wwPDB EM Validation Summary Report (i)

Nov 14, 2023 – 11:34 AM EST

PDB ID	:	8UXG
EMDB ID	:	EMD-42763
Title	:	Structure of PKA phosphorylated human RyR2-R420W in the closed state in the presence of ARM210
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	3.08 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 (1)) were used in the production of this report:

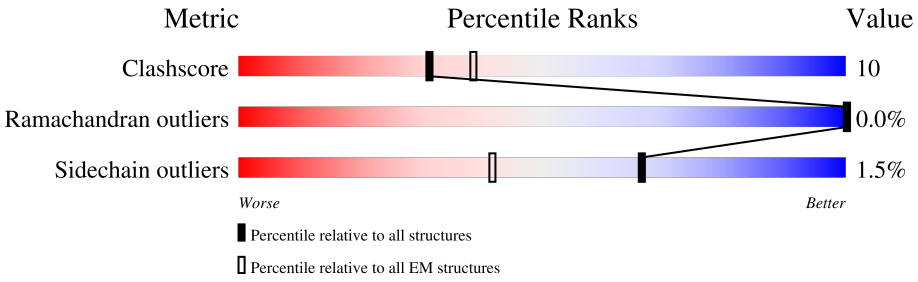
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.08 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	66% 18% • 15%
1	B	4967	66% 18% • 15%
1	C	4967	66% 18% • 15%
1	D	4967	66% 18% • 15%
2	E	108	81% 16% •••
2	F	108	80% 18% •••
2	G	108	81% 17% •••
2	H	108	80% 18% •••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 138712 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 33774	C 21521	N 5743	O 6280	S 230	2	0
1	B	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	C	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	D	4224	Total 33774	C 21521	N 5743	O 6280	S 230	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

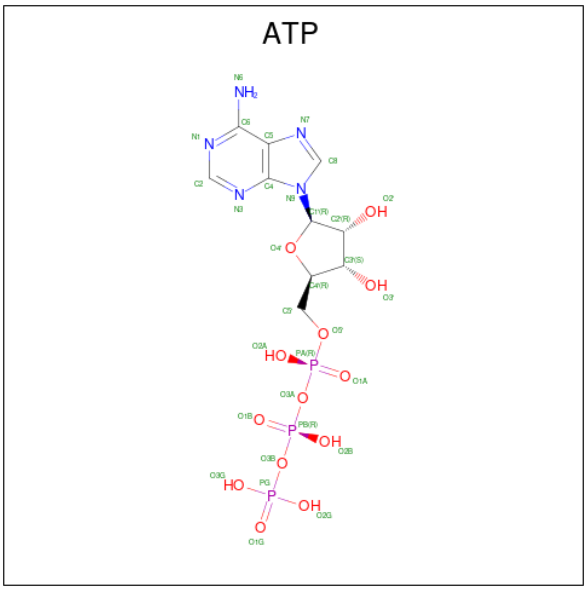
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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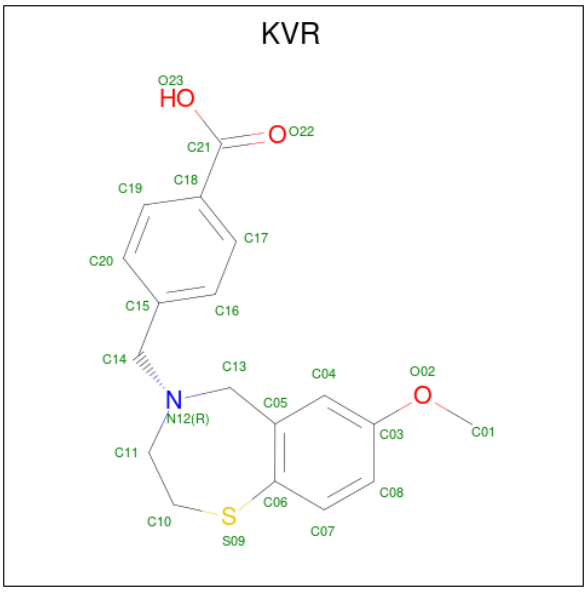
Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: $C_{18}H_{19}NO_3S$) (labeled as "Ligand of Interest" by depositor).



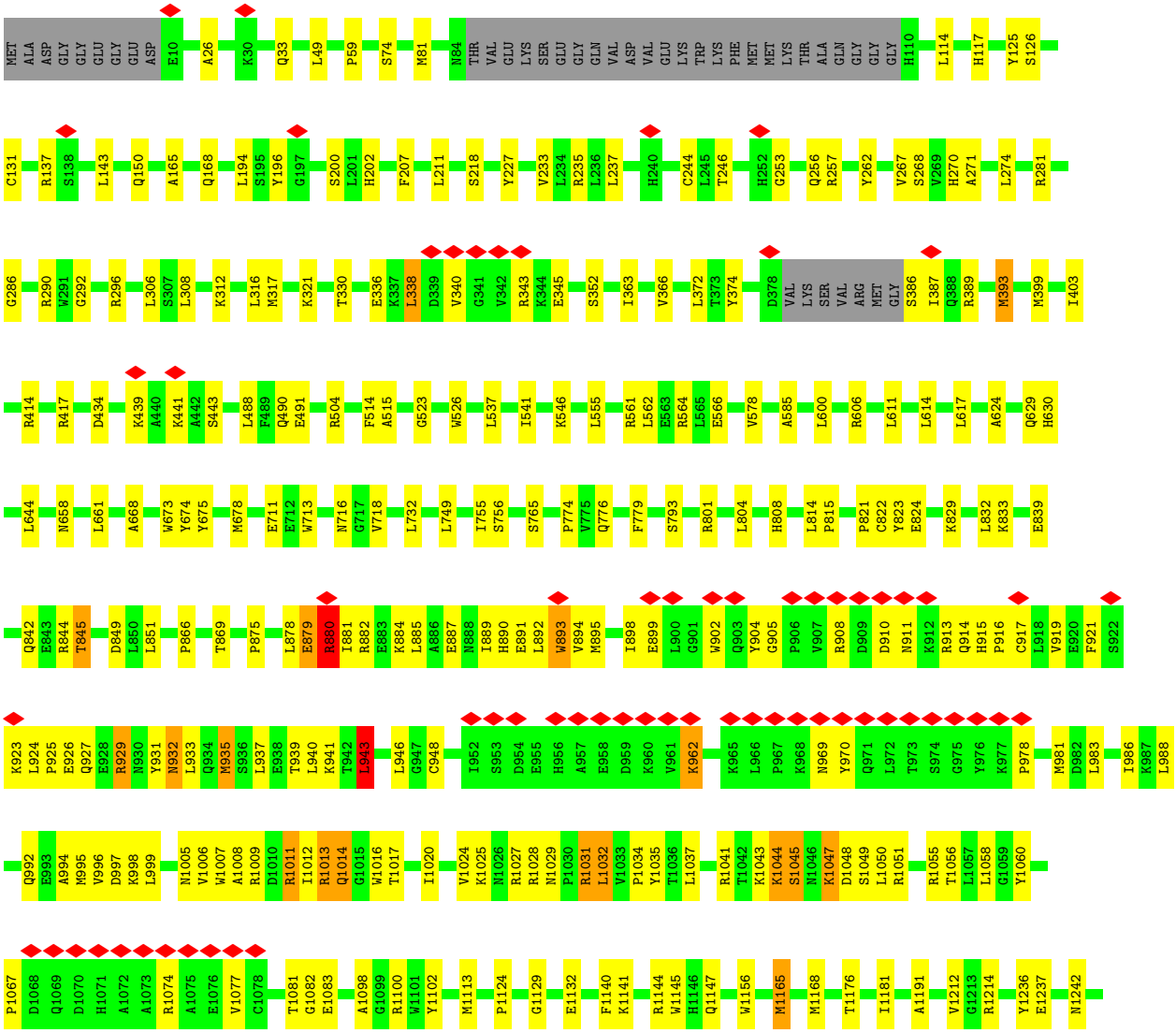
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	C	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	D	1	Total	C	N	O	S	0
			23	18	1	3	1	

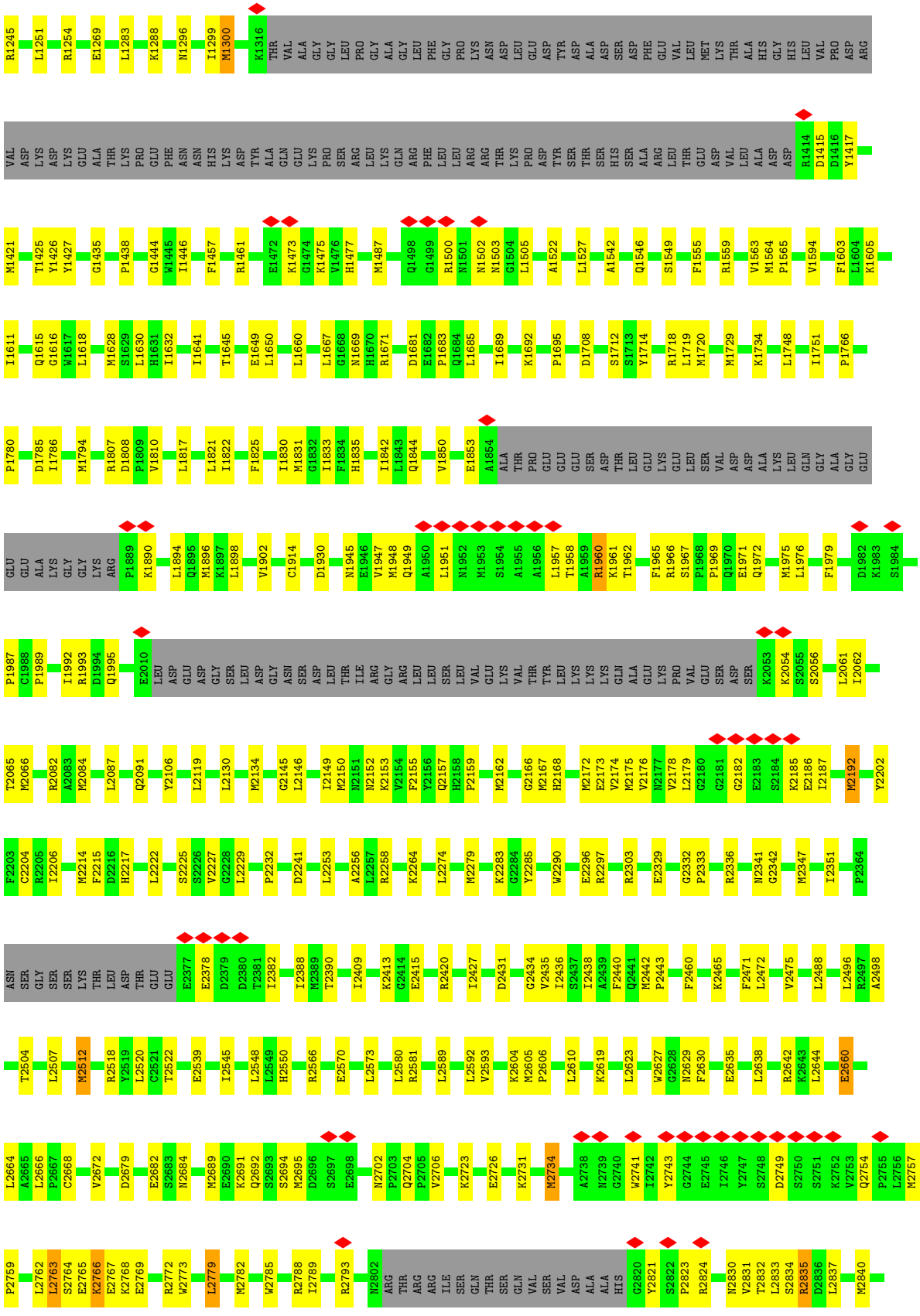
3 Residue-property plots (i)

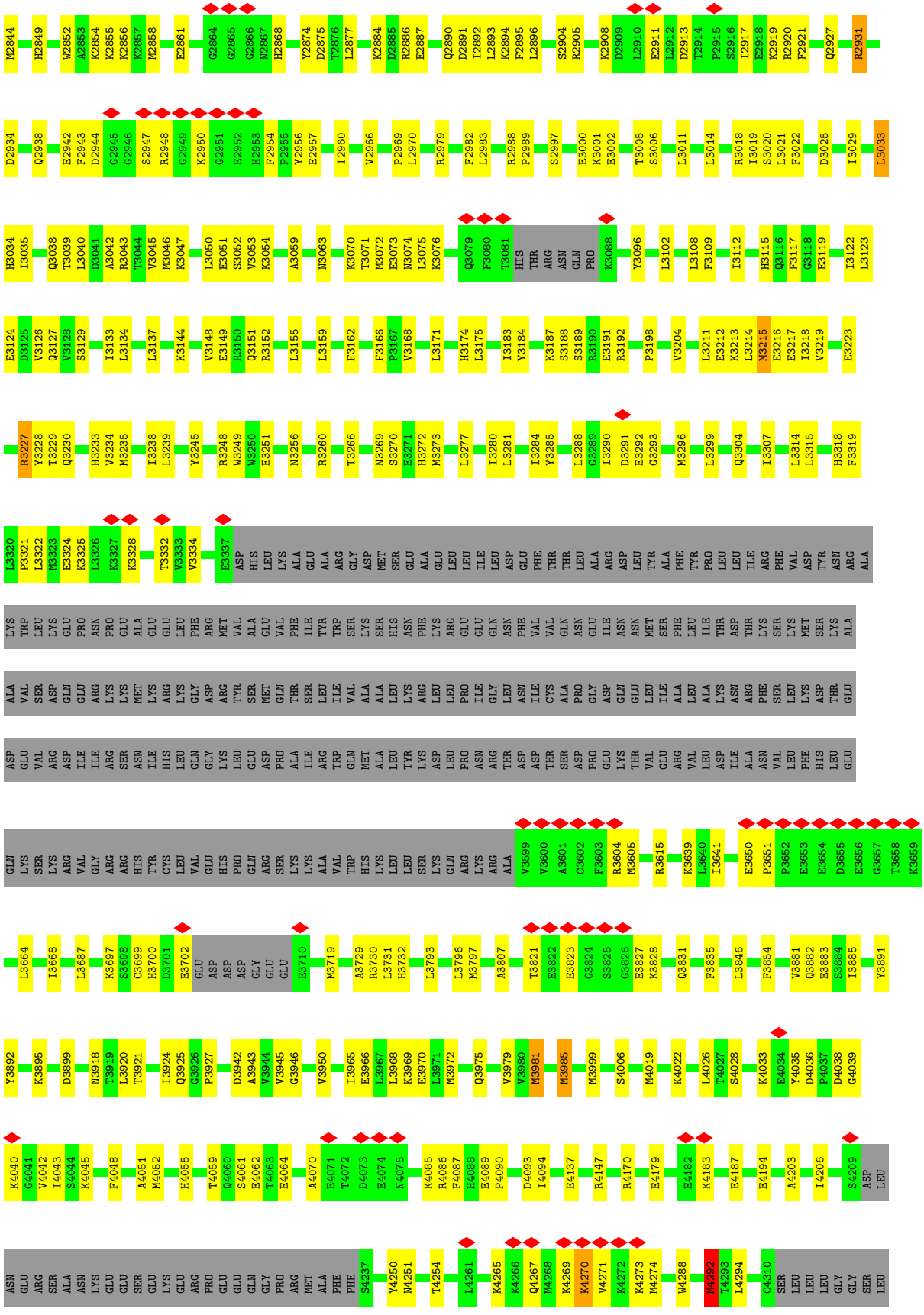
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

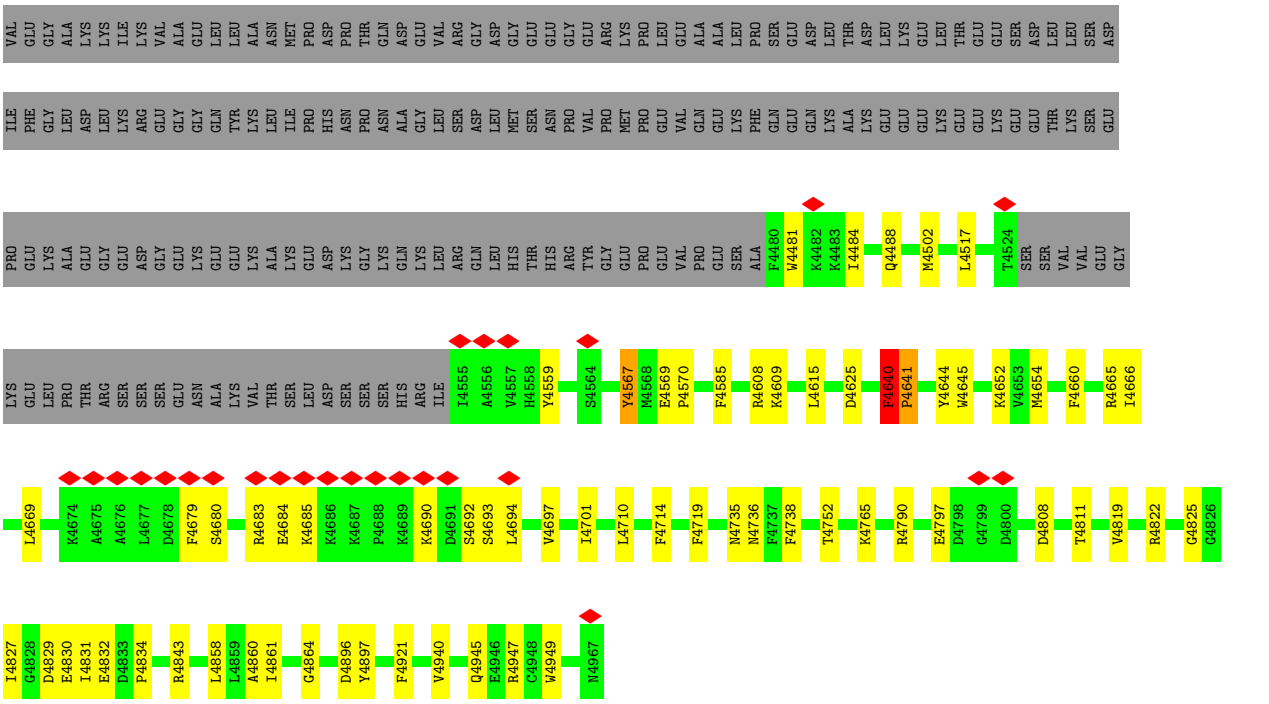
- Molecule 1: Ryanodine receptor 2

Chain A:



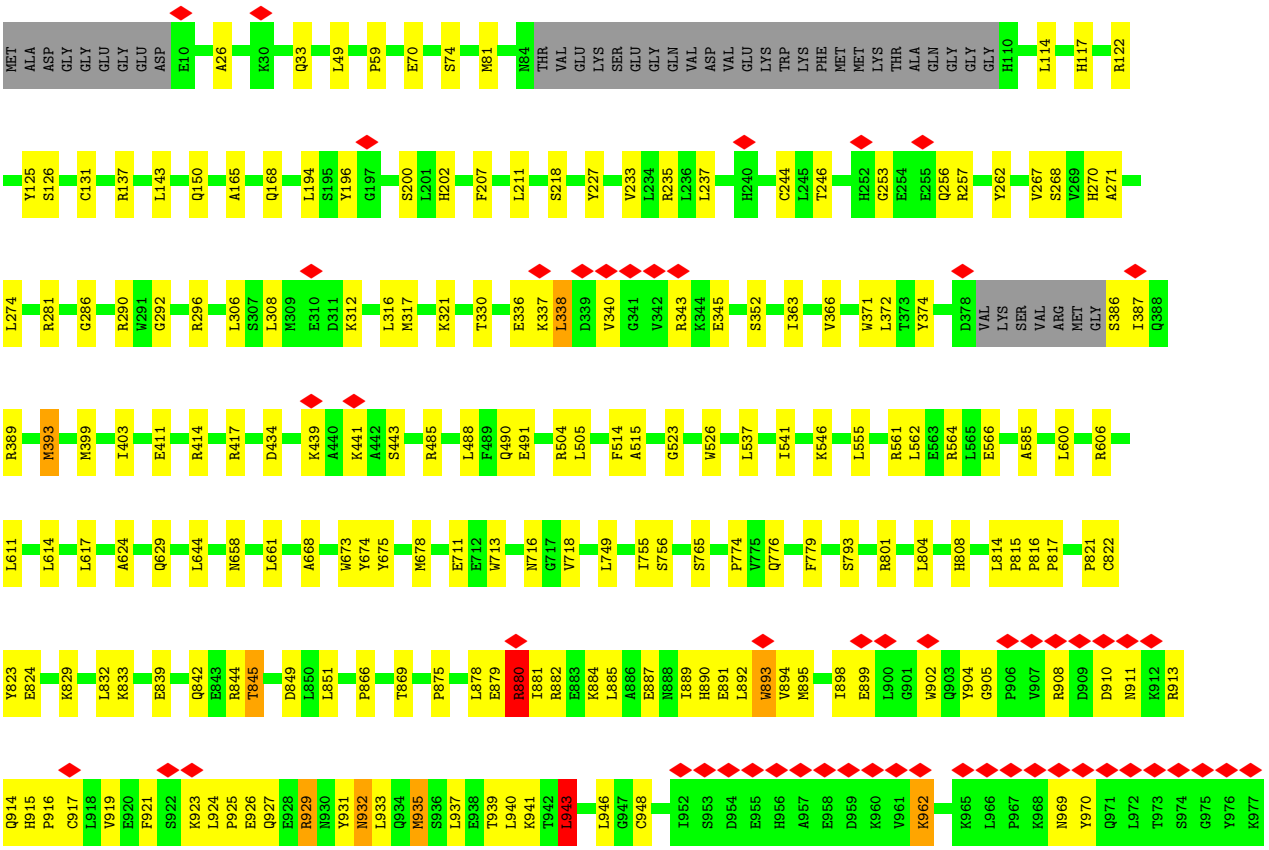

R1245 L1251 R1254 E1269 L1283 K1288 N1296 I1299 M1300 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG
VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA 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 ALA ASP ASP R1414 D1415 D1416 Y1417
M1421 T1425 Y1426 Y1427 G1435 P1438 G1444 W1445 I1446 F1457 R1461 E1472 K1473 G1474 K1475 V1476 H1477 M1487 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1522 L1527 A1542 Q1546 S1549 F1555 R1559 V1563 M1564 P1565 V1594 F1603 L1604 K1605
I1611 Q1615 G1616 W1617 L1618 M1628 S1629 L1630 H1631 I1632 I1641 T1645 E1649 L1650 L1660 L1667 G1668 N1669 H1670 R1671 D1681 E1682 P1683 Q1684 L1685 I1689 K1692 P1695 D1708 S1712 S1713 Y1714 R1718 L1719 M1720 M1729 K1734 L1748 I1751 P1766
P1780 D1785 I1786 M1794 R1807 D1808 P1809 V1810 L1817 L1821 I1822 F1825 I1830 M1831 G1832 I1833 F1834 H1835 I1842 L1843 Q1844 V1850 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 C1914 D1930 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 P1968 P1969 Q1970 E1971 Q1972 M1975 L1976 F1979 D1982 K1983 S1984
P1987 C1988 P1989 I1992 R1993 D1994 Q1995 E2010 LEU ASP GLU ASP GLY SER LEU LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 S2056 L2061 I2062
T2065 M2066 R2082 A2083 M2084 L2087 Q2091 Y2106 L2119 L2130 M2134 G2145 L2146 I2149 M2150 N2151 N2152 K2153 V2154 F2155 Y2156 Q2157 H2158 P2159 M2162 G2166 M2167 H2168 M2172 E2173 V2174 M2175 V2176 N2177 V2178 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 M2192 Y2202
F2203 C2204 R2205 I2206 M2214 F2215 D2216 H2217 L2222 S2225 S2226 V2227 G2228 L2229 P2232 D2241 L2253 A2256 L2257 R2258 K2264 L2274 M2279 K2283 G2284 Y2285 W2290 E2296 R2297 R2303 E2329 G2332 P2333 R2336 N2341 G2342 M2347 I2351 P2364
ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 I2388 M2389 T2390 I2409 K2413 G2414 E2415 R2420 I2427 D2431 G2434 V2435 I2436 S2437 I2438 A2439 F2440 Q2441 M2442 P2443 F2460 K2465 F2471 L2472 V2475 L2488 L2496 R2497 A2498
T2504 L2507 M2512 R2518 Y2519 L2520 C2521 T2522 E2539 I2545 L2548 L2549 H2550 R2566 E2570 L2573 L2580 R2581 L2589 L2592 V2593 K2604 M2605 P2606 L2610 K2619 L2623 W2627 G2628 N2629 F2630 E2635 L2638 R2642 K2643 L2644 E2660
L2664 A2665 L2666 P2667 C2668 V2672 D2679 E2682 S2683 N2684 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 N2702 P2703 Q2704 P2705 V2706 K2723 E2726 K2731 M2734 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758
P2759 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 R2772 W2773 L2779 M2782 W2785 R2788 I2789 R2793 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 M2840

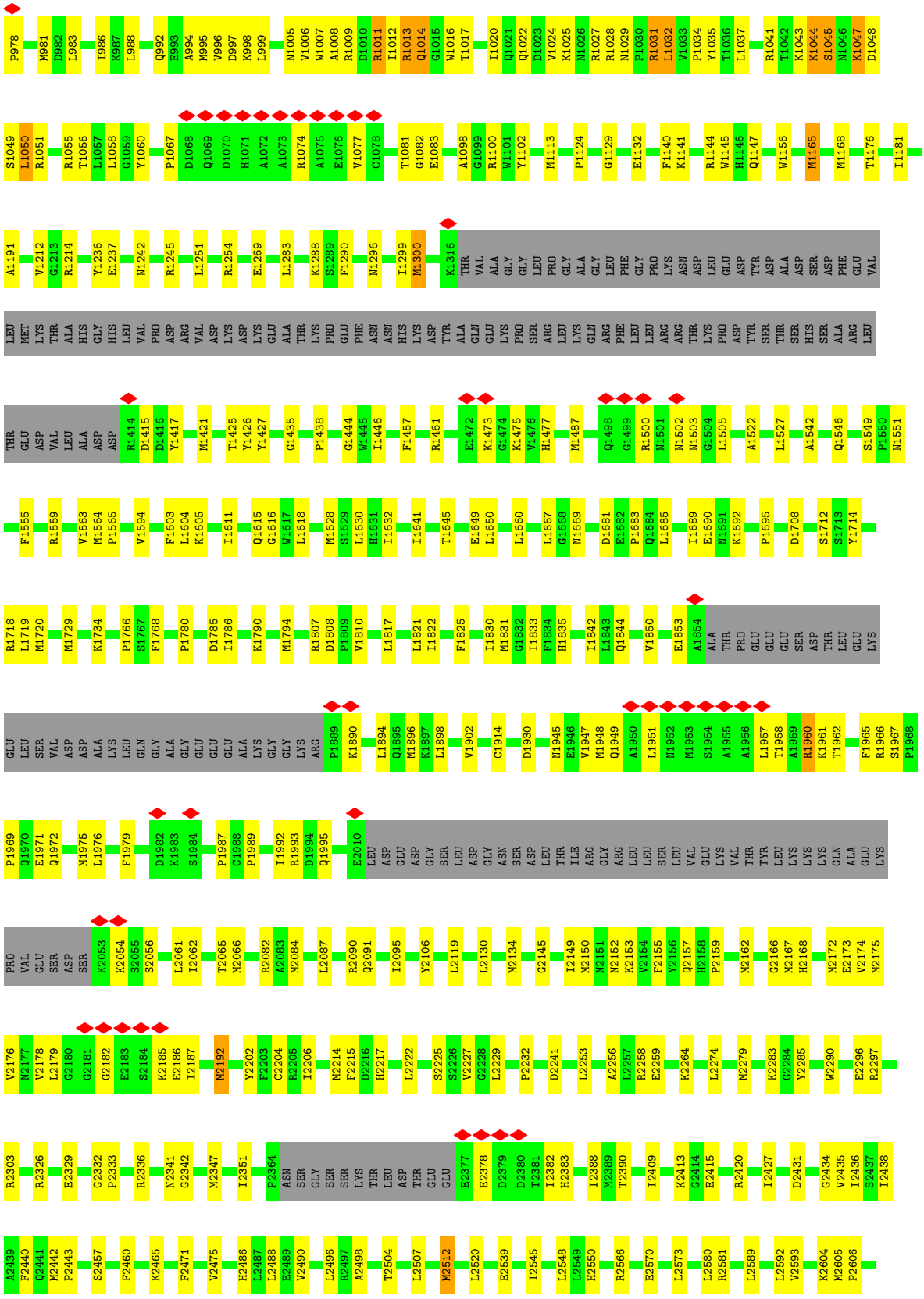


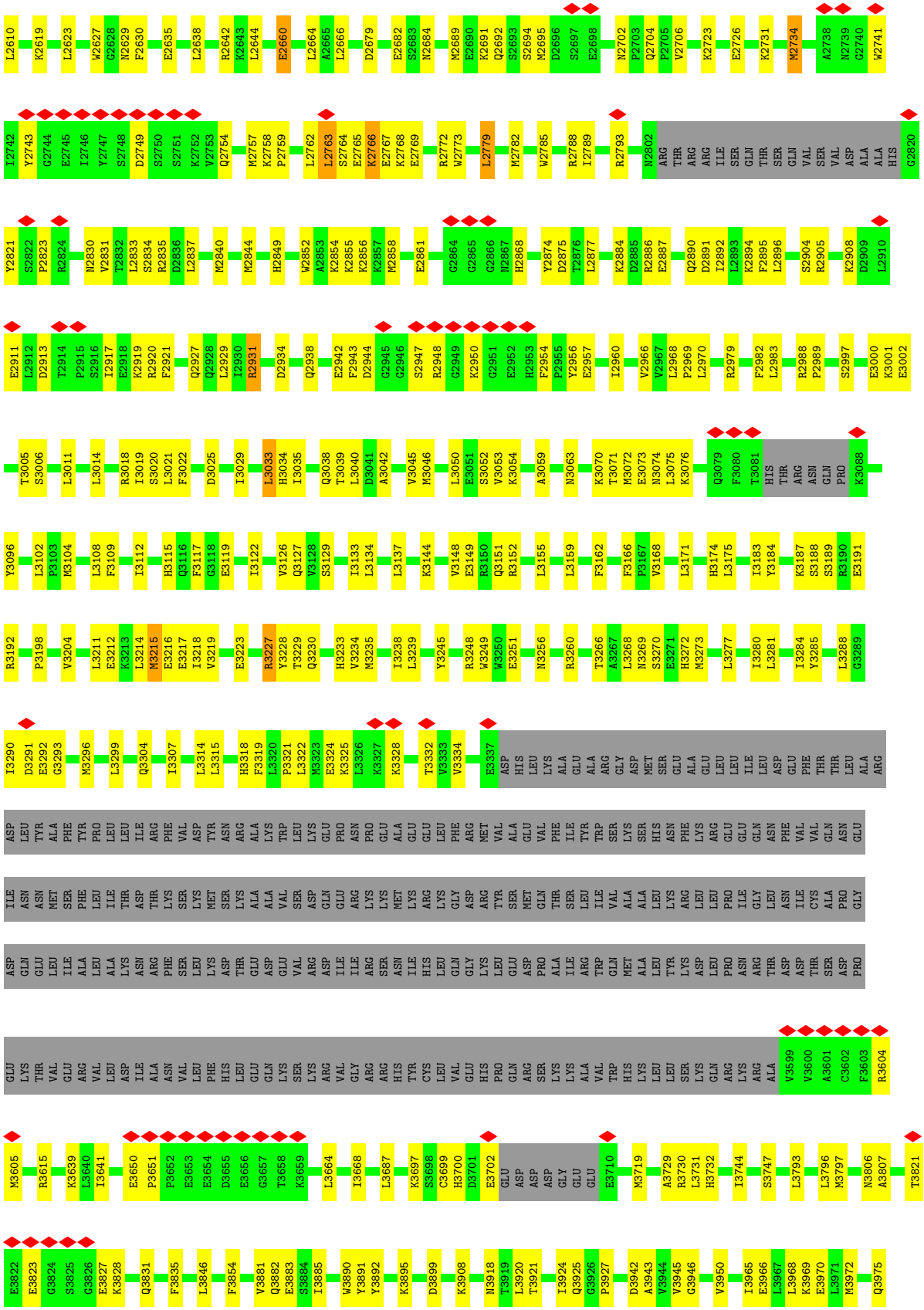


• Molecule 1: Ryanodine receptor 2

Chain B:



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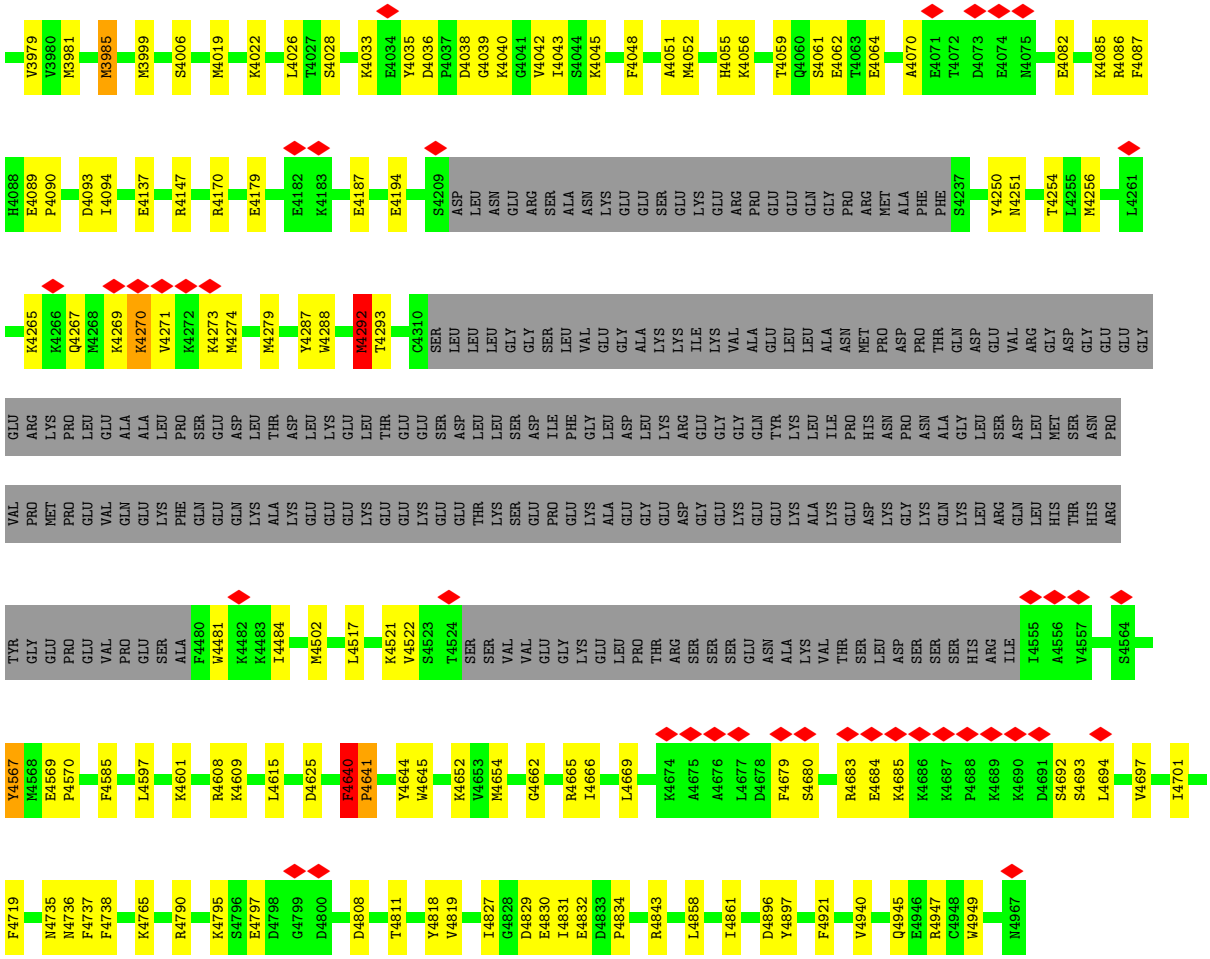
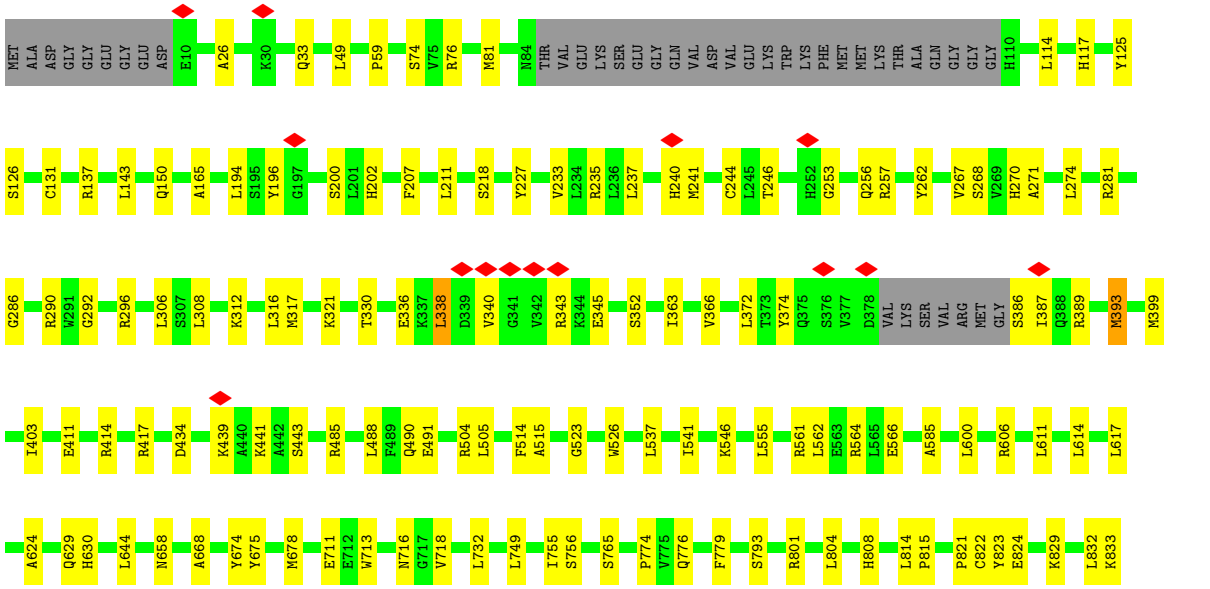
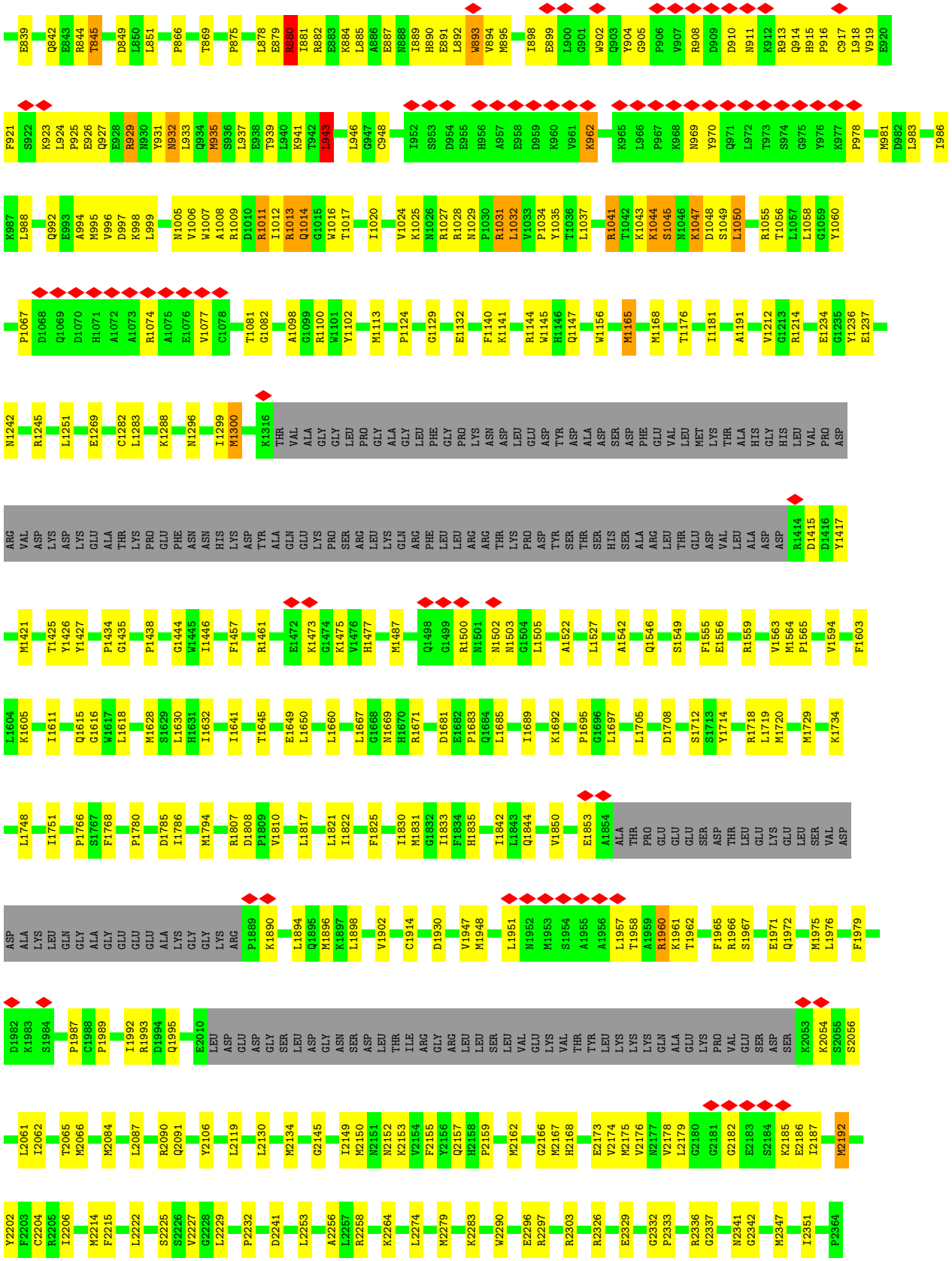
I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 M2757 K2758 P2759 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 R2772 W2773 L2779 M2782 W2785 R2788 I2789 R2793 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820
Y2821 S2822 P2823 R2824 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 M2840 M2844 H2849 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2861 G2864 G2865 G2866 N2867 H2868 Y2874 D2875 T2876 L2877 K2884 D2885 R2886 E2887 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 S2904 R2905 K2908 D2909 L2910
E2911 L2912 D2913 T2914 P2915 S2916 I2917 E2918 K2919 R2920 F2921 Q2927 Q2928 L2929 I2930 R2931 D2934 Q2938 E2942 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 Y2956 E2957 I2960 V2966 V2967 L2968 P2969 L2970 R2979 F2982 L2983 R2988 P2989 S2997 E3000 K3001 E3002
T3005 S3006 L3011 L3014 R3018 I3019 S3020 L3021 F3022 D3025 I3029 L3033 H3034 I3035 Q3038 T3039 L3040 D3041 A3042 V3045 M3046 L3050 E3051 S3052 V3053 K3054 A3059 N3063 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088
Y3096 L3102 P3103 M3104 L3108 F3109 I3112 H3115 Q3116 F3117 G3118 E3119 I3122 V3126 Q3127 V3128 S3129 I3133 L3134 L3137 K3144 V3148 E3149 R3150 Q3151 R3152 L3155 L3159 F3162 F3166 P3167 V3168 L3171 H3174 L3175 I3183 Y3184 K3187 S3188 S3189 R3190 E3191
R3192 P3198 V3204 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3223 R3227 Y3228 T3229 Q3230 H3233 V3234 M3235 I3238 L3239 Y3245 R3248 W3249 W3250 E3251 N3256 R3260 T3266 A3267 L3268 N3269 S3270 E3271 H3272 M3273 L3277 I3280 L3281 I3284 Y3285 L3288 G3289
I3290 D3291 E3292 G3293 M3296 L3299 Q3304 I3307 L3314 L3315 H3318 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 T3332 V3333 V3334 E3337 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 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 GLU ARG LYS MET LYS ARG THR SER 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 LYS 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 LEU TYR LYS ASP LEU PRO ASN ARG THR 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 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 R3615 K3639 L3640 I3641 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 L3664 I3668 L3687 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 M3719 A3729 R3730 L3731 H3732 I3744 S3747 L3793 L3796 M3797 N3806 A3807 T3821
E3822 E3823 G3824 S3825 G3826 E3827 K3828 Q3831 F3835 L3846 F3854 V3881 Q3882 E3883 S3884 I3885 W3890 Y3891 Y3892 K3895 D3899 K3908 N3918 T3919 L3920 T3921 I3924 Q3925 G3926 P3927 D3942 A3943 V3944 V3945 G3946 V3950 I3965 E3966 L3967 L3968 K3969 E3970 L3971 M3972 Q3975



• Molecule 1: Ryanodine receptor 2

Chain C:

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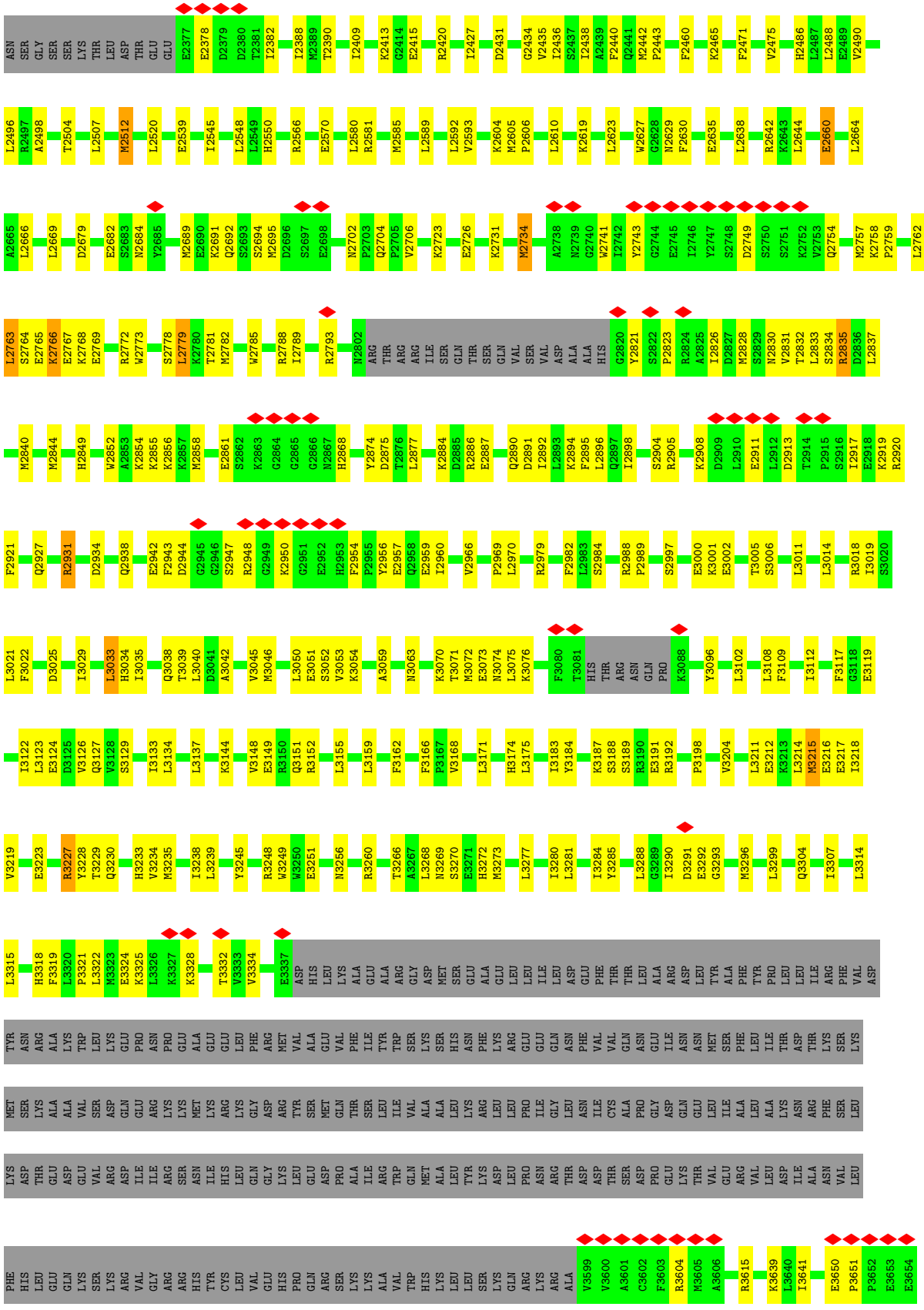
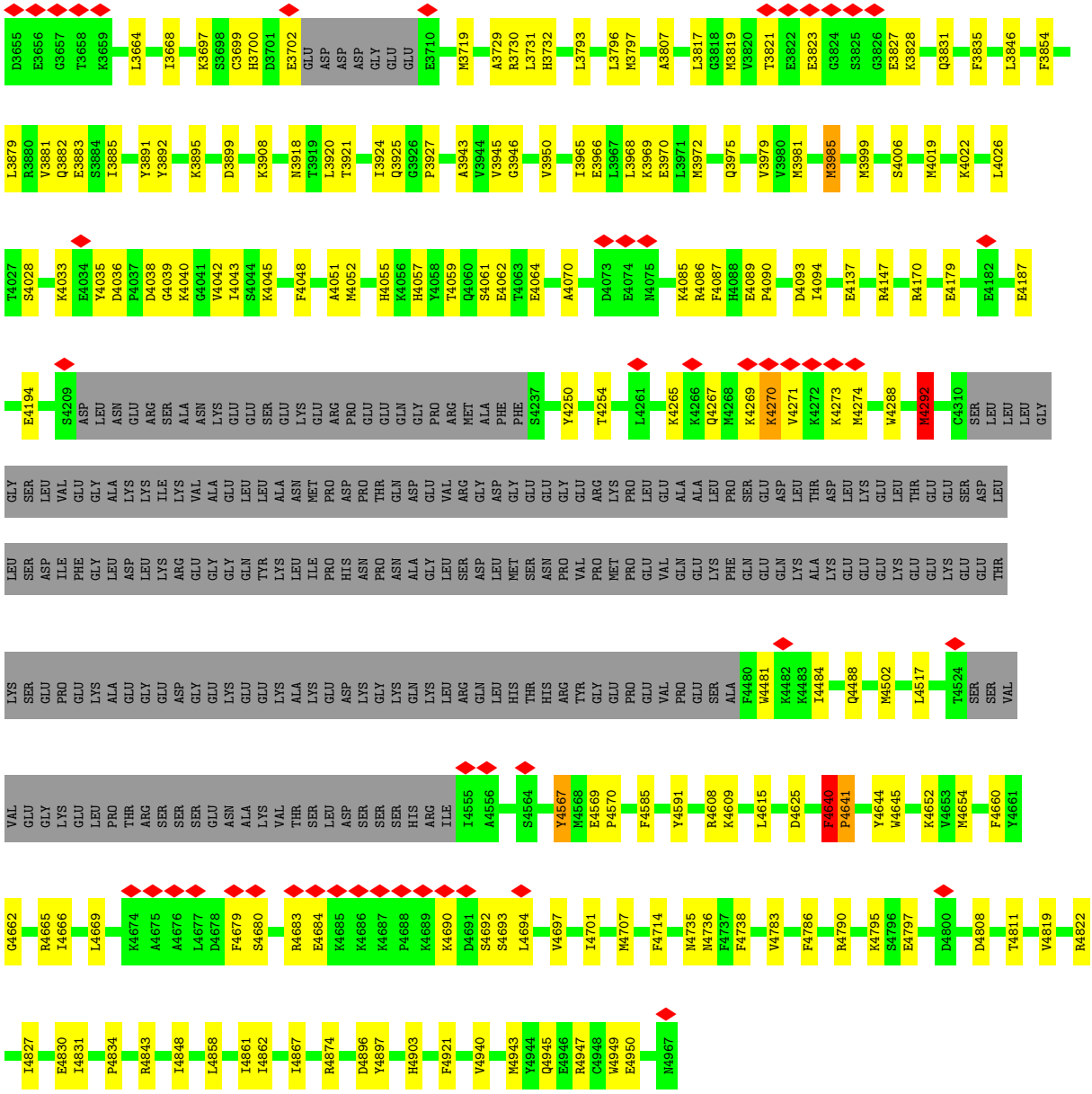
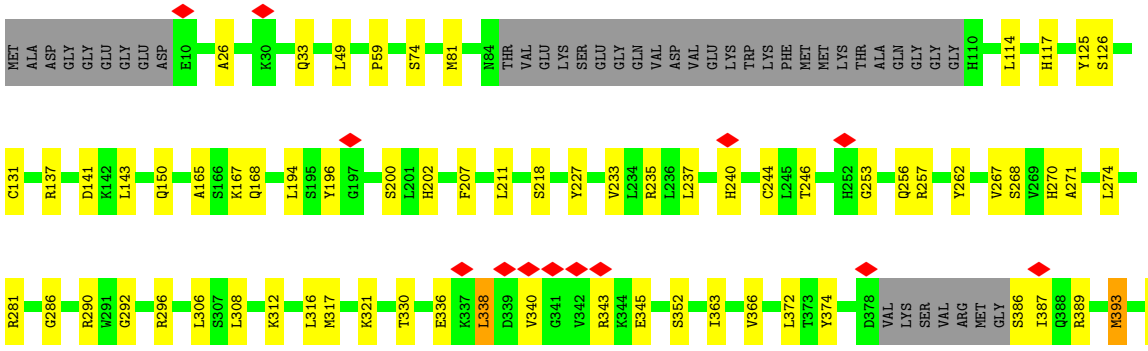
F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L946 G947 C948 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 M981 D982 L983 I986
K987 L988 Q992 E993 A994 M995 V996 D997 K998 L999 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 I1020 V1024 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1055 T1056 L1057 L1058 G1059 Y1060
P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 G1082 A1098 G1099 R1100 W1101 Y1102 M1113 P1124 G1129 E1132 F1140 K1141 R1144 W1145 H1146 Q1147 W1156 M1165 M1168 T1176 I1181 A1191 V1212 G1213 R1214 E1234 G1235 Y1236 E1237
N1242 R1245 L1251 E1269 C1282 L1283 K1288 N1296 I1299 M1300 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
M1421 T1425 Y1426 Y1427 P1434 G1435 P1438 G1444 W1445 I1446 F1457 R1461 E1472 K1473 G1474 K1475 V1476 H1477 M1487 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1522 L1527 A1542 Q1546 S1549 F1555 E1556 R1559 V1563 M1564 P1565 V1594 F1603
L1604 K1605 I1611 Q1615 G1616 W1617 L1618 M1628 S1629 L1630 H1631 I1632 I1641 T1645 E1649 L1650 L1660 L1667 G1668 N1669 H1670 R1671 D1681 E1682 P1683 Q1684 L1685 I1689 K1692 P1695 G1696 L1697 L1705 D1708 S1712 S1713 Y1714 R1718 L1719 M1720 M1729 K1734
L1748 I1751 P1766 S1767 F1768 P1780 D1785 I1786 M1794 R1807 D1808 P1809 V1810 L1817 L1821 I1822 F1825 I1830 M1831 G1832 I1833 F1834 H1835 I1842 L1843 Q1844 V1850 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 ALA LYS GLY GLY LYS ARG P1889 K1890 L1894 Q1895 M1896 K1897 L1898 V1902 C1914 D1930 V1947 M1948 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 E1971 Q1972 M1975 L1976 F1979
D1982 K1983 S1984 P1987 C1988 P1989 I1992 R1993 D1994 Q1995 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 S2056
L2061 I2062 T2065 M2066 M2084 L2087 R2090 Q2091 Y2106 L2119 L2130 M2134 G2145 I2149 M2150 N2151 N2152 K2153 V2154 F2155 Y2156 Q2157 H2158 P2159 M2162 G2166 M2167 H2168 E2173 V2174 M2175 V2176 N2177 V2178 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 M2192
Y2202 F2203 C2204 R2205 I2206 M2214 F2215 L2222 S2225 S2226 V2227 G2228 L2229 P2232 D2241 L2253 A2256 L2257 R2258 K2264 L2274 M2279 K2283 W2290 E2296 R2297 R2303 R2326 E2329 G2332 P2333 R2336 G2337 N2341 G2342 M2347 I2351 P2364

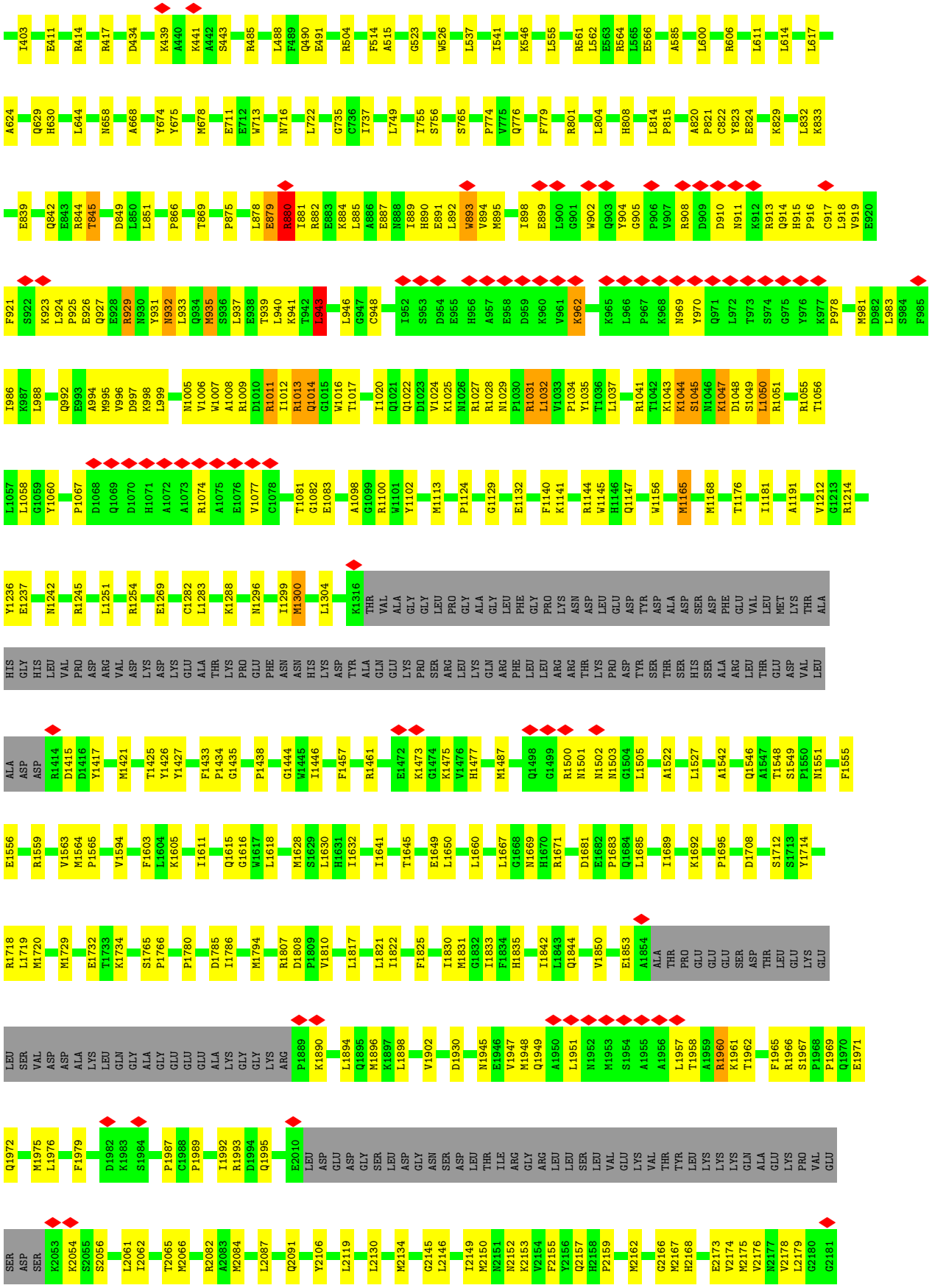




• Molecule 1: Ryanodine receptor 2

Chain D:

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A624 Q629 H630 L644 N658 A668 Y674 Y675 M678 E711 E712 W713 N716 L722 G735 C736 I737 L749 I755 S756 S765 P774 V775 Q776 F779 R801 L804 H808 L814 P815 A820 P821 C822 Y823 E824 K829 L832 K833
E839 Q842 E843 R844 T845 D849 L850 L851 P866 T869 P875 L878 E879 R880 I881 R882 E883 K884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 Y907 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 L946 G947 C948 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 M981 D982 L983 S984 F985
I986 K987 L988 Q992 E993 A994 M995 V996 D997 K998 L999 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 R1055 T1056
L1057 L1058 G1059 Y1060 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 G1082 E1083 A1098 G1099 R1100 W1101 Y1102 M1113 P1124 G1129 E1132 F1140 K1141 R1144 W1145 H1146 Q1147 W1156 M1165 M1168 T1176 I1181 A1191 V1212 G1213 R1214
Y1236 E1237 N1242 R1245 L1251 R1254 E1269 C1282 L1283 K1288 N1296 I1299 M1300 L1304 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA
HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU
ALA ASP ASP R1414 D1415 D1416 Y1417 M1421 T1425 Y1426 Y1427 F1433 P1434 G1435 P1438 G1444 W1445 I1446 F1457 R1461 E1472 K1473 G1474 K1475 V1476 H1477 M1487 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1522 L1527 A1542 Q1546 A1547 T1548 S1549 P1550 N1551 F1555
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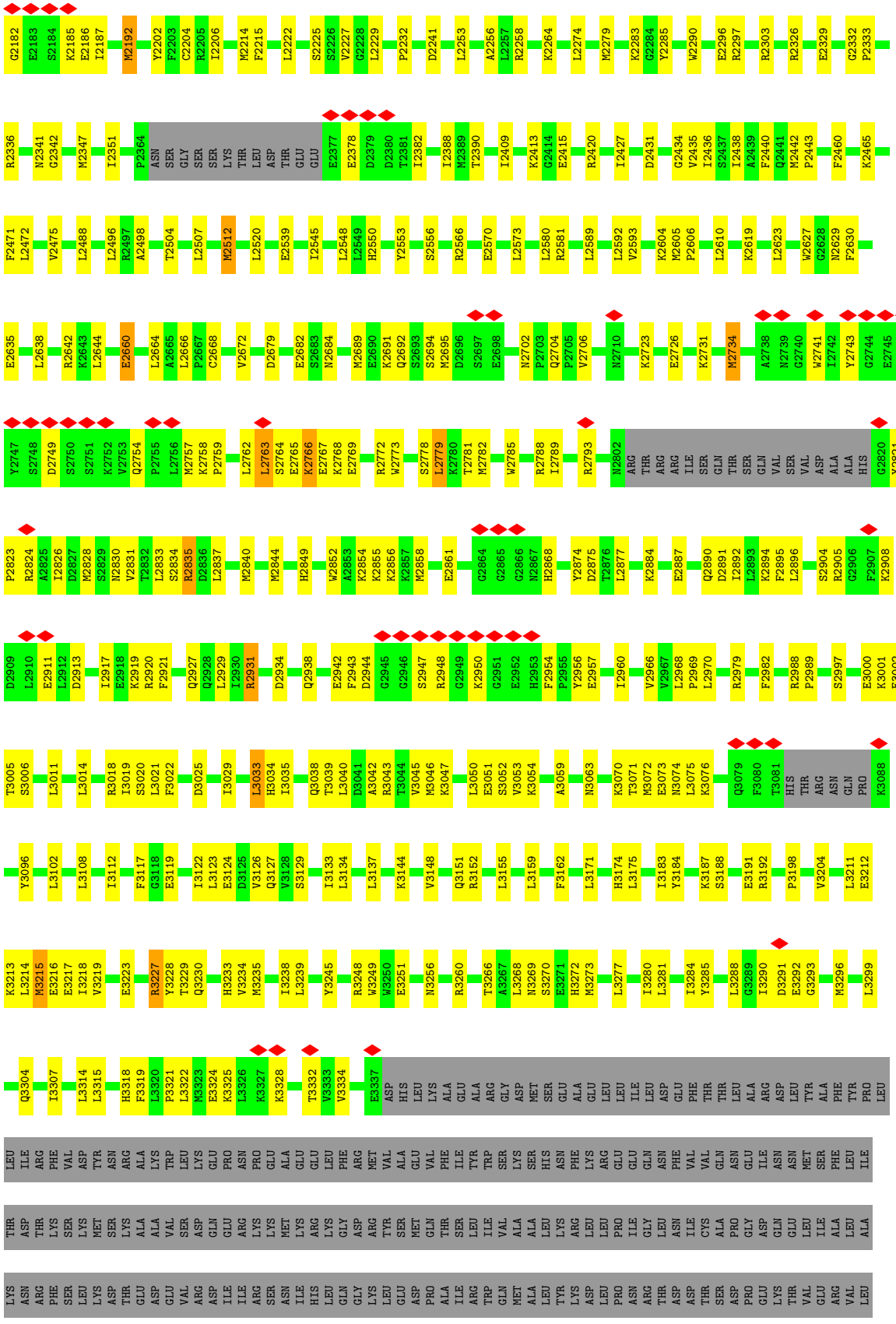
R1718 L1719 M1720 M1729 E1732 T1733 K1734 S1765 P1766 P1780 D1785 I1786 M1794 R1807 D1808 P1809 V1810 L1817 L1821 L1822 F1825 I1830 M1831 G1832 I1833 F1834 H1835 I1842 L1843 Q1844 V1850 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU
LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1894 Q1895 M1896 K1897 L1898 V1902 D1930 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 F1965 R1966 S1967 P1968 P1969 Q1970 E1971
Q1972 M1975 L1976 F1979 D1982 K1983 S1984 P1987 C1988 P1989 I1992 R1993 D1994 Q1995 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU
SER ASP SER K2053 K2054 S2055 S2056 L2061 I2062 T2065 M2066 R2082 A2083 M2084 L2087 Q2091 Y2106 L2119 L2130 M2134 G2145 L2146 I2149 M2150 N2151 N2152 K2153 V2154 F2155 Y2156 Q2157 H2158 P2159 M2162 G2166 M2167 H2168 E2173 V2174 M2175 V2176 N2177 V2178 L2179 G2180 G2181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R2336 N2341 G2342 M2347 I2351 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 I2388 M2389 T2390 I2409 K2413 G2414 E2415 R2420 I2427 D2431 G2434 V2435 I2436 S2437 I2438 A2439 F2440 Q2441 M2442 P2443 F2460 K2465
F2471 L2472 V2475 L2488 L2496 R2497 A2498 T2504 L2507 L2520 E2539 I2545 L2548 L2549 H2550 Y2553 S2556 R2566 E2570 L2573 L2580 R2581 L2589 L2592 V2593 K2604 M2605 P2606 L2610 K2619 L2623 W2627 G2628 N2629 F2630
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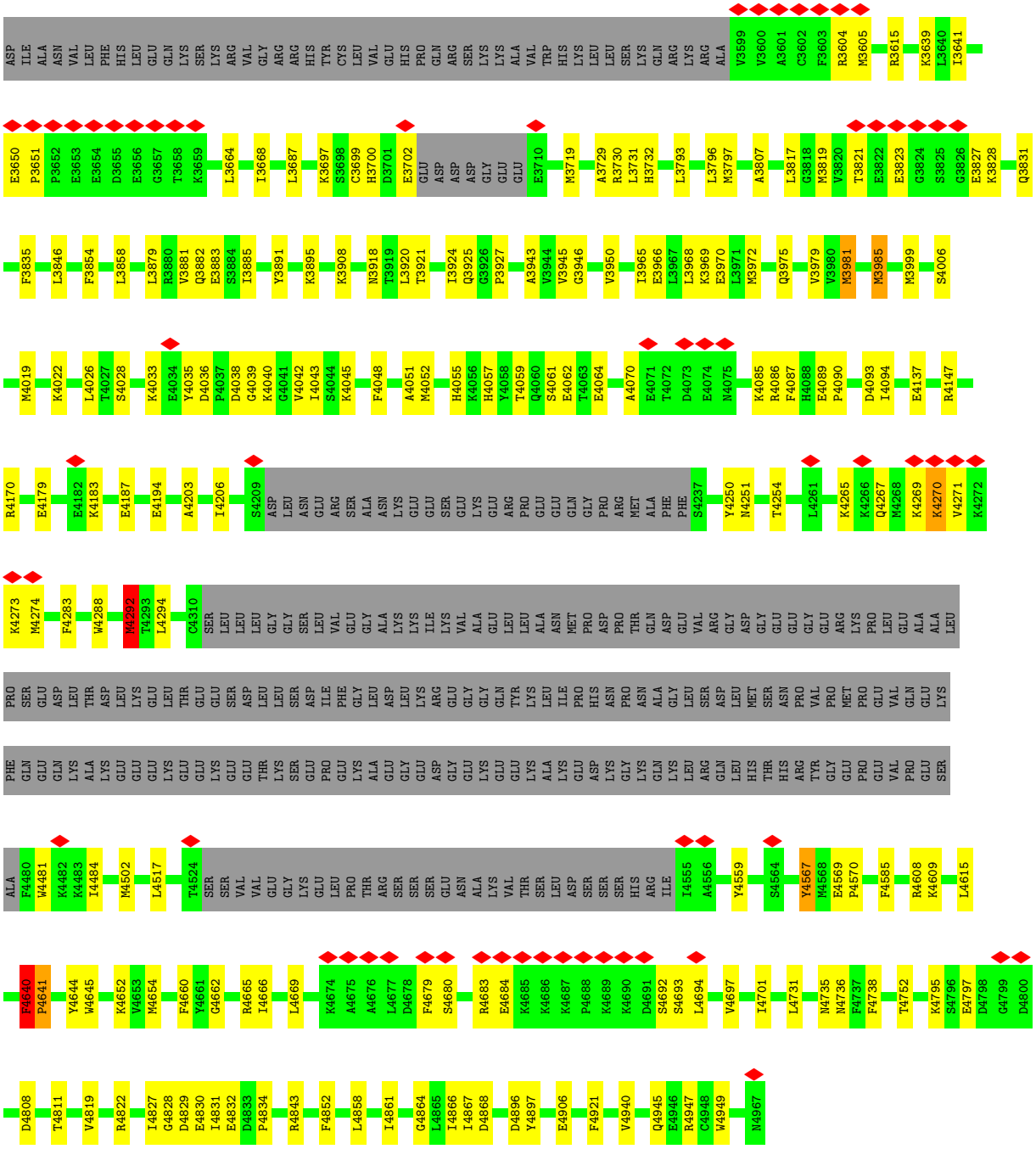
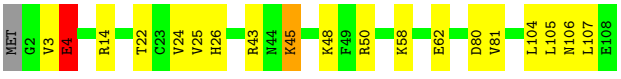
Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 R2772 W2773 S2778 L2779 K2780 T2781 M2782 W2785 R2788 I2789 R2793 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822
P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 M2840 M2844 H2849 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2861 G2864 G2865 G2866 N2867 H2868 Y2874 D2875 T2876 L2877 K2884 E2887 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 S2904 R2905 G2906 F2907 K2908
D2909 L2910 E2911 L2912 D2913 T2917 E2918 K2919 R2920 F2921 Q2927 Q2928 L2929 T2930 R2931 D2934 Q2938 E2942 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 Y2956 E2957 I2960 V2966 V2967 L2968 P2969 L2970 R2979 F2982 R2988 P2989 S2997 E3000 K3001 E3002
T3005 S3006 L3011 L3014 R3018 I3019 S3020 L3021 F3022 D3025 I3029 L3033 H3034 I3035 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 L3050 E3051 S3052 V3053 K3054 A3059 N3063 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088
Y3096 L3102 L3108 I3112 F3117 G3118 E3119 I3122 L3123 E3124 D3125 V3126 Q3127 V3128 S3129 I3133 L3134 L3137 K3144 V3148 Q3151 R3152 L3155 L3159 F3162 L3171 H3174 L3175 I3183 Y3184 K3187 S3188 E3191 R3192 P3198 V3204 L3211 E3212
K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3223 R3227 Y3228 T3229 Q3230 H3233 V3234 M3235 I3238 L3239 Y3245 R3248 W3249 W3250 E3251 N3256 R3260 T3266 A3267 L3268 N3269 S3270 E3271 H3272 M3273 L3277 I3280 L3281 I3284 Y3285 L3288 G3289 I3290 D3291 E3292 G3293 M3296 L3299
Q3304 I3307 L3314 L3315 H3318 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 T3332 V3333 V3334 E3337 ASP HIS LEU LYS ALA GLU ILE ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR 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 LEU VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA ALA LEU
LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU LYS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU



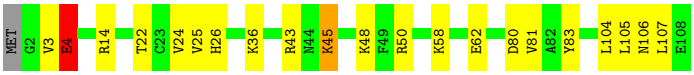
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



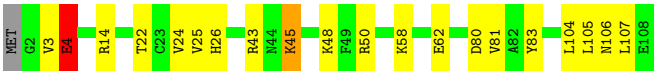
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



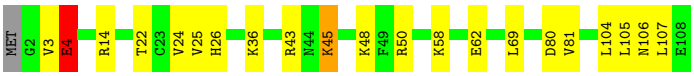
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	181724	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	0.623	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	430.592, 430.592, 430.592	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.841, 0.841, 0.841	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, KVR

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	0/34516	0.50	9/46623 (0.0%)
1	B	0.26	0/34516	0.50	9/46623 (0.0%)
1	C	0.26	0/34516	0.50	9/46623 (0.0%)
1	D	0.26	0/34516	0.50	9/46623 (0.0%)
2	E	0.29	0/834	0.56	1/1123 (0.1%)
2	F	0.29	0/834	0.56	1/1123 (0.1%)
2	G	0.29	0/834	0.56	1/1123 (0.1%)
2	H	0.29	0/834	0.56	1/1123 (0.1%)
All	All	0.26	0/141400	0.51	40/190984 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	943	LEU	CA-CB-CG	12.40	143.83	115.30
1	C	943	LEU	CA-CB-CG	12.39	143.81	115.30
1	D	943	LEU	CA-CB-CG	12.39	143.81	115.30
1	B	943	LEU	CA-CB-CG	12.38	143.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2734	MET	CA-CB-CG	9.25	129.03	113.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2766	LYS	Peptide
1	A	439	LYS	Peptide
1	A	4640	PHE	Peptide
1	A	879	GLU	Peptide
1	A	880	ARG	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	33774	0	33452	652	0
1	B	33774	0	33452	665	0
1	C	33774	0	33452	664	0
1	D	33774	0	33452	671	0
2	E	818	0	821	12	0
2	F	818	0	821	14	0
2	G	818	0	821	13	0
2	H	818	0	821	14	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	23	0	0	1	0
5	B	23	0	0	1	0
5	C	23	0	0	1	0
5	D	23	0	0	1	0
All	All	138712	0	137188	2637	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 10.

The worst 5 of 2637 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2779:LEU:HA	1:A:2782:MET:HG3	1.56	0.88
1:B:2779:LEU:HA	1:B:2782:MET:HG3	1.56	0.87
1:D:2779:LEU:HA	1:D:2782:MET:HG3	1.56	0.86
1:C:2779:LEU:HA	1:C:2782:MET:HG3	1.56	0.85
1:B:4279:MET:HE1	1:C:4488:GLN:HG2	1.57	0.85

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%)	4098 (98%)	98 (2%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4100 (98%)	96 (2%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
2	E	105/108 (97%)	105 (100%)	0	0	100	100
2	F	105/108 (97%)	105 (100%)	0	0	100	100
2	G	105/108 (97%)	105 (100%)	0	0	100	100
2	H	105/108 (97%)	105 (100%)	0	0	100	100
All	All	17212/20300 (85%)	16816 (98%)	388 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3927	PRO

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Mol	Chain	Res	Type
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%)	3653 (98%)	55 (2%)	65 84
1	B	3708/4358 (85%)	3653 (98%)	55 (2%)	65 84
1	C	3708/4358 (85%)	3653 (98%)	55 (2%)	65 84
1	D	3708/4358 (85%)	3653 (98%)	55 (2%)	65 84
2	E	88/89 (99%)	86 (98%)	2 (2%)	50 75
2	F	88/89 (99%)	86 (98%)	2 (2%)	50 75
2	G	88/89 (99%)	86 (98%)	2 (2%)	50 75
2	H	88/89 (99%)	86 (98%)	2 (2%)	50 75
All	All	15184/17788 (85%)	14956 (98%)	228 (2%)	66 84

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4292	MET
1	D	3227	ARG
1	C	1045	SER
1	D	3033	LEU
1	D	1047	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	658	ASN

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Mol	Chain	Res	Type
1	D	3831	GLN
1	D	896	ASN
1	D	1014	GLN
1	B	1014	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, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	KVR	A	5004	-	24,25,25	0.50	0	32,34,34	1.00	2 (6%)
4	ATP	A	5002	-	26,33,33	0.60	0	31,52,52	0.76	2 (6%)
4	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.76	2 (6%)
5	KVR	D	5004	-	24,25,25	0.50	0	32,34,34	1.00	2 (6%)
5	KVR	C	5004	-	24,25,25	0.50	0	32,34,34	1.00	2 (6%)
4	ATP	D	5002	-	26,33,33	0.60	0	31,52,52	0.76	2 (6%)
4	ATP	A	5003	-	26,33,33	0.66	0	31,52,52	0.76	1 (3%)
4	ATP	B	5002	-	26,33,33	0.60	0	31,52,52	0.76	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	KVR	B	5004	-	24,25,25	0.50	0	32,34,34	1.00	2 (6%)
4	ATP	C	5003	-	26,33,33	0.67	0	31,52,52	0.76	1 (3%)
4	ATP	B	5003	-	26,33,33	0.67	0	31,52,52	0.76	1 (3%)
4	ATP	D	5003	-	26,33,33	0.67	0	31,52,52	0.76	1 (3%)

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
5	KVR	A	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	A	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	8/18/38/38	0/3/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	C	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	5004	KVR	C10-S09-C06	3.36	107.46	102.71
5	C	5004	KVR	C10-S09-C06	3.34	107.44	102.71
5	A	5004	KVR	C10-S09-C06	3.34	107.44	102.71
5	B	5004	KVR	C10-S09-C06	3.33	107.42	102.71
5	D	5004	KVR	C14-N12-C11	3.02	115.95	111.06

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C4'-C5'-O5'-PA
4	B	5002	ATP	PB-O3B-PG-O3G

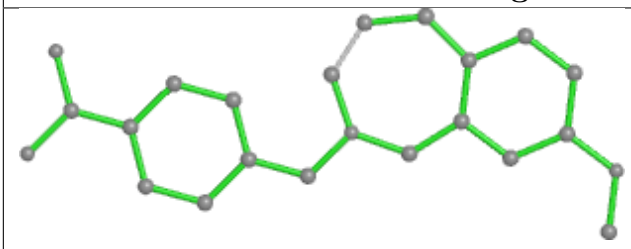
There are no ring outliers.

12 monomers are involved in 12 short contacts:

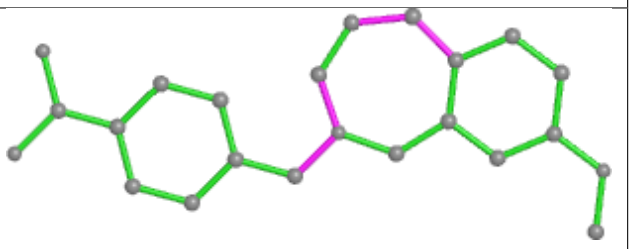
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5004	KVR	1	0
4	A	5002	ATP	1	0
4	C	5002	ATP	1	0
5	D	5004	KVR	1	0
5	C	5004	KVR	1	0
4	D	5002	ATP	1	0
4	A	5003	ATP	1	0
4	B	5002	ATP	1	0
5	B	5004	KVR	1	0
4	C	5003	ATP	1	0
4	B	5003	ATP	1	0
4	D	5003	ATP	1	0

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.

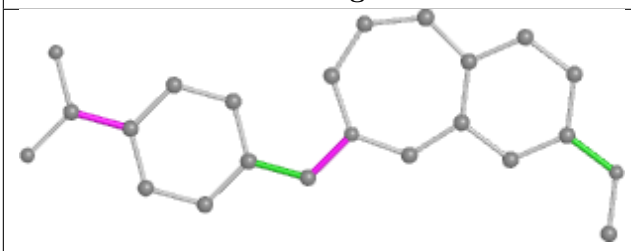
Ligand KVR A 5004



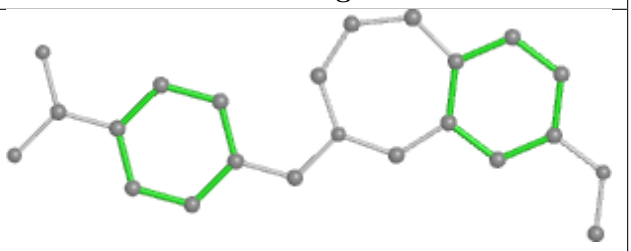
Bond lengths



Bond angles

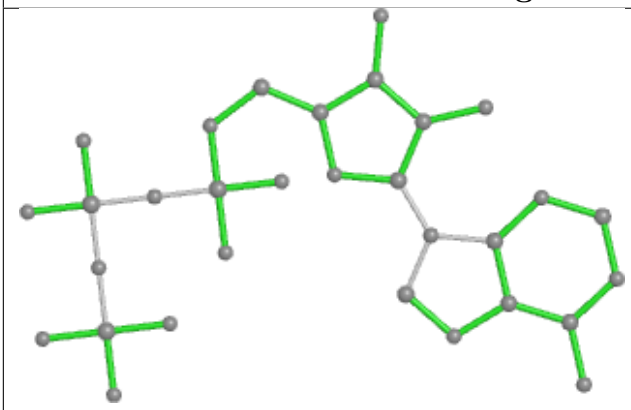


Torsions



Rings

Ligand ATP A 5002



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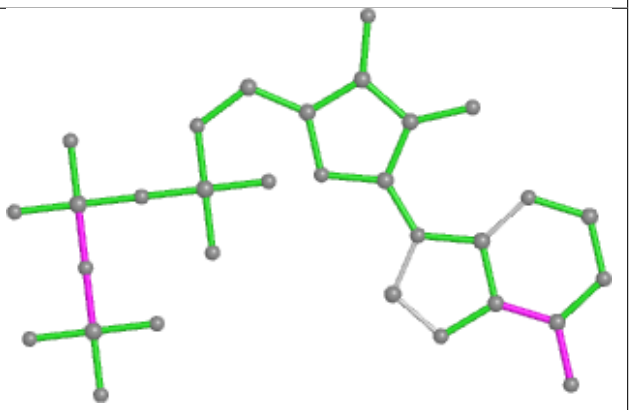

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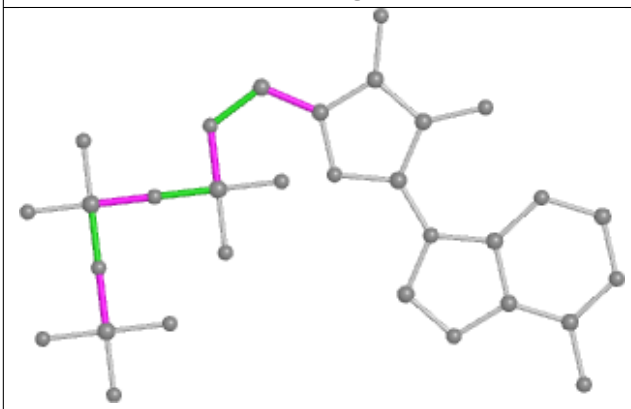

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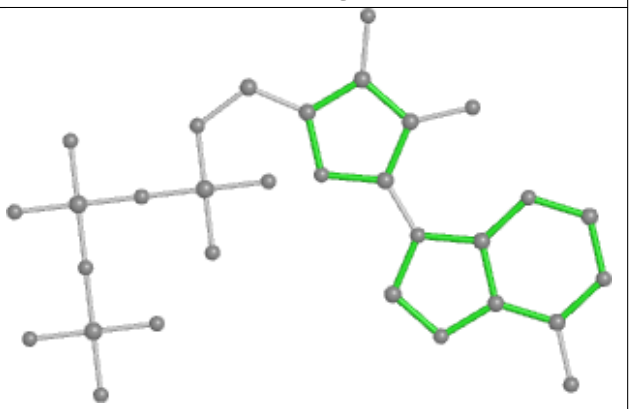
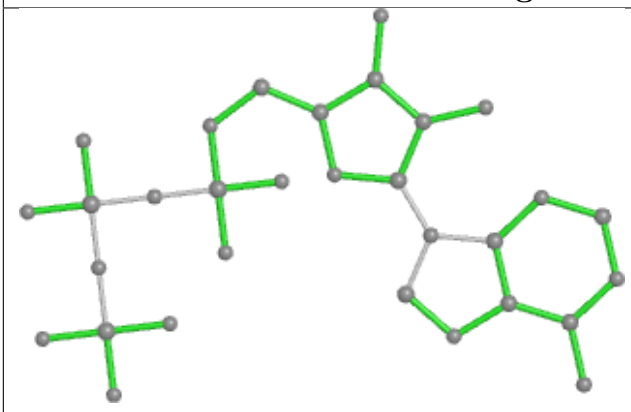


Rings

Ligand ATP C 5002



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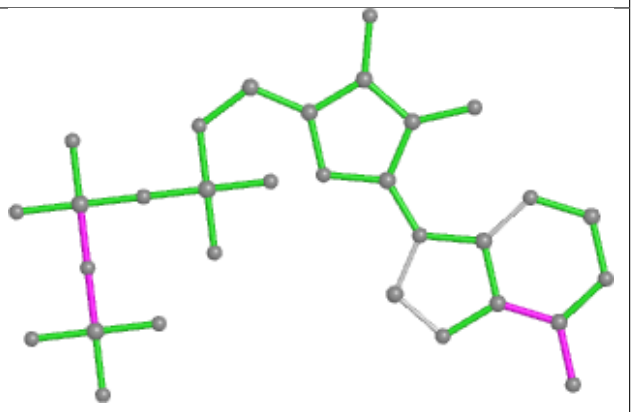

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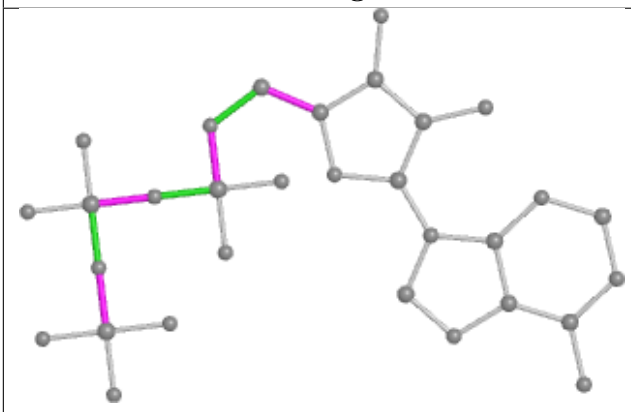

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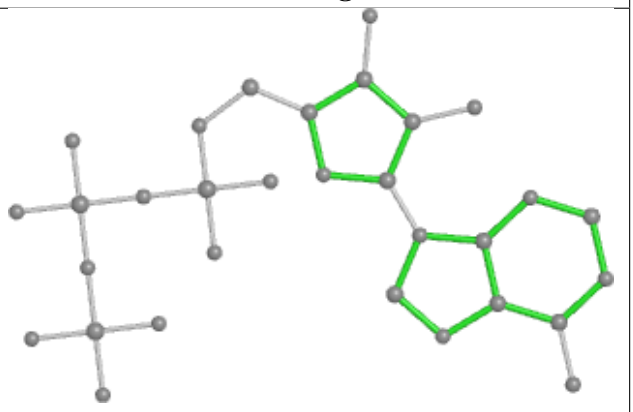
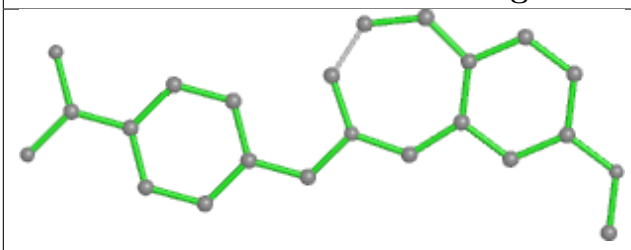


Rings

Ligand KVR D 5004



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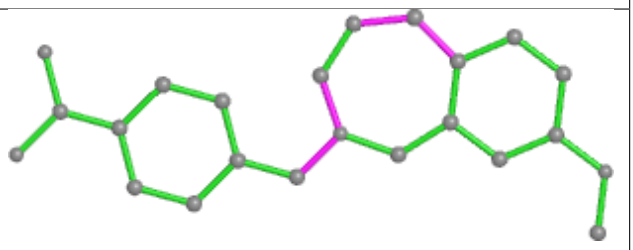

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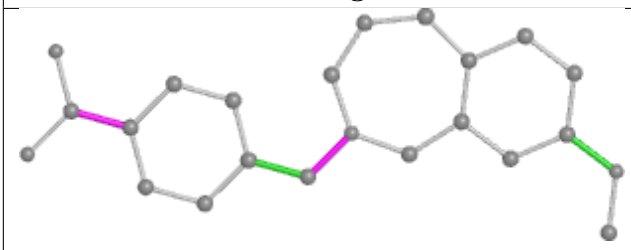

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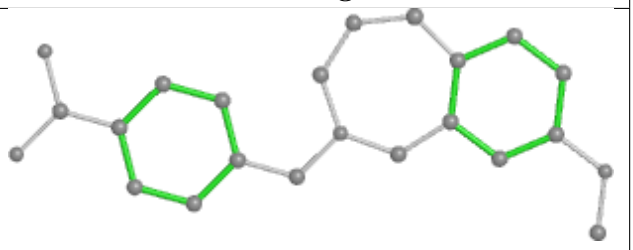
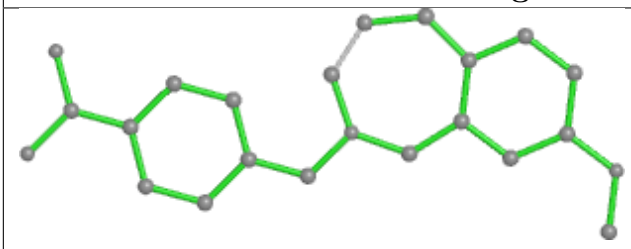


Rings

Ligand KVR C 5004



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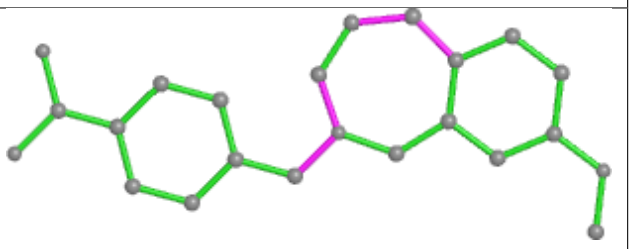

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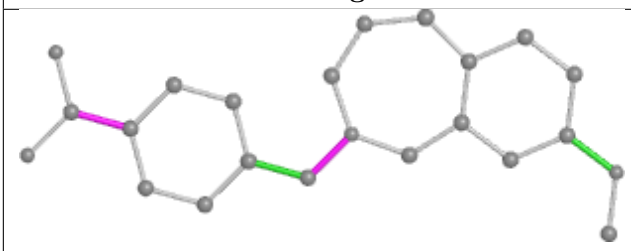

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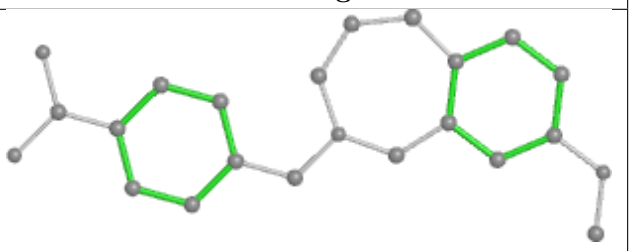
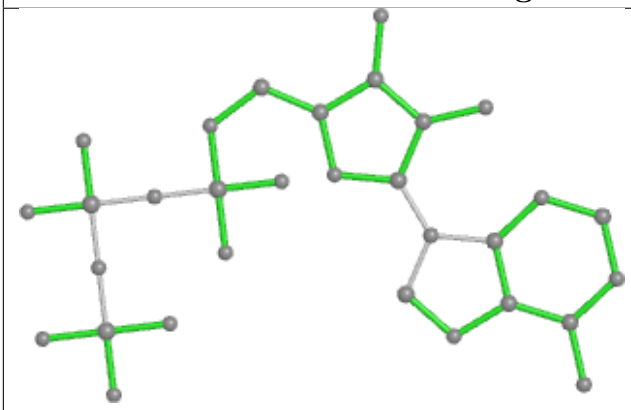


Rings

Ligand ATP D 5002



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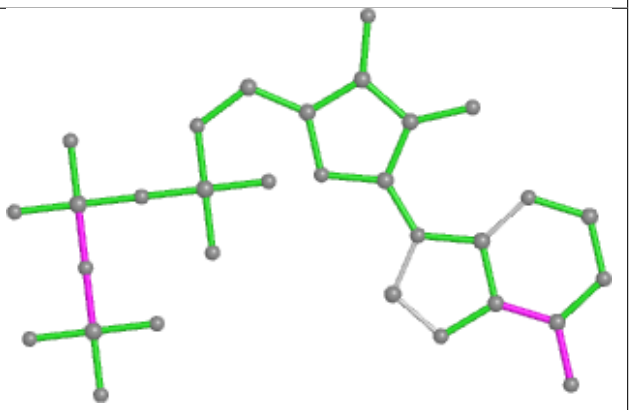

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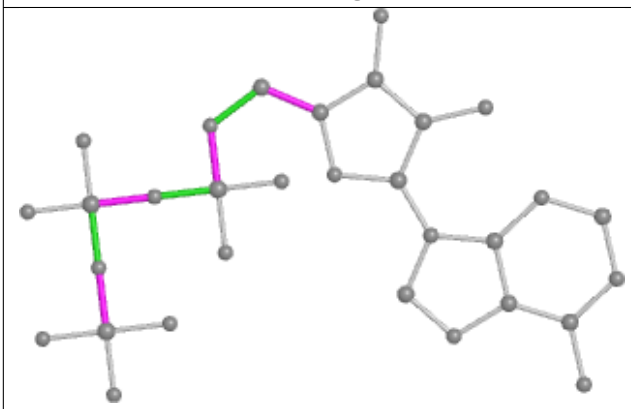

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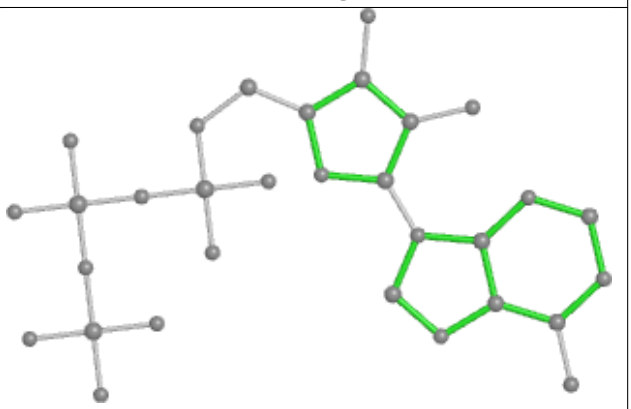
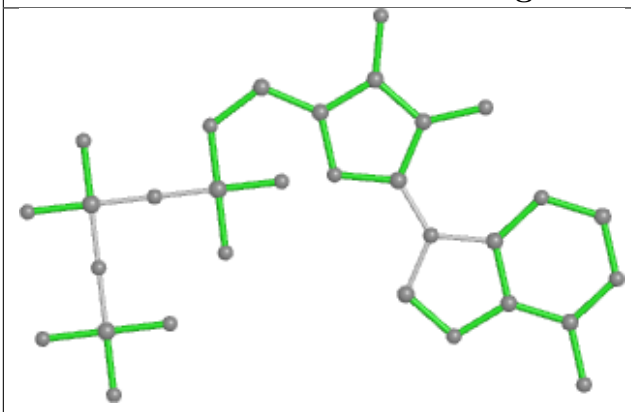


Rings

Ligand ATP A 5003



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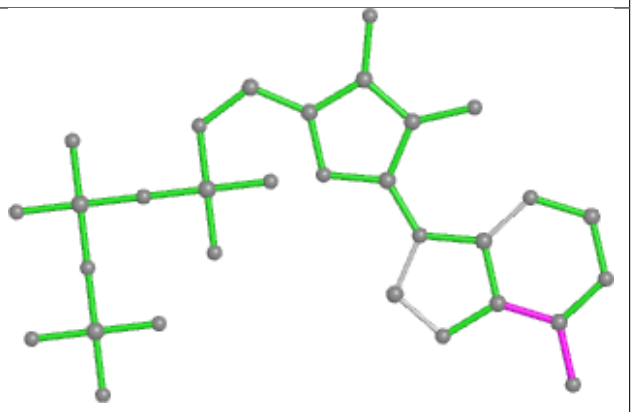

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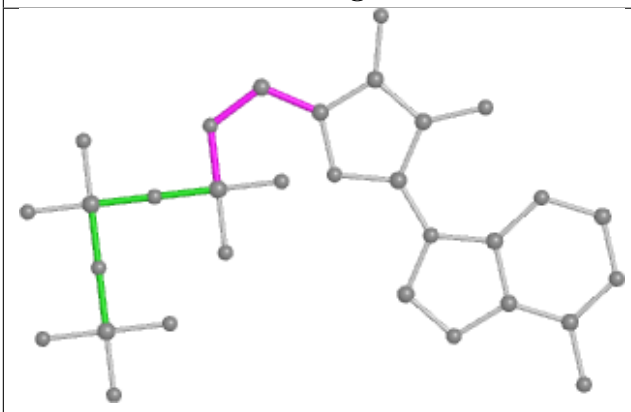

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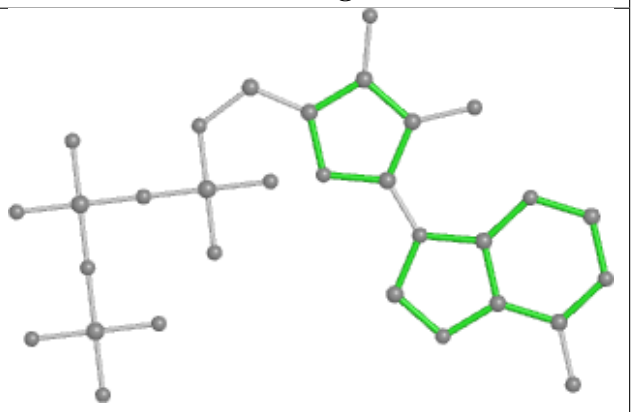
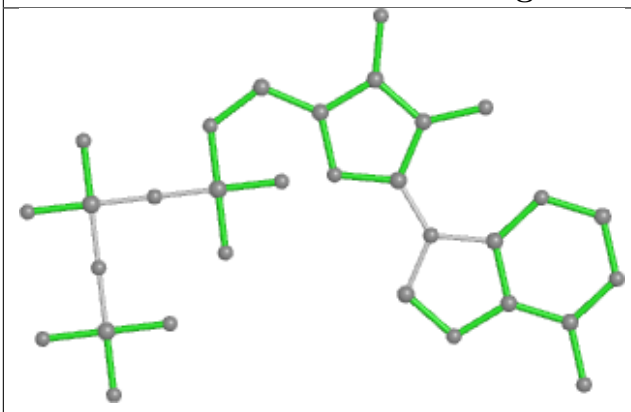
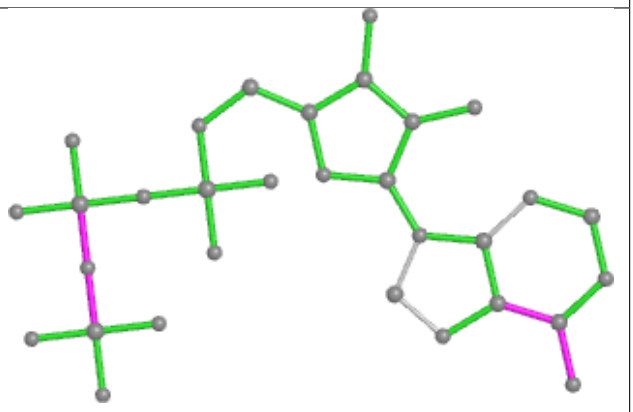


Rings

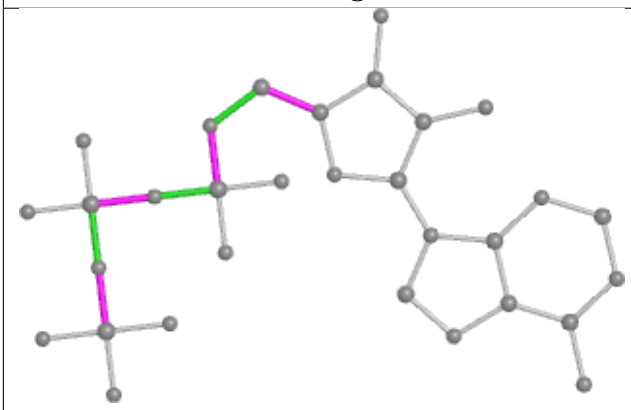
Ligand ATP B 5002



Bond lengths



Bond angles



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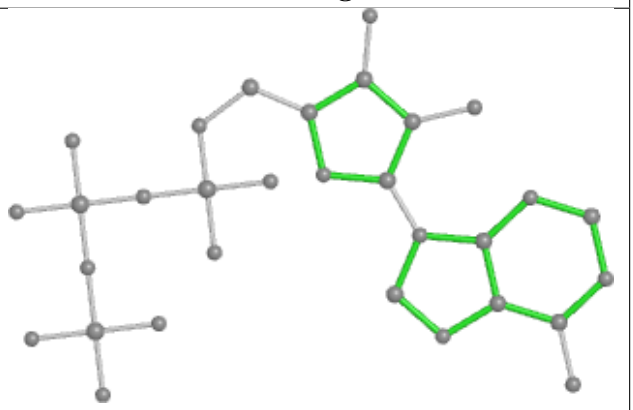
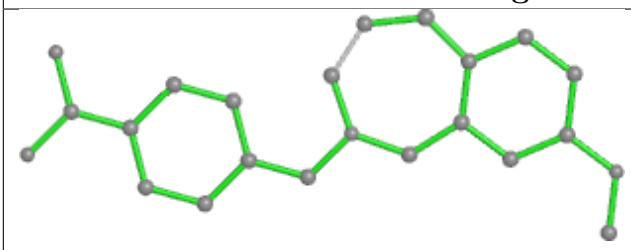
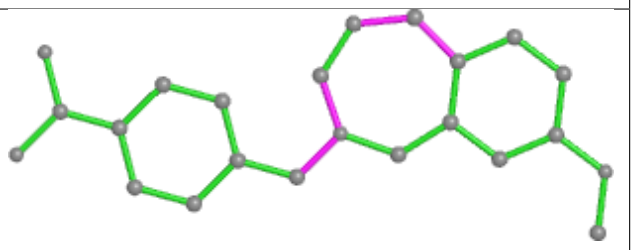


Rings

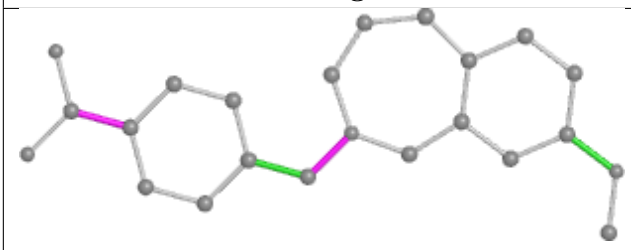
Ligand KVR B 5004



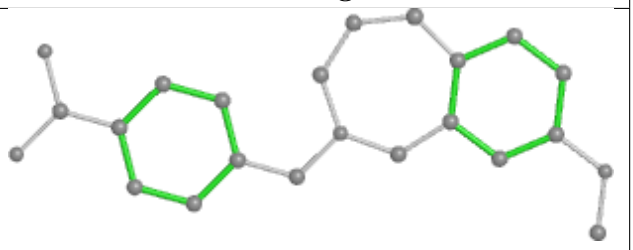
Bond lengths



Bond angles

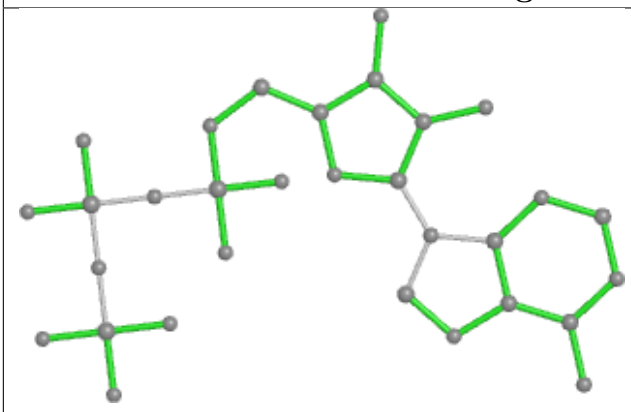


Torsions

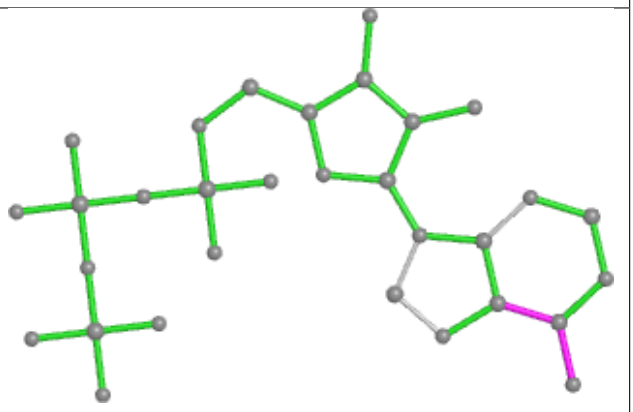


Rings

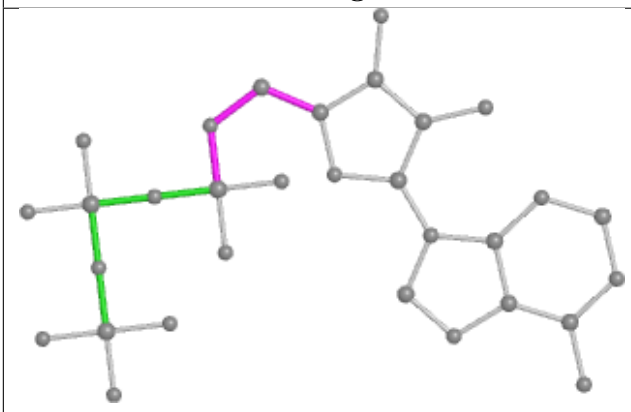
Ligand ATP C 5003



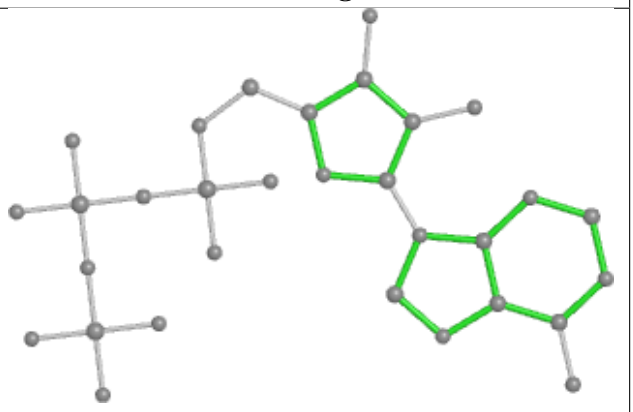
Bond lengths



Bond angles

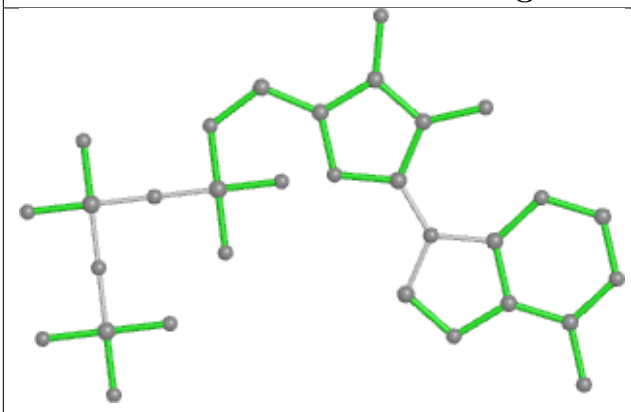


Torsions

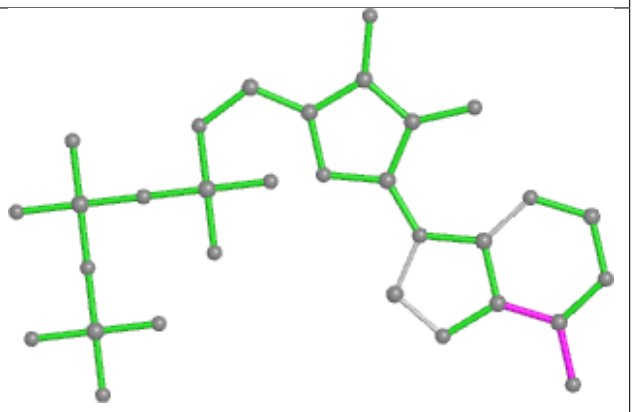


Rings

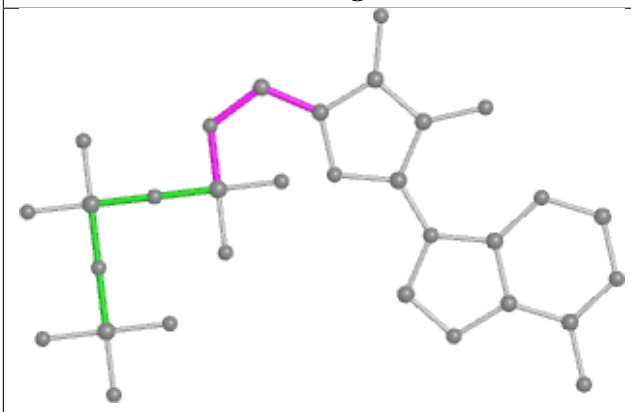
Ligand ATP B 5003



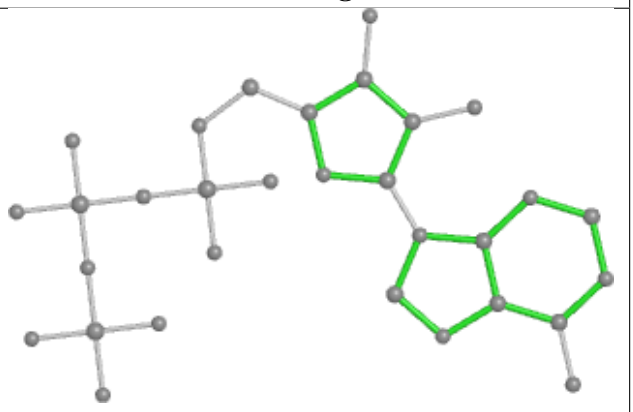
Bond lengths



Bond angles

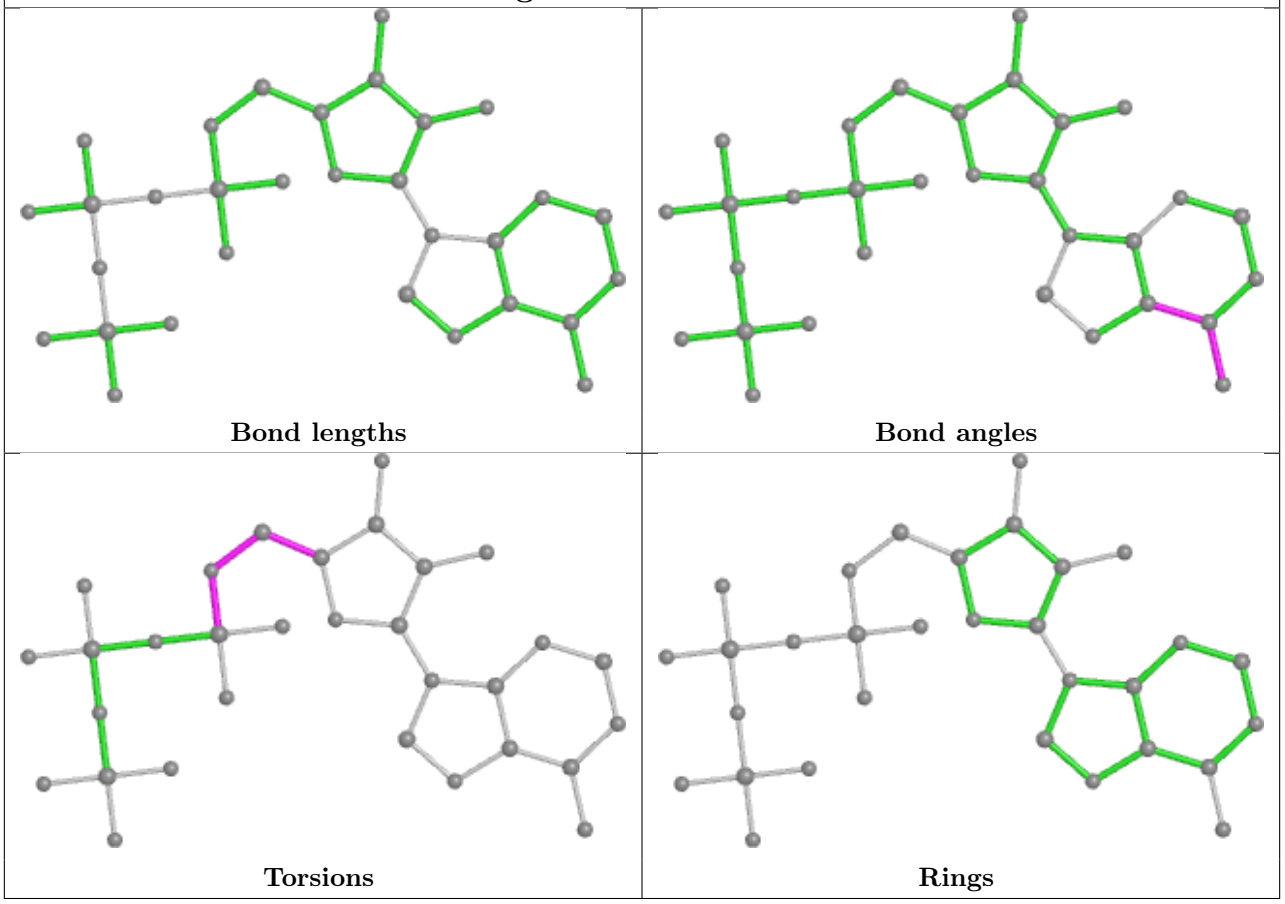


Torsions



Rings

Ligand ATP 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

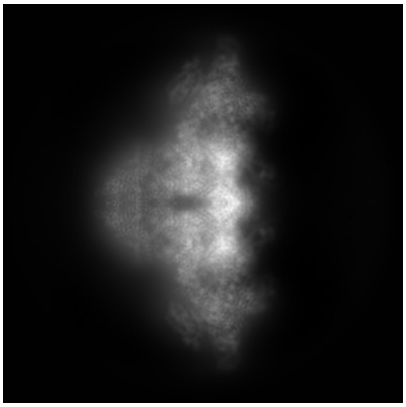
This section contains visualisations of the EMDB entry EMD-42763. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

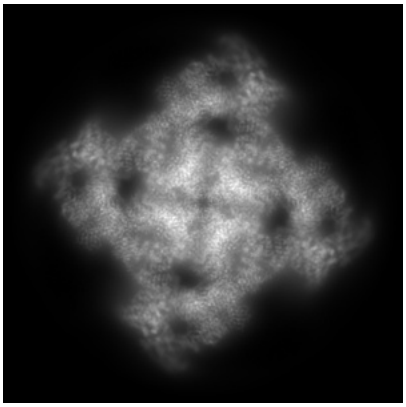
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



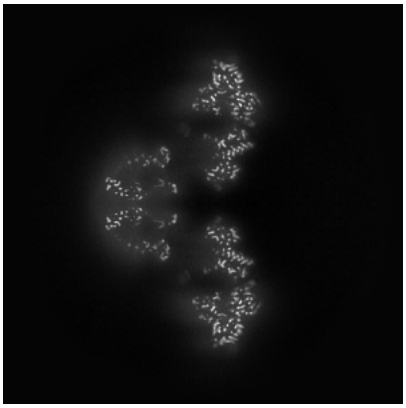
Z

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

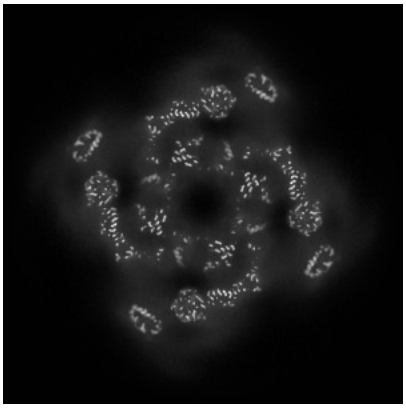
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

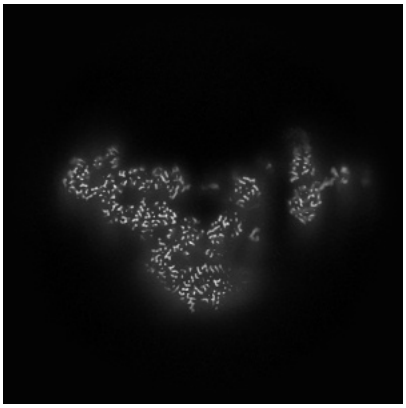


Z Index: 256

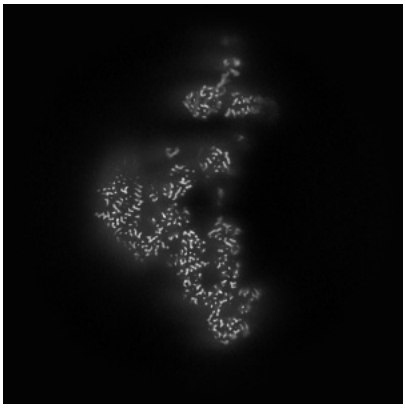
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

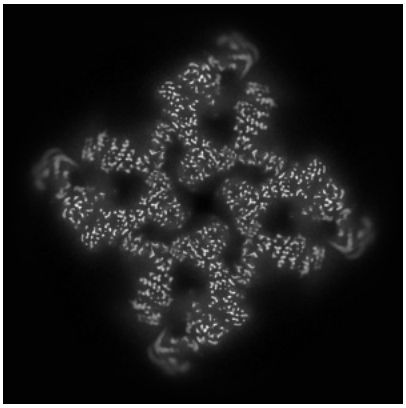
6.3.1 Primary map



X Index: 274



Y Index: 238



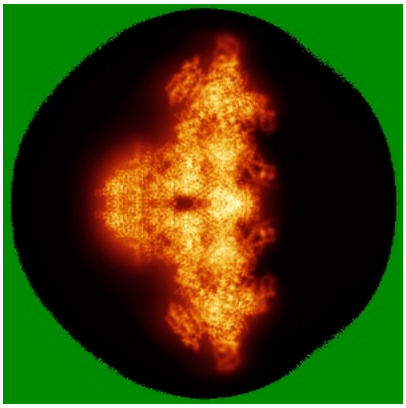
Z Index: 282

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

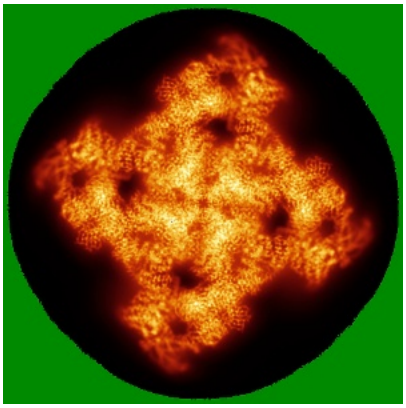
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

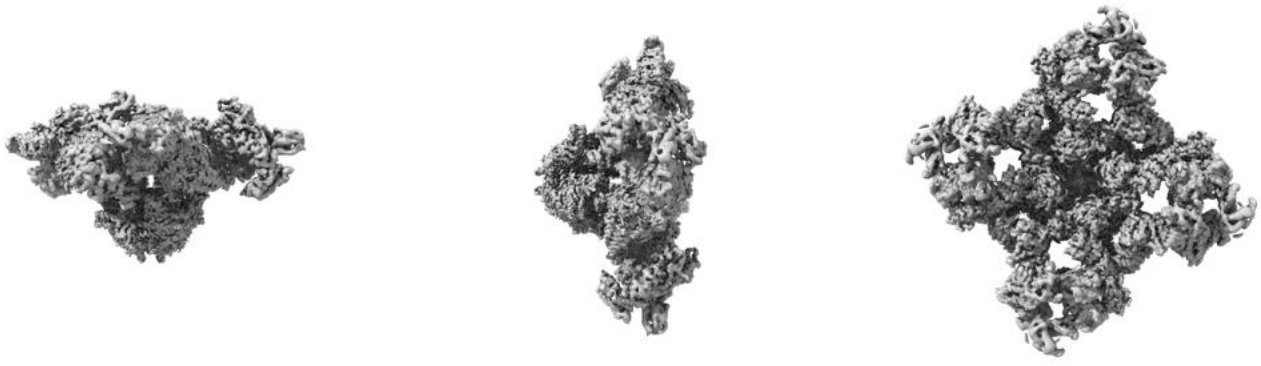


Z

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

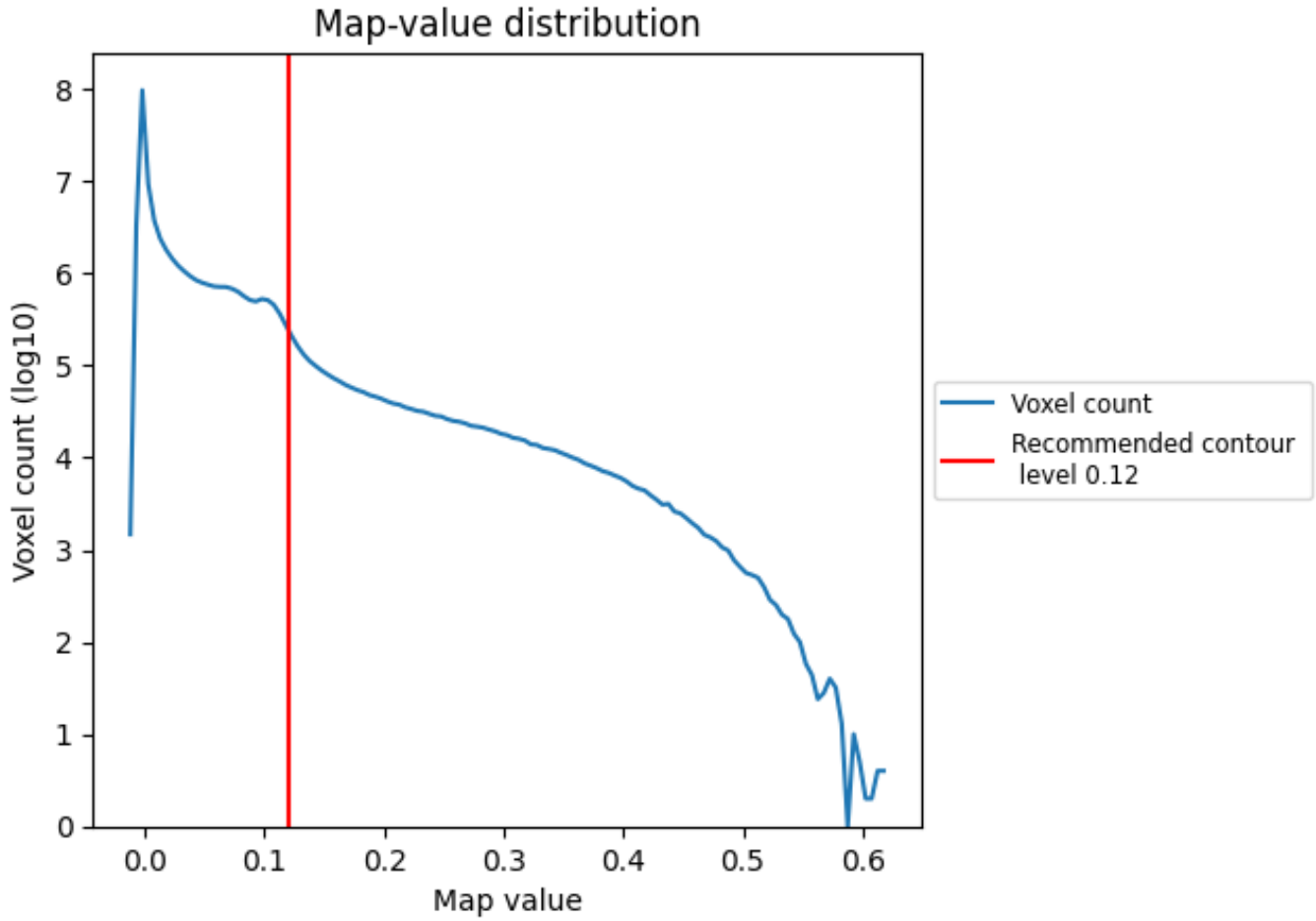
6.6 Mask visualisation (i)

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

7 Map analysis

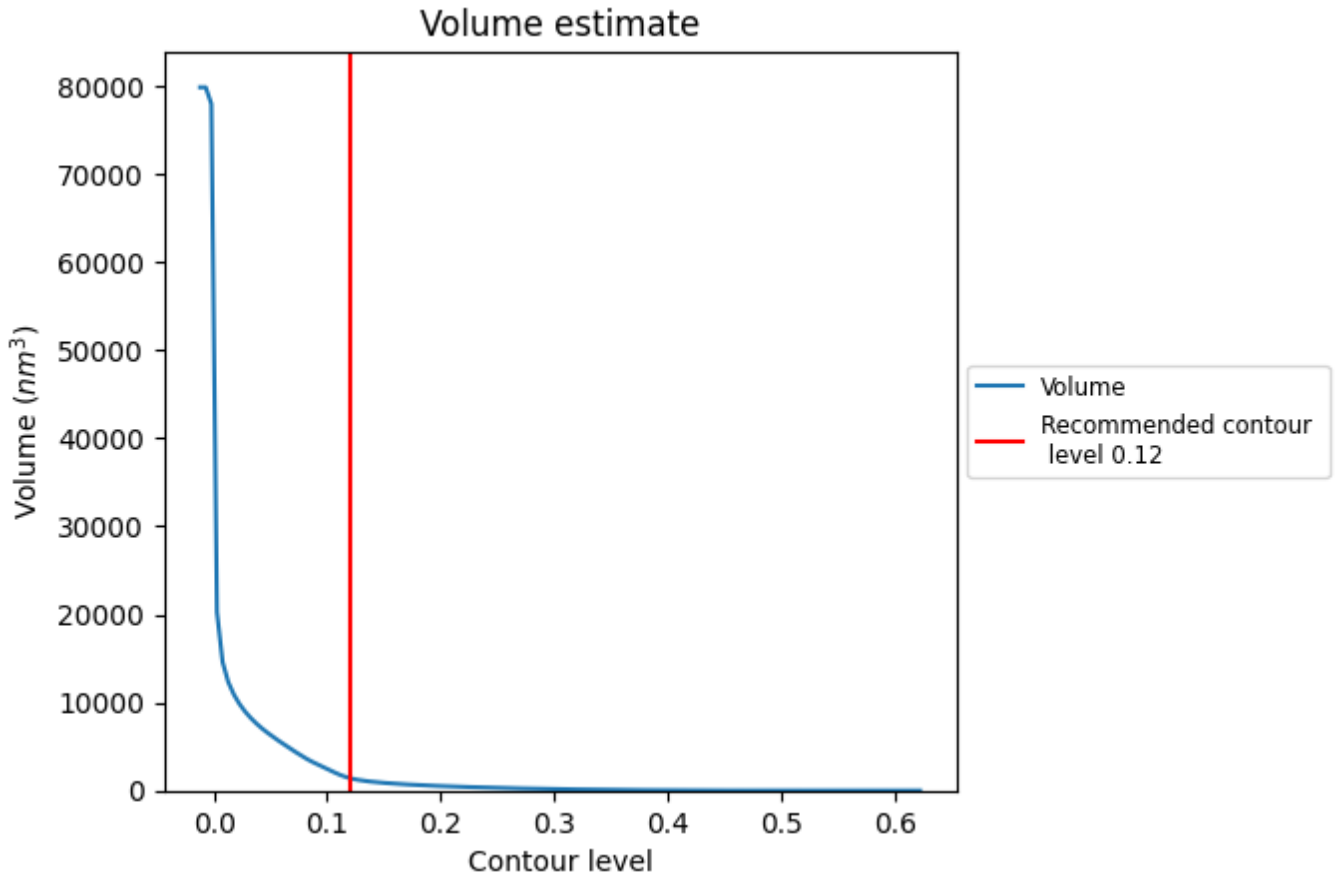
This section contains the results of statistical analysis of the map.

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.

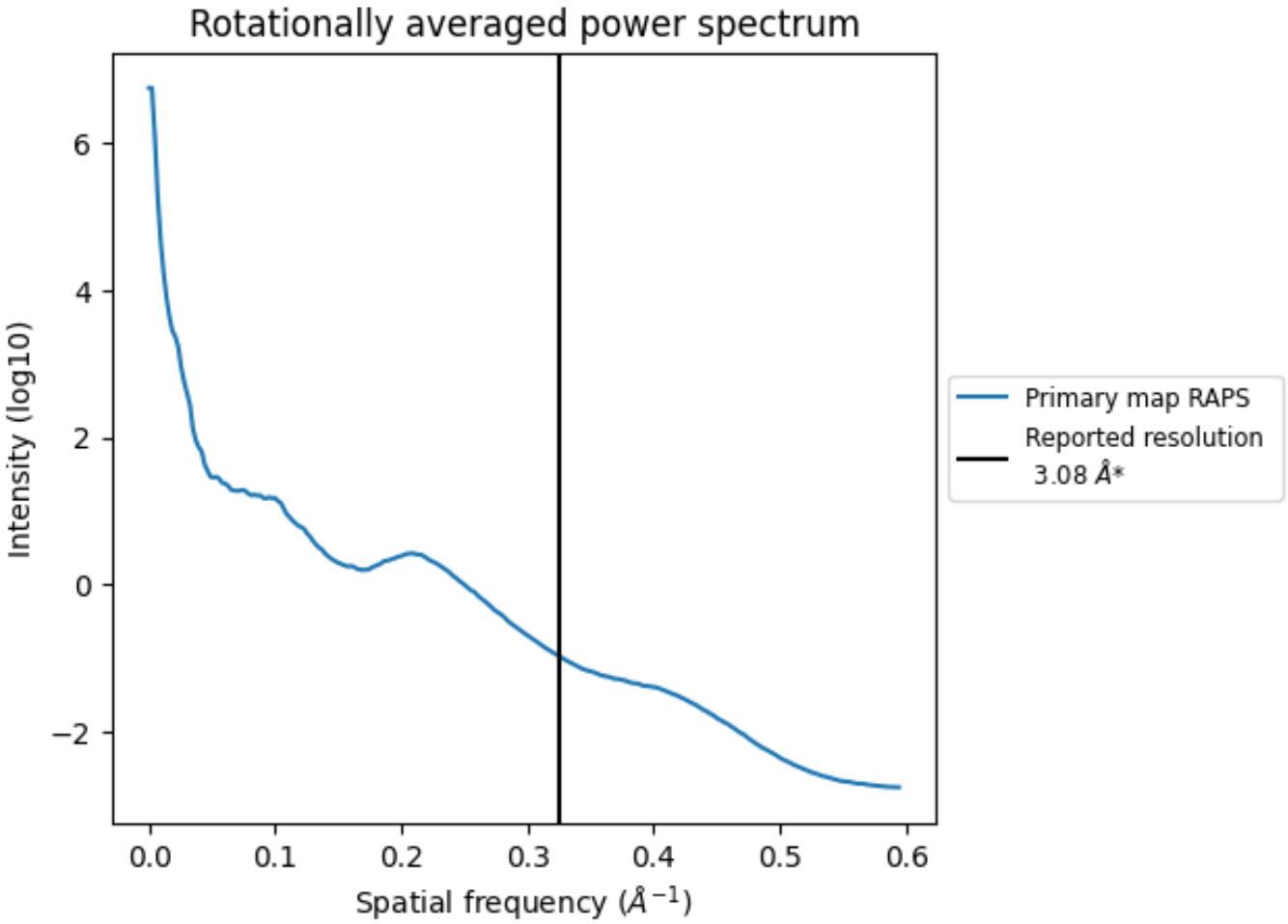
7.2 Volume estimate (i)



The volume at the recommended contour level is 1416 nm^3; this corresponds to an approximate mass of 1279 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 0.325 $Å^{-1}$

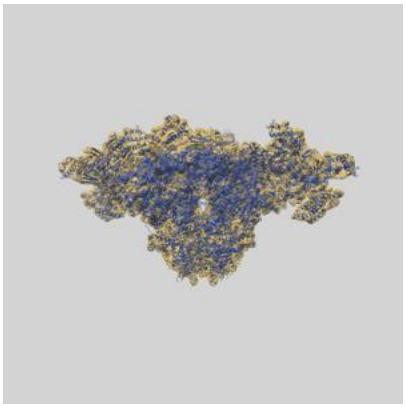
8 Fourier-Shell correlation (i)

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

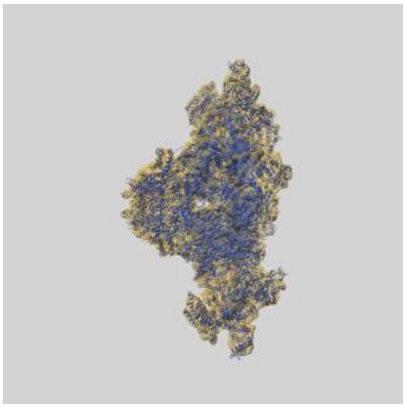
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42763 and PDB model 8UXG. Per-residue inclusion information can be found in section 3 on page 6.

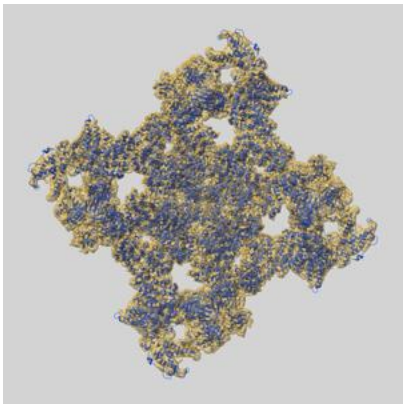
9.1 Map-model overlay



X



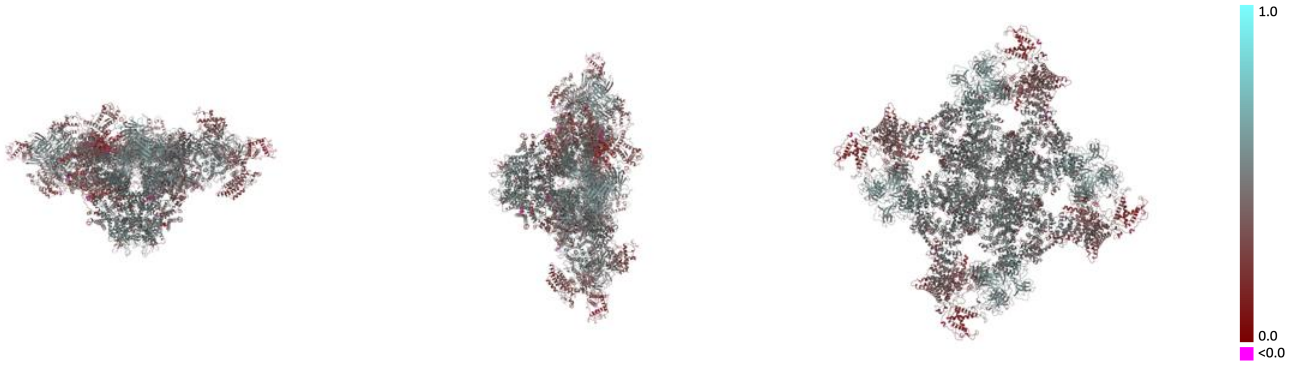
Y



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.

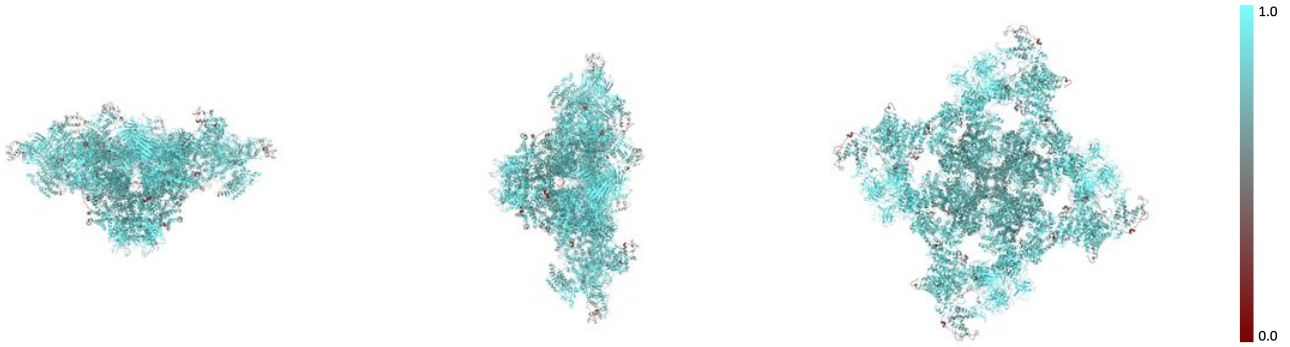
9.2 Q-score mapped to coordinate model (i)



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.

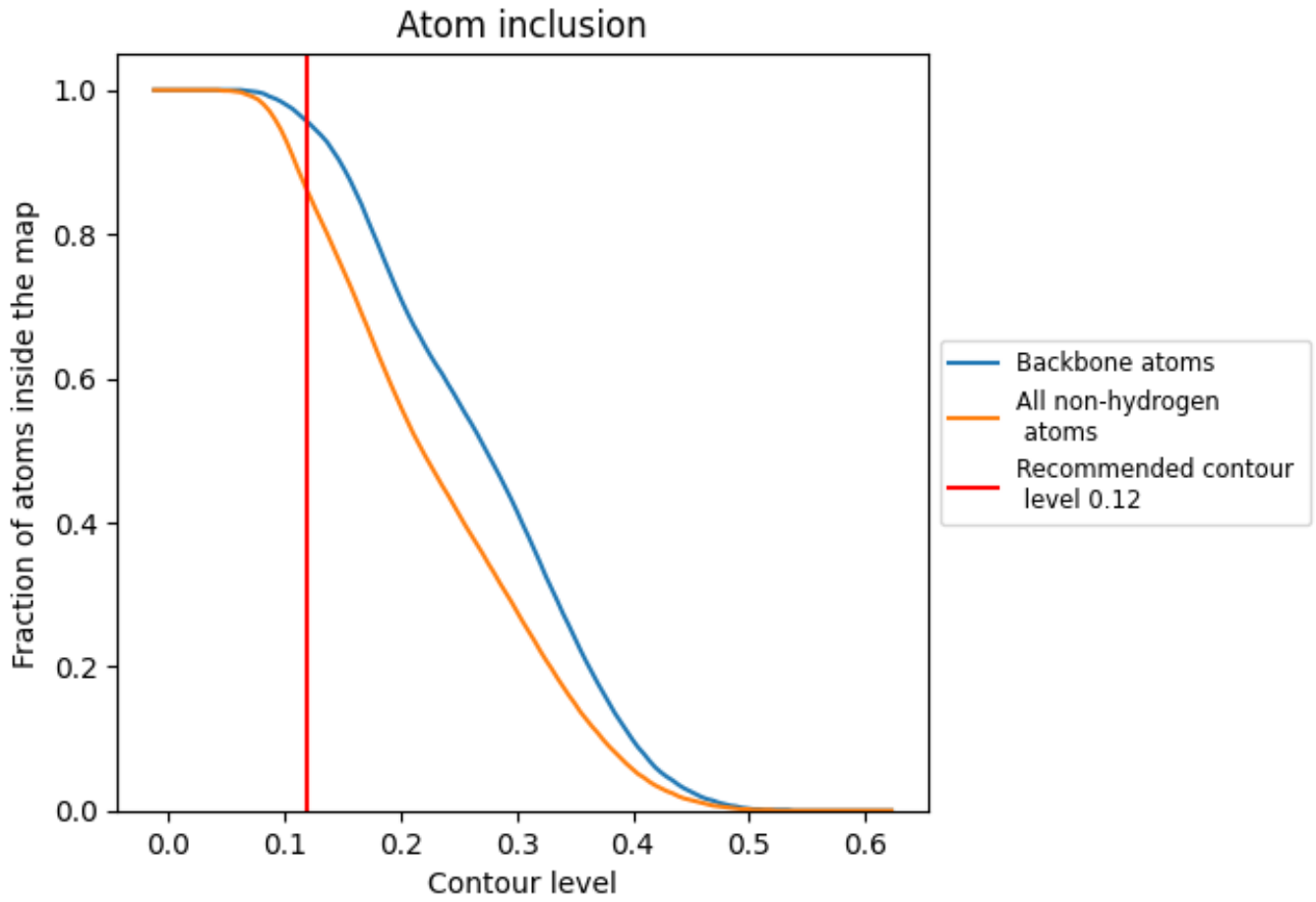
9.3 Atom inclusion mapped to coordinate model (i)



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, 96% of all backbone atoms, 86% 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	0.8590	0.4340
A	0.8580	0.4310
B	0.8580	0.4300
C	0.8590	0.4340
D	0.8560	0.4300
E	0.9330	0.5340
F	0.9290	0.5330
G	0.9340	0.5350
H	0.9340	0.5360