155 F3162
A3163 G3164 A3165 F3166 P3167 V3168 L3171 H3174 L3175 H3178 N3179 I3183 Y3184 K3187 S3188 S3189 R3190 E3191 R3192 A3193 A3194 L3197 P3198 T3199 N3200 V3201 E3202 D3203 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 E3223 I3226 R3227 Y3228 T3229 Q3230 M3231 P3232 H3233 V3234 M3235 E3236 V3237
I3238 L3239 P3240 M3246 S3247 R3248 W3249 W3250 N3256 R3260 A3261 E3262 M3263 C3264 C3265 L3268 N3269 S3270 M3273 L3276 L3277 L3281 K3282 I3283 I3284 Y3285 L3288 G3289 I3290 D3291 E3292 G3293 A3294 W3295 M3296 K3297 R3298 L3299 Q3304 P3305 I3306 I3307 N3308 K3309 V3310 Q3313 L3314 L3315 K3316 T3317

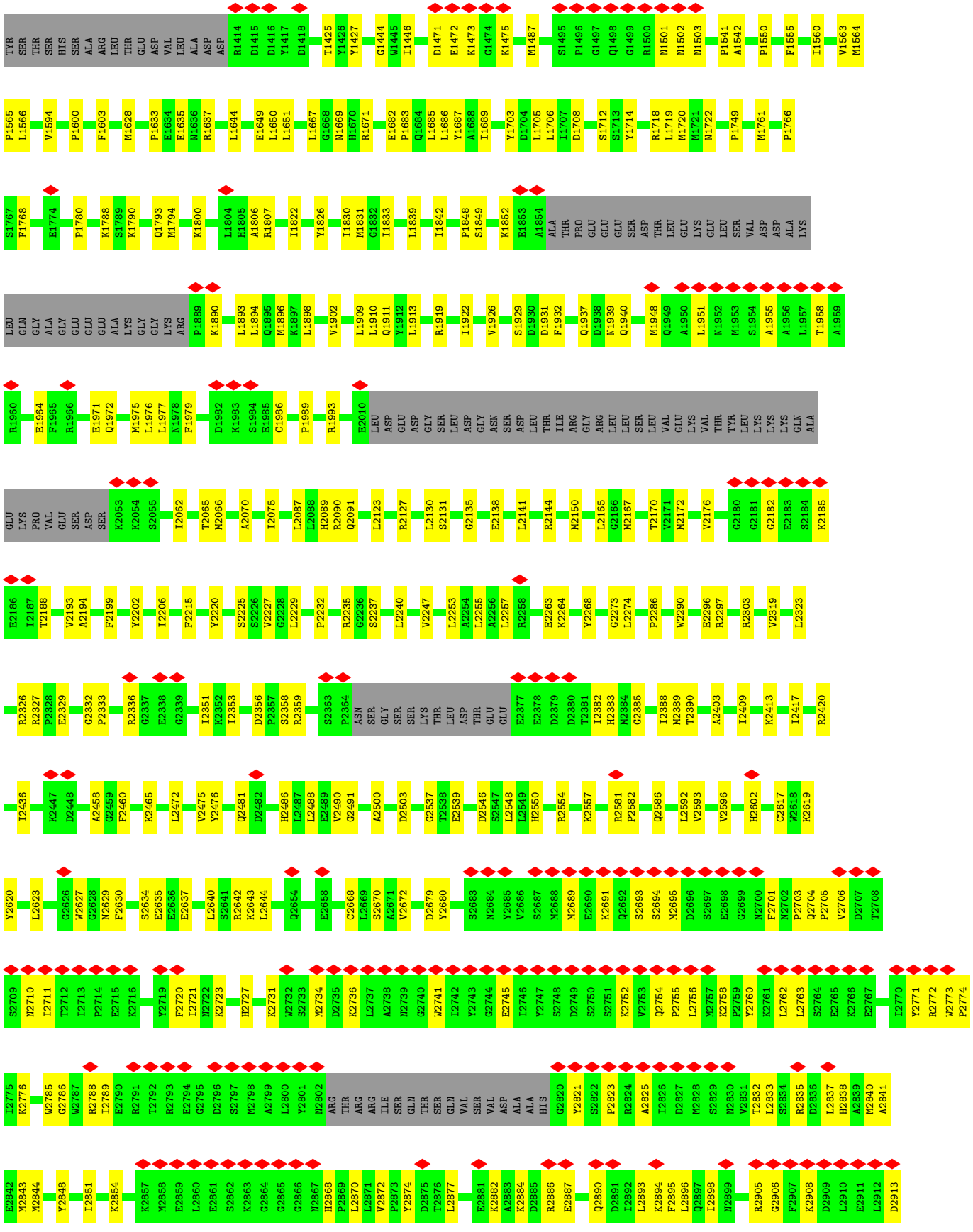




• Molecule 1: Ryanodine receptor 2

Chain C:

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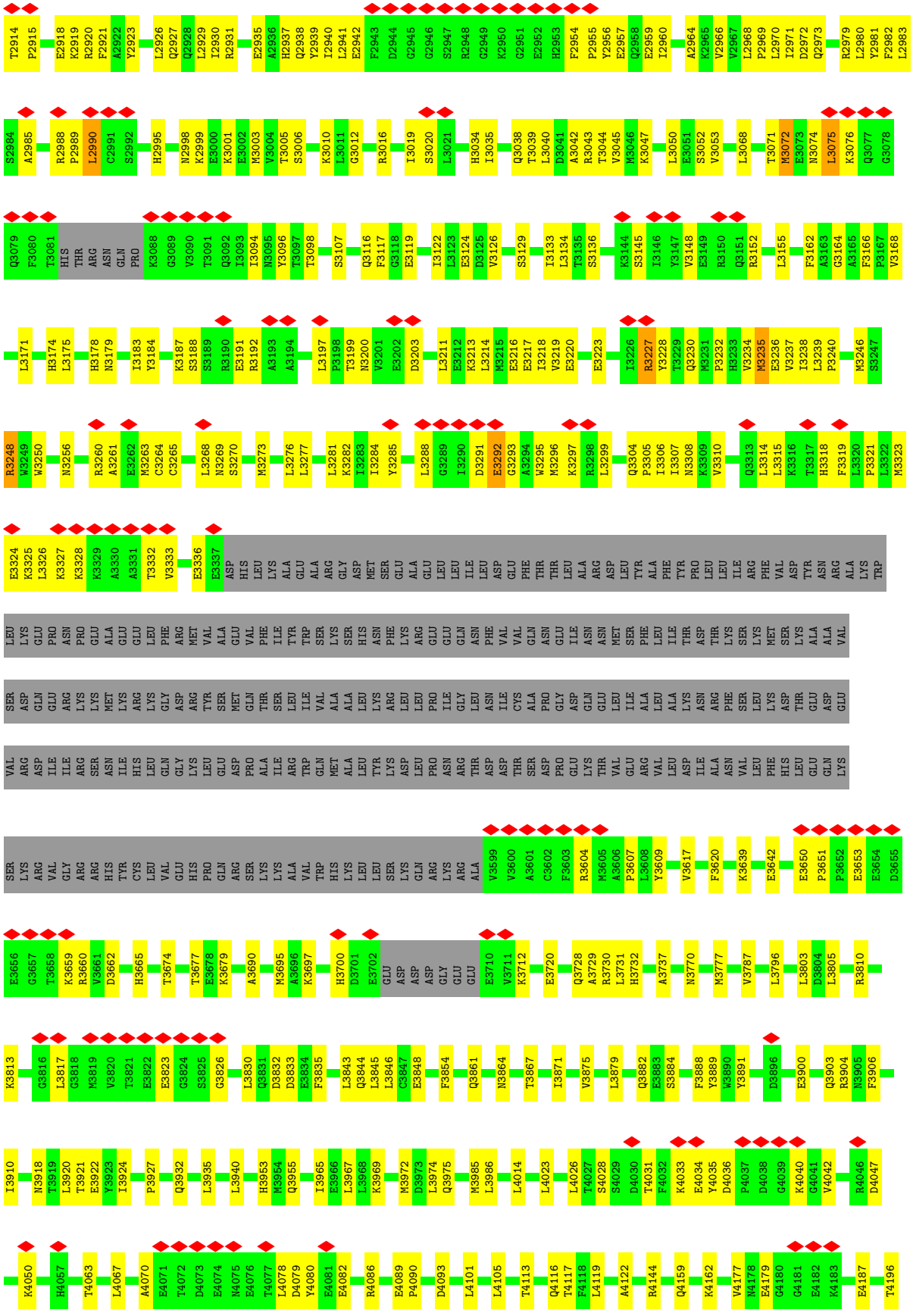
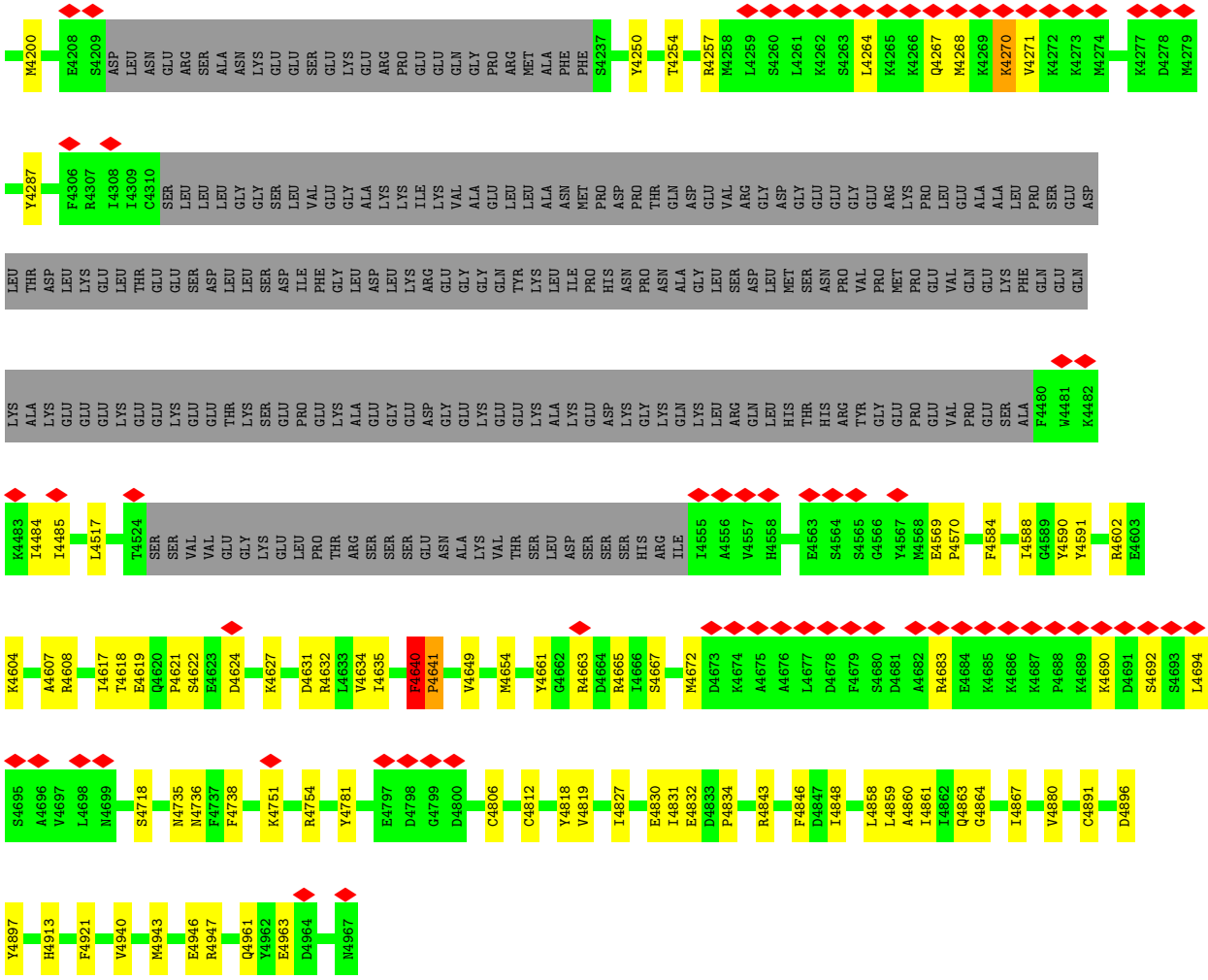
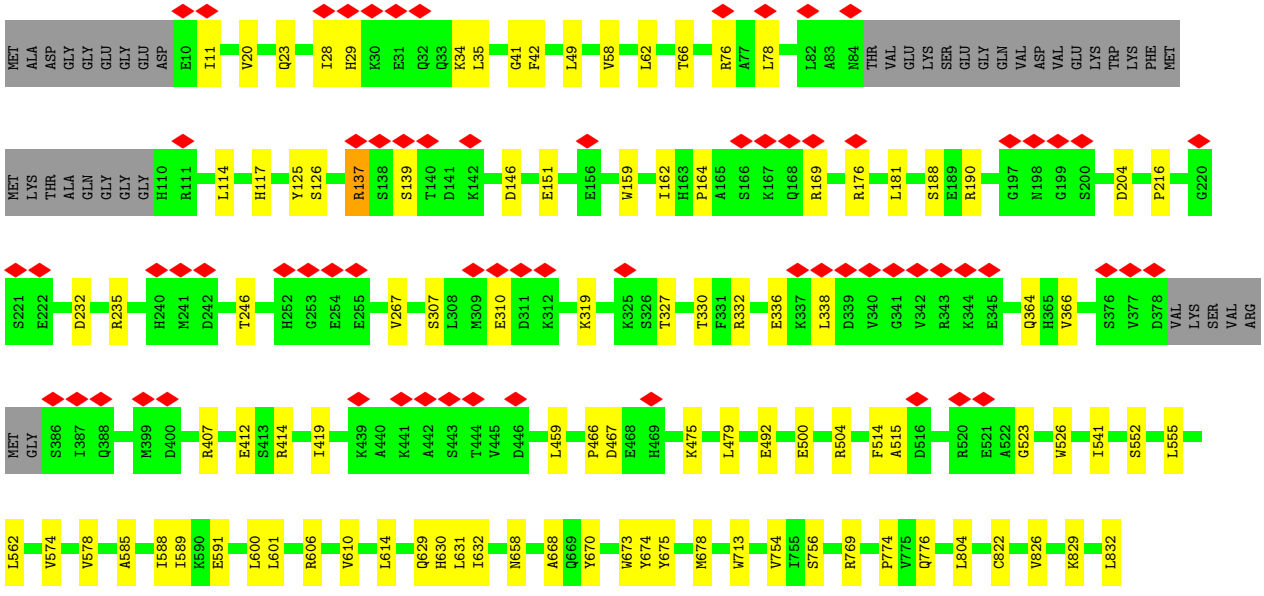
R1414 D1415 D1416 Y1417 D1418 T1425 Y1426 Y1427 G1444 W1445 I1446 D1471 E1472 K1473 G1474 K1475 M1487 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 P1541 A1542 P1550 F1555 I1560 V1563 M1564
P1565 L1566 V1594 P1600 F1603 M1628 P1633 E1634 E1635 N1636 R1637 L1644 E1649 L1650 L1651 L1667 G1668 N1669 H1670 R1671 E1682 P1683 Q1684 L1685 L1686 Y1687 A1688 I1689 Y1703 D1704 L1705 L1706 I1707 D1708 S1712 S1713 Y1714 R1718 L1719 M1720 M1721 N1722 P1749 M1761 P1766
S1767 F1768 E1774 P1780 K1788 S1789 K1790 Q1793 M1794 K1800 L1804 H1805 A1806 R1807 I1822 Y1826 I1830 M1831 G1832 I1833 L1839 I1842 P1848 S1849 K1852 E1853 A1854 ALA THR PRO 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 L1893 L1894 Q1895 M1896 K1897 L1898 V1902 L1909 L1910 Q1911 Y1912 L1913 R1919 I1922 V1926 S1929 D1930 D1931 F1932 Q1937 D1938 N1939 Q1940 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959
R1960 E1964 F1965 R1966 E1971 Q1972 M1975 L1976 L1977 N1978 F1979 D1982 K1983 S1984 E1985 C1986 P1989 R1993 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU 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 I2062 T2065 M2066 A2070 I2075 L2087 L2088 H2089 R2090 Q2091 L2123 R2127 L2130 S2131 G2135 E2138 L2141 R2144 M2150 L2165 G2166 M2167 T2170 V2171 M2172 V2176 G2180 G2181 G2182 E2183 S2184 K2185
E2186 I2187 T2188 V2193 A2194 F2199 Y2202 I2206 F2215 Y2220 S2225 S2226 V2227 G2228 L2229 P2232 R2235 G2236 S2237 L2240 V2247 L2253 A2254 L2255 A2256 L2257 R2258 E2263 K2264 Y2268 G2273 L2274 P2286 W2290 E2296 R2297 R2303 V2319 L2323
R2326 R2327 P2328 E2329 G2332 P2333 R2336 G2337 E2338 G2339 I2351 K2352 I2353 D2356 P2357 S2358 R2359 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 H2383 M2384 G2385 I2388 M2389 T2390 A2403 I2409 K2413 I2417 R2420
I2436 K2447 D2448 A2458 G2459 F2460 K2465 L2472 V2475 Y2476 Q2481 D2482 H2486 L2487 L2488 E2489 V2490 G2491 A2500 D2503 G2537 T2538 E2539 D2546 S2547 L2548 L2549 H2550 R2554 K2557 R2581 P2582 Q2586 L2592 V2593 V2596 H2602 C2617 W2618 K2619
Y2620 L2623 G2626 W2627 G2628 N2629 F2630 S2634 E2635 E2636 E2637 L2640 S2641 R2642 K2643 L2644 Q2654 E2658 C2668 L2669 S2670 A2671 V2672 D2679 Y2680 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 Y2719 F2720 I2721 N2722 K2723 H2727 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 I2770 Y2771 R2772 W2773 P2774
I2775 K2776 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 Y2848 I2851 K2854 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 V2872 P2873 Y2874 D2875 T2876 L2877 E2881 K2882 A2883 K2884 D2885 R2886 E2887 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 Q2897 I2898 N2899 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913

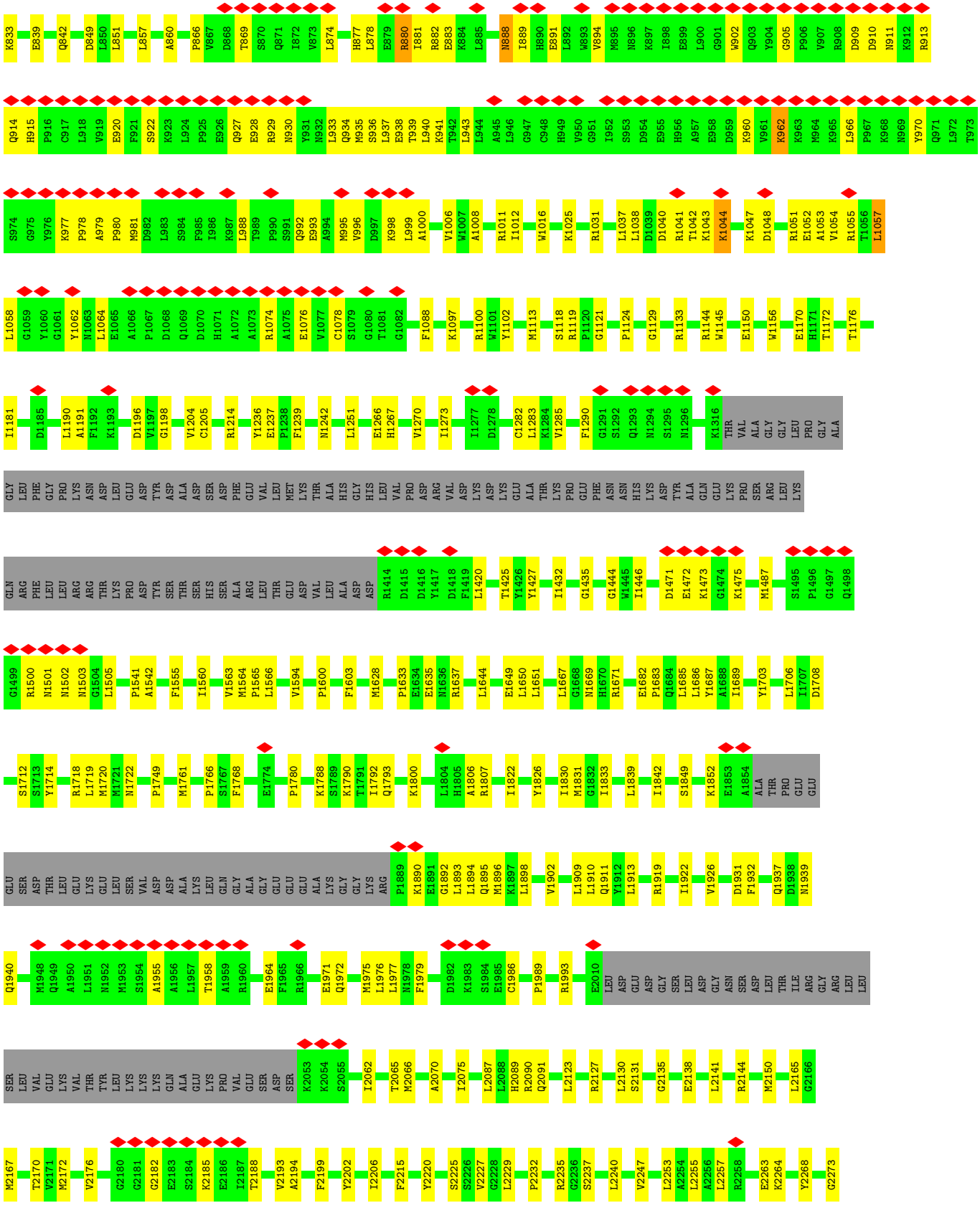




• Molecule 1: Ryanodine receptor 2

Chain D:

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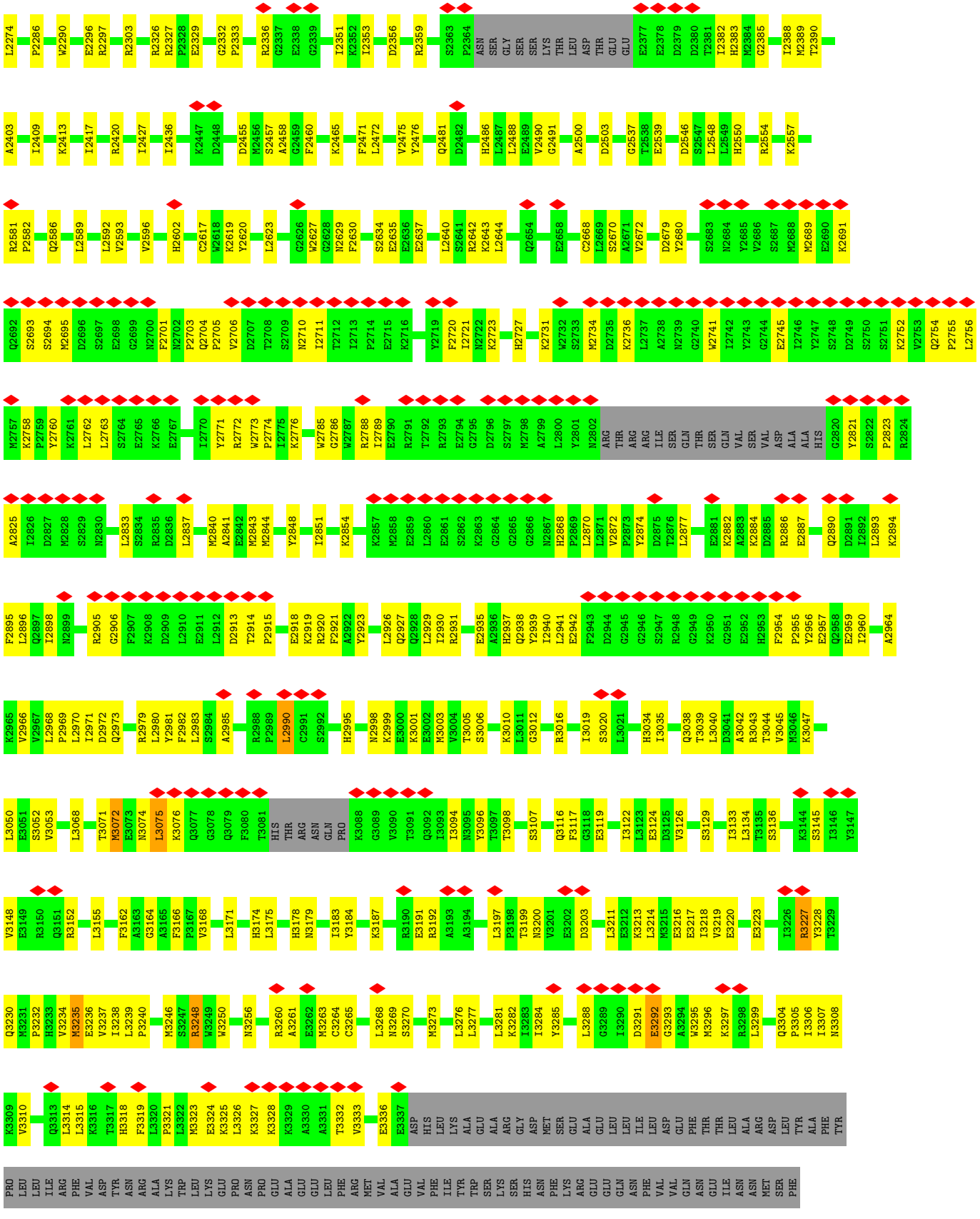
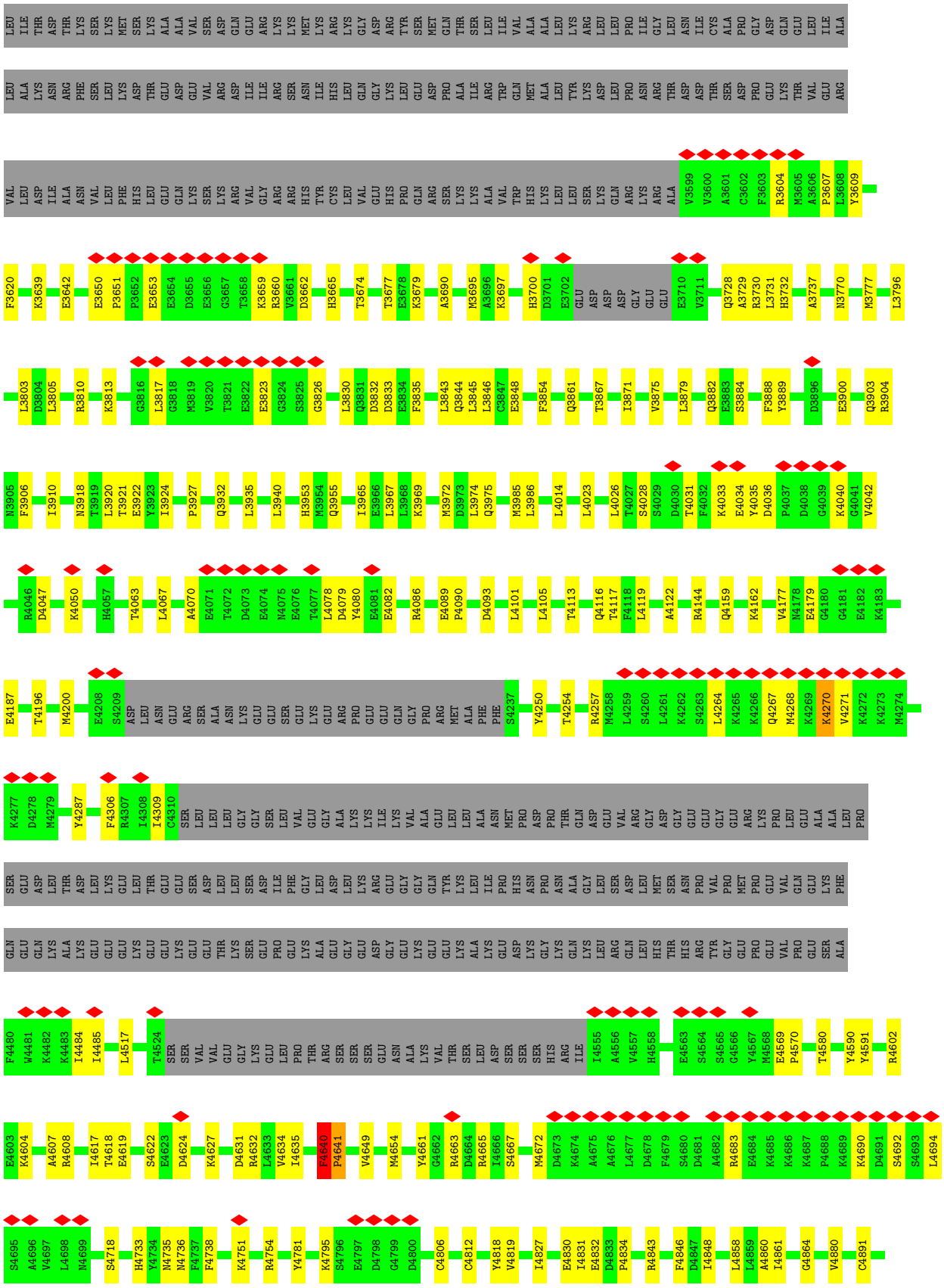
Q914 H915 P916 C917 L918 V919 E920 P921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973
S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 V1006 W1007 A1008 R1011 I1012 W1016 K1025 R1031 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 K1047 D1048 R1051 E1052 A1053 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 F1088 K1097 R1100 W1101 Y1102 M1113 S1118 R1119 P1120 G1121 P1124 G1129 R1133 R1144 W1145 E1150 W1156 E1170 H1171 T1172 T1176
I1181 D1185 L1190 A1191 F1192 K1193 D1196 V1197 G1198 V1204 C1205 R1214 Y1236 E1237 P1238 F1239 N1242 L1251 E1266 H1267 V1270 I1273 I1277 D1278 C1282 L1283 K1284 V1285 F1290 G1291 S1292 Q1293 N1294 S1295 N1296 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 T1425 Y1426 Y1427 I1432 G1435 G1444 W1445 I1446 D1471 E1472 K1473 G1474 K1475 M1487 S1495 P1496 G1497 Q1498
G1499 R1500 N1501 N1502 N1503 G1504 L1505 P1541 A1542 F1555 I1560 V1563 M1564 P1565 L1566 V1594 P1600 F1603 M1628 P1633 E1634 E1635 N1636 R1637 L1644 E1649 L1650 L1651 L1667 G1668 N1669 H1670 R1671 E1682 P1683 Q1684 L1685 L1686 Y1687 A1688 I1689 Y1703 L1706 I1707 D1708
S1712 S1713 Y1714 R1718 L1719 M1720 M1721 N1722 P1749 M1761 P1766 S1767 F1768 E1774 P1780 K1788 S1789 K1790 T1791 I1792 Q1793 K1800 L1804 H1805 A1806 R1807 I1822 Y1826 I1830 M1831 G1832 I1833 L1839 I1842 S1849 K1852 E1853 A1854 ALA THR PRO GLU GLU
GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 G1892 L1893 L1894 Q1895 M1896 K1897 L1898 V1902 L1909 L1910 Q1911 Y1912 L1913 R1919 I1922 V1926 D1931 F1932 Q1937 D1938 N1939
Q1940 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 E1964 F1965 R1966 E1971 Q1972 M1975 L1976 L1977 N1978 F1979 D1982 K1983 S1984 E1985 C1986 P1989 R1993 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 I2062 T2065 M2066 A2070 I2075 L2087 L2088 H2089 R2090 Q2091 L2123 R2127 L2130 S2131 G2135 E2138 L2141 R2144 M2150 L2165 G2166
M2167 T2170 V2171 M2172 V2176 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 T2188 V2193 A2194 F2199 Y2202 I2206 F2215 Y2220 S2225 S2226 V2227 G2228 L2229 P2232 R2235 G2236 S2237 L2240 V2247 L2253 A2254 L2255 A2256 L2257 R2258 E2263 K2264 Y2268 G2273

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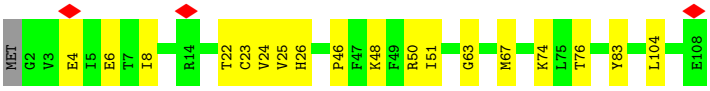
LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG LEU ALA VAL TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP SER ASP PRO GLU LYS THR VAL GLU ARG
VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609
F3620 K3639 E3642 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 V3661 D3662 H3665 T3674 T3677 E3678 K3679 A3690 M3695 A3696 K3697 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 Q3728 A3729 R3730 L3731 H3732 A3737 N3770 M3777 L3796
L3803 D3804 L3805 R3810 K3813 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 L3830 Q3831 D3832 D3833 E3834 F3835 L3843 Q3844 L3845 L3846 C3847 E3848 F3854 Q3861 T3867 I3871 V3875 L3879 Q3882 E3883 S3884 F3888 Y3889 D3896 E3900 Q3903 R3904
N3905 F3906 I3910 N3918 T3919 L3920 T3921 E3922 Y3923 I3924 P3927 Q3932 L3935 L3940 H3953 M3954 Q3955 I3965 E3966 L3967 L3968 K3969 M3972 D3973 L3974 Q3975 M3985 L3986 L4014 L4023 L4026 T4027 S4028 S4029 D4030 T4031 F4032 K4033 E4034 Y4035 D4036 P4037 D4038 G4039 K4040 G4041 V4042
R4046 D4047 K4050 H4057 T4063 L4067 A4070 E4071 T4072 D4073 E4074 N4075 E4076 T4077 L4078 D4079 Y4080 E4081 E4082 R4086 E4089 P4090 D4093 L4101 L4105 T4113 Q4116 T4117 F4118 L4119 A4122 R4144 Q4159 K4162 V4177 N4178 E4179 G4180 G4181 E4182 K4183
E4187 T4196 M4200 E4208 S4209 ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU GLU ARG PRO GLU GLU GLN GLY PRO ARG MET ALA PHE PHE S4237 Y4250 T4254 R4257 M4258 L4259 S4260 L4261 K4262 S4263 L4264 K4265 K4266 Q4267 M4268 K4269 K4270 V4271 K4272 K4273 M4274
K4277 D4278 M4279 Y4287 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLU GLY GLU ARG LYS PRO LEU GLU ALA ALA LEU PRO
SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER ASN PRO VAL PRO MET PRO GLU VAL GLN GLU LYS PHE
GLN GLU GLN LYS ALA LYS GLU GLU GLU LYS GLU GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU LYS GLU LYS ALA LYS GLU ASP LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU GLU SER ALA
F4480 W4481 K4482 K4483 I4484 I4485 L4517 T4524 SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG SER SER SER GLU GLU ASN ALA LYS VAL THR SER LEU ASP SER SER SER HIS ARG ILE I4555 A4556 V4557 H4558 E4563 S4564 S4565 G4566 Y4567 M4568 E4569 P4570 T4580 Y4590 Y4591 R4602
E4603 K4604 A4607 R4608 I4617 T4618 E4619 S4622 E4623 D4624 K4627 D4631 R4632 L4633 V4634 I4635 F4640 P4641 V4649 M4654 Y4661 G4662 R4663 D4664 R4665 I4666 S4667 M4672 D4673 K4674 A4675 A4676 L4677 D4678 F4679 S4680 D4681 A4682 R4683 E4684 K4685 K4686 K4687 P4688 K4689 K4690 D4691 S4692 S4693 L4694
S4695 A4696 V4697 L4698 N4699 S4718 H4733 Y4734 N4735 N4736 F4737 F4738 K4751 R4754 Y4781 K4795 S4796 E4797 D4798 G4799 D4800 C4606 C4812 Y4818 V4819 I4827 E4830 I4831 E4832 D4833 P4834 R4843 F4846 D4847 I4848 L4858 L4859 A4860 I4861 G4864 V4880 C4891

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

Chain E:



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

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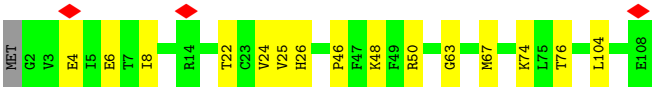

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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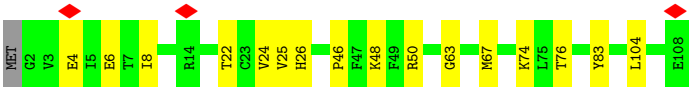
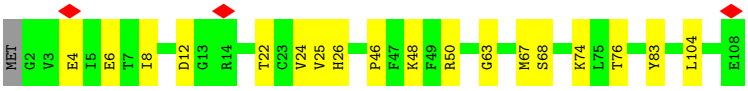


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143933	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	0.730	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/34509	0.48	6/46612 (0.0%)
1	B	0.25	0/34509	0.48	6/46612 (0.0%)
1	C	0.25	0/34509	0.48	6/46612 (0.0%)
1	D	0.25	0/34509	0.48	6/46612 (0.0%)
2	E	0.26	0/834	0.48	0/1123
2	F	0.27	0/834	0.48	0/1123
2	G	0.27	0/834	0.48	0/1123
2	H	0.27	0/834	0.48	0/1123
All	All	0.25	0/141372	0.48	24/190940 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4640	PHE	C-N-CD	-6.73	105.79	120.60
1	C	4640	PHE	C-N-CD	-6.71	105.83	120.60
1	A	4640	PHE	C-N-CD	-6.71	105.84	120.60
1	D	4640	PHE	C-N-CD	-6.70	105.86	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2990	LEU	CA-CB-CG	6.38	129.96	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4640	PHE	Peptide
1	B	4640	PHE	Peptide
1	C	4640	PHE	Peptide
1	D	4640	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33769	0	33450	598	0
1	B	33769	0	33450	602	0
1	C	33769	0	33450	599	0
1	D	33769	0	33450	592	0
2	E	818	0	821	13	0
2	F	818	0	821	11	0
2	G	818	0	821	11	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	1	0
4	B	62	0	24	1	0
4	C	62	0	24	1	0
4	D	62	0	24	1	0
All	All	138600	0	137180	2407	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 9.

The worst 5 of 2407 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:D:3293:GLY:H	1:D:3296:MET:HE1	1.32	0.94
1:C:3293:GLY:H	1:C:3296:MET:HE1	1.33	0.94
1:A:3293:GLY:H	1:A:3296:MET:HE1	1.33	0.93
1:B:3293:GLY:H	1:B:3296:MET:HE1	1.32	0.91
1:C:1940:GLN:HE22	1:C:1972:GLN:HE21	1.16	0.90

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4198/4967 (84%)	4086 (97%)	109 (3%)	3 (0%)	51 79
1	B	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	51 79
1	C	4198/4967 (84%)	4086 (97%)	109 (3%)	3 (0%)	51 79
1	D	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	51 79
2	E	105/108 (97%)	104 (99%)	1 (1%)	0	100 100
2	F	105/108 (97%)	104 (99%)	1 (1%)	0	100 100
2	G	105/108 (97%)	104 (99%)	1 (1%)	0	100 100
2	H	105/108 (97%)	104 (99%)	1 (1%)	0	100 100
All	All	17212/20300 (85%)	16762 (97%)	438 (2%)	12 (0%)	54 79

5 of 12 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3708/4358 (85%)	3691 (100%)	17 (0%)	88 96
1	B	3708/4358 (85%)	3691 (100%)	17 (0%)	88 96
1	C	3708/4358 (85%)	3691 (100%)	17 (0%)	88 96
1	D	3708/4358 (85%)	3691 (100%)	17 (0%)	88 96
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%)	15116 (100%)	68 (0%)	91 96

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1025	LYS
1	D	1473	LYS
1	D	3227	ARG
1	B	1044	LYS
1	B	1025	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	934	GLN
1	C	3955	GLN
1	C	1267	HIS
1	C	2704	GLN
1	D	658	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	A	5002	-	26,33,33	0.61	0	31,52,52	0.77	2 (6%)
4	ATP	B	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	C	5002	-	26,33,33	0.61	0	31,52,52	0.76	2 (6%)
4	ATP	B	5002	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
4	ATP	C	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	A	5003	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	D	5002	-	26,33,33	0.61	0	31,52,52	0.77	2 (6%)
4	ATP	D	5003	-	26,33,33	0.60	0	31,52,52	0.73	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	5002	-	-	4/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	4/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	4/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	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	A	5002	ATP	C5-C6-N6	2.33	123.89	120.35
4	B	5003	ATP	C5-C6-N6	2.33	123.89	120.35
4	D	5003	ATP	C5-C6-N6	2.31	123.87	120.35
4	A	5003	ATP	C5-C6-N6	2.31	123.86	120.35
4	C	5002	ATP	C5-C6-N6	2.29	123.84	120.35

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O3A
4	B	5003	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

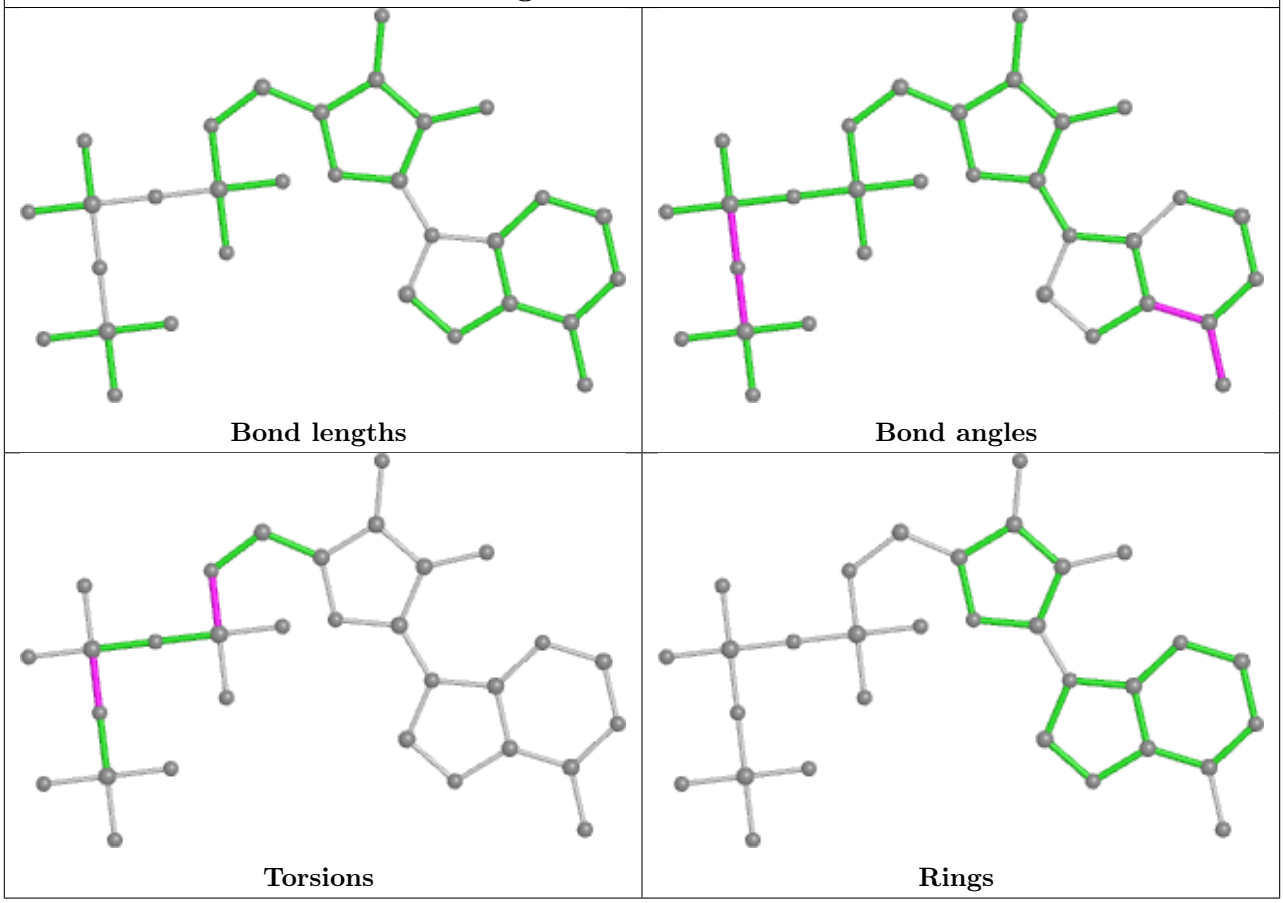
4 monomers are involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

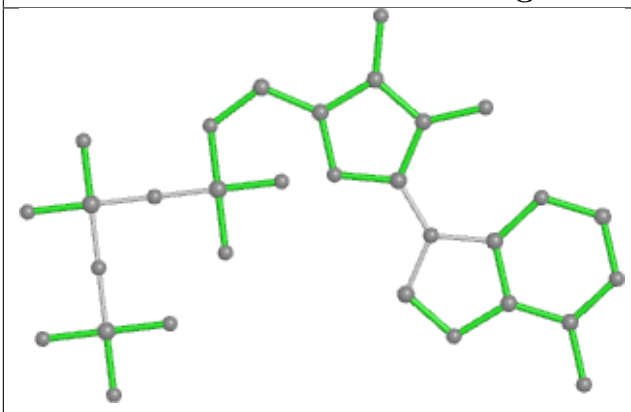
Ligand ATP A 5002



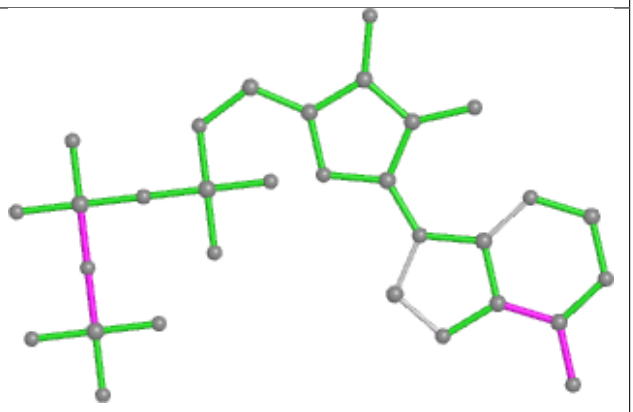
Bond lengths | **Bond angles**

Torsions | **Rings**

Ligand ATP B 5003



Bond lengths



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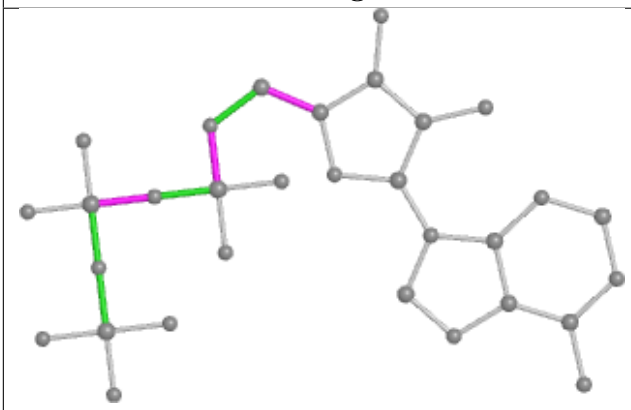
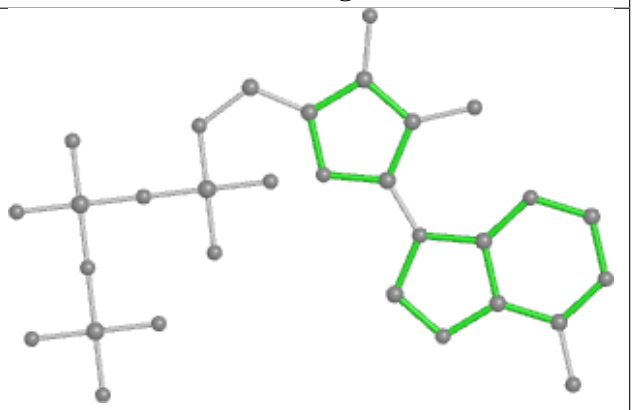
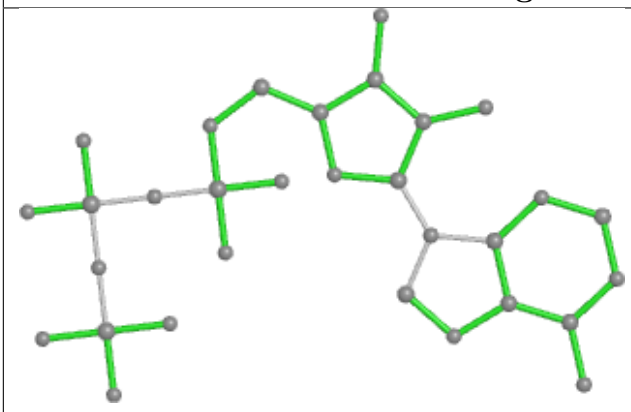


Torsions



Rings

Ligand ATP C 5002



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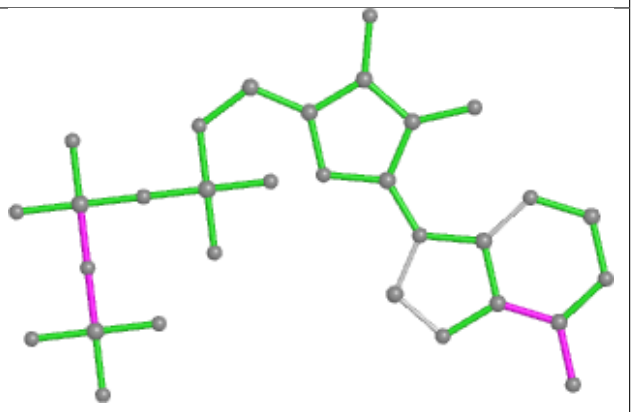

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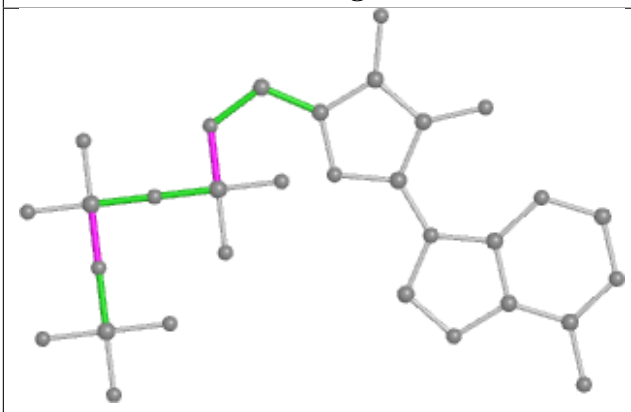

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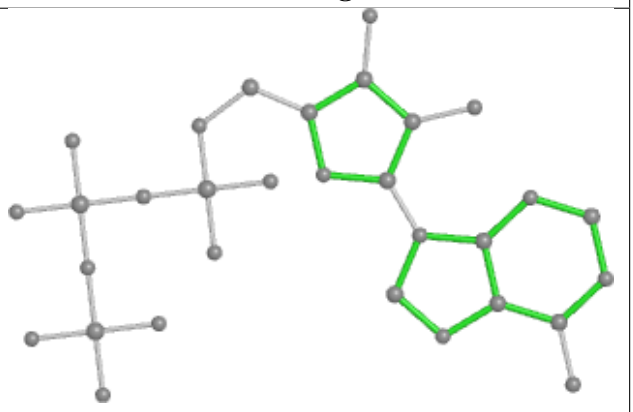
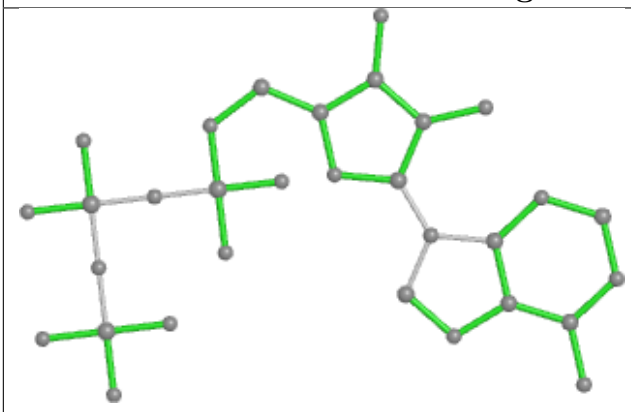


Rings

Ligand ATP B 5002



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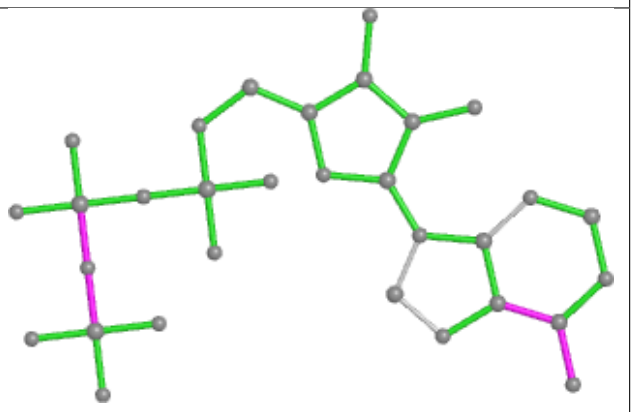
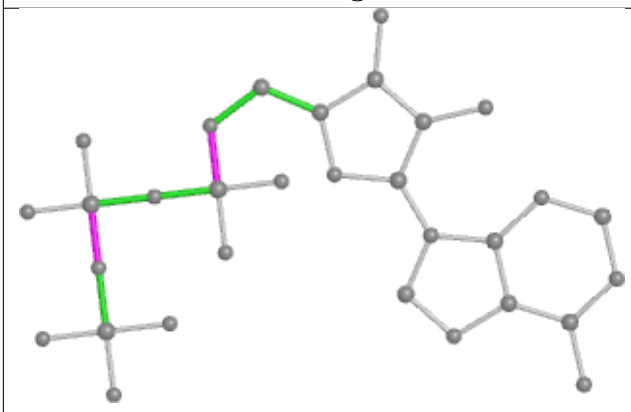
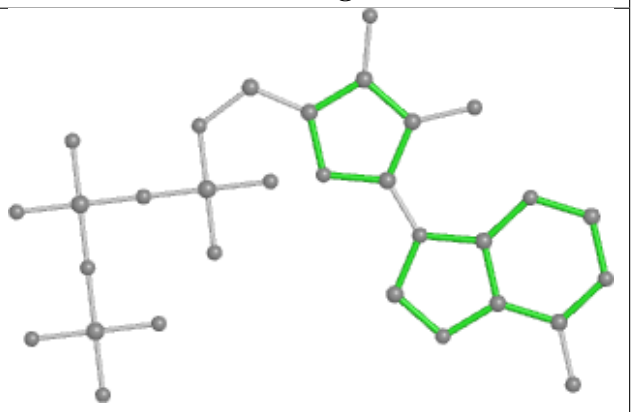


Bond angles

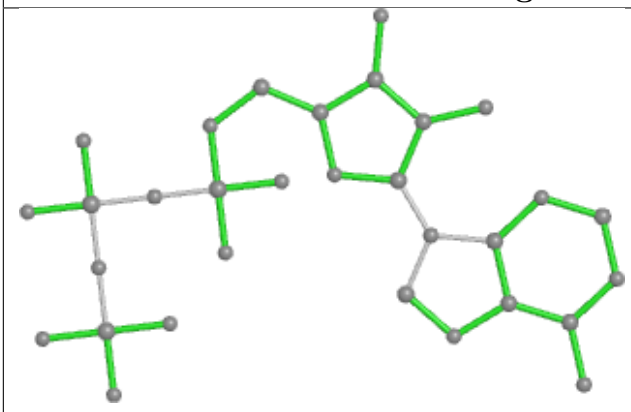


Torsions



Rings

Ligand ATP C 5003



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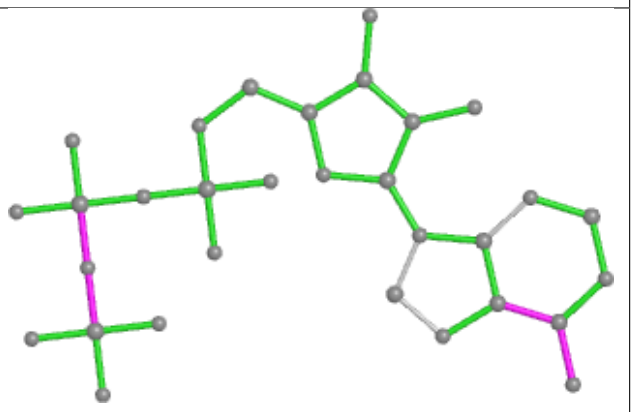
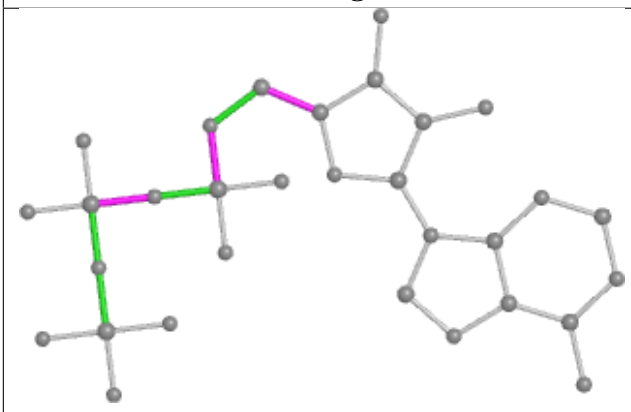
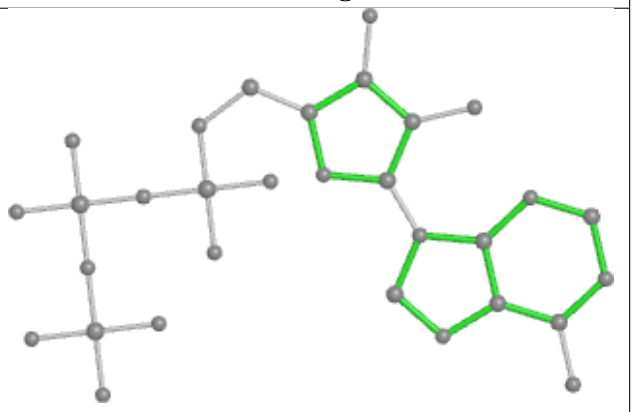


Bond angles

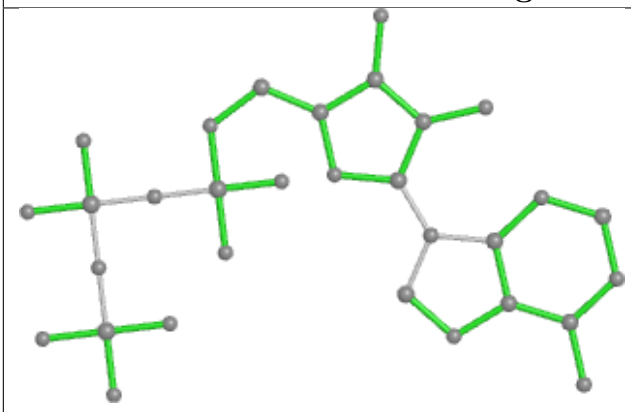


Torsions



Rings

Ligand ATP A 5003



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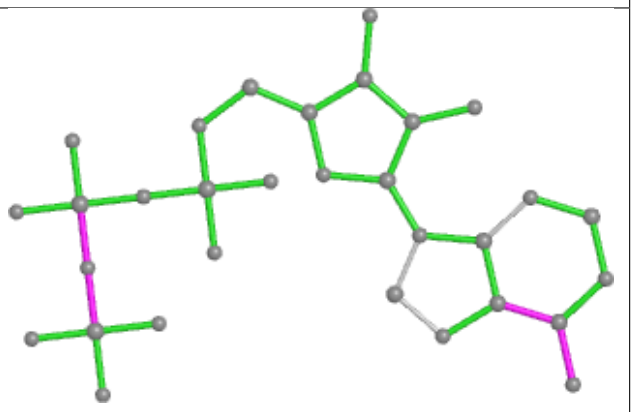
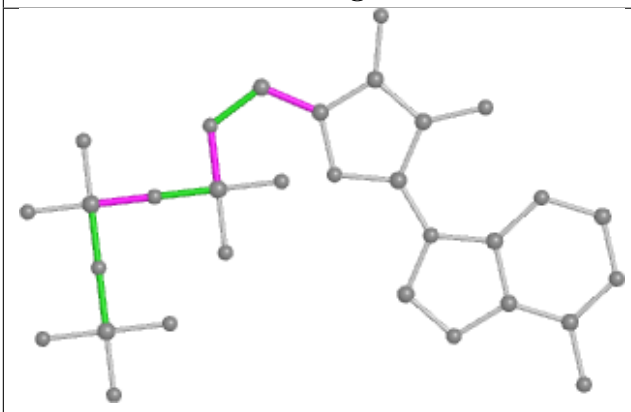


Bond angles



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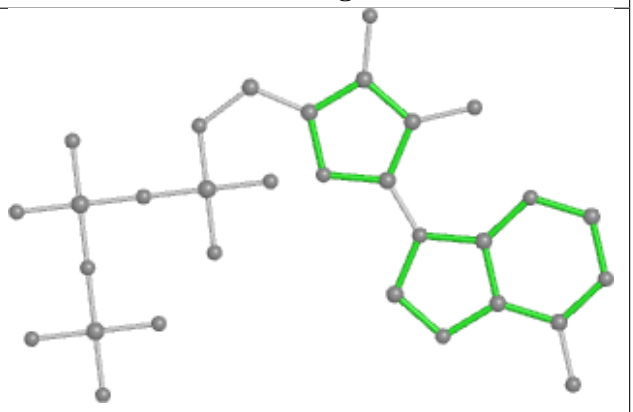
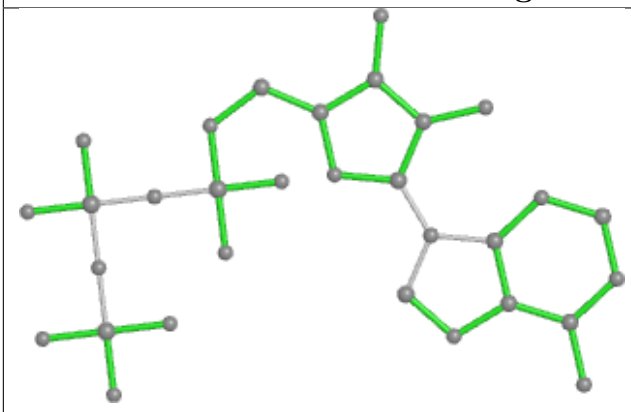
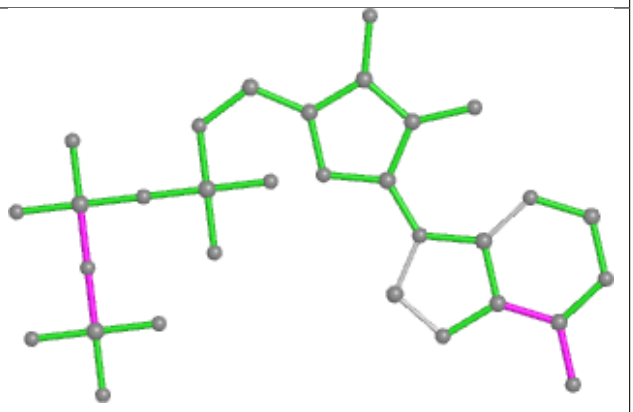


Rings

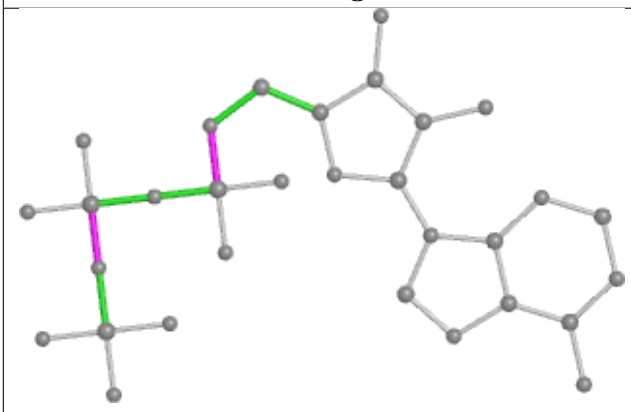
Ligand ATP D 5002



Bond lengths



Bond angles



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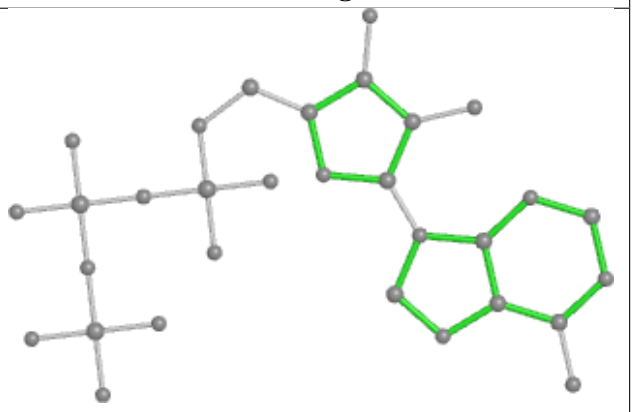
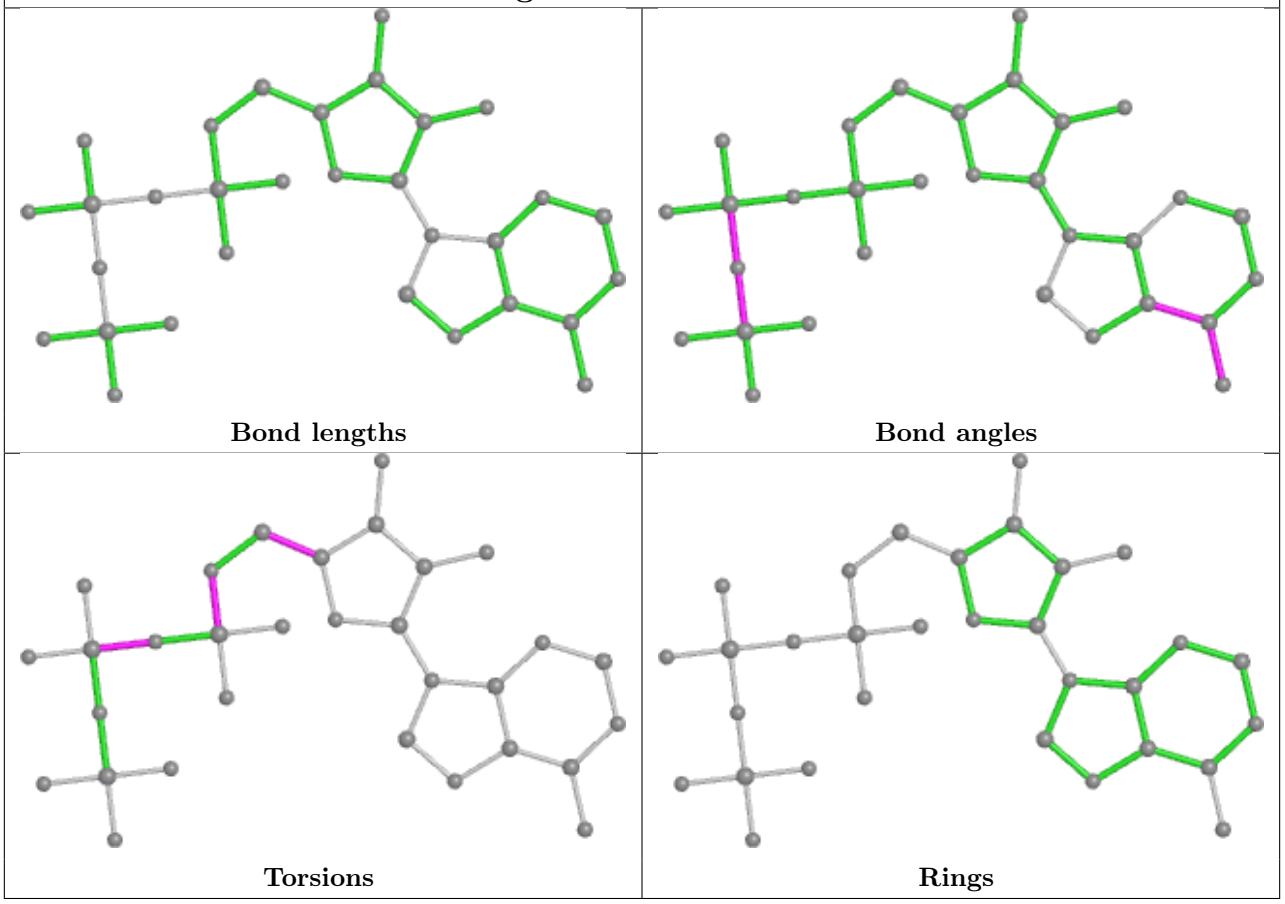


Rings

Ligand ATP D 5003



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

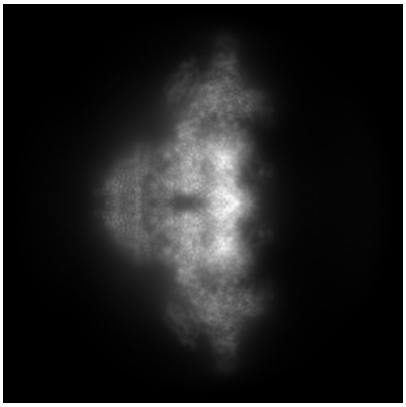
This section contains visualisations of the EMDB entry EMD-42759. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

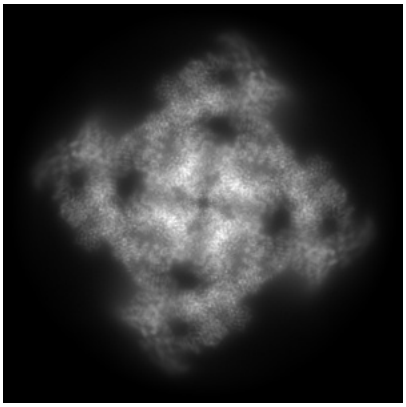
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

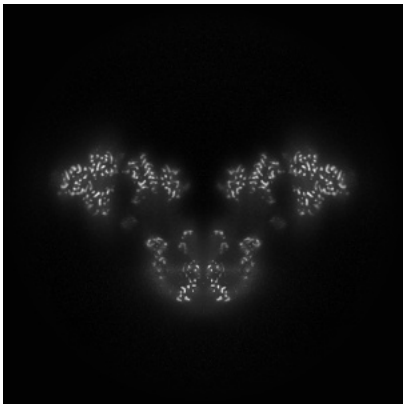


Z

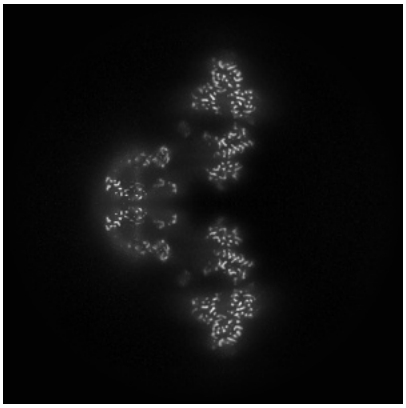
The images above show the map projected in three orthogonal directions.

6.2 Central slices

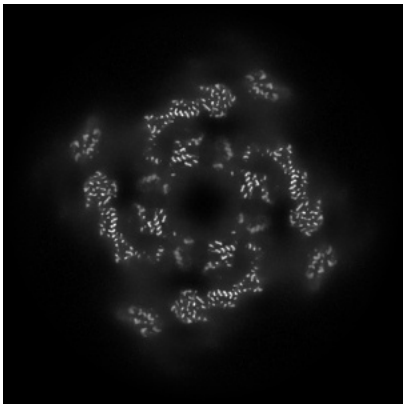
6.2.1 Primary map



X Index: 256



Y Index: 256

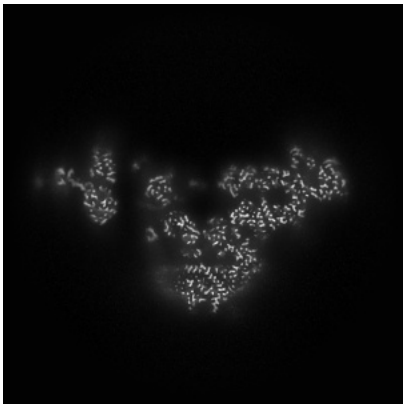


Z Index: 256

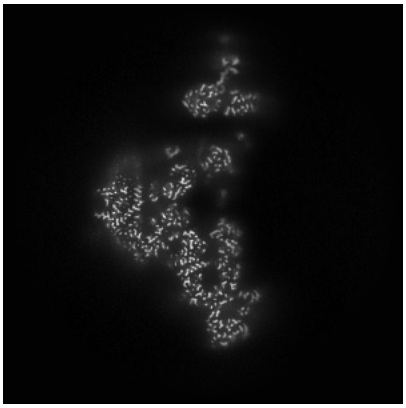
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

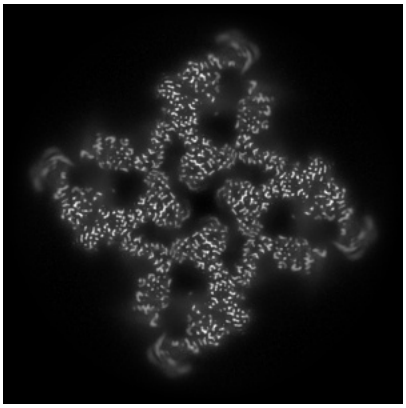
6.3.1 Primary map



X Index: 238



Y Index: 238



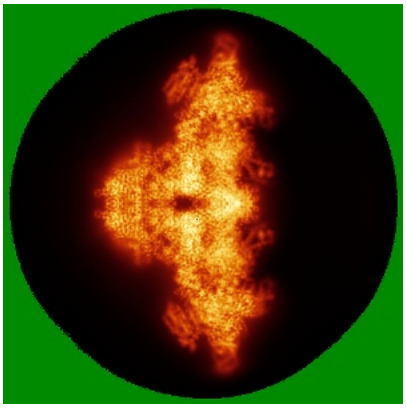
Z Index: 282

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

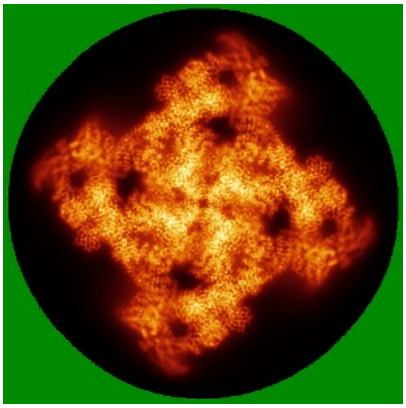
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

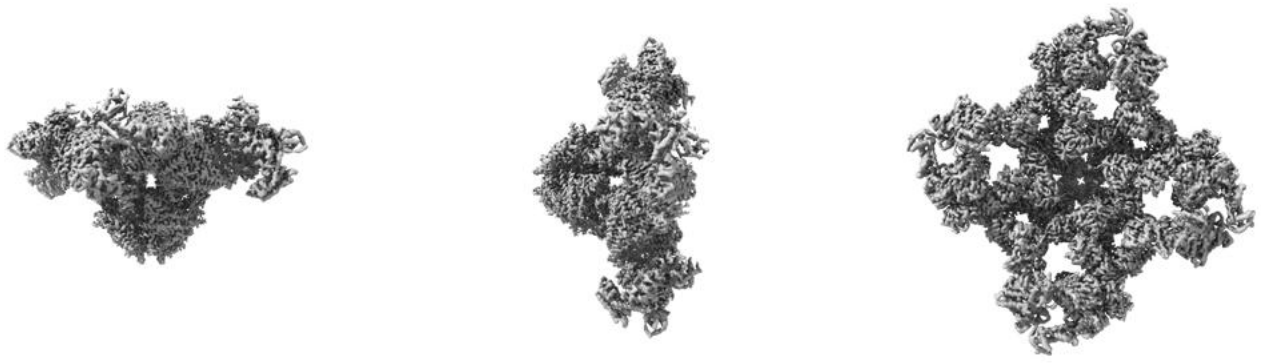


Z

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

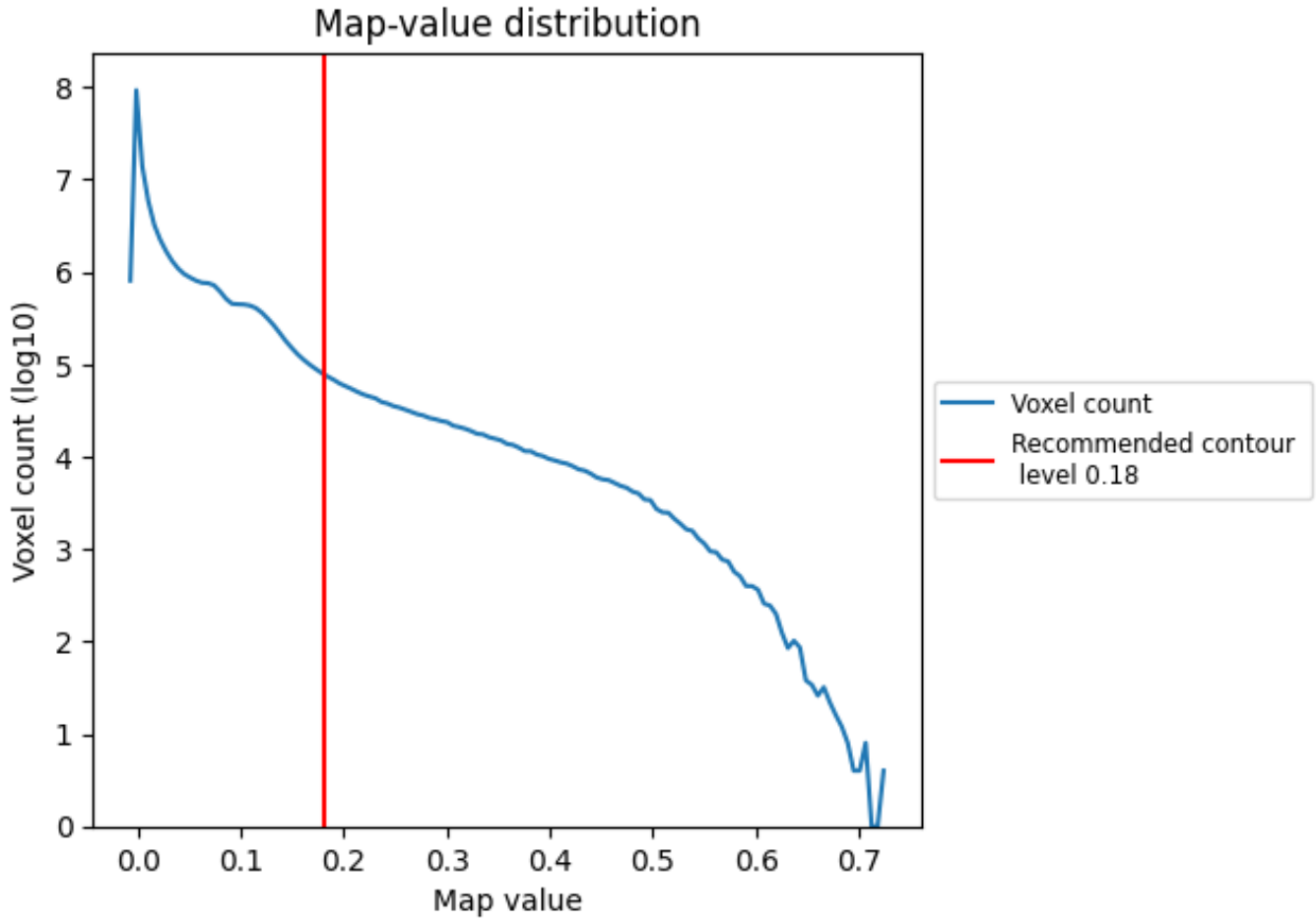
6.6 Mask visualisation (i)

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

7 Map analysis

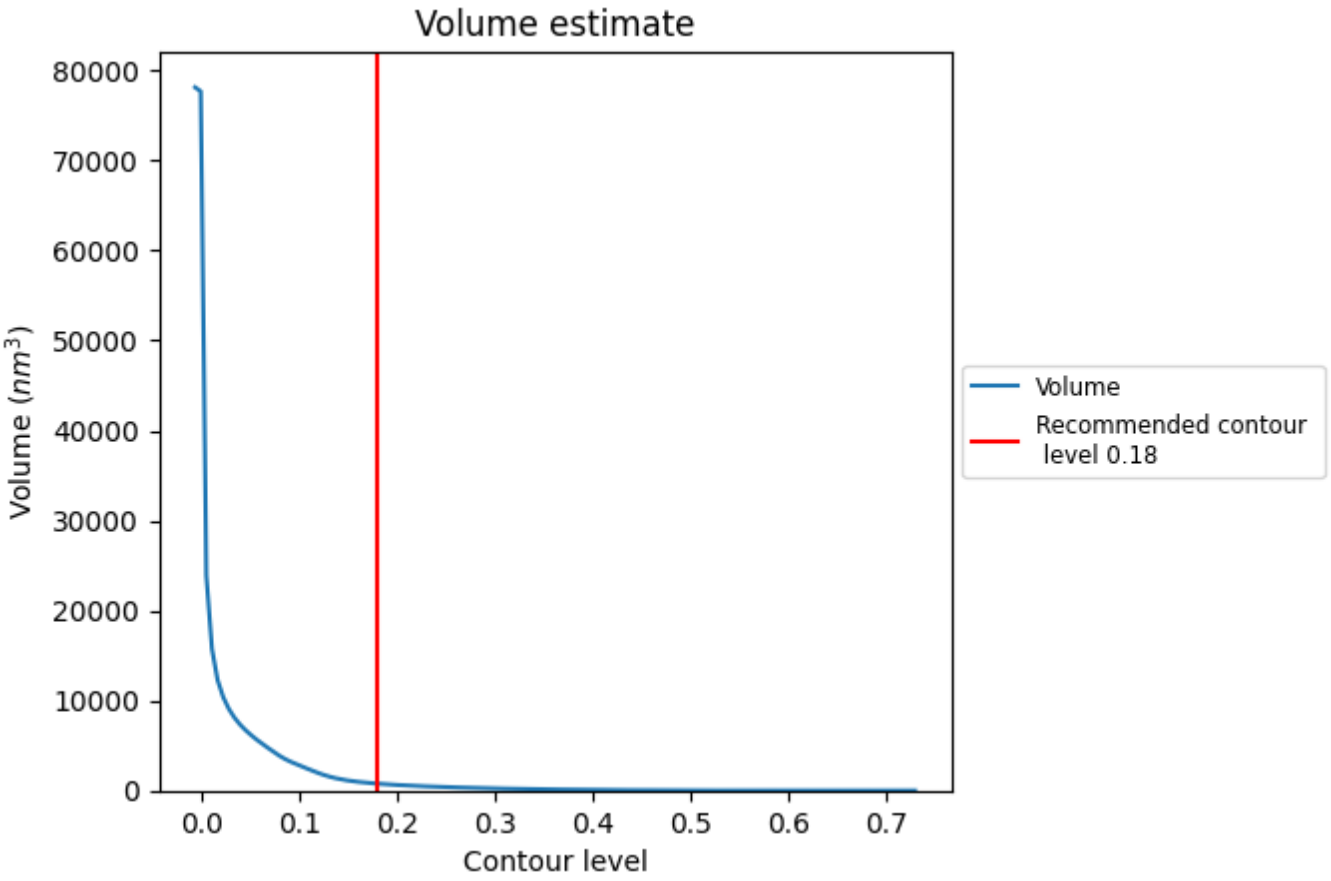
This section contains the results of statistical analysis of the map.

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.

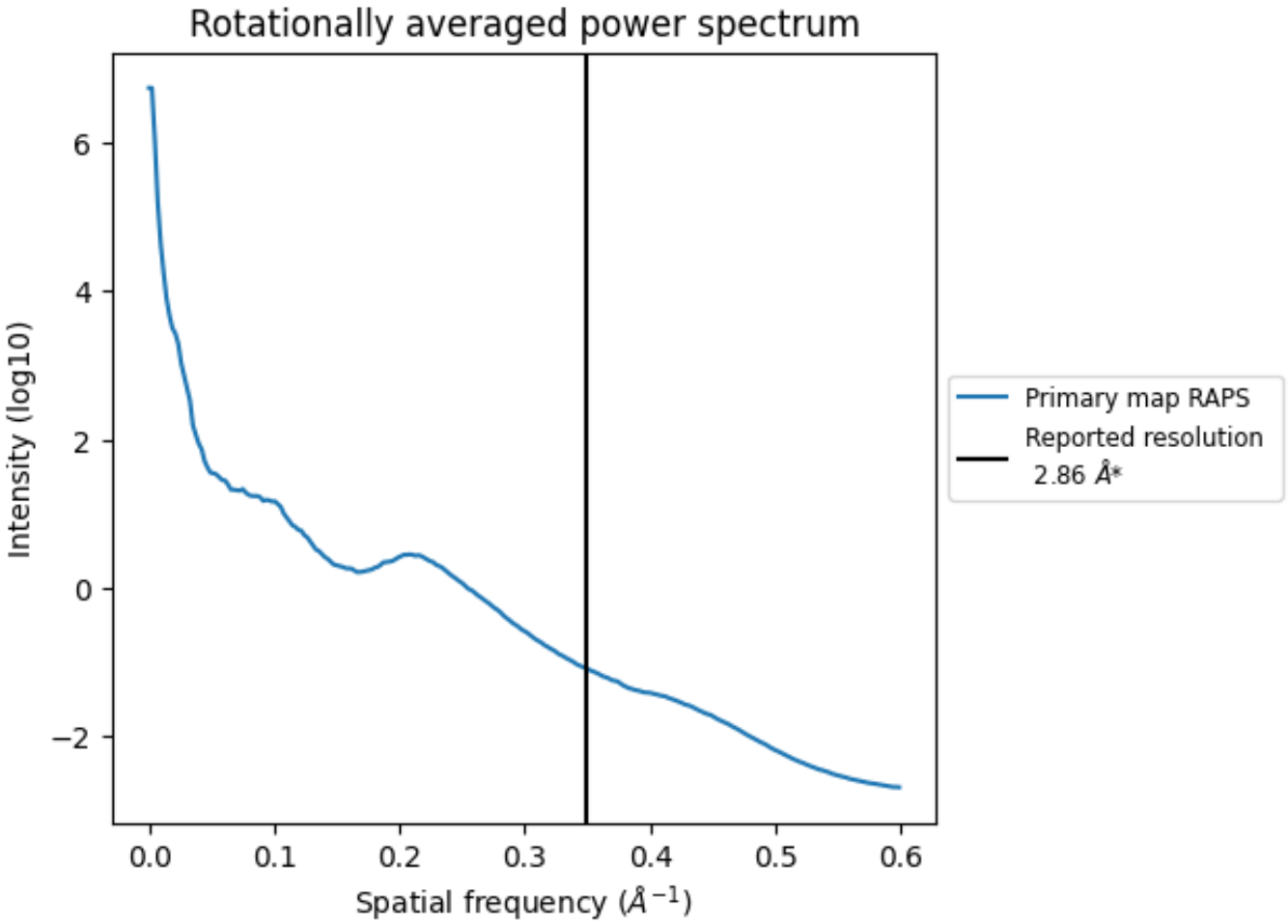
7.2 Volume estimate (i)



The volume at the recommended contour level is 763 nm^3; this corresponds to an approximate mass of 689 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 0.350 Å^{-1}

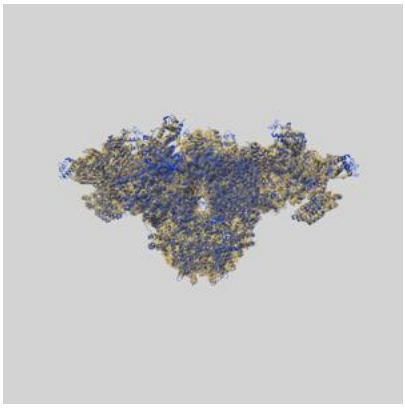
8 Fourier-Shell correlation (i)

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

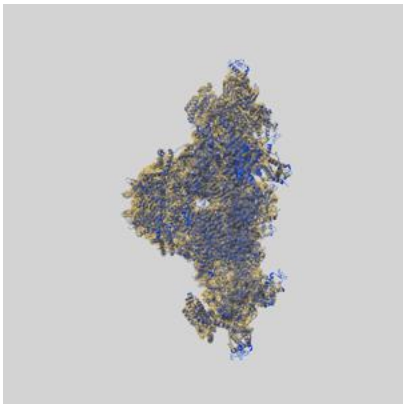
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42759 and PDB model 8UXC. Per-residue inclusion information can be found in section 3 on page 6.

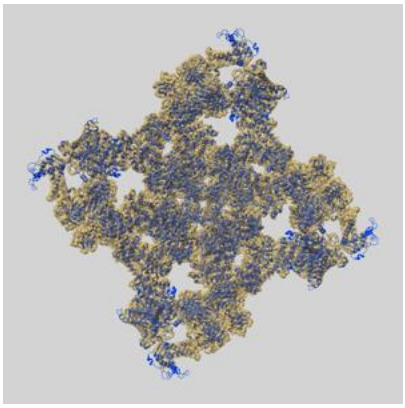
9.1 Map-model overlay



X



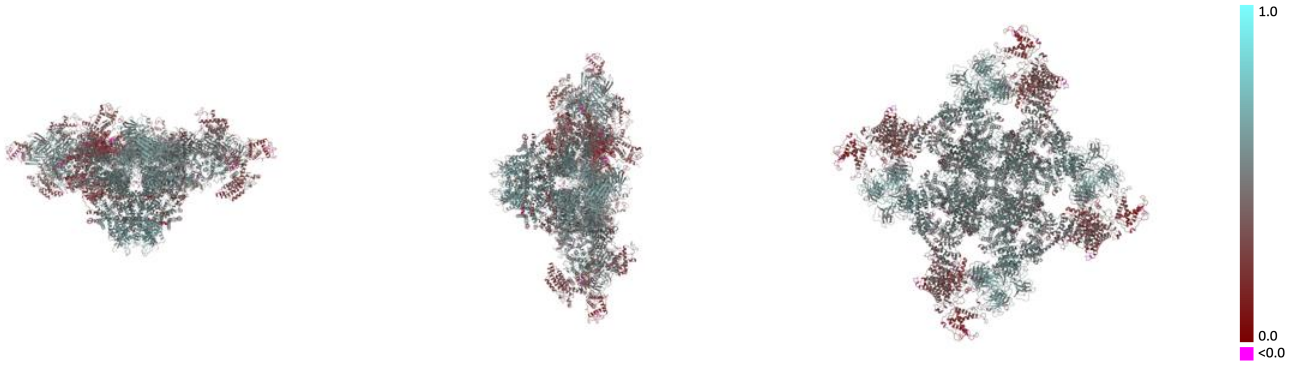
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

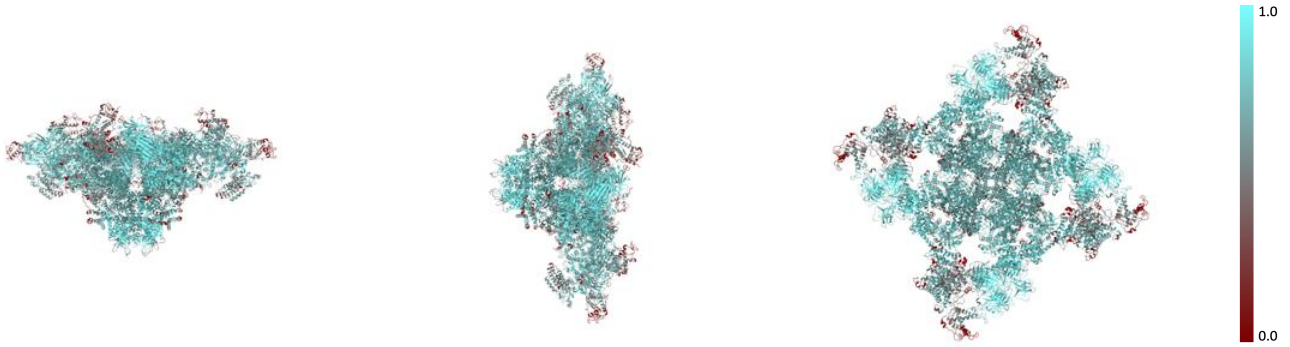
9.2 Q-score mapped to coordinate model



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.

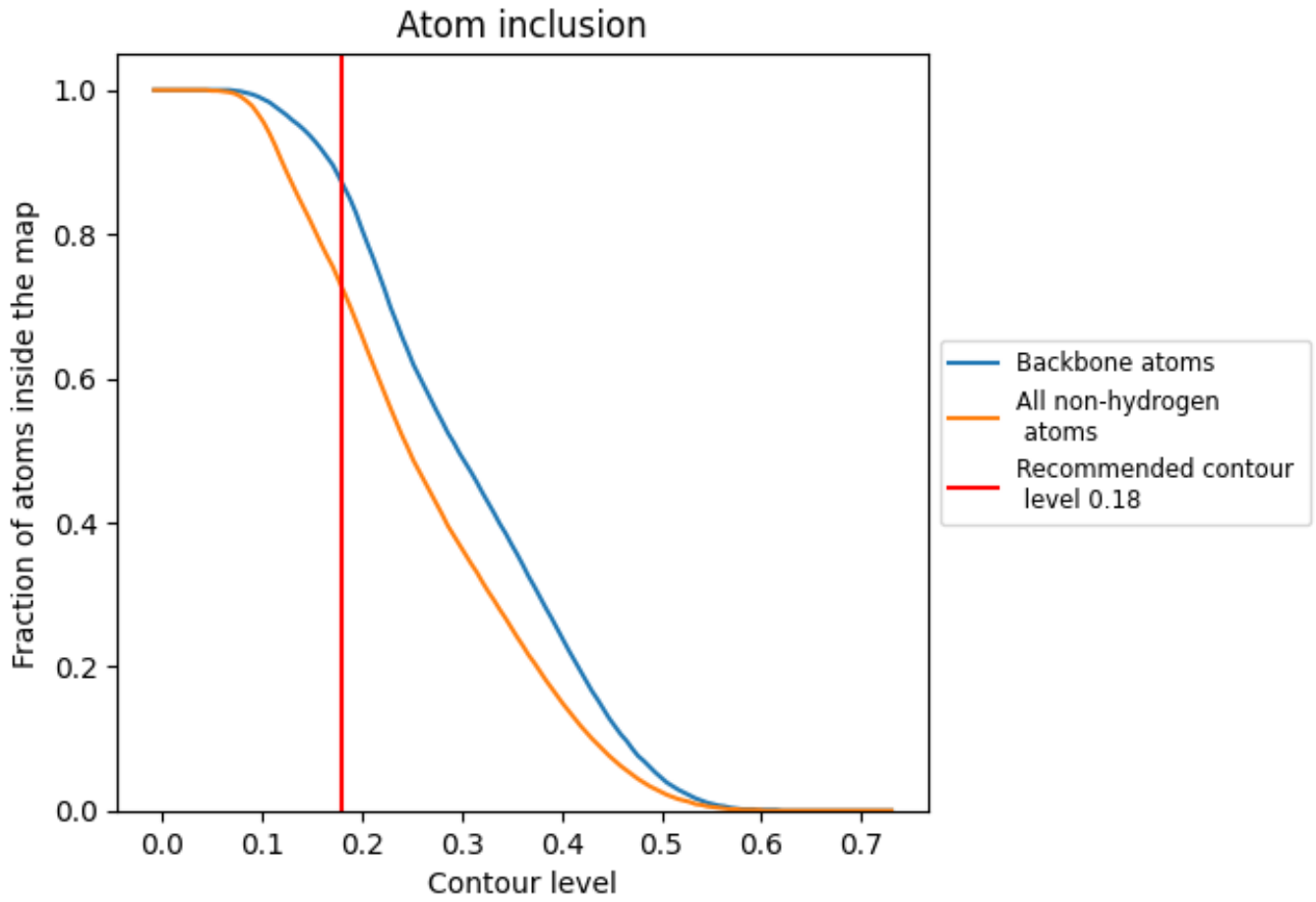
9.3 Atom inclusion mapped to coordinate model



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 (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 87% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.4660
A	0.7240	0.4640
B	0.7240	0.4640
C	0.7240	0.4640
D	0.7240	0.4640
E	0.8490	0.5520
F	0.8440	0.5520
G	0.8500	0.5520
H	0.8500	0.5510