wwPDB EM Validation Summary Report (i)

Nov 8, 2023 – 03:31 PM EST

PDB ID	:	8UQ5
EMDB ID	:	EMD-42461
Title	:	Structure of human RyR2-S2808D in the primed state in the presence of Rapamycin
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-10-23
Resolution	:	3.96 Å(reported)
Based on initial model	:	7UA5

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

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

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

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

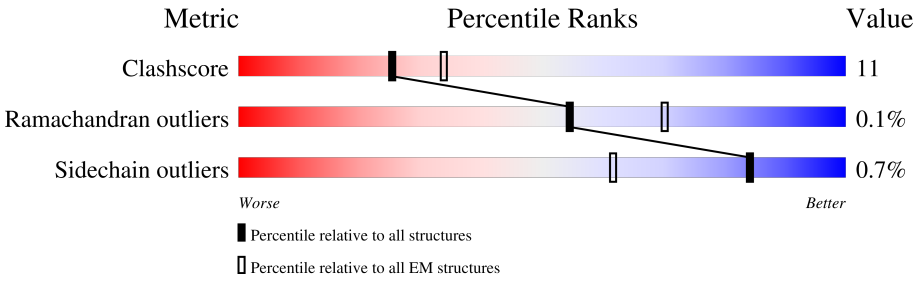
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.96 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	16% 62% 23% 15%
1	B	4967	16% 62% 23% 15%
1	C	4967	16% 62% 23% 15%
1	D	4967	16% 62% 23% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 135336 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0
1	B	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0
1	C	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0
1	D	4224	Total 33771	C 21516	N 5745	O 6280	S 230	2	0

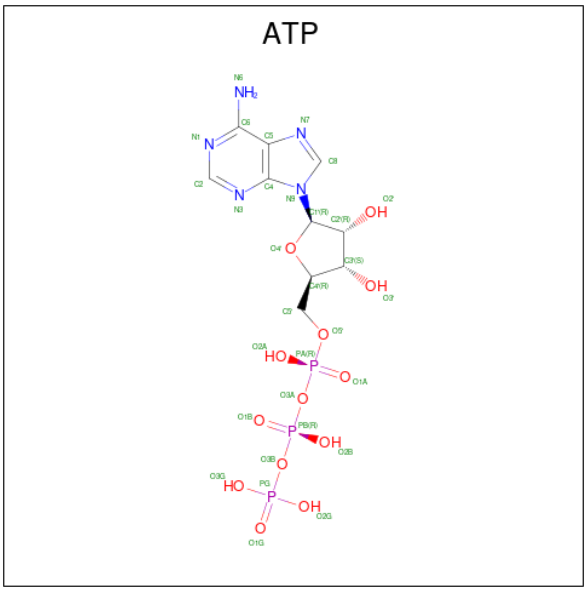
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 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).

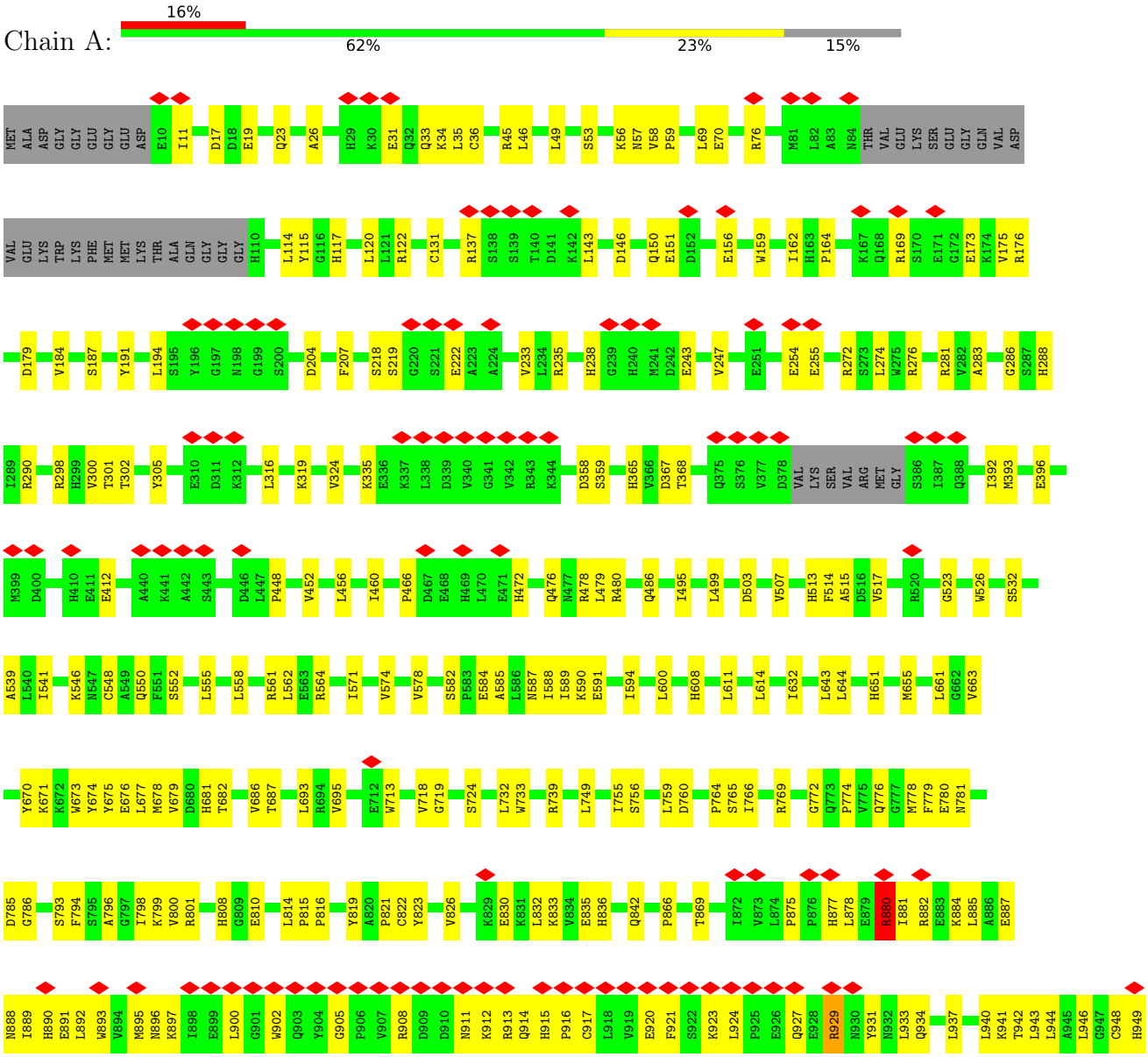


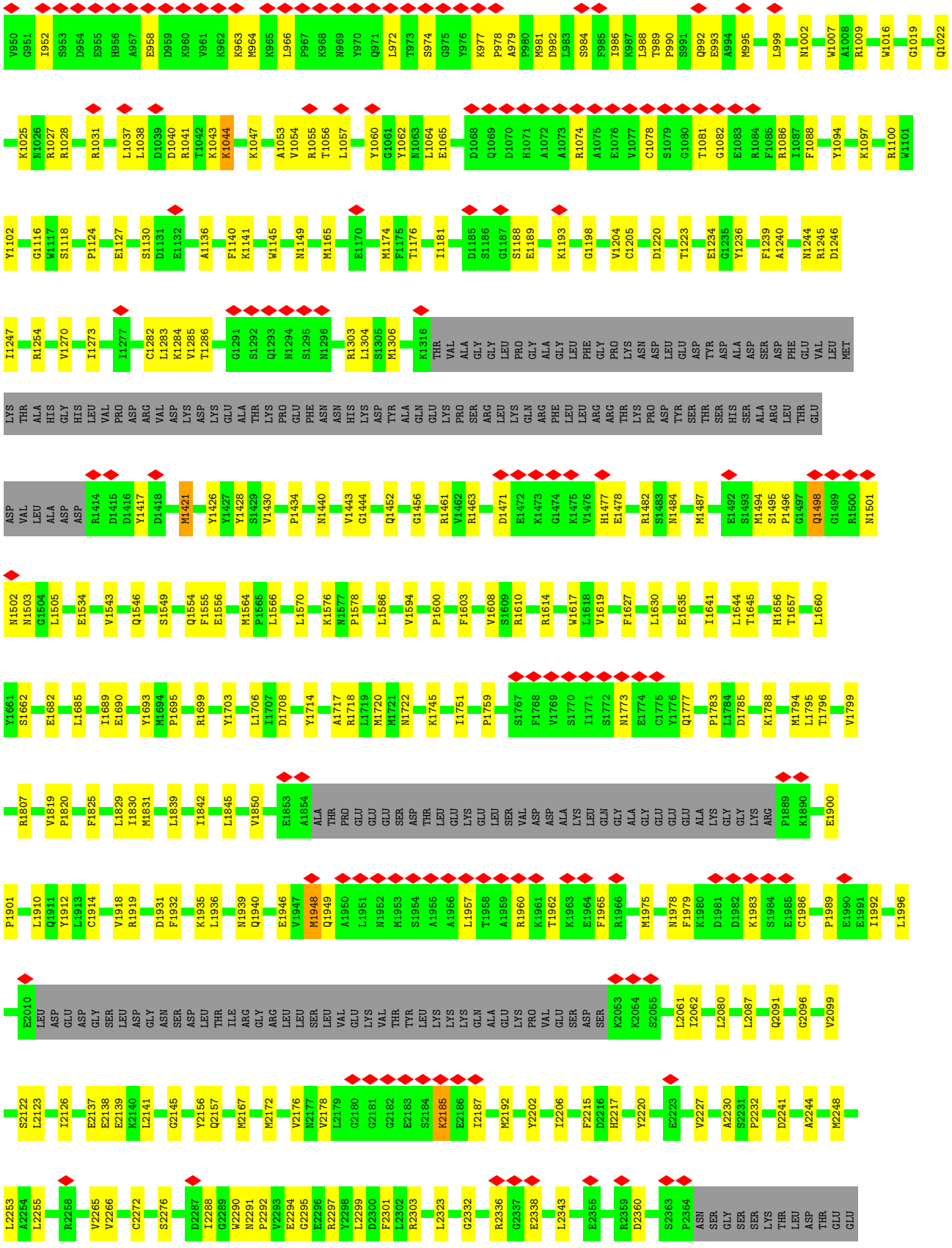
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10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

3 Residue-property plots (i)

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

- Molecule 1: Ryanodine receptor 2

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K1025 N1026 R1027 R1028 R1031 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 K1047 A1053 V1054 R1055 T1056 L1057 Y1060 G1061 Y1062 N1063 L1064 E1065 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 F1085 R1086 I1087 F1088 Y1094 K1097 R1100 W1101
Y1102 G1116 W1117 S1118 P1124 E1127 S1130 D1131 E1132 A1136 F1140 K1141 W1145 N1149 M1165 E1170 M1174 F1175 T1176 I1181 D1185 S1186 G1187 S1188 E1189 K1193 G1198 V1204 C1205 D1220 T1223 E1234 G1235 Y1236 F1239 A1240 N1244 R1245 D1246
I1247 R1254 V1270 I1273 I1277 C1282 L1283 K1284 V1285 T1286 G1291 S1292 Q1293 N1294 S1295 N1296 R1303 L1304 S1305 M1306 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 M1421 Y1426 Y1427 Y1428 S1429 V1430 P1434 N1440 V1443 G1444 Q1452 G1456 R1461 V1462 R1463 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 R1482 S1483 N1484 M1487 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501
N1502 N1503 G1504 L1505 E1534 V1543 Q1546 S1549 Q1554 F1555 E1556 M1564 P1565 L1566 L1570 K1576 N1577 P1578 L1586 V1594 P1600 F1603 V1608 S1609 R1610 R1614 W1617 L1618 V1619 F1627 L1630 E1635 I1641 L1644 T1645 H1656 T1657 L1660
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R1807 V1819 P1820 F1825 L1829 I1830 M1831 L1839 I1842 L1845 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 E1900
P1901 L1910 Q1911 Y1912 K1913 C1914 V1918 R1919 D1931 F1932 K1935 L1936 N1939 Q1940 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 E1964 F1965 R1966 M1975 N1978 F1979 K1980 D1981 D1982 K1983 S1984 E1985 C1986 P1989 E1990 E1991 I1992 L1996
E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 L2061 I2062 L2080 L2087 Q2091 G2096 V2099
S2122 L2123 I2126 E2137 E2138 E2139 K2140 L2141 G2145 Y2156 Q2157 M2167 M2172 V2176 N2177 V2178 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 M2192 Y2202 I2206 F2215 D2216 H2217 Y2220 E2223 V2227 A2230 S2231 P2232 D2241 A2244 M2248
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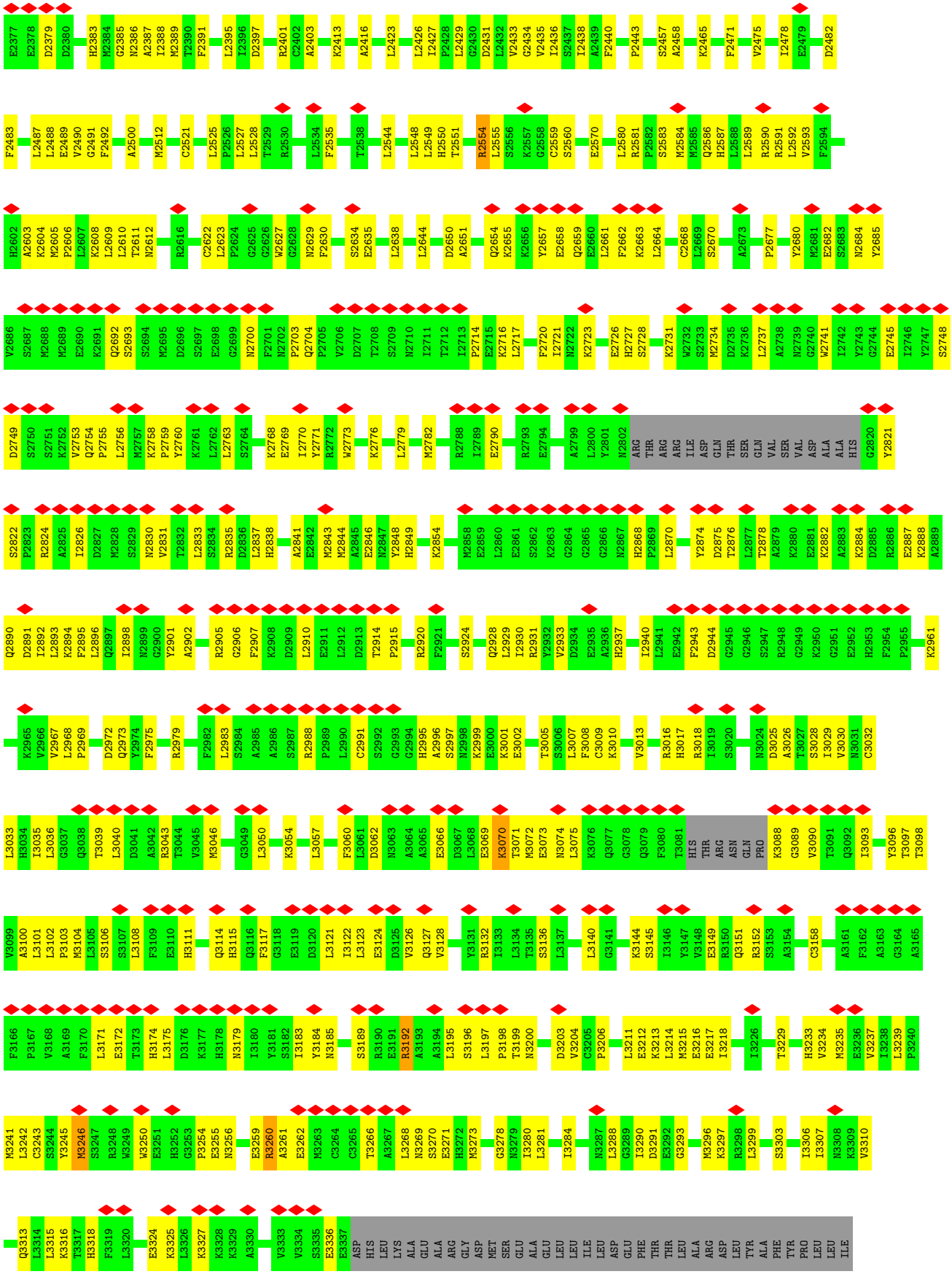
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F2483 L2487 L2488 E2489 V2490 G2491 F2492 A2500 M2512 C2521 L2525 P2526 L2527 L2528 T2529 R2530 L2534 F2535 T2538 L2544 L2548 L2549 H2550 T2551 R2564 L2555 S2556 K2557 G2558 C2559 S2560 E2570 L2580 R2581 P2582 S2583 M2584 M2585 Q2586 H2587 L2588 L2589 R2590 R2591 L2592 V2593 F2594
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V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 F2720 I2721 N2722 K2723 E2726 H2727 S2728 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 K2768 E2769 I2770 Y2771 R2772 W2773 K2776 L2779 M2782 R2788 I2789 E2790 R2793 E2794 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE ASP 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 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 H2849 K2854 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 Y2874 D2875 T2876 L2877 T2878 A2879 K2880 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889
Q2890 D2891 I2892 L2893 K2894 P2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 R2920 F2921 S2924 Q2928 L2929 I2930 R2931 Y2932 V2933 D2934 E2935 A2936 H2937 I2940 L2941 E2942 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2963 P2954 P2955 K2961
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L3033 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 G3049 L3050 K3054 L3057 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 Y3096 T3097 T3098
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F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 L3175 D3176 K3177 H3178 N3179 I3180 Y3181 S3182 I3183 Y3184 N3185 S3189 R3190 E3191 R3192 A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 D3203 V3204 C3205 P3206 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 I3226 T3229 H3233 V3234 M3235 E3236 V3237 I3238 L3239 P3240
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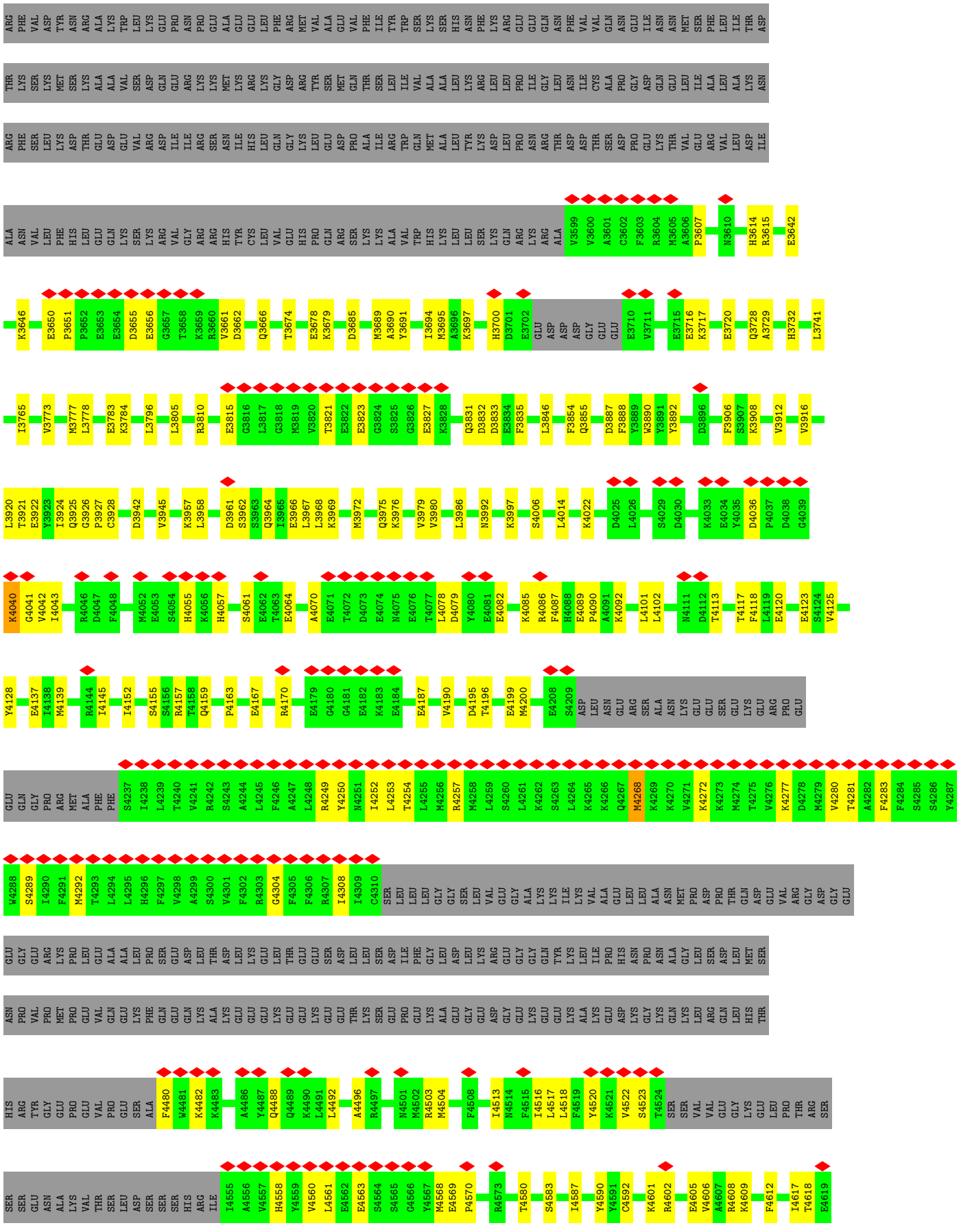
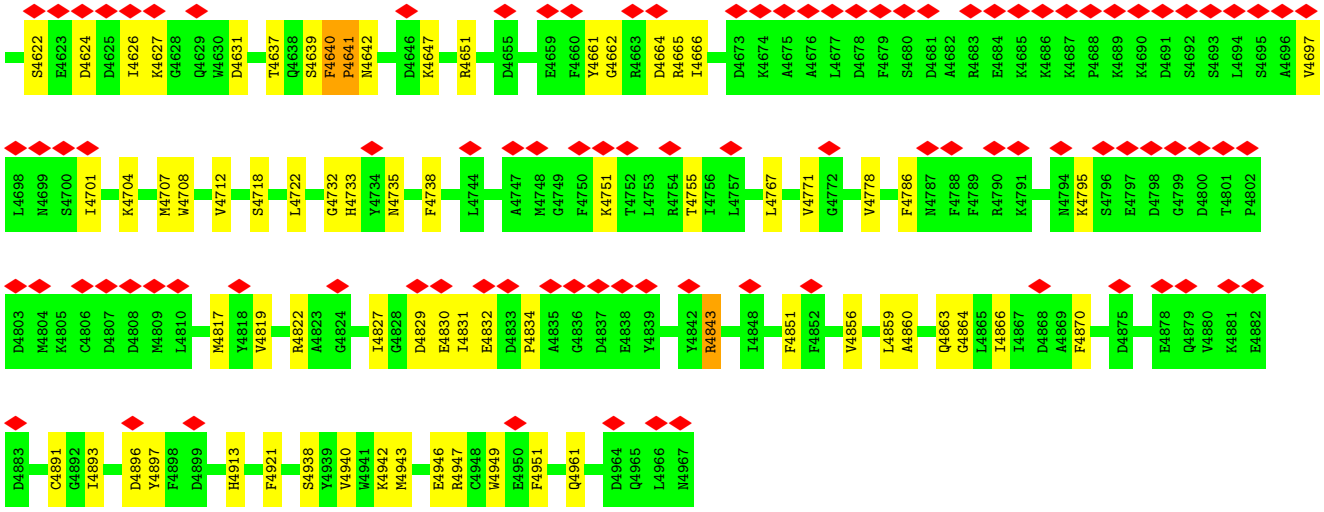
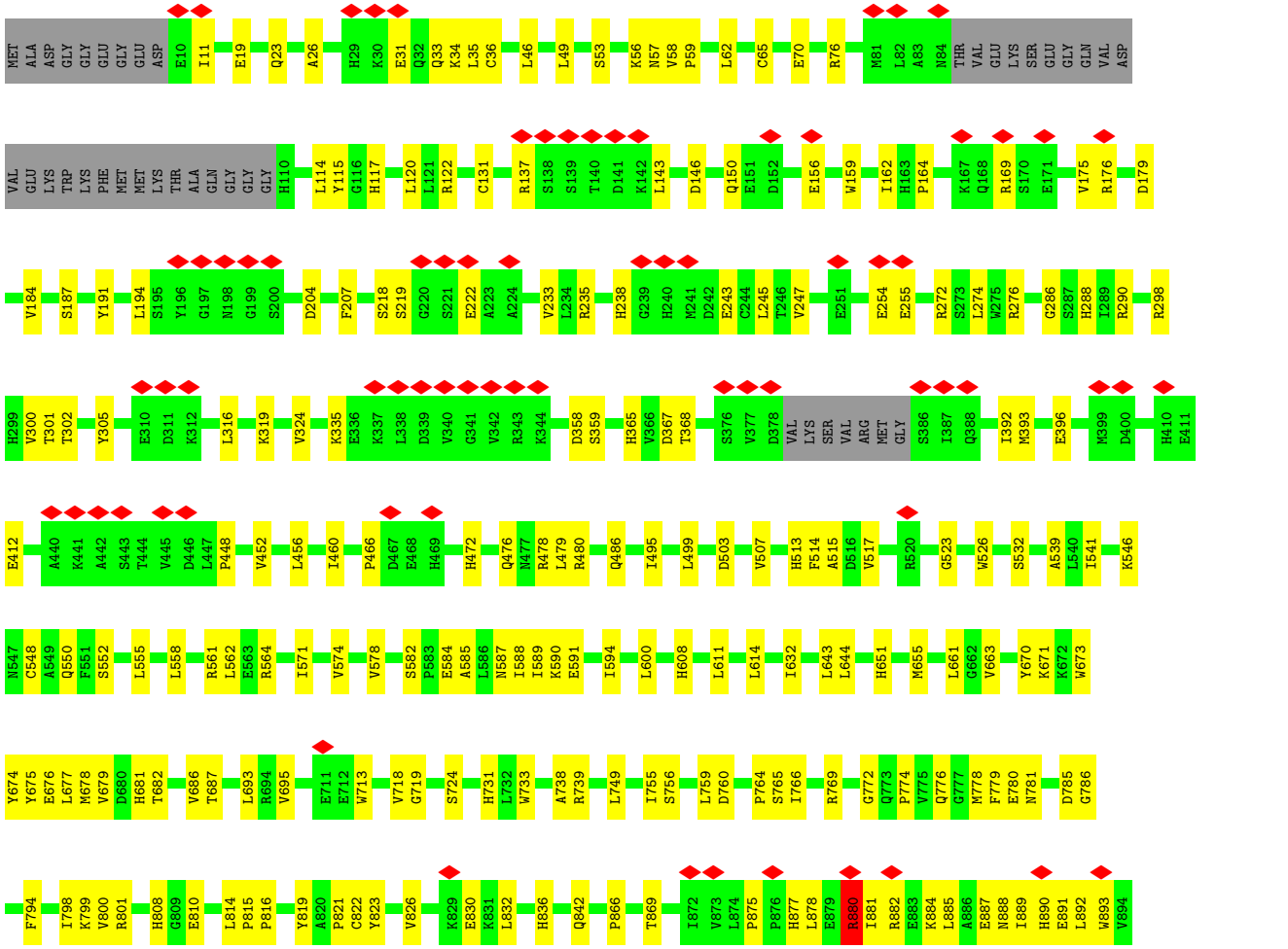
Q3313 L3314 L3315 K3316 T3317 H3318 F3319 L3320 E3324 K3325 L3326 K3327 K3328 K3329 A3330 V3333 V3334 S3335 E3336 E3337 ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE

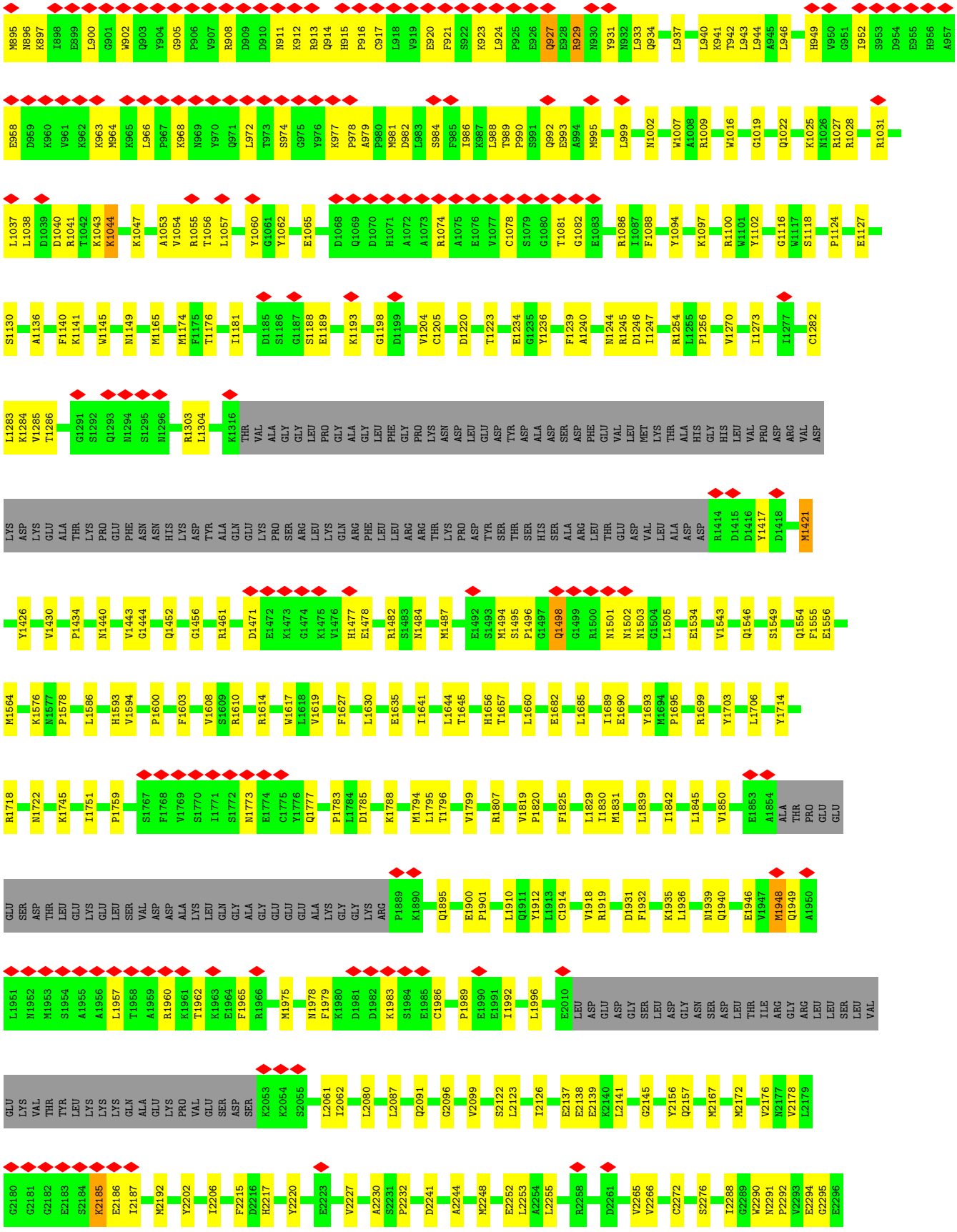




• Molecule 1: Ryanodine receptor 2

Chain B:

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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 L999 N1002 W1007 A1008 R1009 W1016 G1019 Q1022 K1025 N1026 R1027 R1028 R1031
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L1283 K1284 V1285 T1286 G1291 S1292 Q1293 N1294 S1295 N1296 R1303 L1304 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP
LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 M1421
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GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 Q1895 E1900 P1901 L1910 Q1911 Y1912 L1913 C1914 V1918 R1919 D1931 F1932 K1935 L1936 N1939 Q1940 E1946 V1947 M1948 Q1949 A1950
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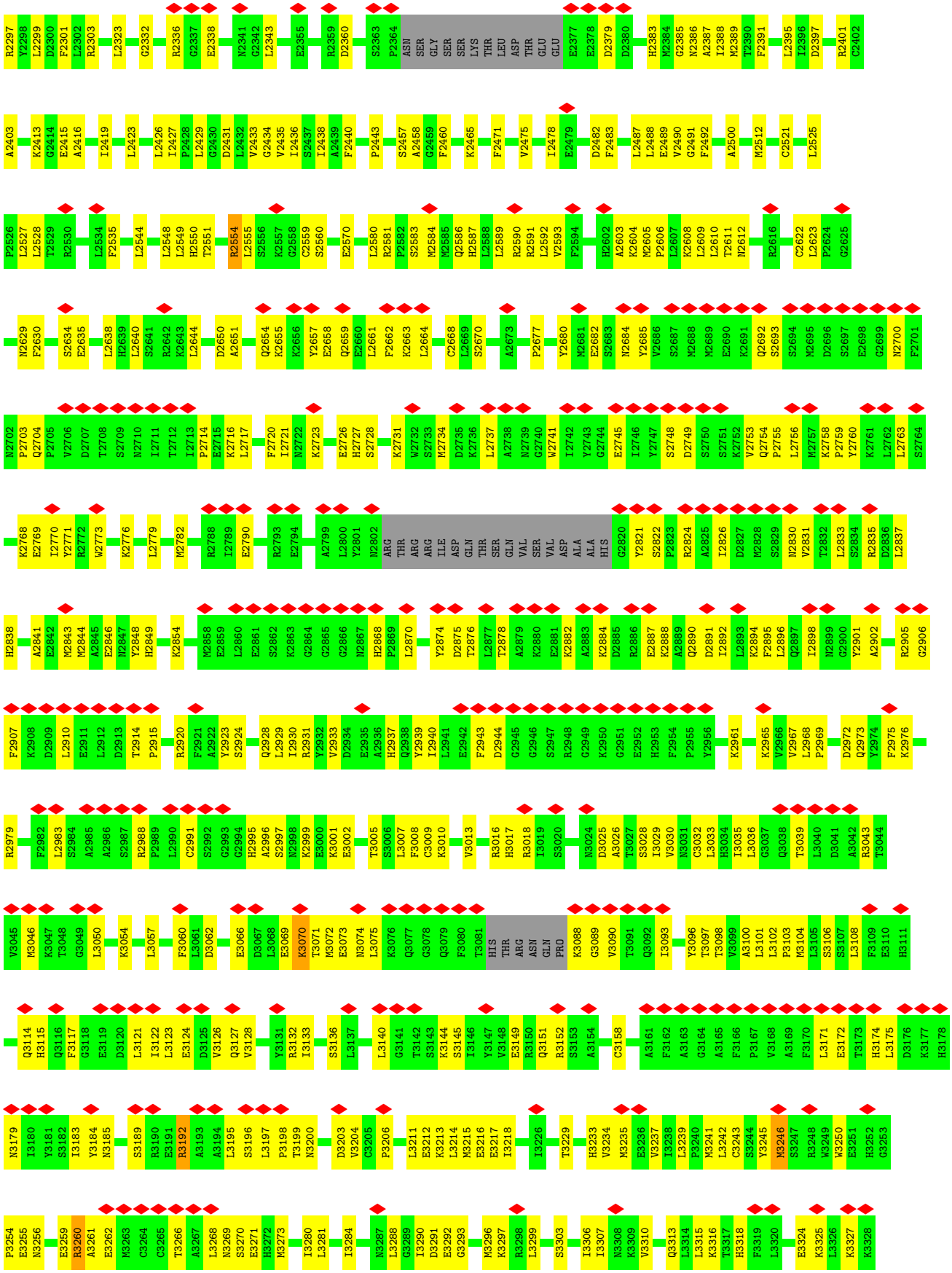
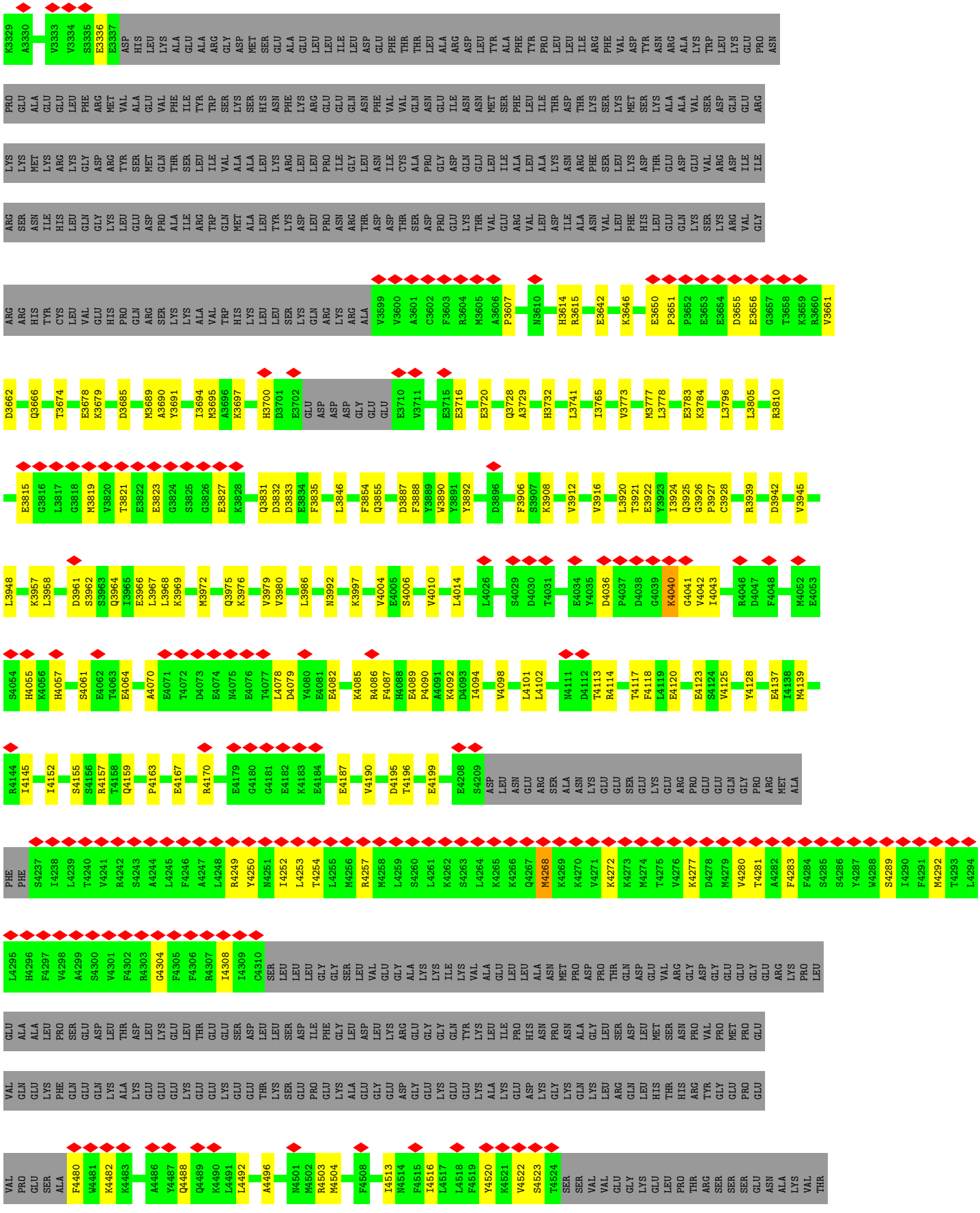
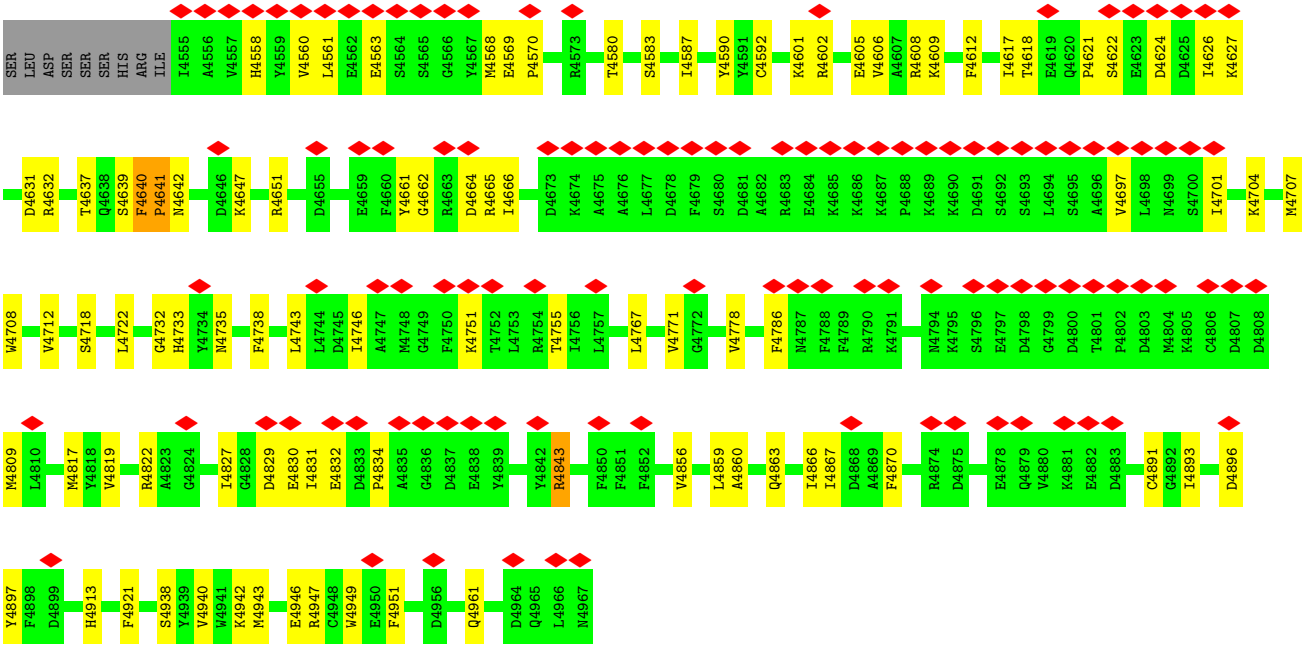
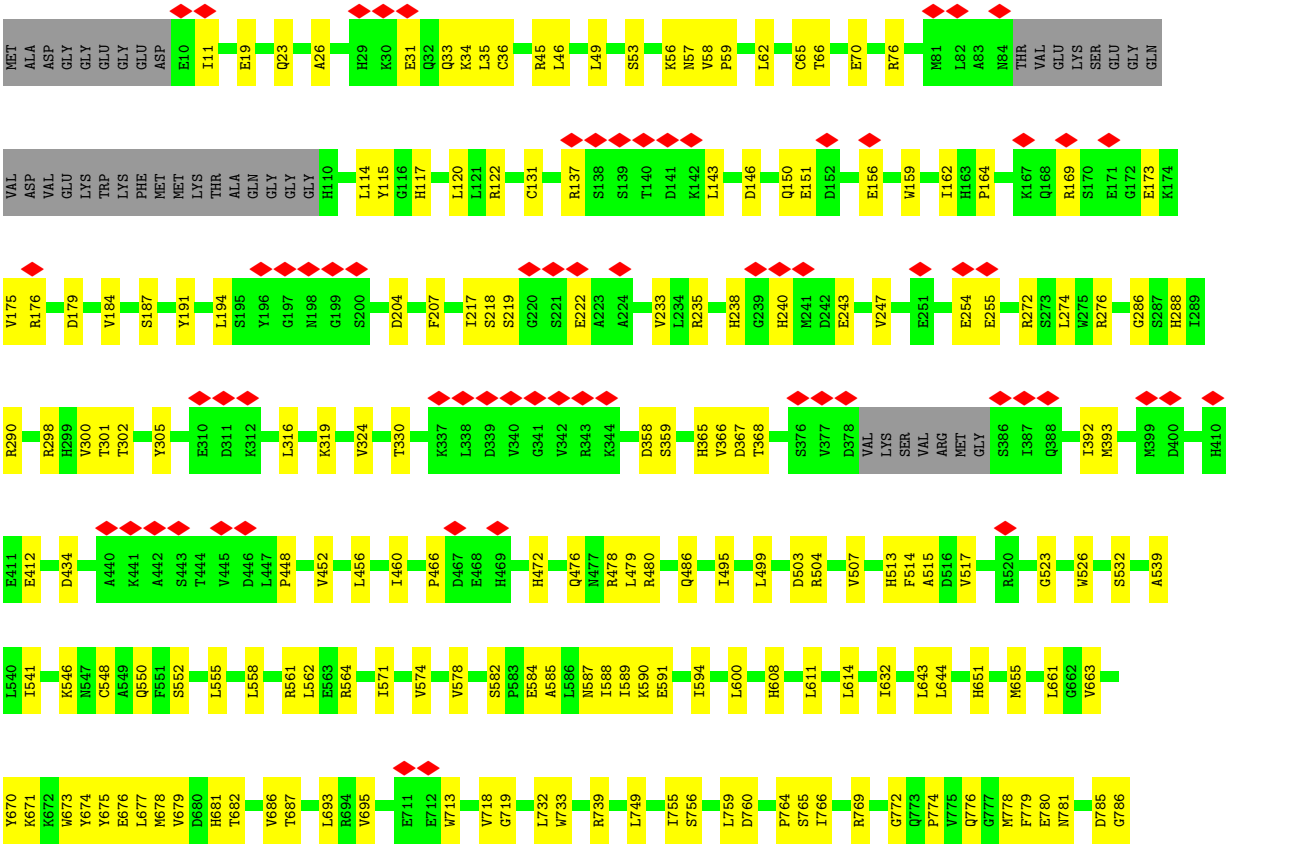


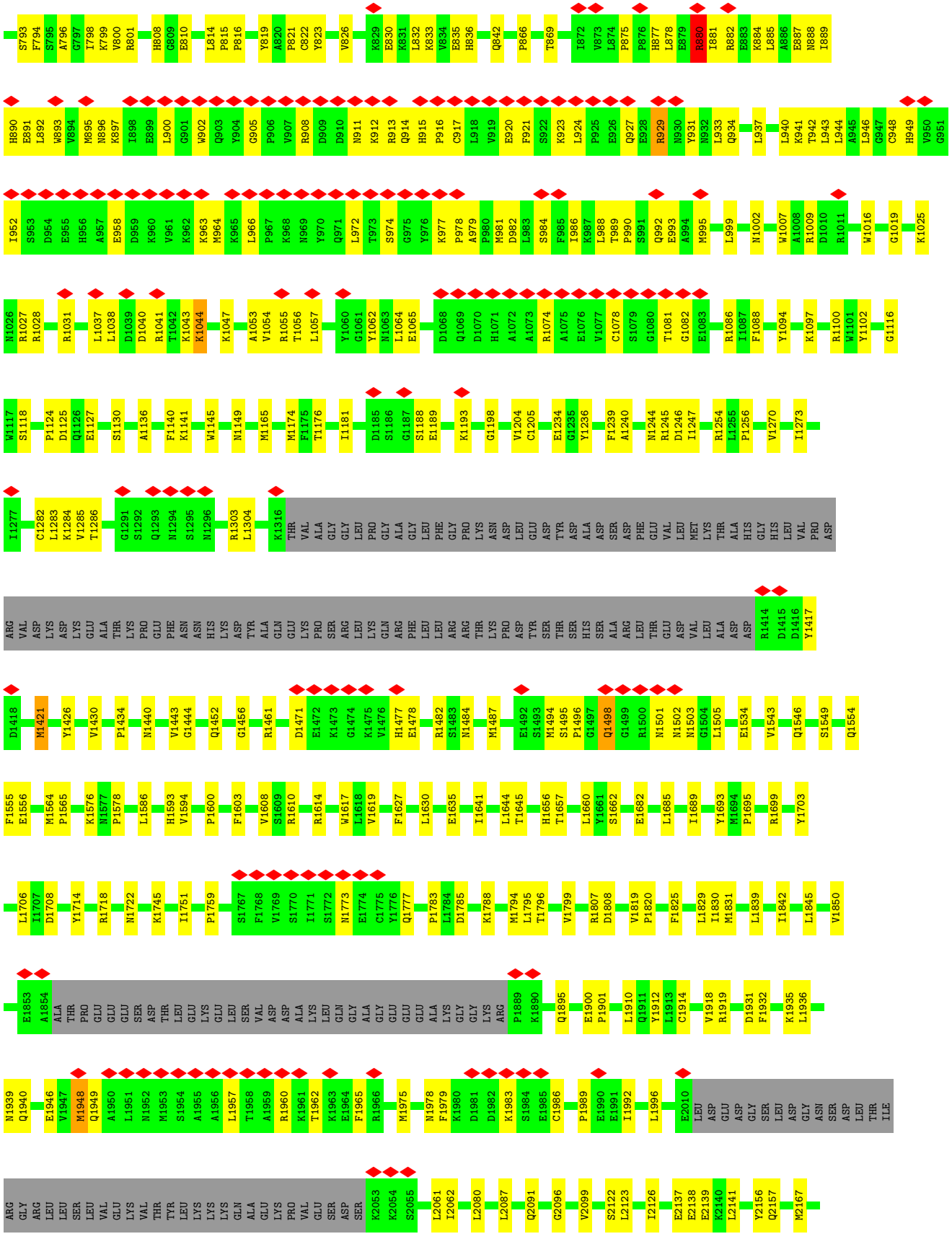




• Molecule 1: Ryanodine receptor 2

Chain C:

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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 R1414 D1415 D1416 Y1417
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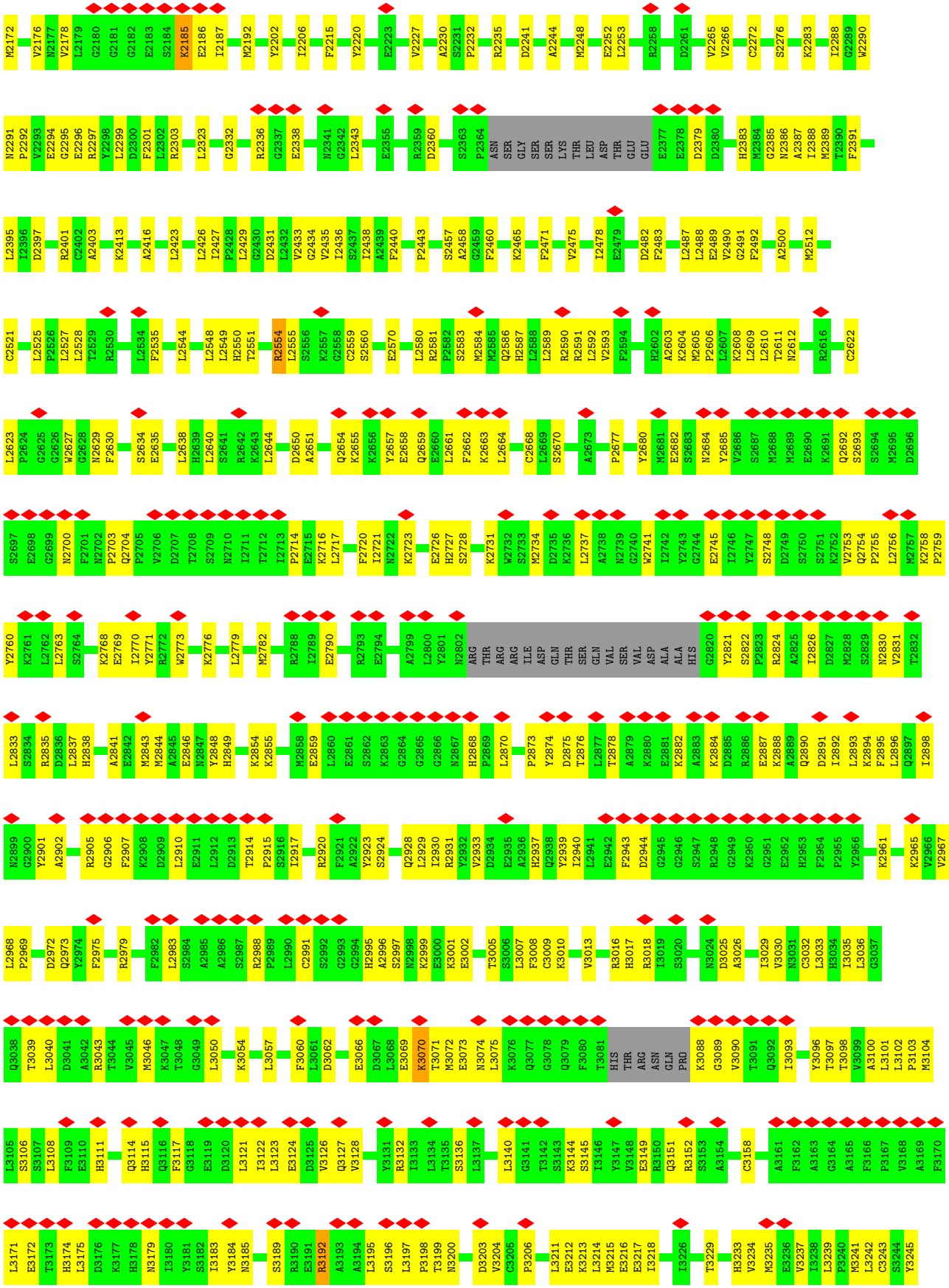
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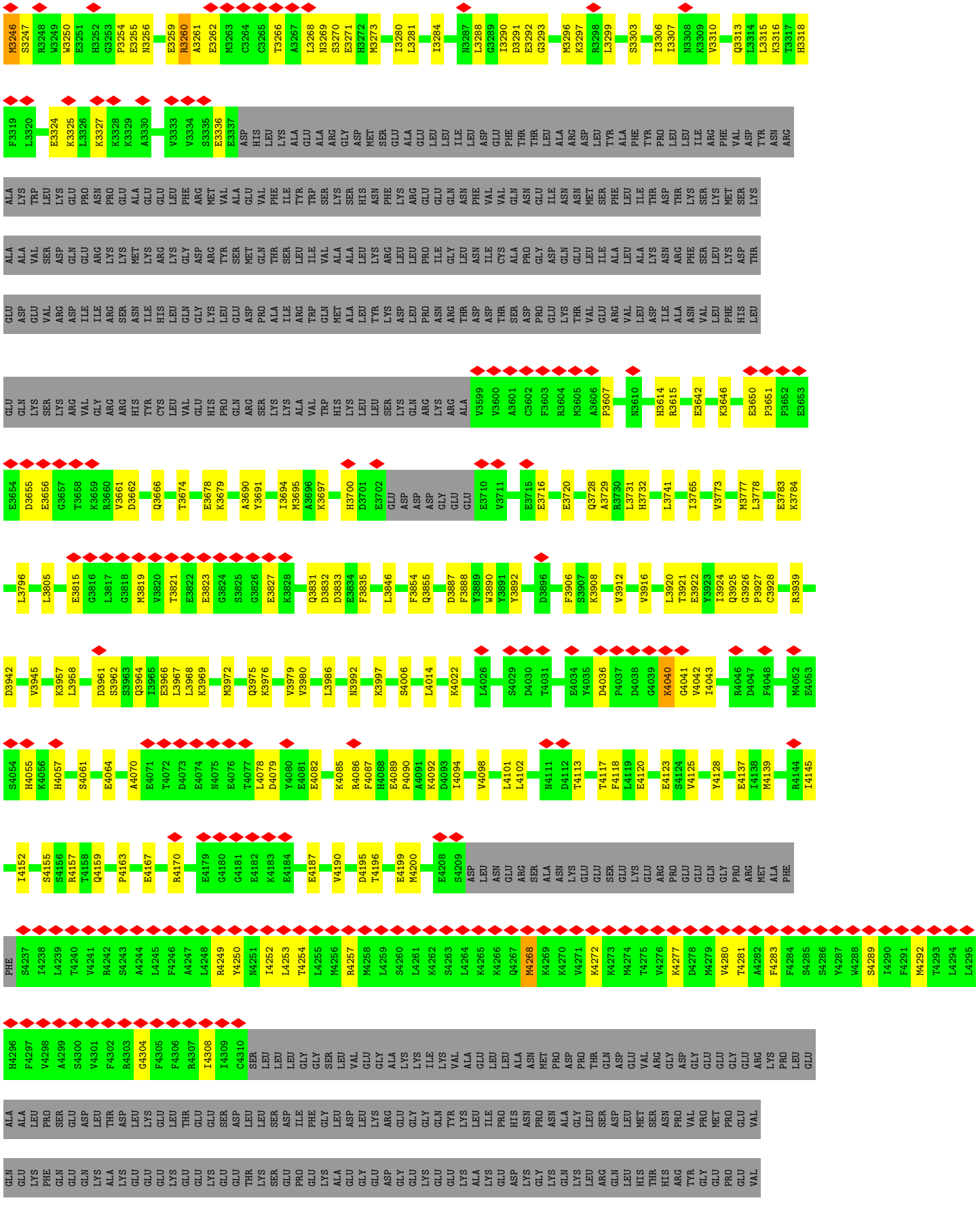
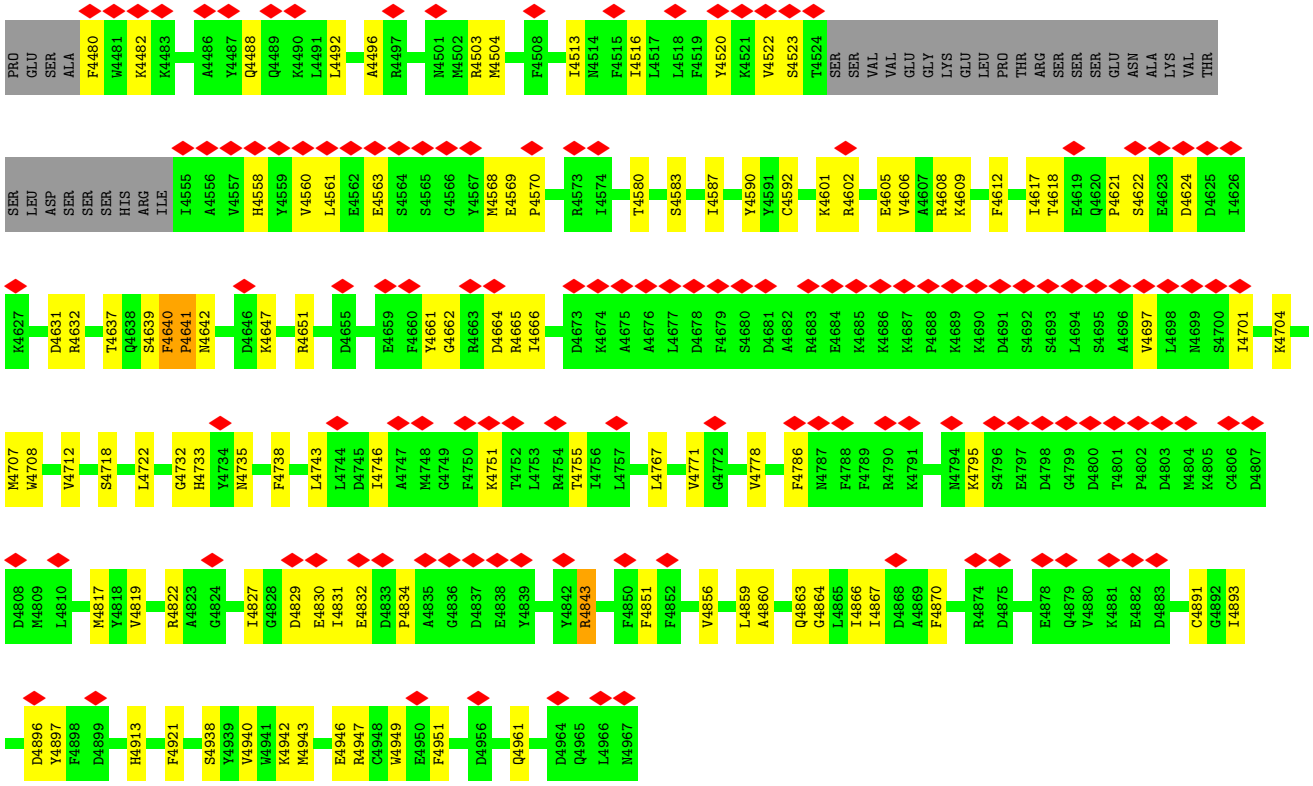
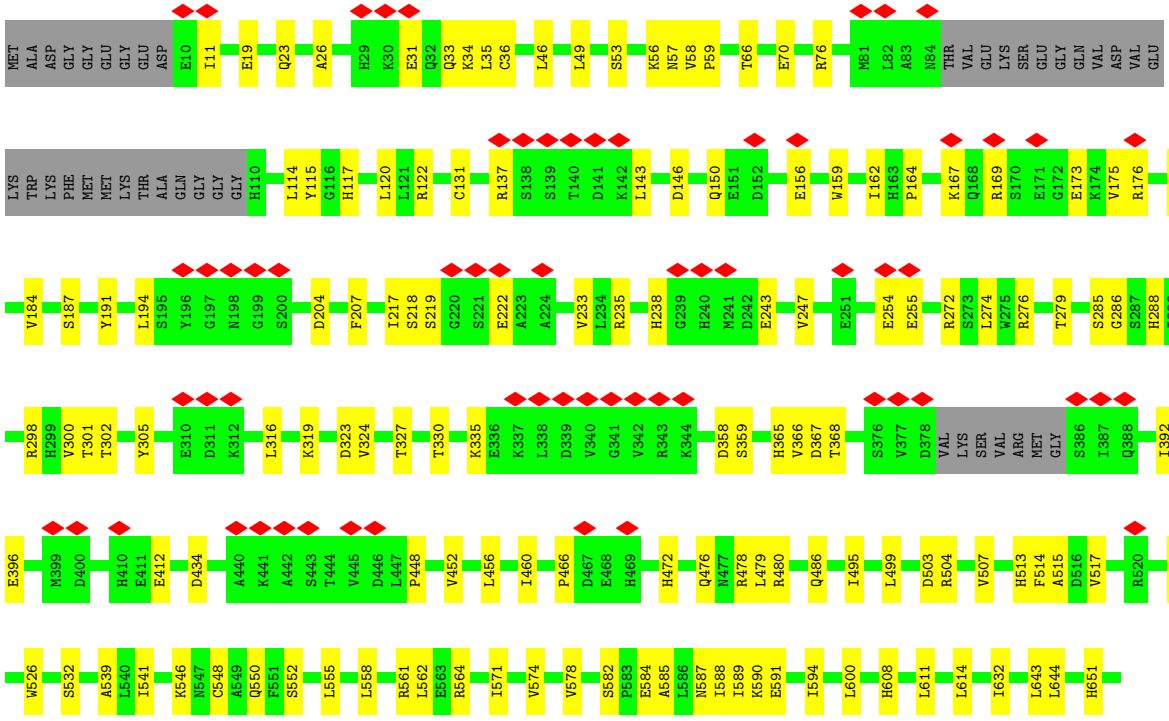
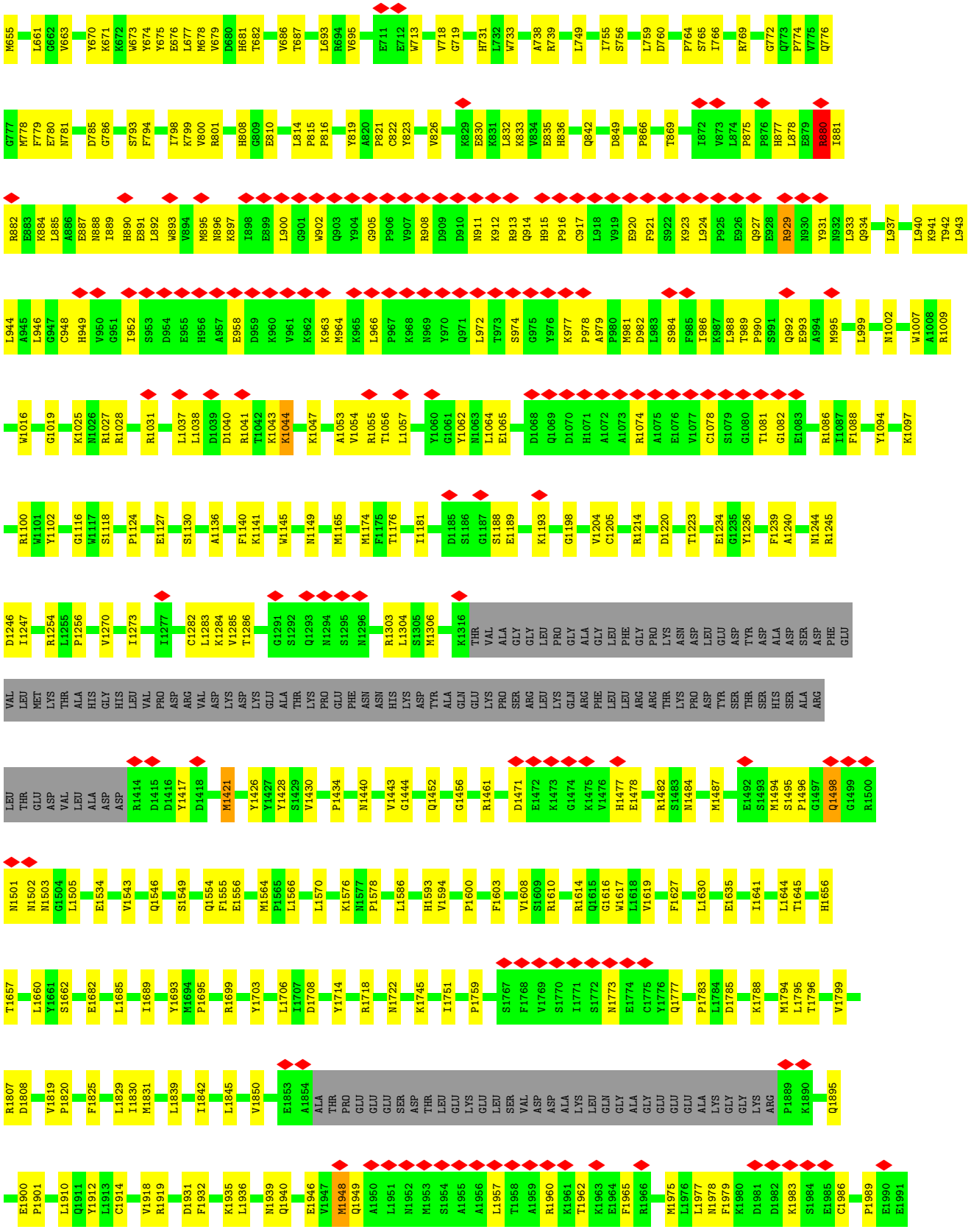




• Molecule 1: Ryanodine receptor 2

Chain D:

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D1246 I1247 R1254 L1255 P1256 V1270 I1273 I1277 C1282 L1283 K1284 V1285 T1286 G1291 S1292 Q1293 N1294 S1295 N1296 R1303 L1304 S1305 M1306 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
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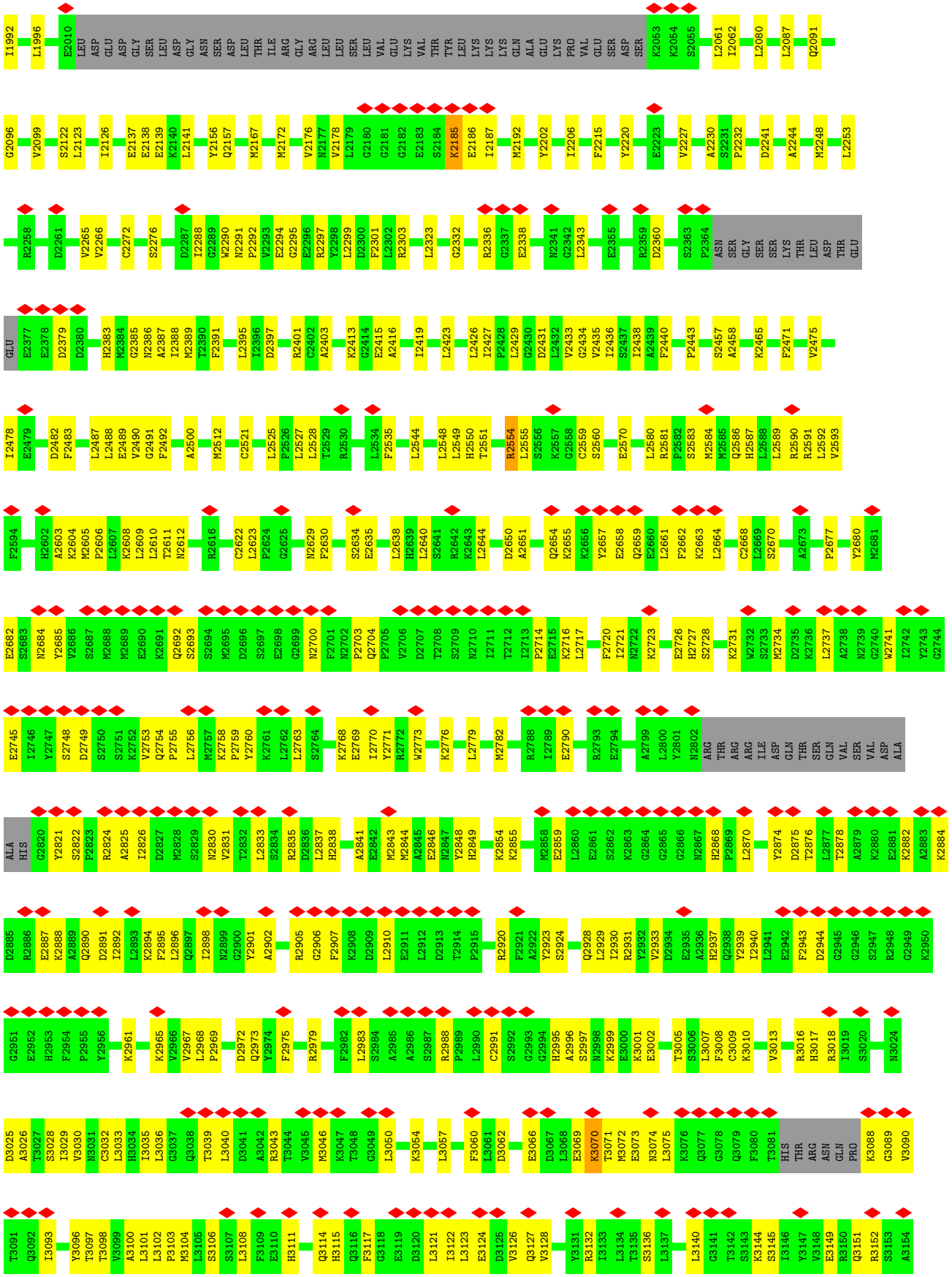
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D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 F2895 L2896 Q2897 I2898 N2899 G2900 Y2901 A2902 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 R2920 F2921 A2922 Y2923 S2924 Q2928 L2929 I2930 R2931 Y2932 V2933 D2934 E2935 A2936 H2937 Q2938 Y2939 I2940 L2941 E2942 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950
G2951 E2952 H2953 F2954 P2955 Y2956 K2961 K2965 V2966 V2967 L2968 P2969 D2972 Q2973 Y2974 F2975 R2979 F2982 L2983 S2984 A2985 A2986 S2987 R2988 P2989 L2990 C2991 S2992 G2993 G2994 H2995 A2996 S2997 N2998 K2999 E3000 K3001 E3002 T3005 S3006 L3007 F3008 C3009 K3010 V3013 R3016 H3017 R3018 I3019 S3020 N3024
D3025 A3026 T3027 S3028 I3029 V3030 M3031 C3032 L3033 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 K3064 L3057 F3060 L3061 D3062 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 Q3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090
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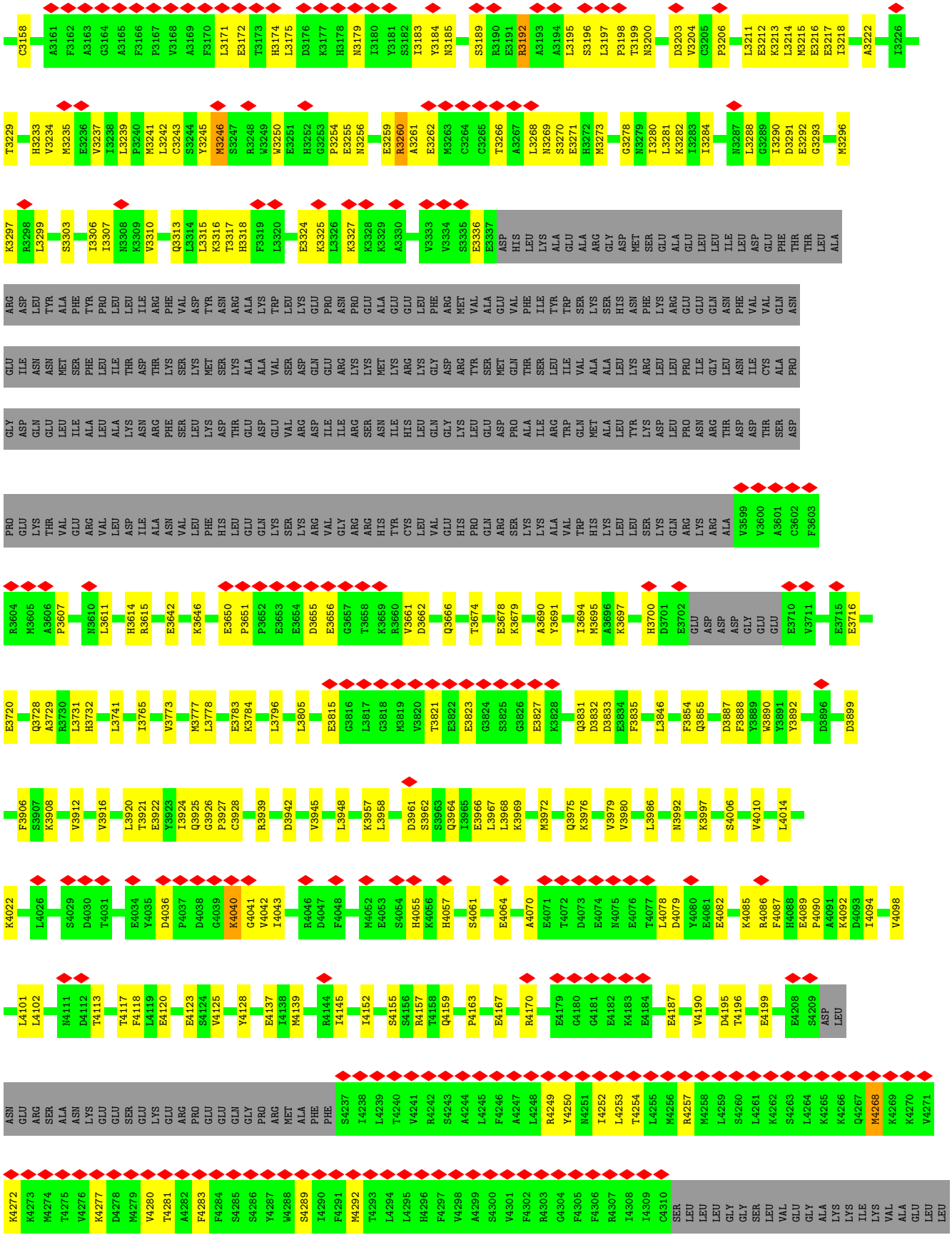
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T3229 H3233 V3234 M3235 E3236 V3237 I3238 L3239 P3240 M3241 L3242 C3243 S3244 Y3245 M3246 S3247 R3248 W3249 W3250 E3251 H3252 G3253 P3254 E3255 N3256 E3259 R3260 A3261 E3262 M3263 C3264 C3265 T3266 A3267 L3268 N3269 S3270 E3271 H3272 M3273 G3278 N3279 I3280 L3281 K3282 I3283 I3284 N3287 L3288 G3289 I3290 D3291 E3292 G3293 M3296
K3297 R3298 L3299 S3303 I3306 T3307 N3308 K3309 V3310 Q3313 L3314 L3315 K3316 T3317 H3318 F3319 L3320 E3324 K3325 L3326 K3327 K3328 K3329 A3330 V3333 V3334 S3335 E3336 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 ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN
GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO
GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP
PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603
R3604 M3605 A3606 P3607 N3610 L3611 H3614 R3615 E3642 K3646 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 V3661 D3662 Q3666 T3674 E3678 K3679 A3690 Y3691 I3694 M3695 A3696 K3697 H3700 D3701 E3702 GLU ASP ASP GLY GLU GLU E3710 V3711 E3715 E3716
E3720 Q3728 A3729 R3730 L3731 H3732 L3741 I3765 V3773 M3777 L3778 E3783 K3784 L3796 L3805 E3815 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 K3828 Q3831 D3832 D3833 E3834 F3835 L3846 F3854 Q3855 D3887 F3888 Y3889 W3890 Y3891 Y3892 D3896 D3899
F3906 S3907 K3908 V3912 V3916 L3920 T3921 E3922 Y3923 I3924 Q3925 G3926 P3927 C3928 R3939 D3942 V3945 L3948 K3957 L3958 D3961 S3962 S3963 Q3964 I3965 E3966 L3967 L3968 K3969 M3972 Q3975 K3976 V3979 V3980 L3986 N3992 K3997 S4006 V4010 L4014
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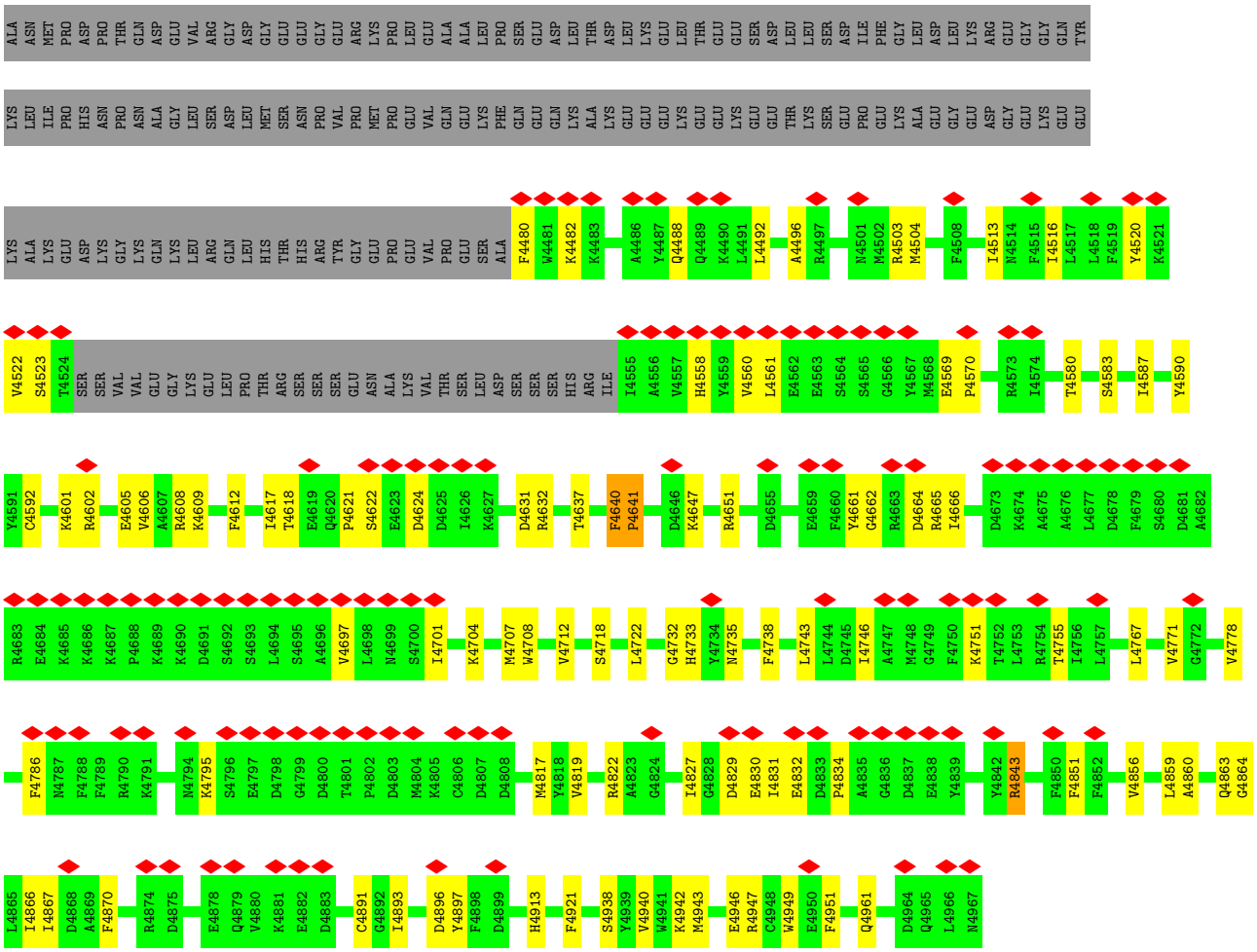
L4101 L4102 N4111 D4112 T4113 T4117 F4118 L4119 E4120 E4123 S4124 V4125 Y4128 E4137 I4138 M4139 R4144 I4145 I4152 S4155 S4156 R4157 T4158 Q4159 P4163 E4167 R4170 E4179 G4180 G4181 E4182 K4183 E4184 E4187 V4190 D4195 T4196 E4199 E4208 S4209 ASP LEU
ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU GLU LYS GLU ARG PRO GLU GLU GLN GLY PRO ARG MET ALA PHE PHE S4237 I4238 L4239 T4240 V4241 R4242 S4243 A4244 L4245 F4246 A4247 L4248 R4249 Y4250 N4251 I4252 L4253 T4254 L4255 M4256 R4257 M4258 L4259 S4260 L4261 K4262 S4263 L4264 K4265 K4266 Q4267 M4268 K4269 K4270 V4271
K4272 K4273 M4274 T4275 V4276 K4277 D4278 M4279 V4280 T4281 A4282 F4283 F4284 S4285 S4286 Y4287 W4288 A4289 I4290 F4291 M4292 T4293 L4294 L4295 H4296 F4297 V4298 A4299 S4300 V4301 F4302 R4303 G4304 F4305 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU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LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER ASN PRO VAL PRO MET PRO GLU VAL GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU SER GLU GLU GLU GLY GLU GLU LYS GLU GLU
LYS ALA LYS GLU ASP LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA F4480 W4481 K4482 K4483 A4486 Y4487 Q4488 Q4489 K4490 L4491 L4492 A4496 R4497 N4501 M4502 R4503 M4504 F4508 I4513 N4514 F4515 I4516 L4517 L4518 F4519 Y4520 K4521
V4522 S4523 T4524 SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG SER SER SER GLU ASN ALA LYS VAL THR SER LEU ASP SER SER SER HIS ARG ILE I4555 A4556 V4557 H4558 Y4559 V4560 L4561 E4562 E4563 S4564 S4565 G4566 Y4567 M4568 E4569 P4570 R4573 I4574 T4580 S4583 I4587 Y4590
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F4786 N4787 F4788 F4789 R4790 K4791 N4794 K4795 S4796 E4797 D4798 G4799 D4800 T4801 P4802 D4803 M4804 K4805 C4806 D4807 D4808 M4817 Y4818 V4819 R4822 A4823 G4824 I4827 G4828 D4829 E4830 I4831 E4832 D4833 P4834 A4835 G4836 D4837 E4838 Y4839 Y4842 R4843 F4850 F4851 F4852 V4856 L4859 A4860 Q4863 G4864
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18232	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	0.473	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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

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	0/34511	0.50	4/46614 (0.0%)
1	B	0.25	0/34511	0.50	4/46614 (0.0%)
1	C	0.25	0/34511	0.50	4/46614 (0.0%)
1	D	0.25	0/34511	0.50	4/46614 (0.0%)
All	All	0.25	0/138044	0.50	16/186456 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1948	MET	CB-CG-SD	7.23	134.09	112.40
1	B	1948	MET	CB-CG-SD	7.22	134.07	112.40
1	C	1948	MET	CB-CG-SD	7.22	134.07	112.40
1	A	1948	MET	CB-CG-SD	7.22	134.06	112.40
1	A	880	ARG	CA-CB-CG	6.59	127.90	113.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3192	ARG	Sidechain
1	A	4640	PHE	Peptide
1	A	880	ARG	Sidechain
1	B	3192	ARG	Sidechain
1	B	880	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33771	0	33455	790	0
1	B	33771	0	33455	785	0
1	C	33771	0	33455	790	0
1	D	33771	0	33455	800	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	62	0	24	1	0
3	B	62	0	24	2	0
3	C	62	0	24	1	0
3	D	62	0	24	1	0
All	All	135336	0	133916	3086	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 3086 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4891:CYS:SG	1:B:4913:HIS:CE1	2.51	1.04
1:A:4891:CYS:SG	1:A:4913:HIS:CE1	2.51	1.02
1:D:4891:CYS:SG	1:D:4913:HIS:CE1	2.51	1.00
1:C:4891:CYS:SG	1:C:4913:HIS:CE1	2.51	1.00
1:A:4860:ALA:CB	1:D:4863:GLN:OE1	2.15	0.94

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%)	4085 (97%)	109 (3%)	4 (0%)	51	83
1	B	4198/4967 (84%)	4085 (97%)	109 (3%)	4 (0%)	51	83
1	C	4198/4967 (84%)	4085 (97%)	109 (3%)	4 (0%)	51	83
1	D	4198/4967 (84%)	4084 (97%)	110 (3%)	4 (0%)	51	83
All	All	16792/19868 (84%)	16339 (97%)	437 (3%)	16 (0%)	54	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2770	ILE
1	A	3927	PRO
1	A	4641	PRO
1	B	2770	ILE
1	B	3927	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3708/4358 (85%)	3682 (99%)	26 (1%)	84	90
1	B	3708/4358 (85%)	3682 (99%)	26 (1%)	84	90
1	C	3708/4358 (85%)	3682 (99%)	26 (1%)	84	90
1	D	3708/4358 (85%)	3682 (99%)	26 (1%)	84	90
All	All	14832/17432 (85%)	14728 (99%)	104 (1%)	84	90

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1044	LYS
1	C	3327	LYS
1	D	4085	LYS
1	C	1498	GLN
1	C	2884	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3949	HIS
1	D	3114	GLN
1	C	2550	HIS
1	D	2928	GLN
1	D	3949	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\|>2$
3	ATP	D	5002	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
3	ATP	D	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
3	ATP	C	5002	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
3	ATP	B	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
3	ATP	A	5003	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
3	ATP	B	5002	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
3	ATP	A	5002	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
3	ATP	C	5003	-	26,33,33	0.59	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
3	ATP	D	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	D	5003	-	-	5/18/38/38	0/3/3/3
3	ATP	C	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	B	5003	-	-	5/18/38/38	0/3/3/3
3	ATP	A	5003	-	-	5/18/38/38	0/3/3/3
3	ATP	B	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	A	5002	-	-	4/18/38/38	0/3/3/3
3	ATP	C	5003	-	-	5/18/38/38	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})
3	A	5003	ATP	C5-C6-N6	2.30	123.85	120.35
3	B	5003	ATP	C5-C6-N6	2.30	123.85	120.35
3	C	5003	ATP	C5-C6-N6	2.30	123.85	120.35
3	B	5002	ATP	C5-C6-N6	2.30	123.85	120.35
3	C	5002	ATP	C5-C6-N6	2.30	123.85	120.35

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5002	ATP	O4'-C4'-C5'-O5'
3	A	5002	ATP	C3'-C4'-C5'-O5'
3	A	5003	ATP	O4'-C4'-C5'-O5'
3	B	5002	ATP	O4'-C4'-C5'-O5'
3	B	5002	ATP	C3'-C4'-C5'-O5'

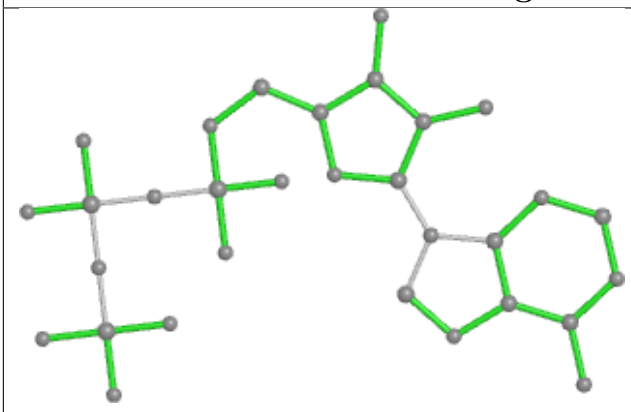
There are no ring outliers.

4 monomers are involved in 5 short contacts:

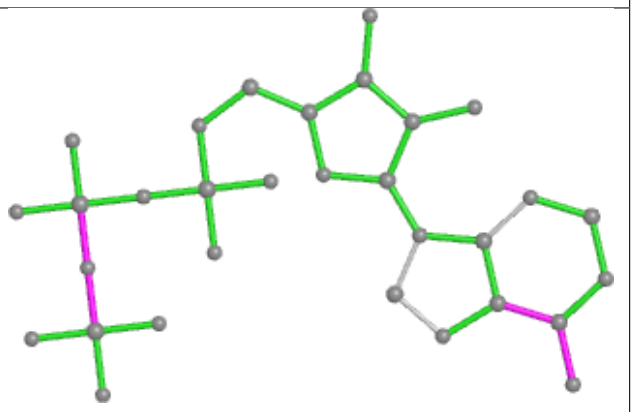
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5003	ATP	1	0
3	B	5003	ATP	2	0
3	A	5003	ATP	1	0
3	C	5003	ATP	1	0

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.

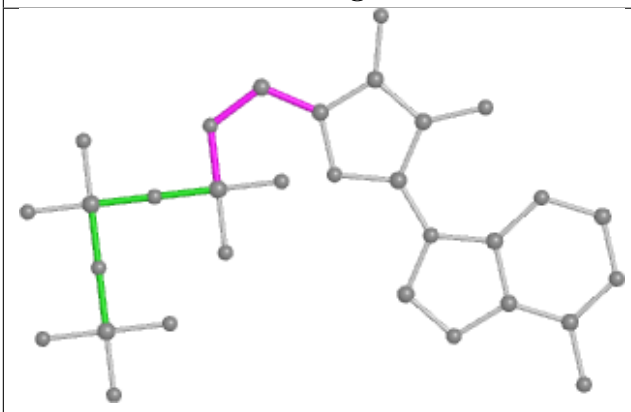
Ligand ATP D 5002



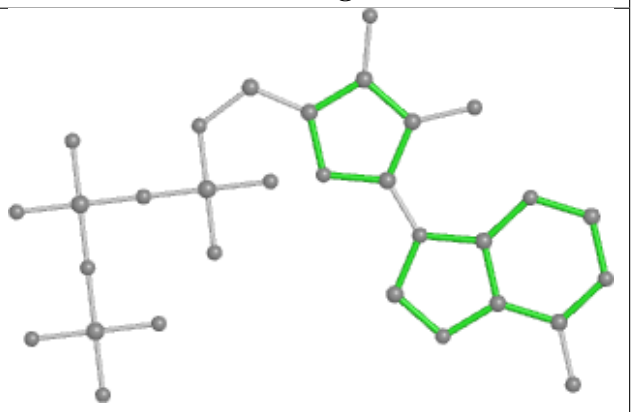
Bond lengths



Bond angles

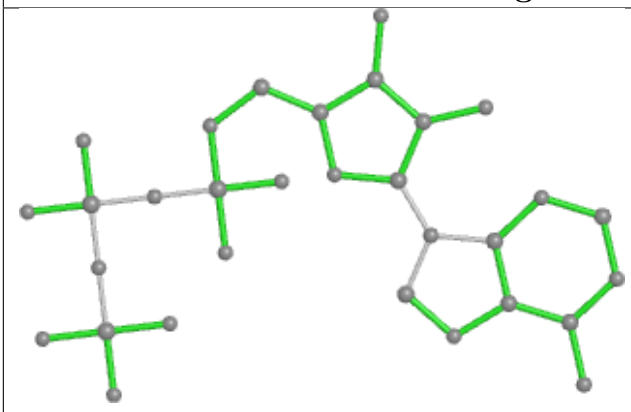


Torsions

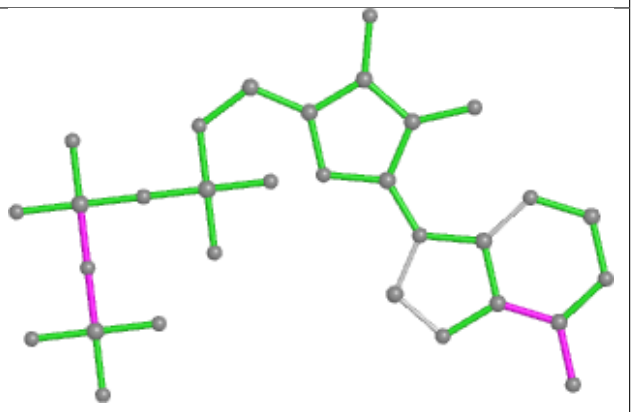


Rings

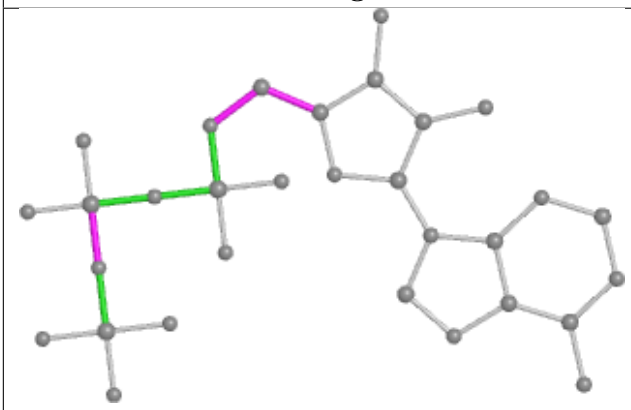
Ligand ATP D 5003



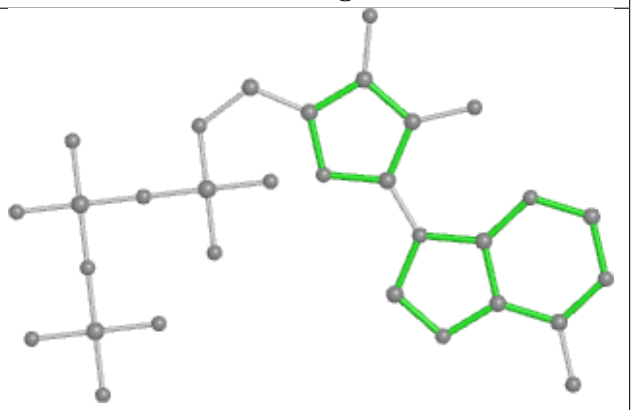
Bond lengths



Bond angles

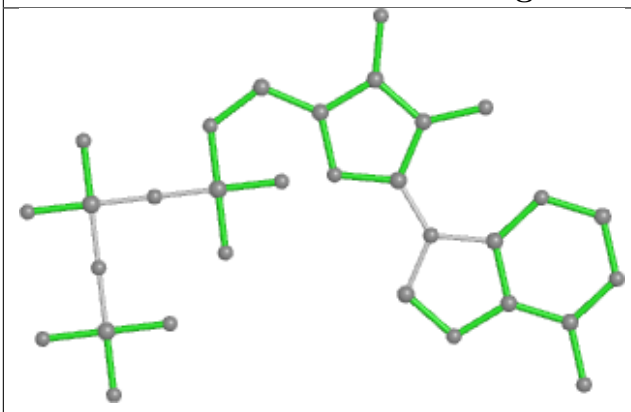


Torsions

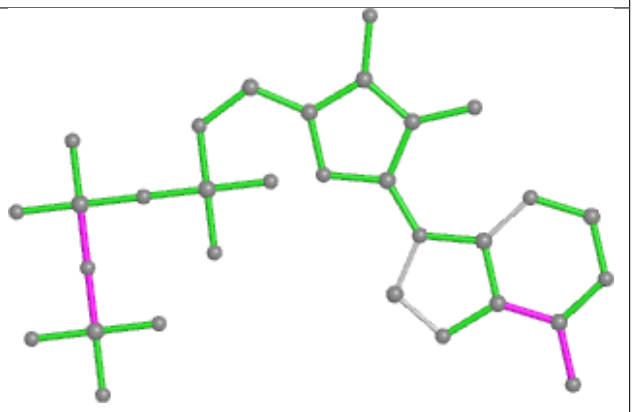


Rings

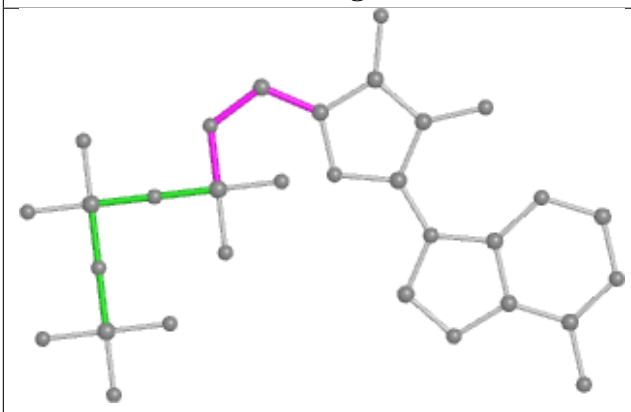
Ligand ATP C 5002



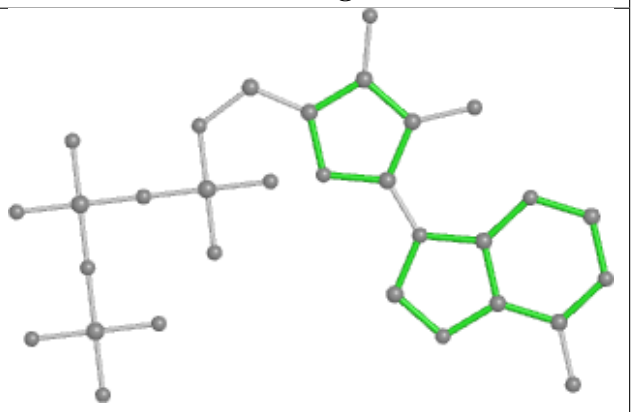
Bond lengths



Bond angles

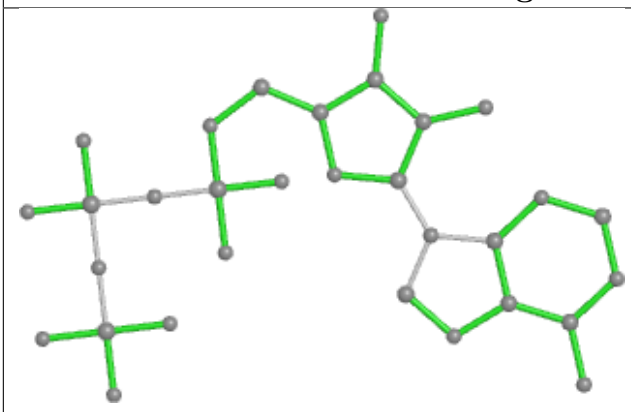


Torsions

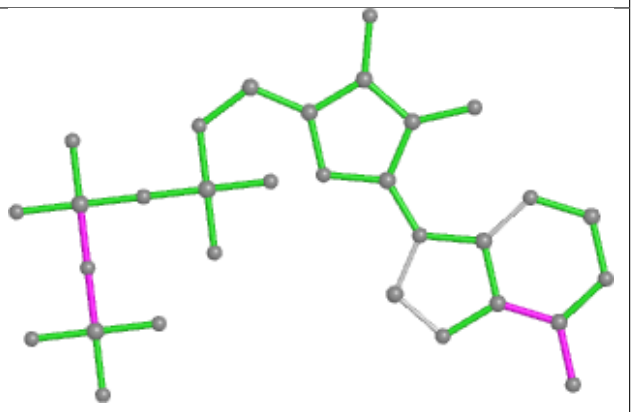


Rings

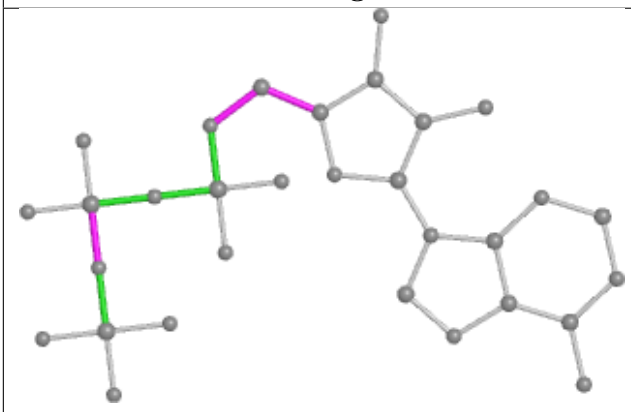
Ligand ATP B 5003



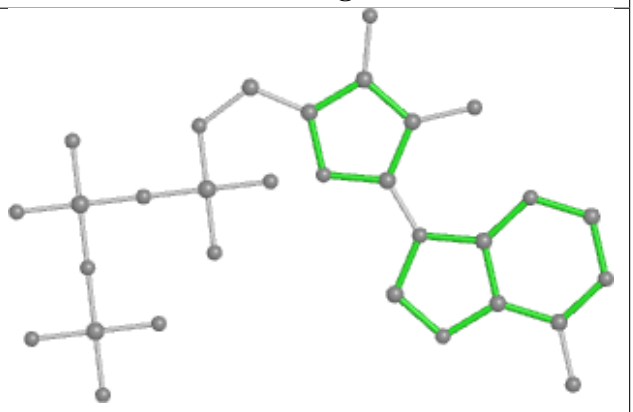
Bond lengths



Bond angles

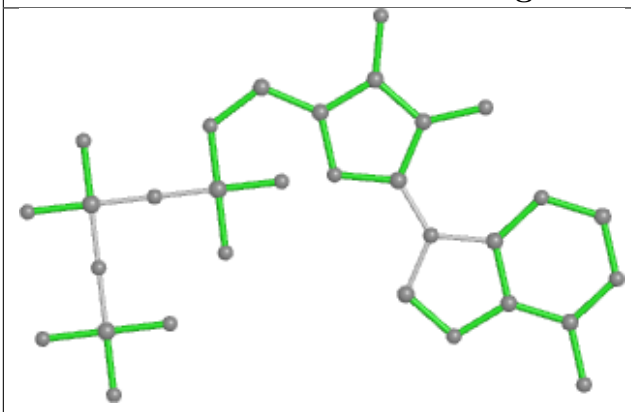


Torsions

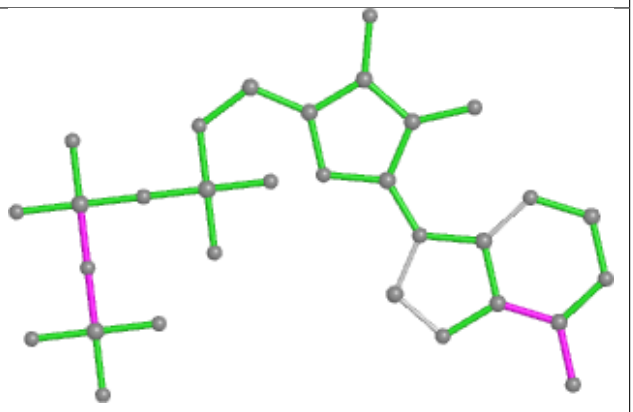


Rings

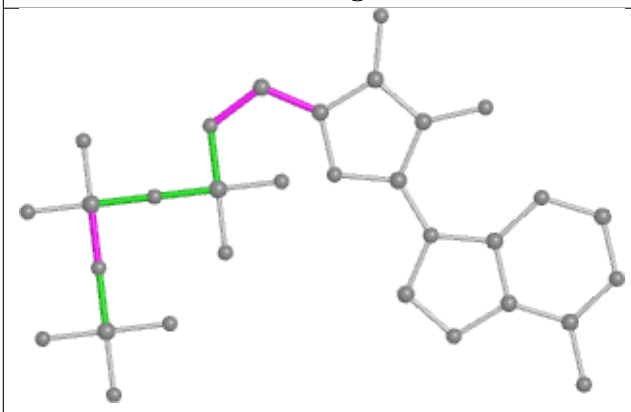
Ligand ATP A 5003



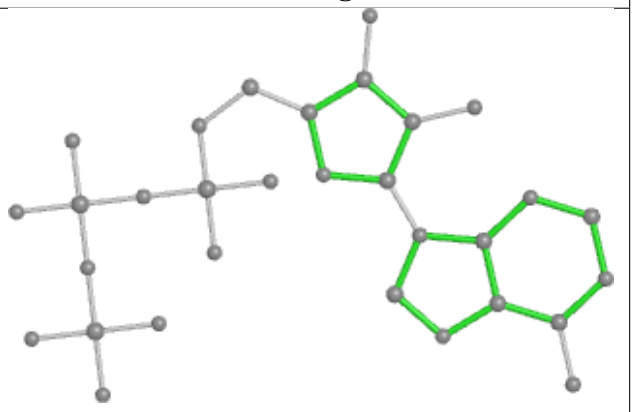
Bond lengths



Bond angles

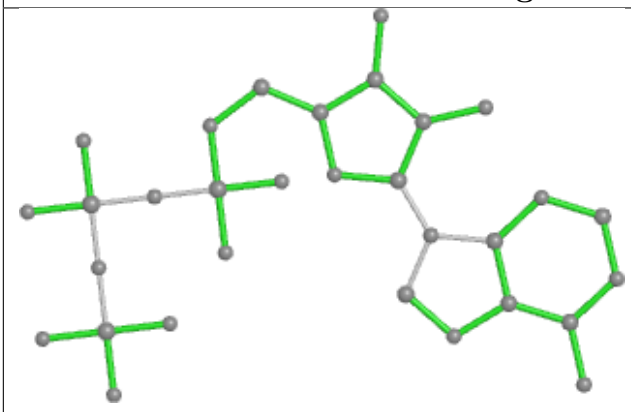


Torsions

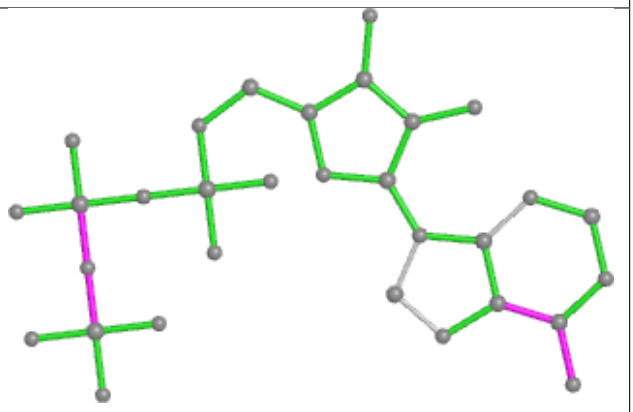


Rings

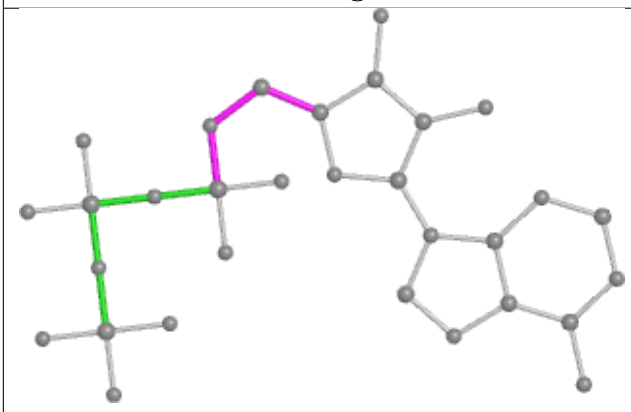
Ligand ATP B 5002



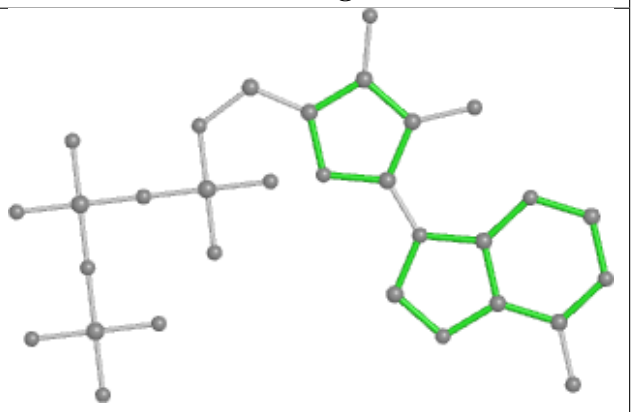
Bond lengths



Bond angles

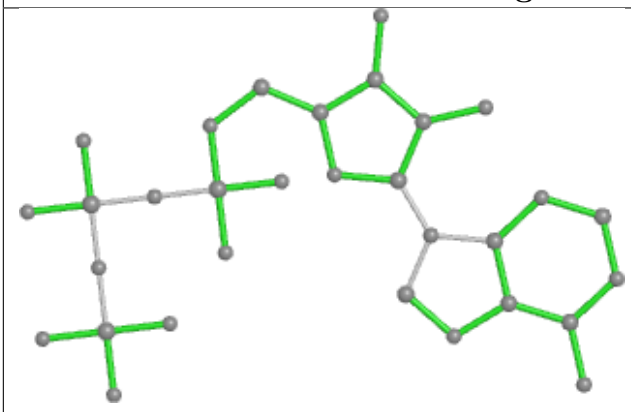


Torsions

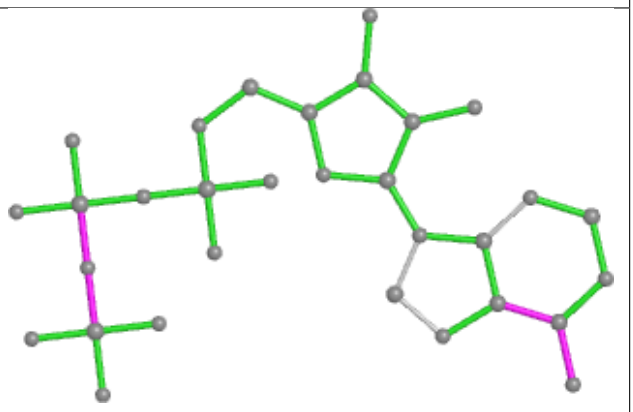


Rings

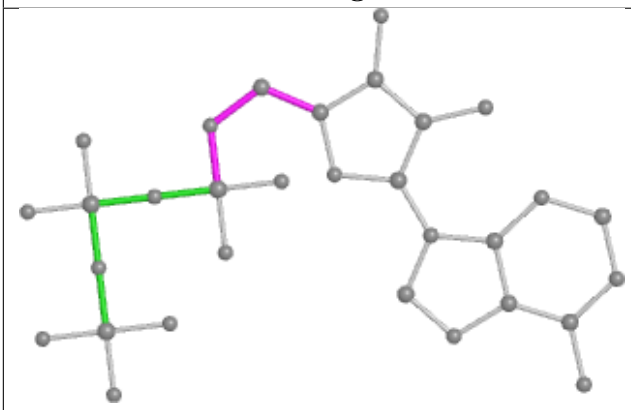
Ligand ATP A 5002



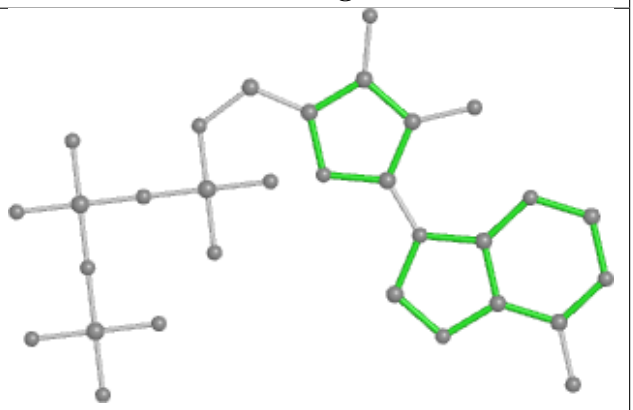
Bond lengths



Bond angles

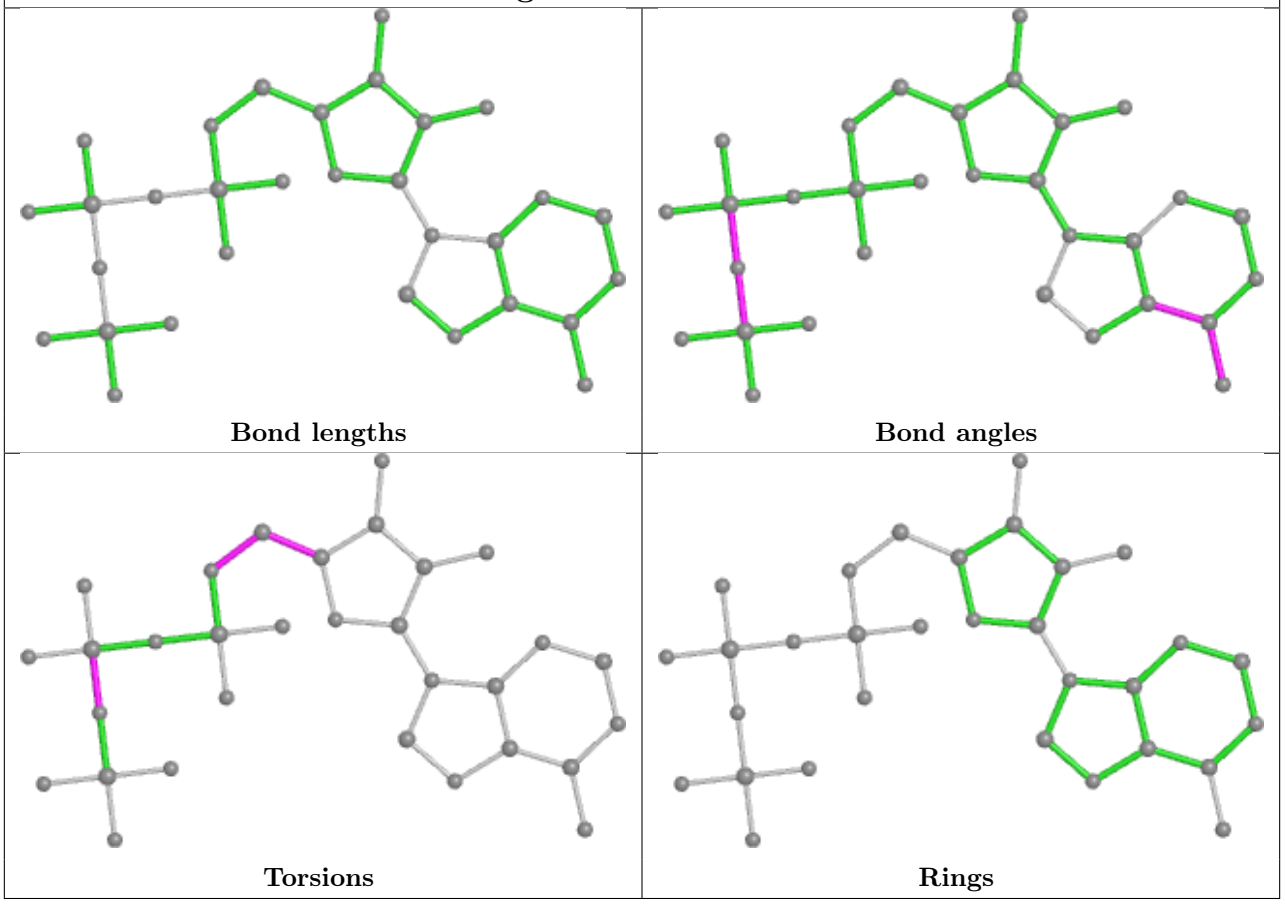


Torsions



Rings

Ligand ATP C 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.

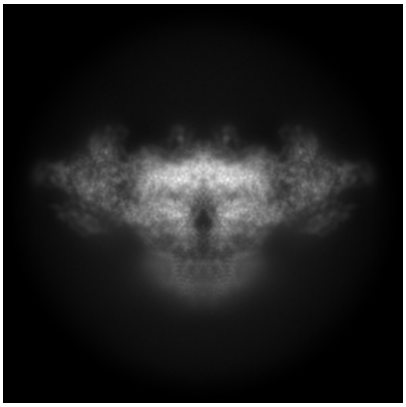
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42461. These allow visual inspection of the internal detail of the map and identification of artifacts.

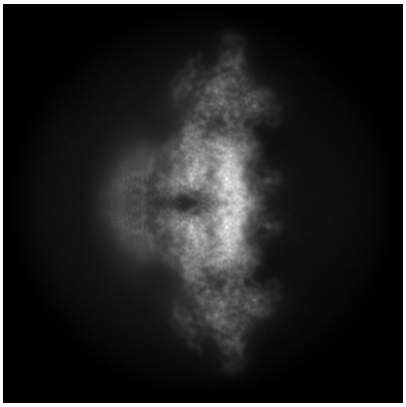
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

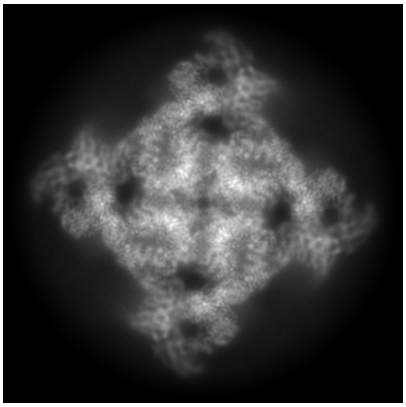
6.1.1 Primary map



X



Y

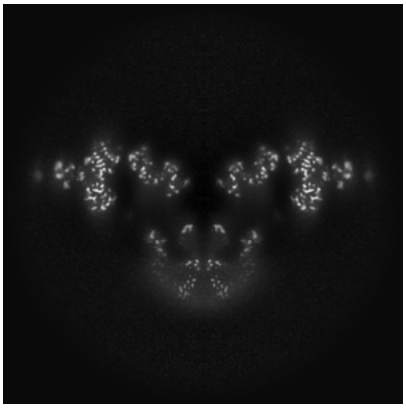


Z

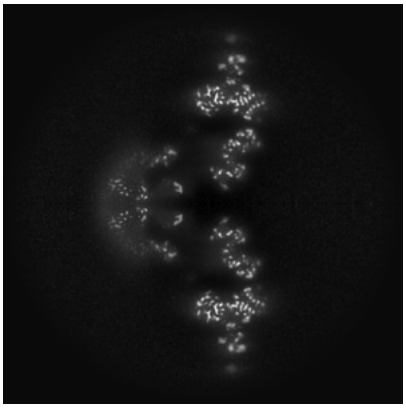
The images above show the map projected in three orthogonal directions.

6.2 Central slices

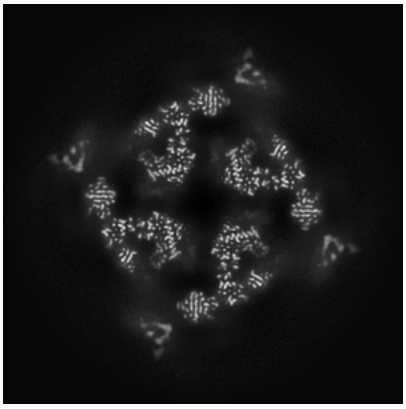
6.2.1 Primary map



X Index: 256



Y Index: 256

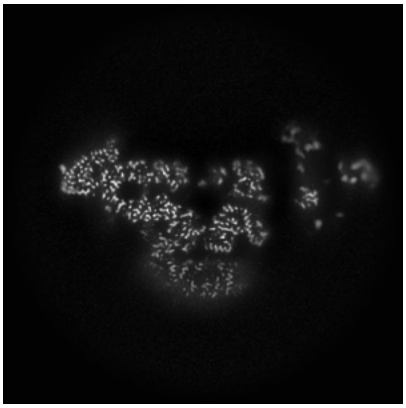


Z Index: 256

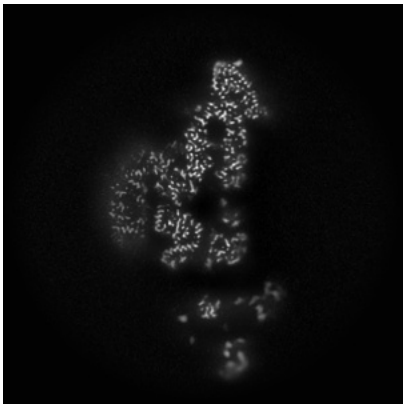
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

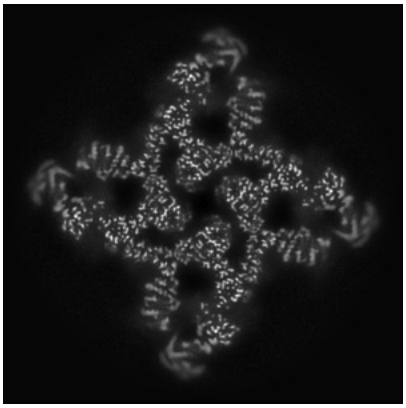
6.3.1 Primary map



X Index: 279



Y Index: 279

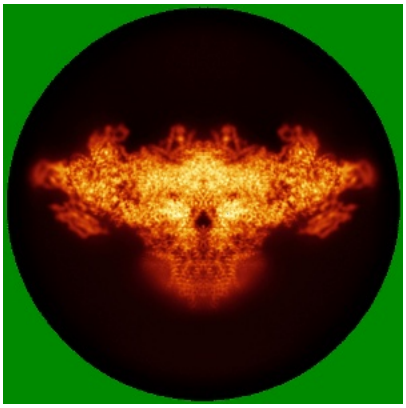


Z Index: 289

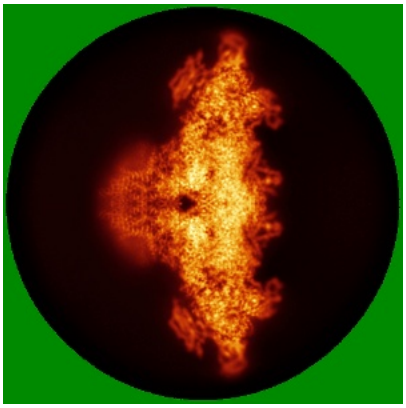
The images above show the largest variance slices of the map in three orthogonal directions.

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

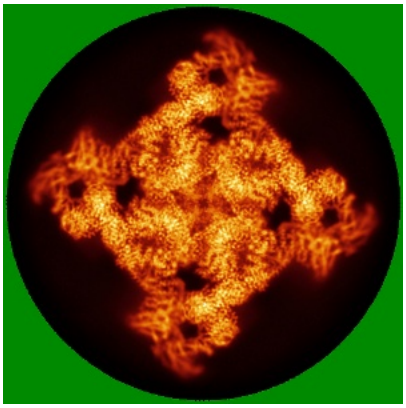
6.4.1 Primary map



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.

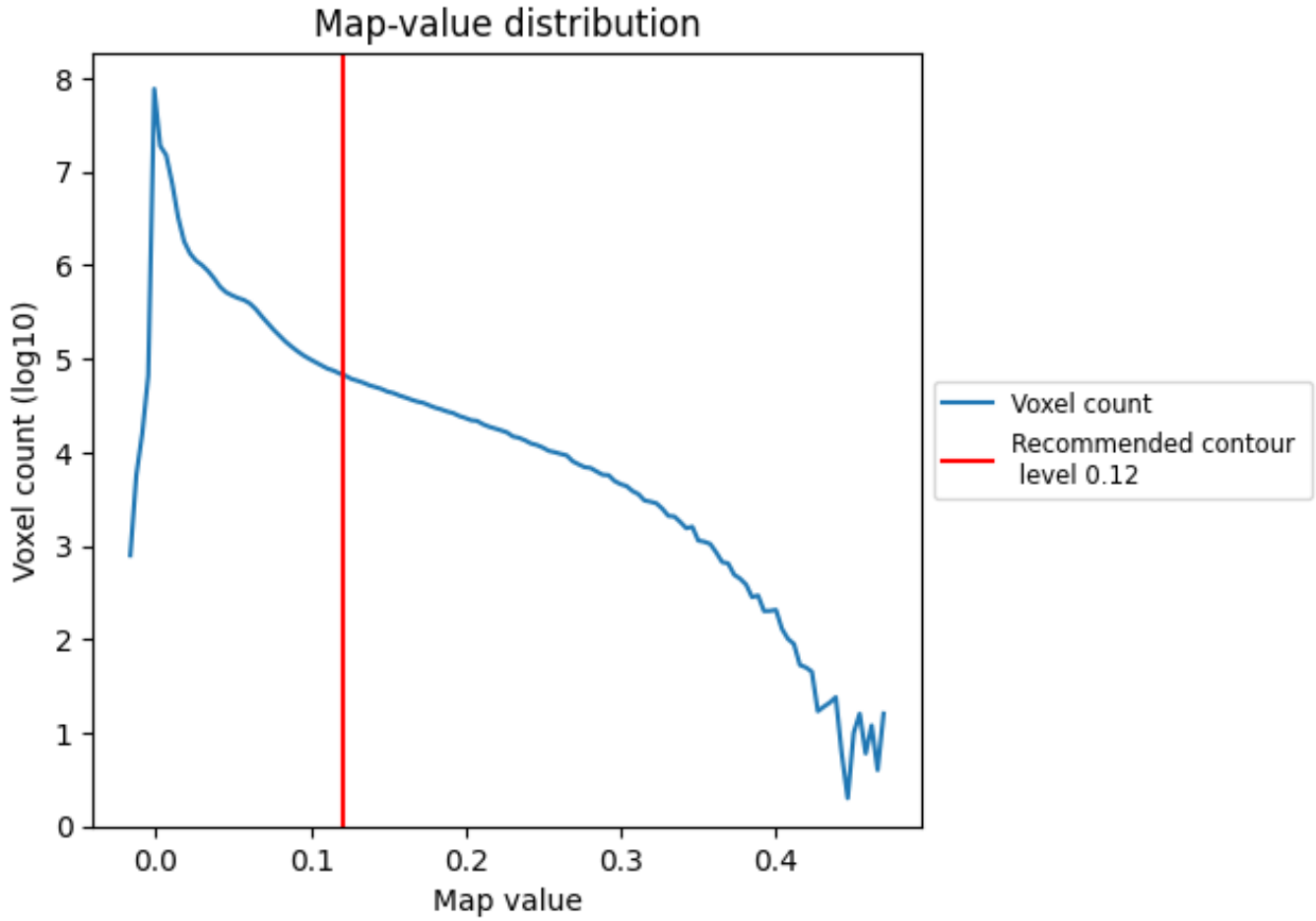
6.6 Mask visualisation (i)

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

7 Map analysis

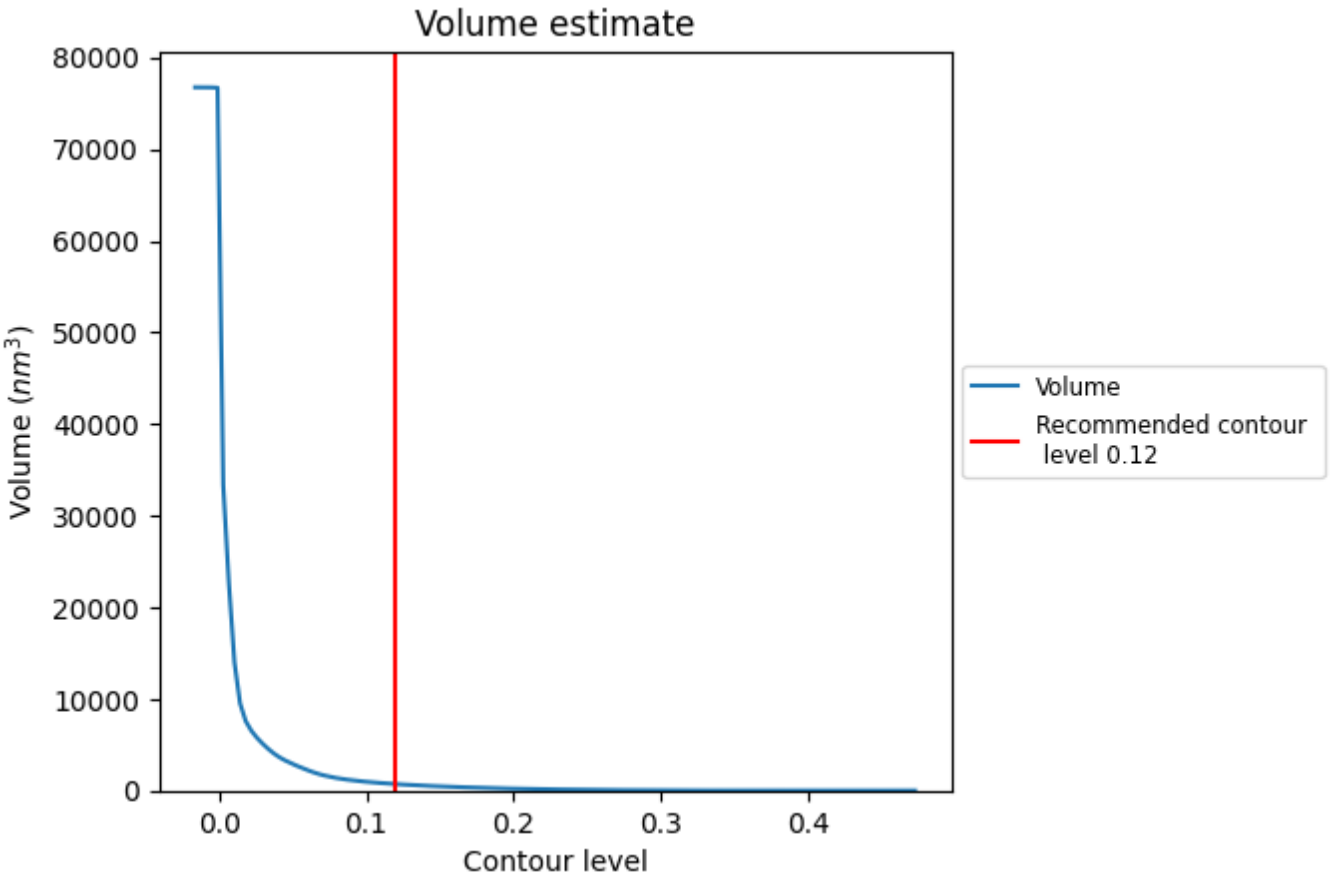
This section contains the results of statistical analysis of the map.

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.

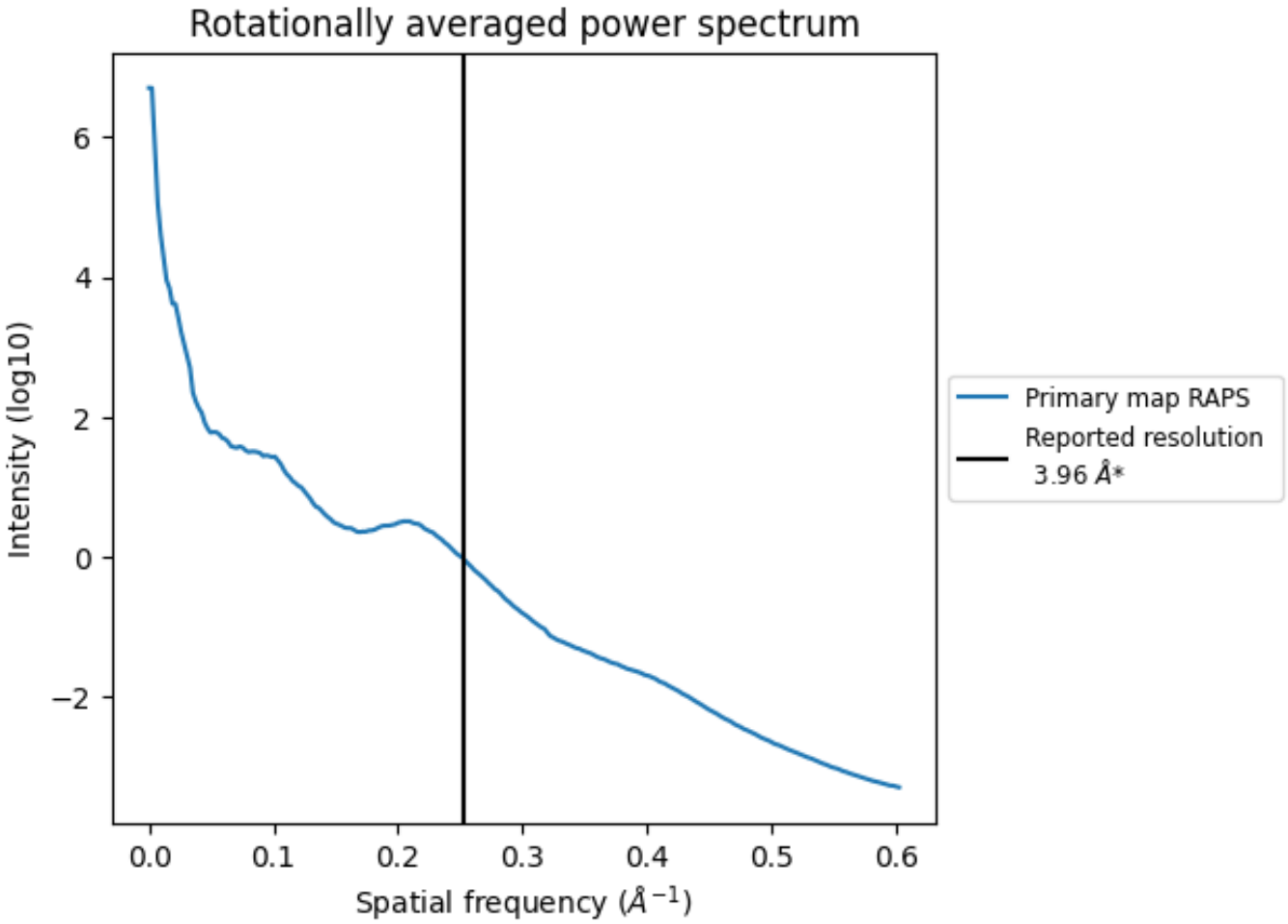
7.2 Volume estimate (i)



The volume at the recommended contour level is 708 nm^3; this corresponds to an approximate mass of 640 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 0.253 Å^{-1}

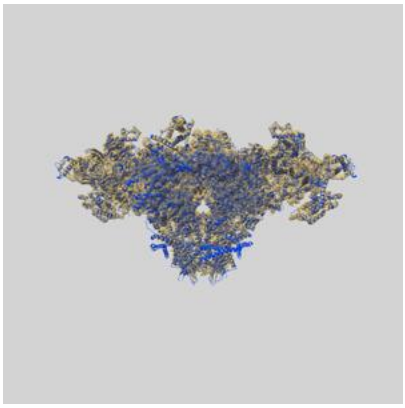
8 Fourier-Shell correlation

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

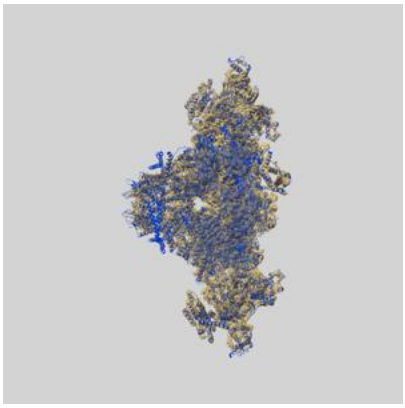
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42461 and PDB model 8UQ5. Per-residue inclusion information can be found in section 3 on page 5.

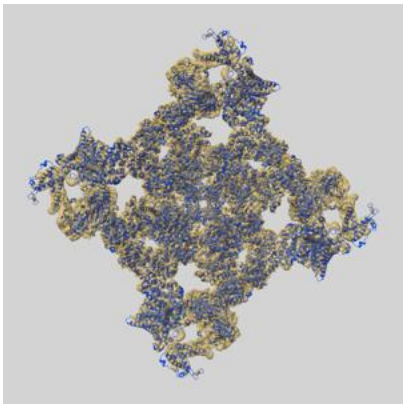
9.1 Map-model overlay



X



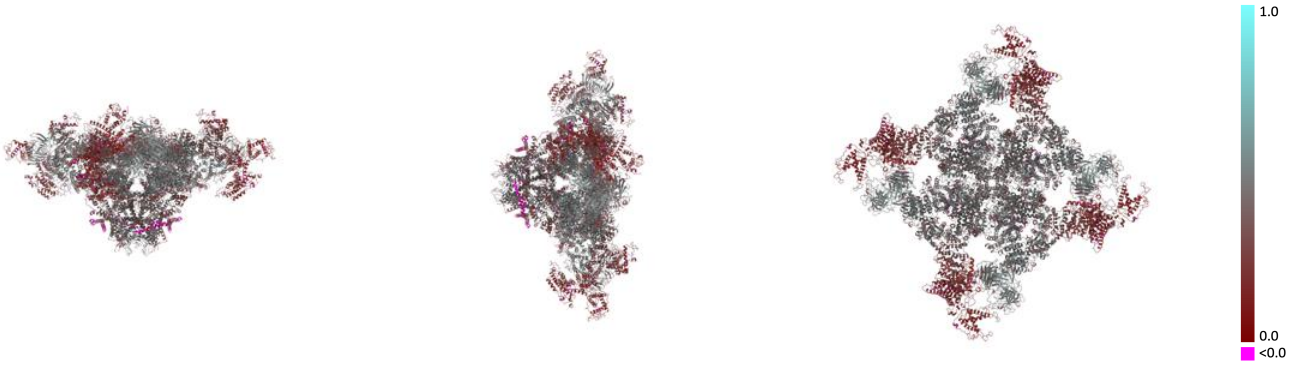
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

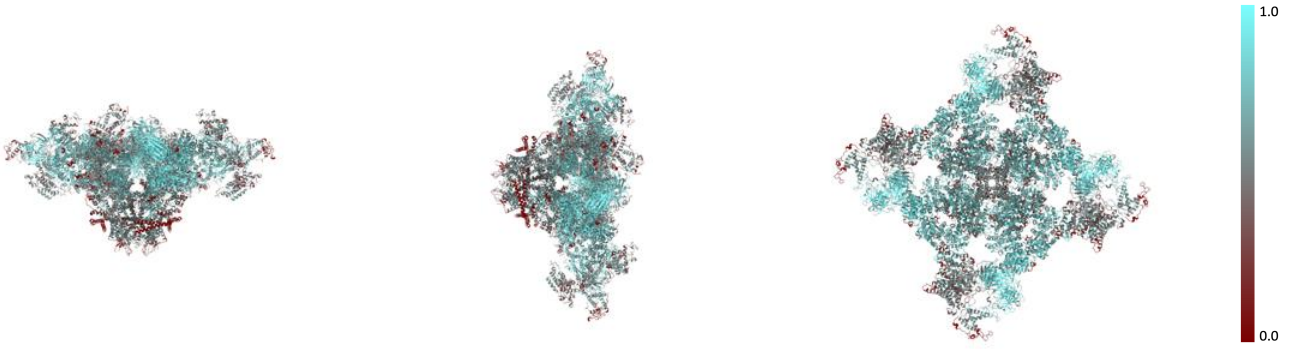
9.2 Q-score mapped to coordinate model



X Y Z

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

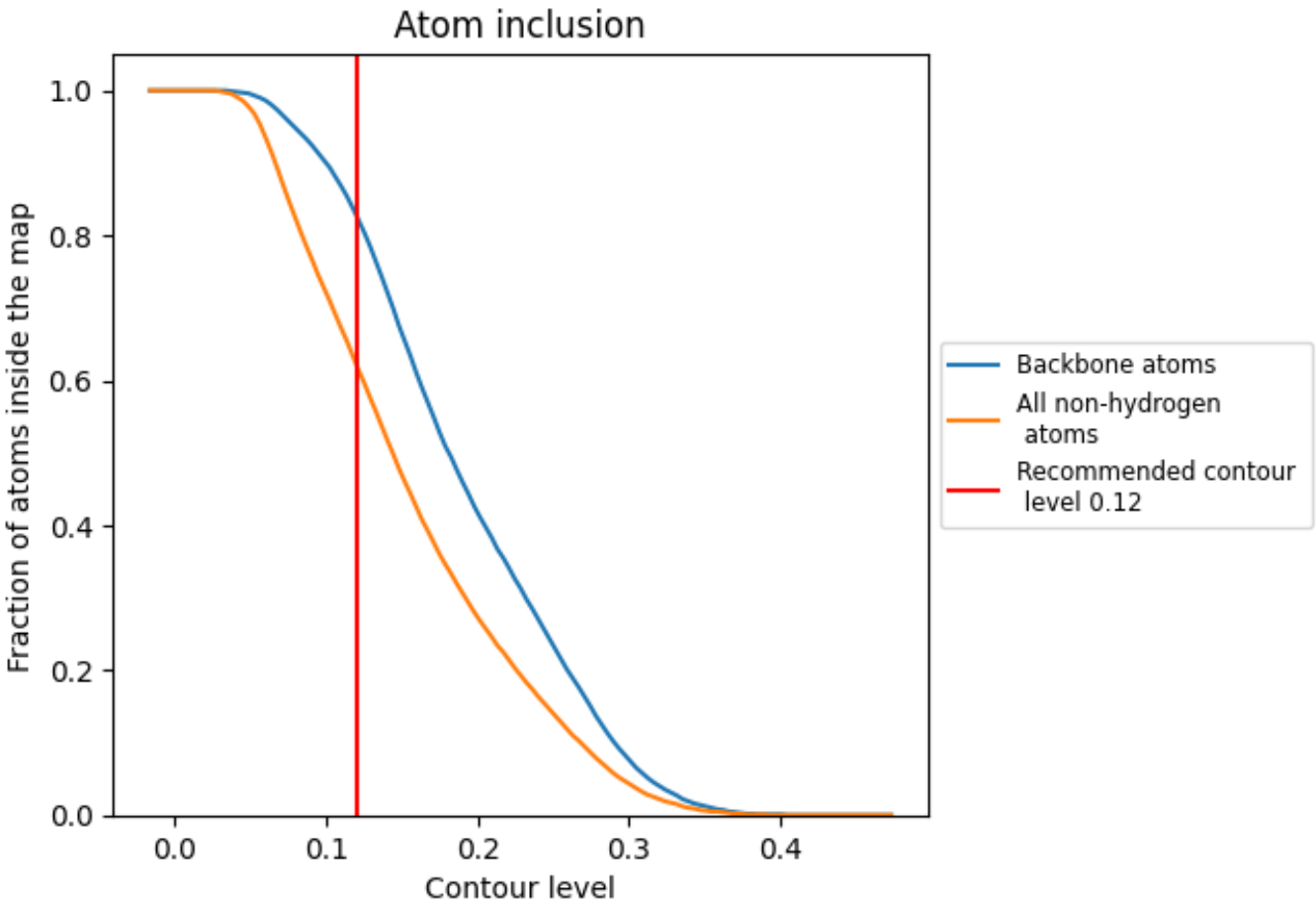
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 62% 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	0.6210	0.3710
A	0.6200	0.3710
B	0.6220	0.3710
C	0.6220	0.3710
D	0.6210	0.3720