wwPDB EM Validation Summary Report (i)

Oct 7, 2024 – 04:58 AM EDT

PDB ID	:	8UXL
EMDB ID	:	EMD-42768
Title	:	Structure of PKA phosphorylated human RyR2-R420W in the primed state in the presence of calcium and calmodulin
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	3.12 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:

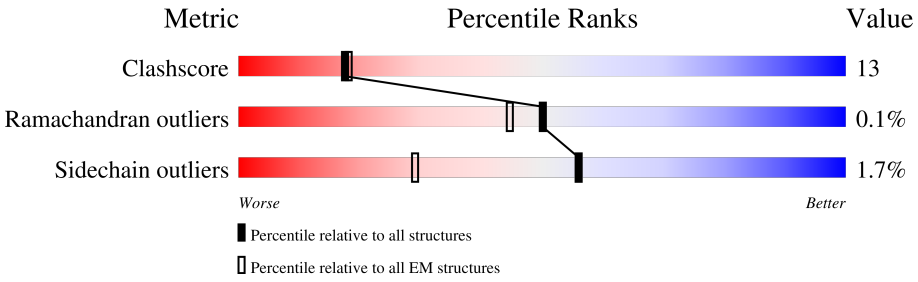
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.12 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4967	7% 63% 21% • 15%
1	B	4967	7% 63% 21% • 15%
1	C	4967	7% 64% 21% • 15%
1	D	4967	7% 63% 21% • 15%
2	E	108	76% 21% • •
2	F	108	78% 19% • •
2	G	108	78% 19% • •
2	H	108	75% 22% • •

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Mol	Chain	Length	Quality of chain
3	I	149	59% 32% 5%
3	J	149	56% 34% 6%
3	K	149	57% 34% 5%
3	L	149	56% 34% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 143500 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	4232	Total 33858	C 21578	N 5766	O 6284	S 230	2	0
1	B	4232	Total 33858	C 21578	N 5766	O 6284	S 230	2	0
1	C	4232	Total 33858	C 21578	N 5766	O 6284	S 230	2	0
1	D	4232	Total 33858	C 21578	N 5766	O 6284	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

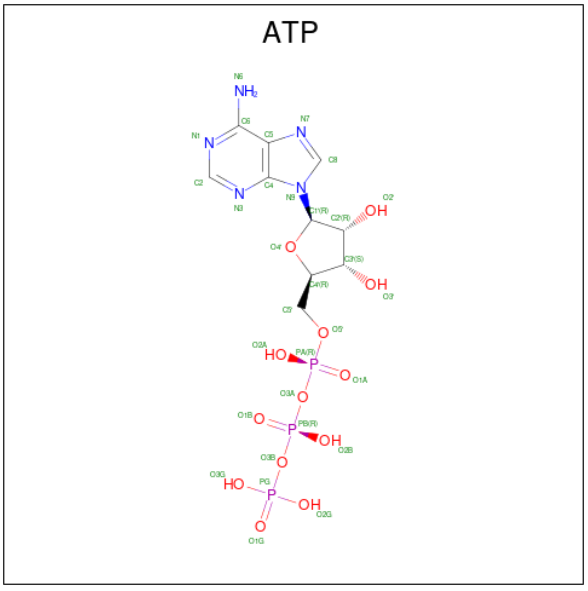
- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
3	J	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
3	L	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
3	K	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 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
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

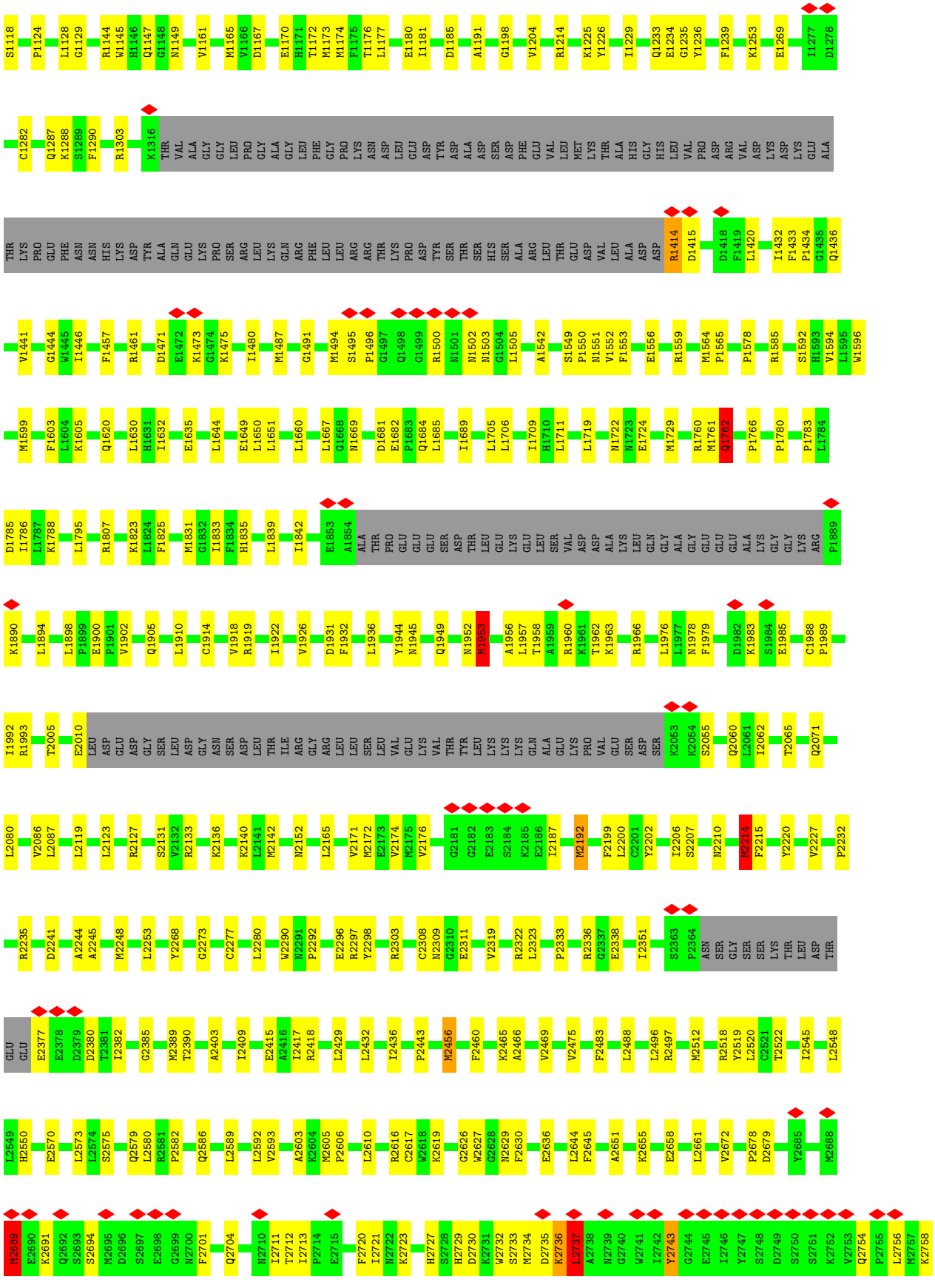
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	I	4	Total	Ca	0
			4	4	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	J	4	Total	Ca	0
			4	4	
6	L	4	Total	Ca	0
			4	4	
6	K	4	Total	Ca	0
			4	4	

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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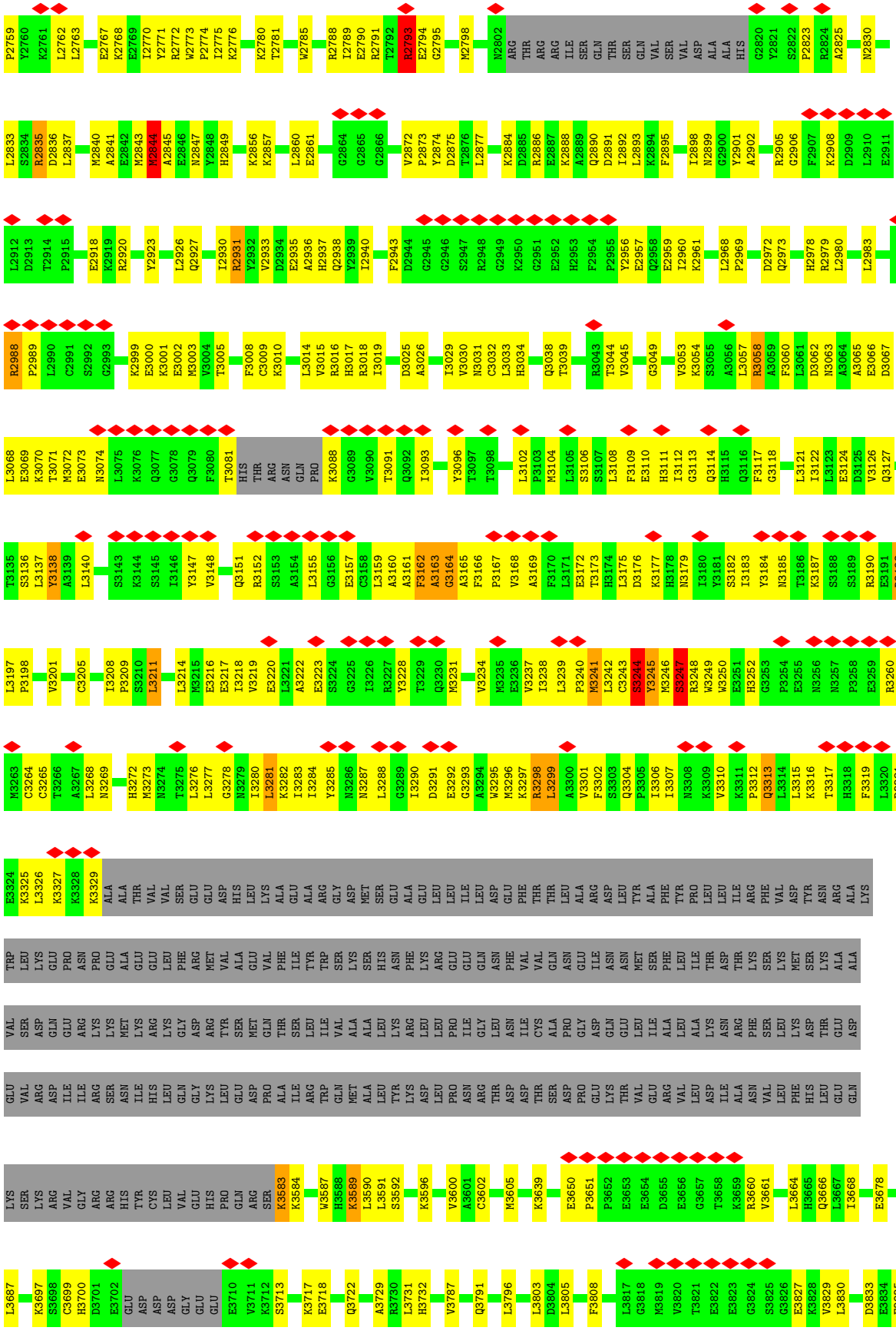
C1282 Q1287 K1288 S1289 F1290 R1303 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA
THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO 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 R1414 D1415 D1418 F1419 L1420 I1432 F1433 P1434 G1435 Q1436
V1441 G1444 W1445 I1446 F1457 R1461 D1471 E1472 K1473 G1474 K1475 I1480 M1487 G1491 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1542 S1549 P1550 N1551 V1552 F1553 E1556 R1559 M1564 P1565 P1578 R1585 S1592 H1593 V1594 L1595 W1596
M1599 F1603 L1604 K1605 Q1620 L1630 H1631 I1632 E1635 L1644 E1649 L1650 L1651 L1660 L1667 G1668 N1669 D1681 E1682 P1683 Q1684 L1685 I1689 L1705 L1706 I1709 H1710 L1711 L1719 N1722 N1723 E1724 M1729 R1760 M1761 Q1762 P1766 P1780 P1783 L1784
D1785 I1786 L1787 K1788 L1795 R1807 K1823 L1824 F1825 M1831 G1832 I1833 F1834 H1835 L1839 I1842 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 L1898 P1899 E1900 P1901 V1902 Q1905 L1910 C1914 V1918 R1919 I1922 V1926 D1931 F1932 L1936 Y1944 N1945 Q1949 N1952 M1953 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 R1966 L1976 L1977 N1978 F1979 D1982 K1983 S1984 E1985 C1988 P1989
I1992 R1993 T2005 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 GLY LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 Q2060 L2061 I2062 T2065 Q2071
L2080 V2086 L2087 L2119 L2123 R2127 S2131 V2132 R2133 K2136 K2140 L2141 M2142 N2152 L2165 V2171 M2172 E2173 V2174 M2175 V2176 G2181 G2182 E2183 S2184 K2185 E2186 I2187 M2192 F2199 L2200 C2201 Y2202 I2206 S2207 N2210 M2214 F2215 Y2220 V2227 P2232
R2235 D2241 A2244 A2245 M2248 L2253 Y2268 G2273 C2277 L2280 W2290 N2291 P2292 E2296 R2297 Y2298 R2303 C2308 N2309 G2310 E2311 V2319 R2322 L2323 P2333 R2336 G2337 E2338 I2351 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR
GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 G2385 M2389 T2390 A2403 I2409 E2415 A2416 I2417 R2418 L2429 L2432 I2436 P2443 M2456 F2460 K2465 A2466 V2469 V2475 F2483 L2488 L2496 R2497 M2512 R2518 Y2519 L2520 C2521 T2522 I2545 L2548
L2549 H2550 E2570 L2573 L2574 S2575 Q2579 L2580 R2581 P2582 Q2586 L2589 L2592 V2593 A2603 K2604 M2605 P2606 L2610 R2616 C2617 W2618 K2619 G2626 W2627 C2628 N2629 F2630 E2636 L2644 F2645 A2651 K2655 E2658 L2661 V2672 P2678 D2679 Y2685 M2688
M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 Q2704 N2710 I2711 T2712 I2713 P2714 E2715 F2720 I2721 N2722 K2723 H2727 S2728 H2729 D2730 K2731 W2732 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758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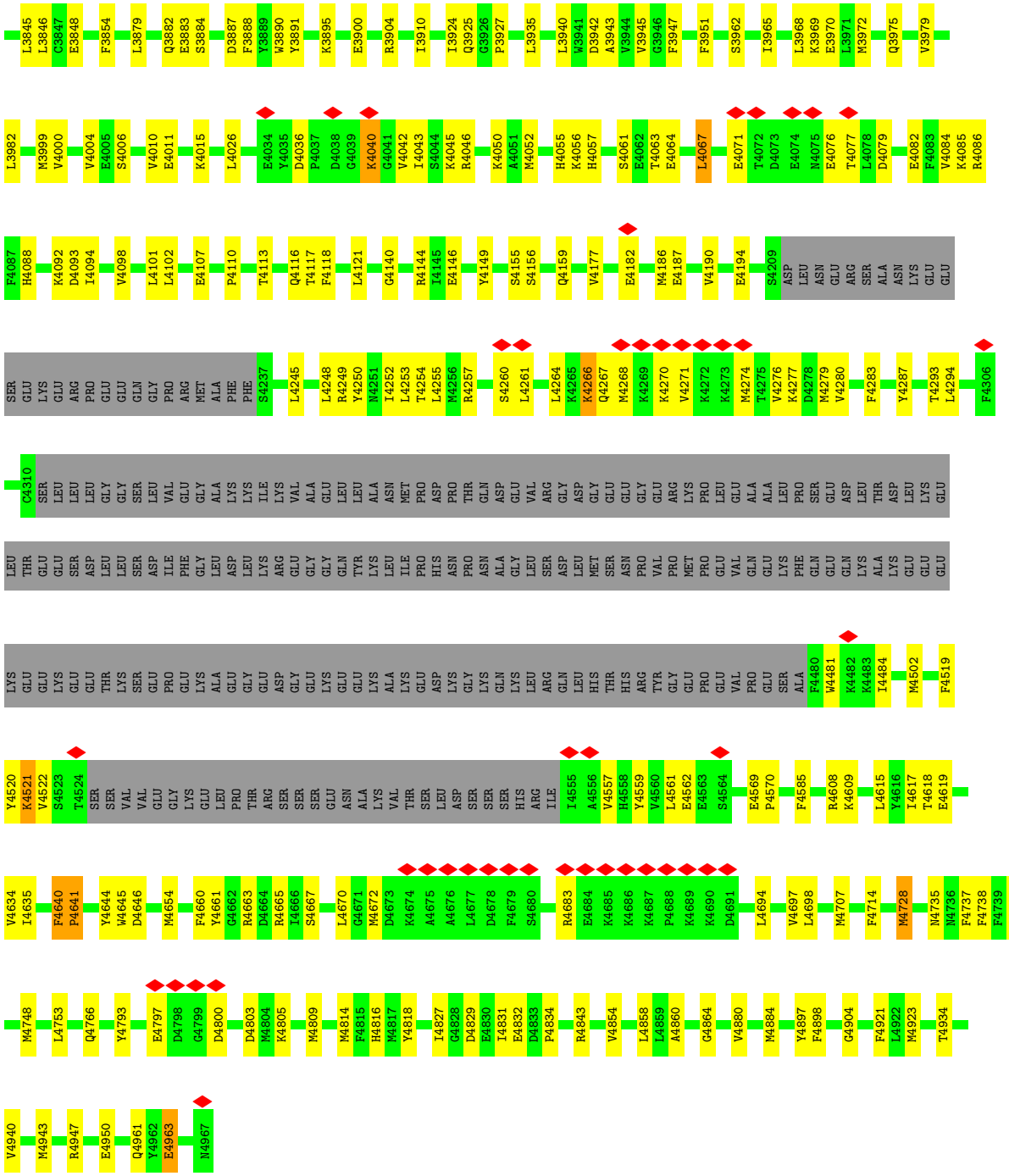
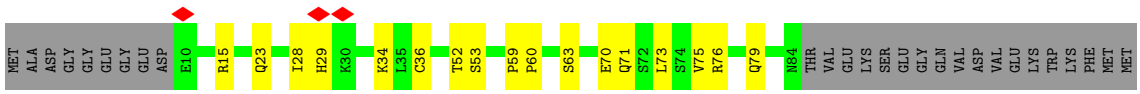
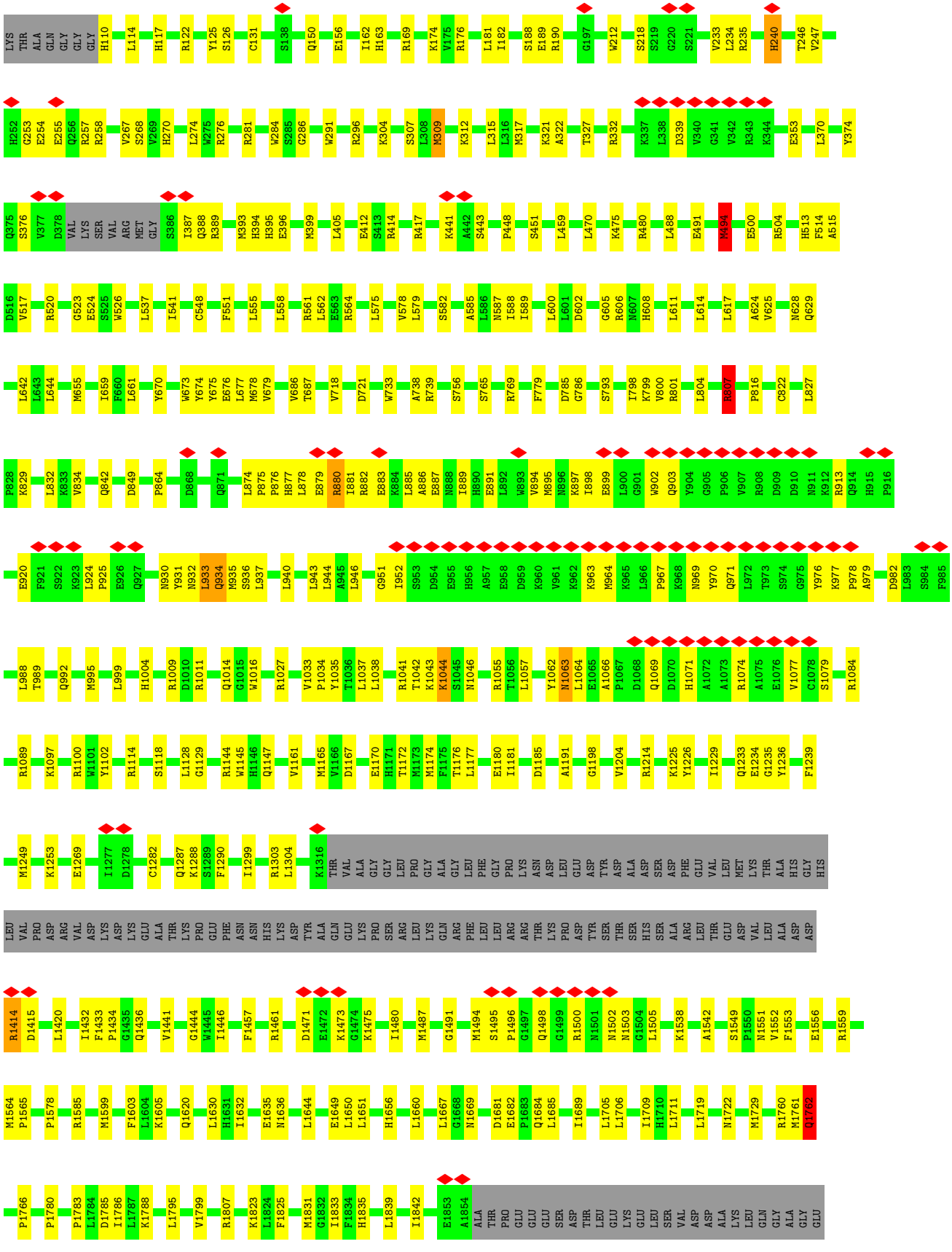
L2833 S2834 R2835 D2836 L2837 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 H2849 K2856 K2857 L2860 E2861 G2864 G2865 G2866 V2872 P2873 Y2874 D2875 T2876 L2877 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 F2895 I2898 N2899 G2900 Y2901 A2902 R2905 G2906 F2907 K2908 D2909 L2910 E2911
L2912 D2913 T2914 P2915 E2918 K2919 R2920 Y2923 L2926 Q2927 I2930 R2931 Y2932 V2933 D2934 E2935 A2936 H2937 Q2938 Y2939 I2940 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 Y2956 E2957 Q2958 E2959 I2960 K2961 L2968 P2969 D2972 Q2973 H2978 R2979 L2980 L2983 A2986 S2987
R2988 P2989 L2990 C2991 S2992 G2993 K2999 E3000 K3001 E3002 N3003 V3004 T3005 F3008 C3009 K3010 L3014 V3015 R3016 H3017 R3018 I3019 D3025 A3026 I3029 V3030 N3031 C3032 L3033 H3034 Q3038 T3039 R3043 T3044 V3045 G3049 V3053 K3054 S3055 A3056 L3057 R3058 A3059 F3060 L3061 D3062 N3063 A3064 A3065 E3066 D3067
L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 Y3096 T3097 T3098 L3102 P3103 M3104 L3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 G3118 L3121 I3122 L3123 E3124 D3125 V3126 Q3127 R3132 I3133 L3134
T3135 S3136 L3137 Y3138 A3139 L3140 S3143 K3144 S3145 I3146 Y3147 V3148 Q3151 R3152 S3153 A3154 L3155 G3156 E3157 C3158 L3159 A3160 A3161 F3162 A3163 G3164 A3165 F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 L3175 D3176 K3177 H3178 N3179 I3180 Y3181 S3182 I3183 Y3184 N3185 T3186 K3187 S3188 S3189 R3190 E3191 R3192 A3193 A3194 L3195 S3196
L3197 P3198 V3201 C3205 I3208 P3209 S3210 L3211 L3214 M3215 E3216 E3217 I3218 V3219 E3220 E3221 A3222 E3223 S3224 G3225 I3226 R3227 Y3228 T3229 Q3230 M3231 V3234 M3235 E3236 V3237 I3238 L3239 P3240 M3241 L3242 C3243 S3244 Y3245 M3246 S3247 R3248 W3249 W3250 E3251 H3252 G3253 P3254 E3255 N3256 N3257 P3258 E3259 R3260 A3261 E3262
M3263 C3264 C3265 T3266 A3267 L3268 N3269 H3272 M3273 N3274 T3275 L3276 L3277 G3278 N3279 I3280 L3281 K3282 I3283 I3284 Y3285 N3286 N3287 L3288 G3289 I3290 D3291 E3292 G3293 A3294 W3295 M3296 K3297 R3298 L3299 A3300 V3301 F3302 S3303 Q3304 P3305 I3306 I3307 N3308 K3309 V3310 K3311 P3312 Q3313 L3314 L3315 K3316 T3317 H3318 F3319 L3320 P3321 L3322 M3323
E3324 K3325 L3326 K3327 K3328 K3329 ALA ALA THR VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE THR ASP THR LYS SER LEU LYS MET SER LYS GLU ALA 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 GLU 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 ILE ASN 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 ALA LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN
LYS SER LYS ARG VAL GLY HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER K3583 K3584 W3587 H3588 K3589 L3590 L3591 S3592 K3596 V3600 A3601 C3602 M3605 K3639 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 V3661 L3664 H3665 Q3666 L3667 I3668 E3678
L3687 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP GLY GLU GLU E3710 V3711 K3712 S3713 K3717 E3718 Q3722 A3729 R3730 L3731 H3732 V3787 Q3791 L3796 L3803 D3804 L3805 F3808 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 K3828 V3829 L3830 D3833 E3834 F3835



• Molecule 1: Ryanodine receptor 2

Chain B:

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H252 G253 E254 E255 Q256 R257 R258 V267 S268 V269 H270 L274 W275 R276 R281 W284 S285 Q286 W291 R296 K304 S307 L308 M309 K312 L315 L316 M317 K321 A322 T327 R332 K337 L338 D339 Y340 G341 V342 R343 K344 E353 L370 Y374
Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 M393 H394 H395 E396 M399 L405 E412 S413 R414 R417 K441 A442 S443 P448 S451 L459 L470 K475 R480 L488 E491 M494 E500 R504 H513 F514 A515
D516 V517 R520 G523 E524 S525 W526 L537 I541 C548 F551 L555 L558 R561 L562 E563 R564 L575 V578 L579 S582 A585 L586 N587 I588 I589 L600 L601 D602 G605 R606 N607 H608 L611 L614 L617 A624 V625 N628 Q629
L642 L643 L644 M655 I659 F660 L661 Y670 W673 Y674 Y675 E676 L677 M678 V679 V686 T687 V718 D721 W733 A738 R739 S756 S765 R769 F779 D785 G786 S793 I798 K799 V800 R801 L804 R807 P816 C822 L827
P828 K829 L832 K833 V834 Q842 D849 P864 D868 Q871 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916
E920 F921 S922 K923 L924 P925 E926 Q927 N930 Y931 N932 L933 Q934 M935 S936 L937 L940 L943 L944 A945 L946 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 D982 L983 S984 F985
L988 T989 Q992 M995 L999 H1004 R1009 D1010 R1011 Q1014 G1015 W1016 R1027 V1033 P1034 Y1035 T1036 L1037 L1038 R1041 T1042 K1043 K1044 S1045 N1046 R1055 T1056 L1057 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 R1084
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M1249 K1253 E1269 I1277 D1278 C1282 Q1287 K1288 S1289 F1290 I1299 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 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 L1420 I1432 F1433 P1434 G1435 Q1436 V1441 G1444 W1445 I1446 F1457 R1461 D1471 E1472 K1473 G1474 K1475 I1480 M1487 G1491 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 K1538 A1542 S1549 P1550 N1551 V1552 F1553 E1556 R1559
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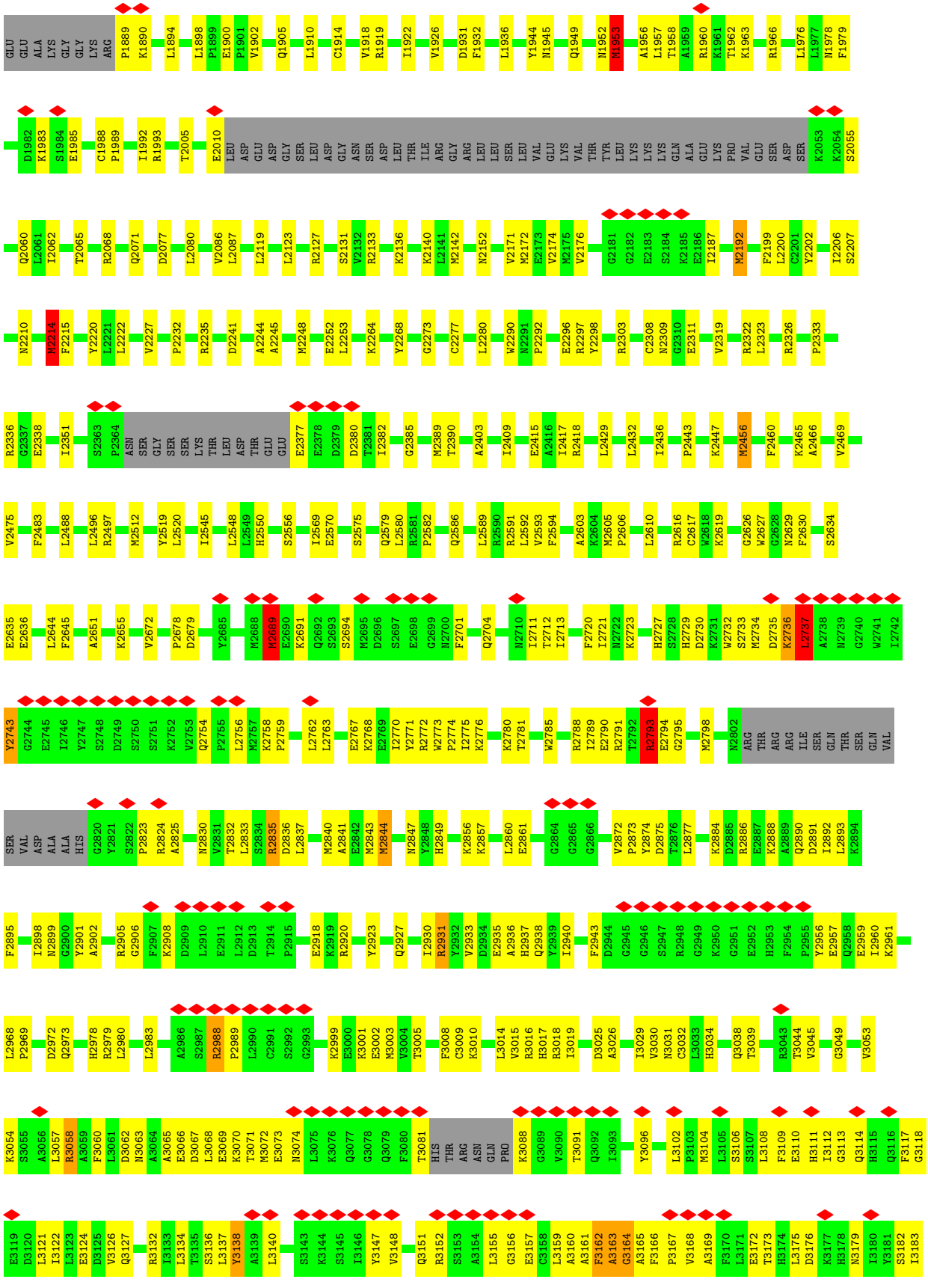
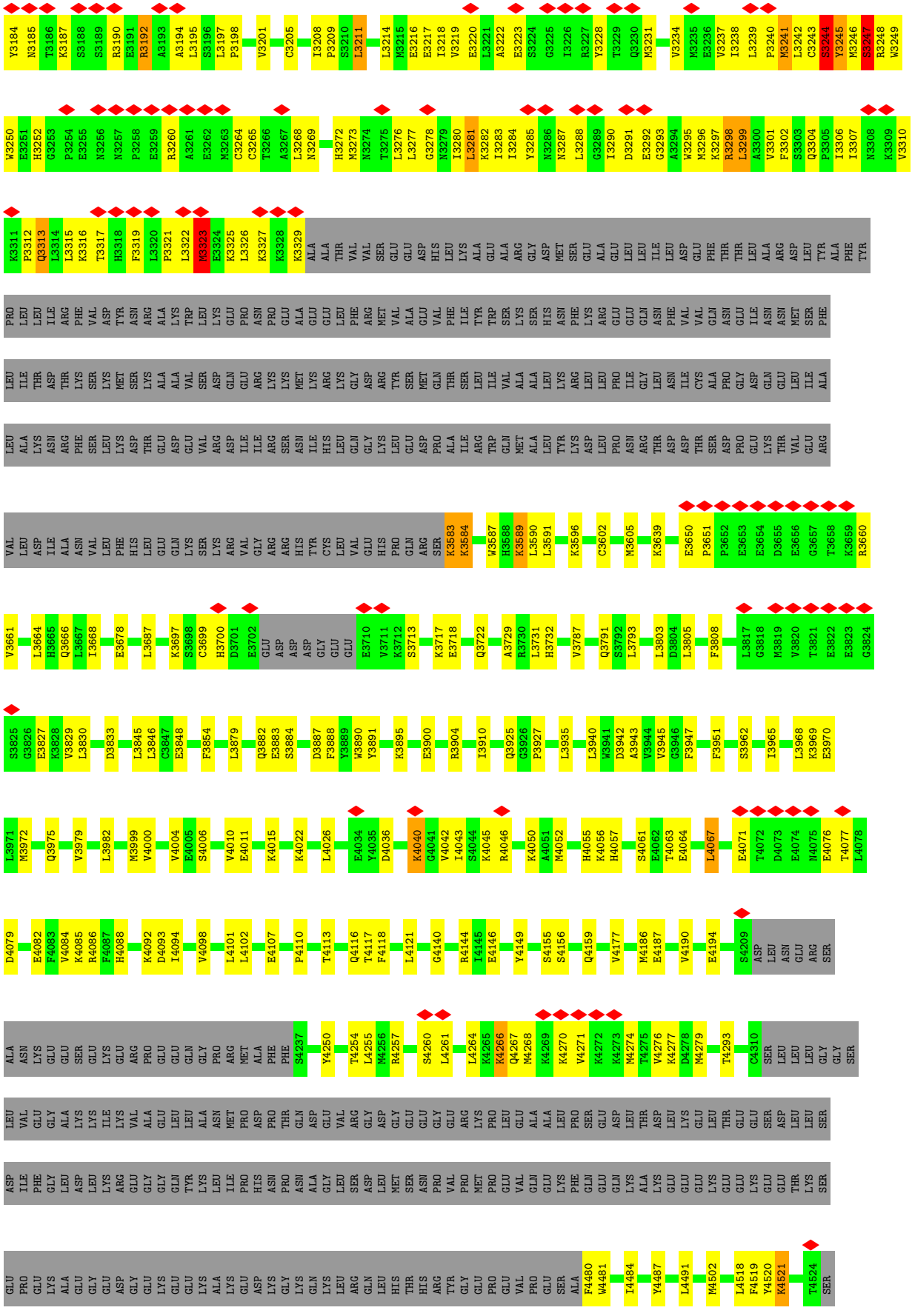
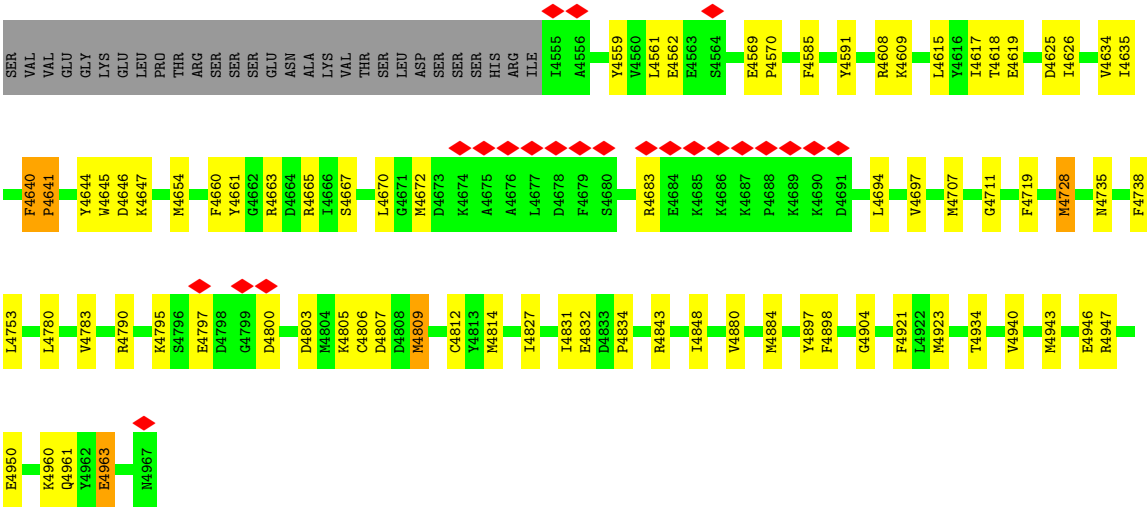
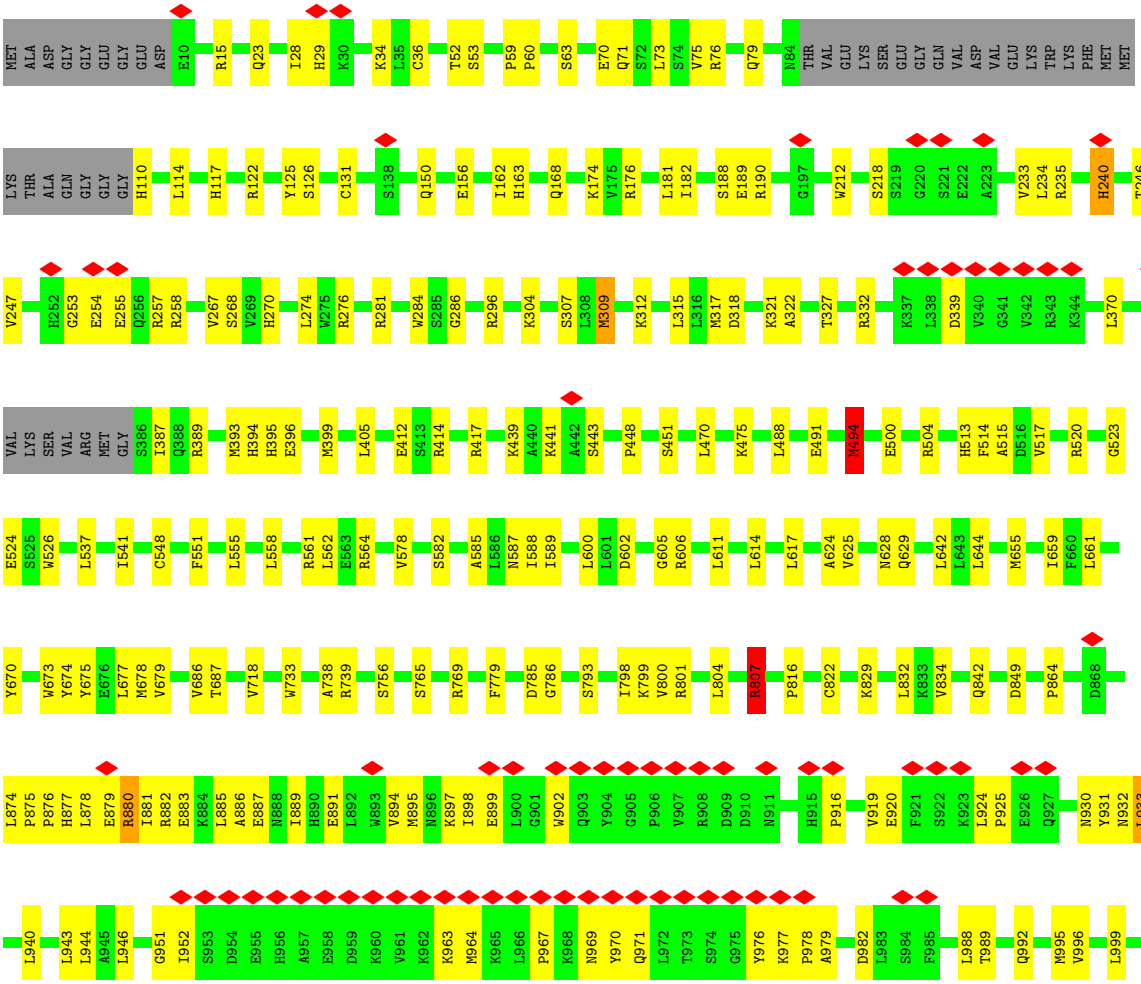


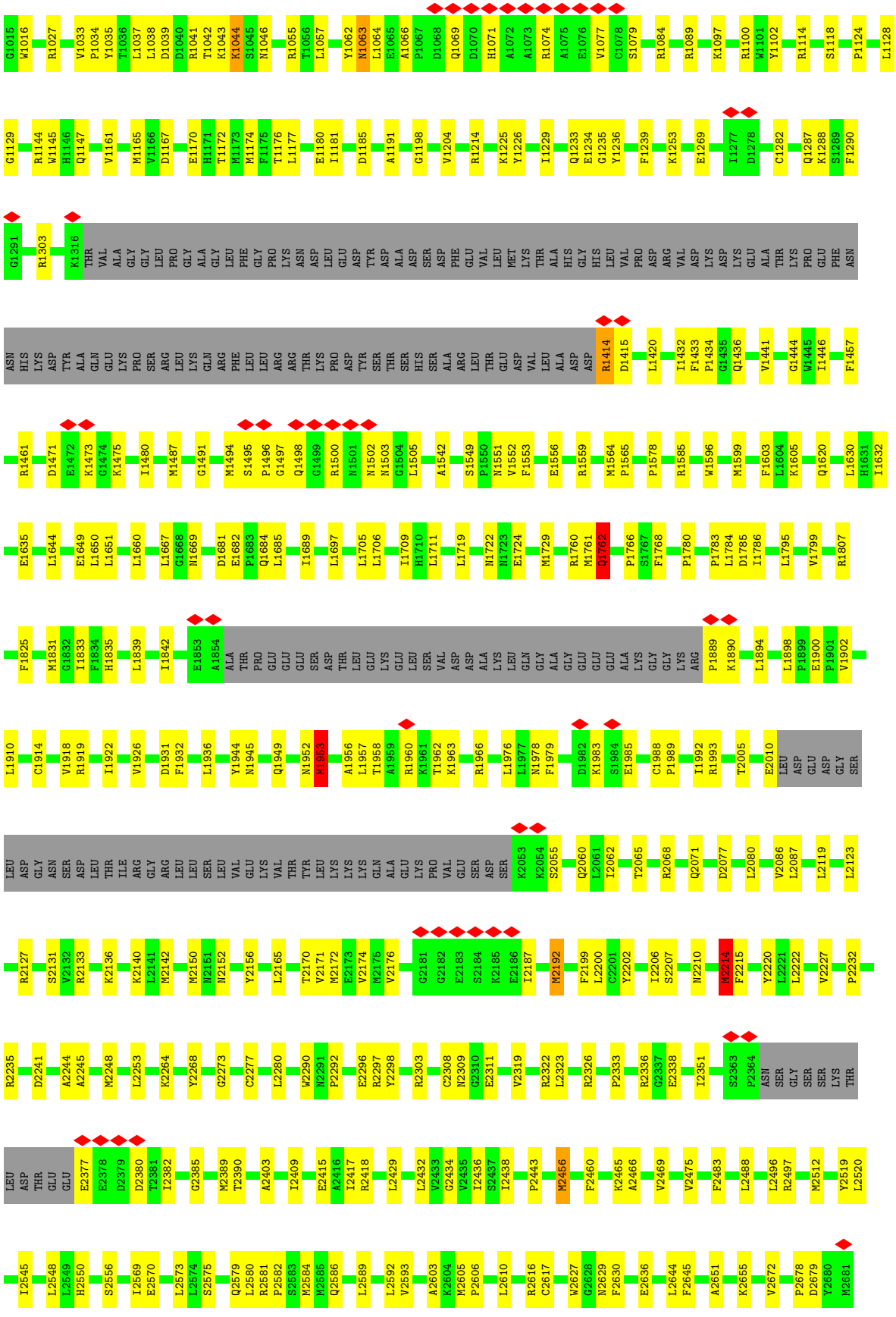




• Molecule 1: Ryanodine receptor 2

Chain C:

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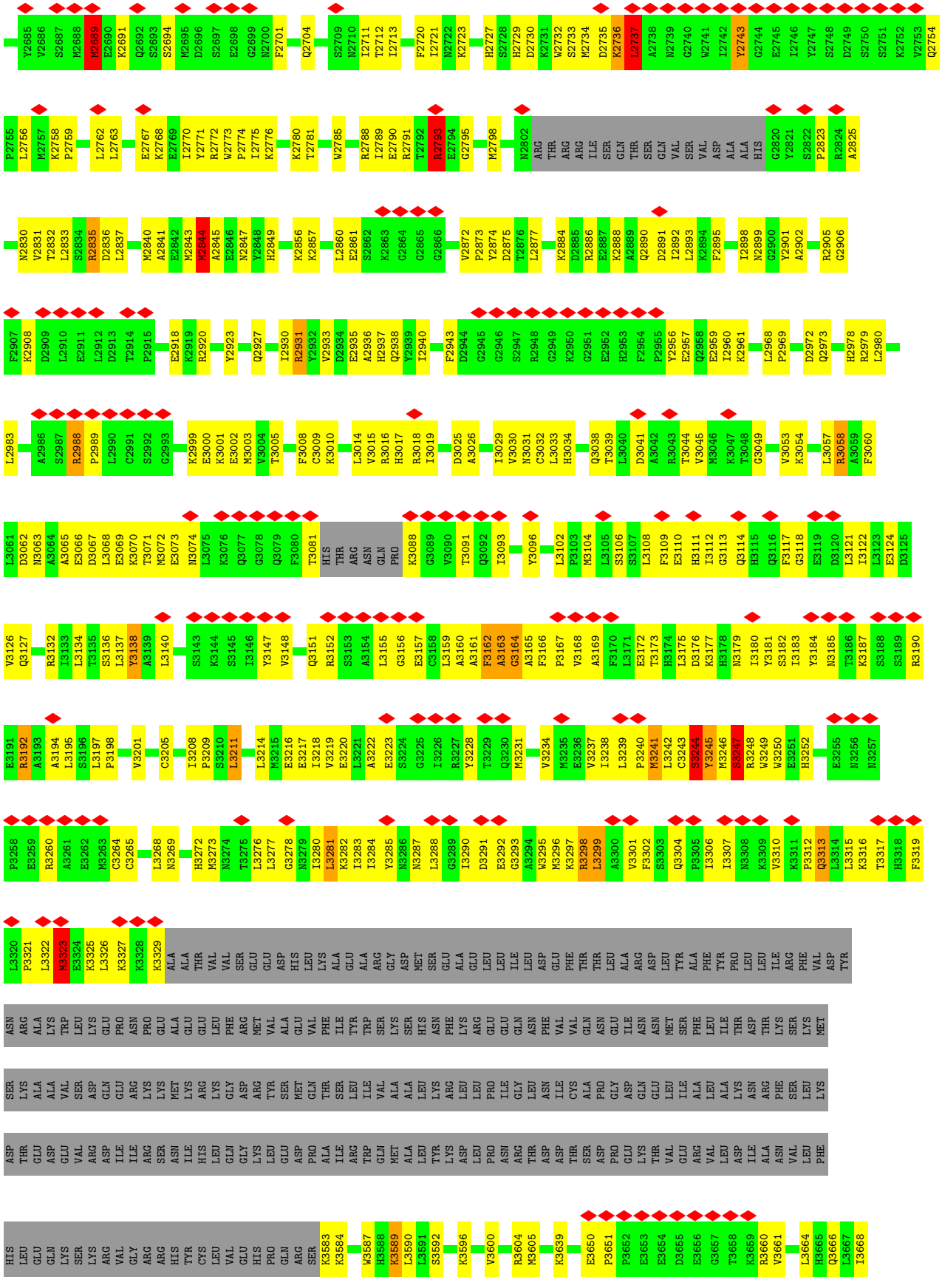
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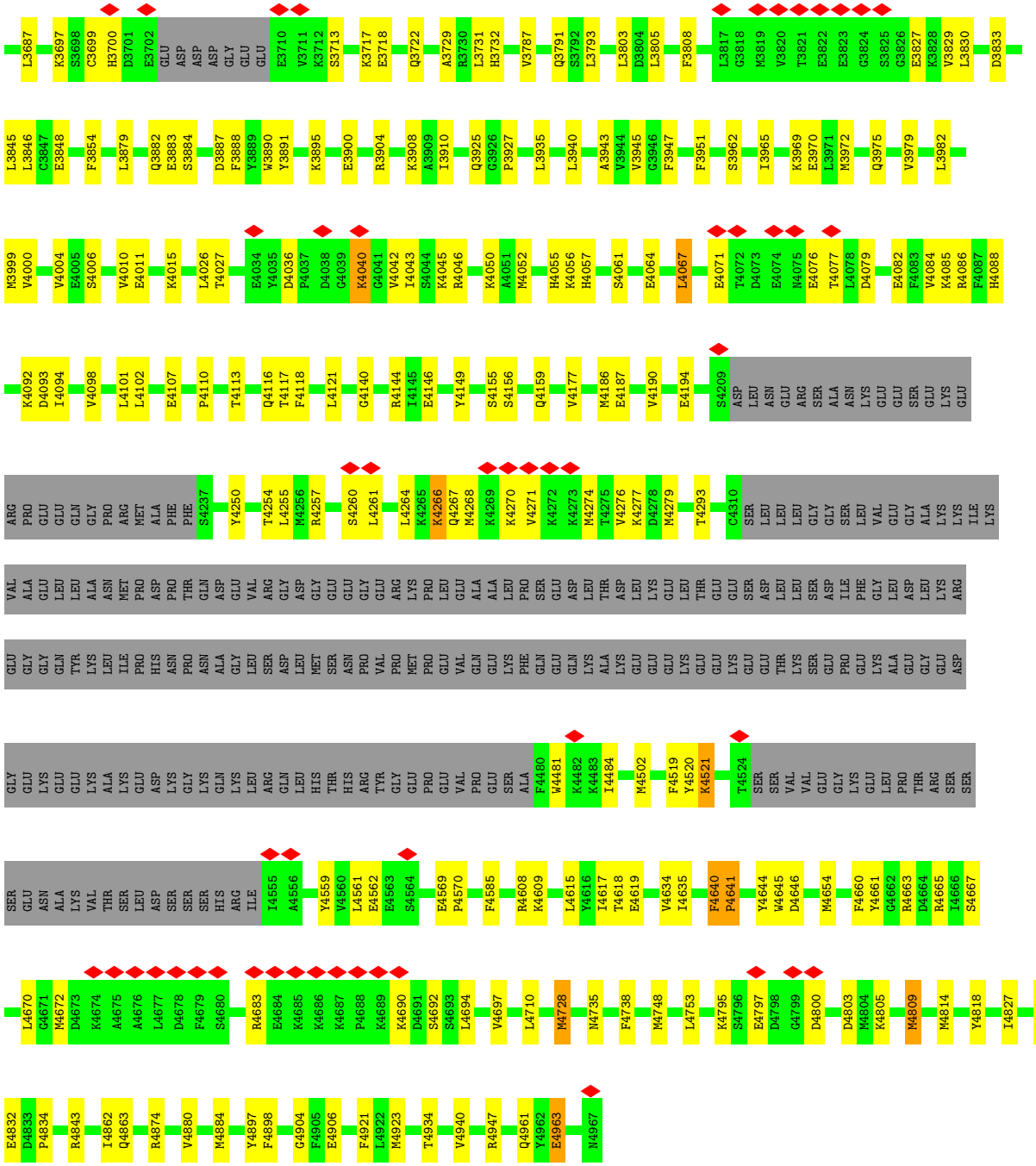
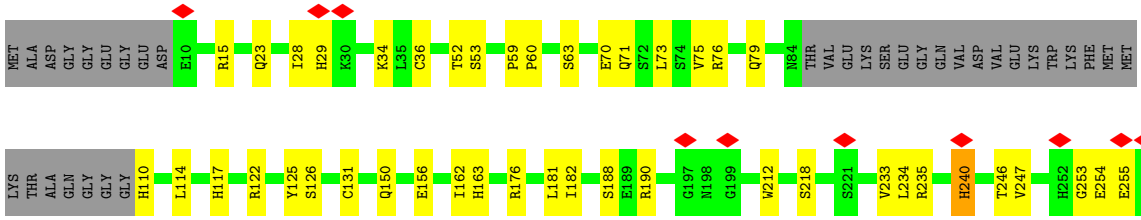
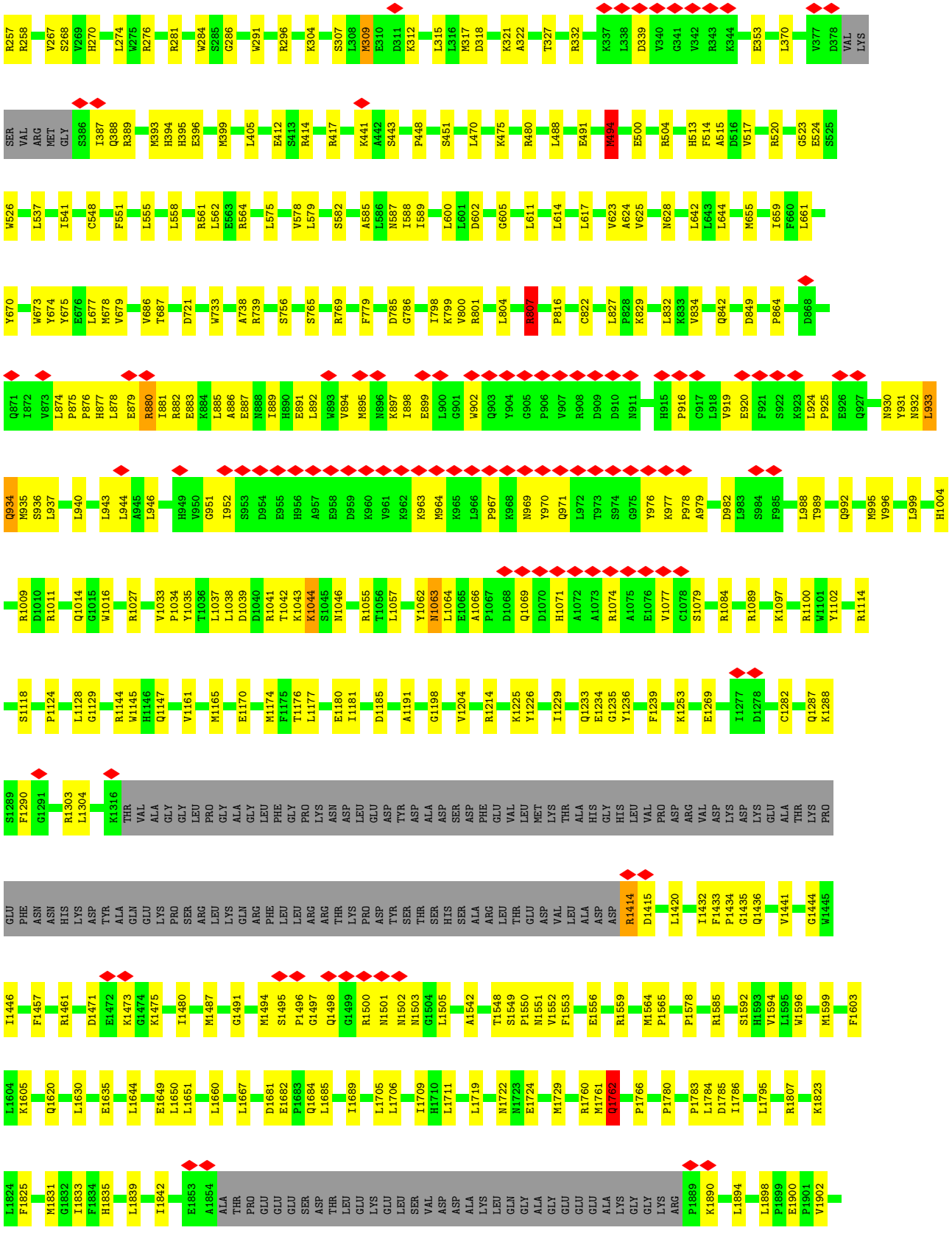
ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET LEU TYR SER PHE LEU ILE THR ASP THR LYS SER LYS MET
SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET ARG 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 PRO GLU LYS THR VAL GLU ARG LEU LEU ASP ILE ALA ASN ARG PHE SER LEU 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 PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ARG ASN VAL LEU LEU PHE
HIS LEU GLU GLN LYS SER ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER K3583 K3584 W3587 H3588 K3589 L3590 L3591 S3592 K3596 V3600 R3604 M3605 K3639 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 V3661 L3664 H3665 Q3666 L3667 I3668



• Molecule 1: Ryanodine receptor 2

Chain D:

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S1289 F1290 G1291 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 R1414 D1415 L1420 I1432 F1433 P1434 G1435 Q1436 V1441 G1444 W1445
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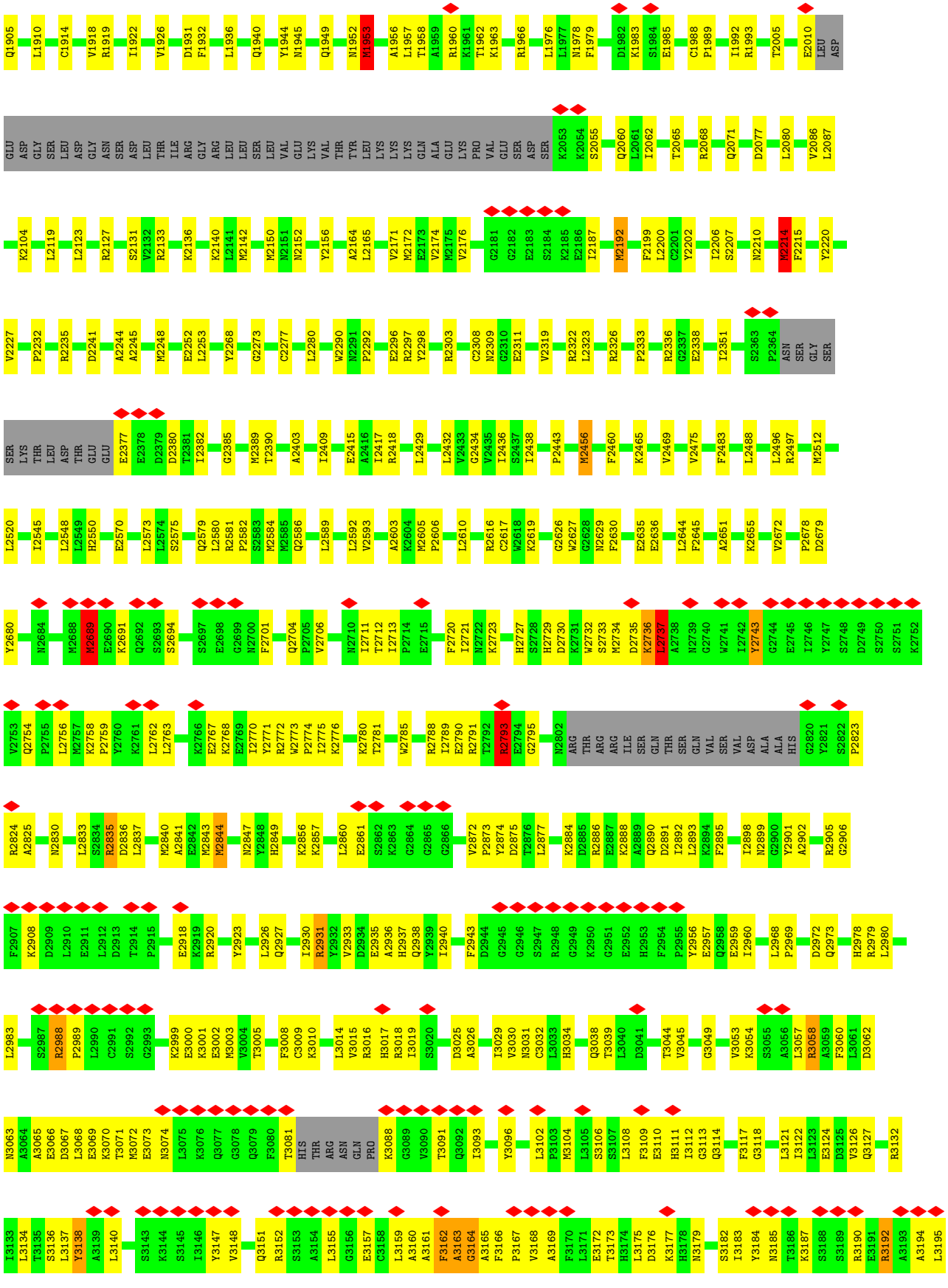
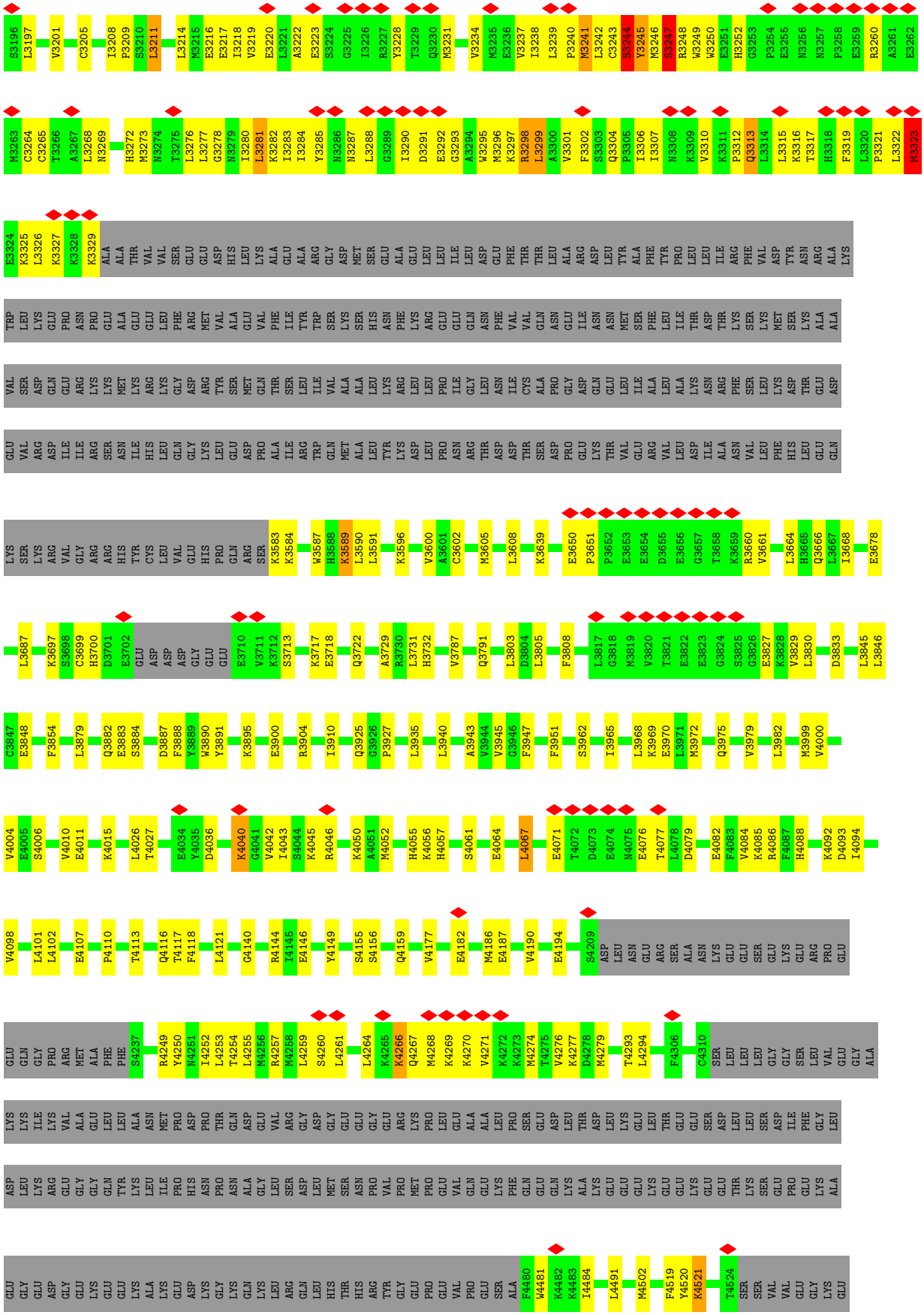
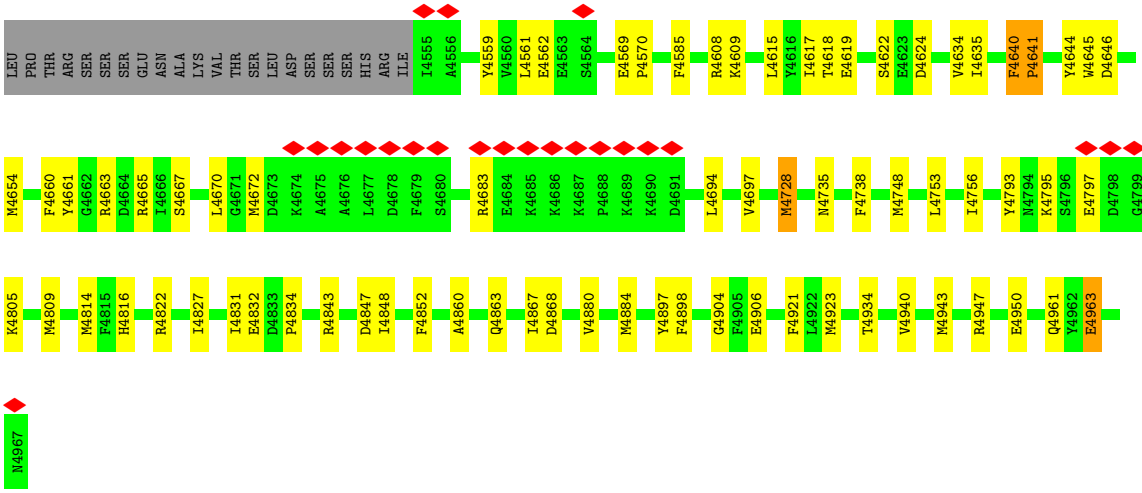
L1824 F1825 M1831 G1832 I1833 F1834 H1835 L1839 I1842 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1894 L1898 P1899 E1900 P1901 V1902

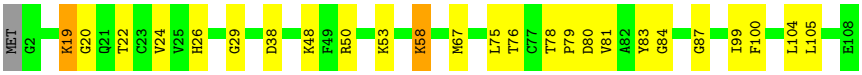






• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



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

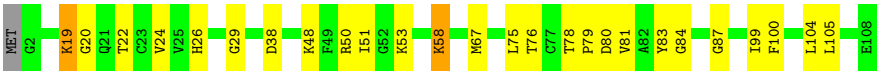
Chain F:

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

Chain G:

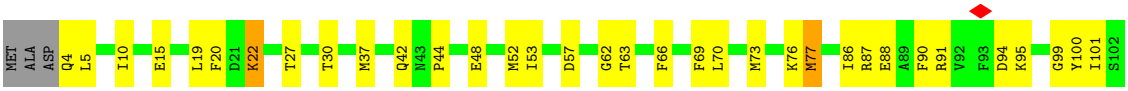
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



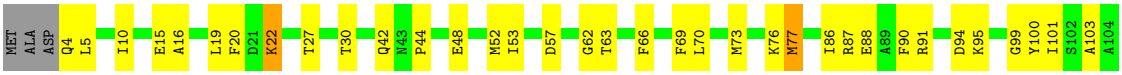
• Molecule 3: Calmodulin-1

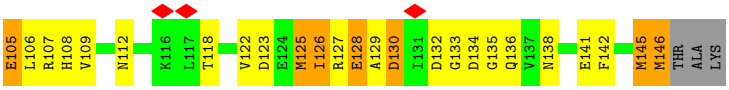
Chain I:



• Molecule 3: Calmodulin-1

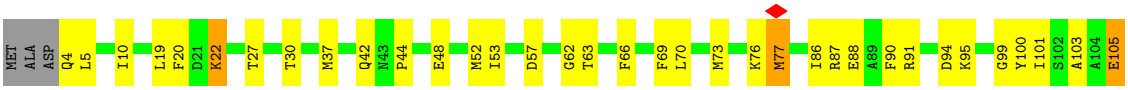
Chain J:

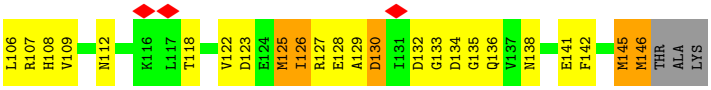




• Molecule 3: Calmodulin-1

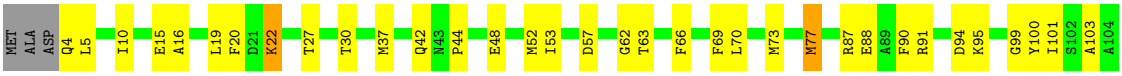
Chain L:

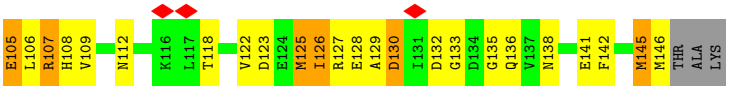




• Molecule 3: Calmodulin-1

Chain K:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77625	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	0.637	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.14	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: ATP, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	5/34603 (0.0%)	0.55	29/46734 (0.1%)
1	B	0.29	5/34603 (0.0%)	0.55	29/46734 (0.1%)
1	C	0.29	5/34603 (0.0%)	0.55	29/46734 (0.1%)
1	D	0.29	5/34603 (0.0%)	0.55	29/46734 (0.1%)
2	E	0.29	0/834	0.55	0/1123
2	F	0.29	0/834	0.55	0/1123
2	G	0.29	0/834	0.55	0/1123
2	H	0.29	0/834	0.56	0/1123
3	I	0.33	0/1143	0.62	2/1534 (0.1%)
3	J	0.34	0/1143	0.62	2/1534 (0.1%)
3	K	0.33	0/1143	0.62	2/1534 (0.1%)
3	L	0.33	0/1143	0.62	2/1534 (0.1%)
All	All	0.29	20/146320 (0.0%)	0.55	124/197564 (0.1%)

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	8
1	B	0	8
1	C	0	8
1	D	0	8
All	All	0	32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3164	GLY	N-CA	9.24	1.59	1.46
1	B	3164	GLY	N-CA	9.23	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3164	GLY	N-CA	9.23	1.59	1.46
1	C	3164	GLY	N-CA	9.22	1.59	1.46
1	B	3164	GLY	CA-C	9.05	1.66	1.51

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2737	LEU	CA-CB-CG	11.85	142.56	115.30
1	C	2737	LEU	CA-CB-CG	11.84	142.54	115.30
1	A	2737	LEU	CA-CB-CG	11.84	142.53	115.30
1	B	2737	LEU	CA-CB-CG	11.83	142.51	115.30
1	A	2844	MET	CA-CB-CG	10.67	131.44	113.30

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3058	ARG	Sidechain
1	A	3162	PHE	Peptide
1	A	3163	ALA	Peptide
1	A	3244	SER	Peptide,Mainchain
1	A	3247	SER	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	33858	0	33562	919	0
1	B	33858	0	33562	925	0
1	C	33858	0	33562	916	0
1	D	33858	0	33562	912	0
2	E	818	0	821	16	0
2	F	818	0	821	16	0
2	G	818	0	821	17	0
2	H	818	0	821	18	0
3	I	1131	0	1059	42	0
3	J	1131	0	1059	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1131	0	1059	50	0
3	L	1131	0	1059	46	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	62	0	24	0	0
5	B	62	0	24	0	0
5	C	62	0	24	0	0
5	D	62	0	24	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	4	0	0	2	0
6	J	4	0	0	2	0
6	K	4	0	0	2	0
6	L	4	0	0	2	0
All	All	143500	0	141864	3788	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 13.

The worst 5 of 3788 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:C:3165:ALA:N	1:C:3244:SER:O	1.63	1.32
1:B:3165:ALA:N	1:B:3244:SER:O	1.63	1.31
1:D:3165:ALA:N	1:D:3244:SER:O	1.63	1.29
1:A:3165:ALA:N	1:A:3244:SER:O	1.63	1.26
1:A:3165:ALA:H	1:A:3244:SER:C	1.39	1.25

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	4206/4967 (85%)	4072 (97%)	130 (3%)	4 (0%)	48	78
1	B	4206/4967 (85%)	4072 (97%)	130 (3%)	4 (0%)	48	78
1	C	4206/4967 (85%)	4074 (97%)	128 (3%)	4 (0%)	48	78
1	D	4206/4967 (85%)	4073 (97%)	129 (3%)	4 (0%)	48	78
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
3	I	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	J	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	K	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
3	L	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
All	All	17808/20896 (85%)	17243 (97%)	549 (3%)	16 (0%)	50	78

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2793	ARG
1	A	2988	ARG
1	A	3927	PRO
1	A	4641	PRO
1	B	2793	ARG

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	3716/4358 (85%)	3663 (99%)	53 (1%)	62	79
1	B	3716/4358 (85%)	3663 (99%)	53 (1%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	3716/4358 (85%)	3663 (99%)	53 (1%)	62 79
1	D	3716/4358 (85%)	3663 (99%)	53 (1%)	62 79
2	E	88/89 (99%)	86 (98%)	2 (2%)	45 68
2	F	88/89 (99%)	86 (98%)	2 (2%)	45 68
2	G	88/89 (99%)	86 (98%)	2 (2%)	45 68
2	H	88/89 (99%)	86 (98%)	2 (2%)	45 68
3	I	123/127 (97%)	113 (92%)	10 (8%)	9 31
3	J	123/127 (97%)	113 (92%)	10 (8%)	9 31
3	K	123/127 (97%)	113 (92%)	10 (8%)	9 31
3	L	123/127 (97%)	113 (92%)	10 (8%)	9 31
All	All	15708/18296 (86%)	15448 (98%)	260 (2%)	56 76

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	77	MET
3	J	145	MET
1	B	2743	TYR
1	B	2712	THR
3	L	107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	79	GLN
1	D	3850	HIS
1	C	2927	GLN
1	D	3179	ASN
1	D	2847	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 24 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	$\#\|Z\| > 2$
5	ATP	B	5004	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
5	ATP	D	5004	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
5	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
5	ATP	A	5004	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
5	ATP	D	5002	-	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
5	ATP	C	5004	-	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
5	ATP	C	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
5	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	5004	-	-	7/18/38/38	0/3/3/3
5	ATP	D	5004	-	-	7/18/38/38	0/3/3/3
5	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
5	ATP	A	5004	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
5	ATP	C	5004	-	-	7/18/38/38	0/3/3/3
5	ATP	C	5002	-	-	8/18/38/38	0/3/3/3
5	ATP	A	5002	-	-	8/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	5004	ATP	C5-C6-N6	2.37	123.93	120.31
5	C	5002	ATP	C5-C6-N6	2.37	123.92	120.31
5	D	5004	ATP	C5-C6-N6	2.35	123.89	120.31
5	A	5004	ATP	C5-C6-N6	2.34	123.88	120.31
5	B	5002	ATP	C5-C6-N6	2.33	123.86	120.31

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

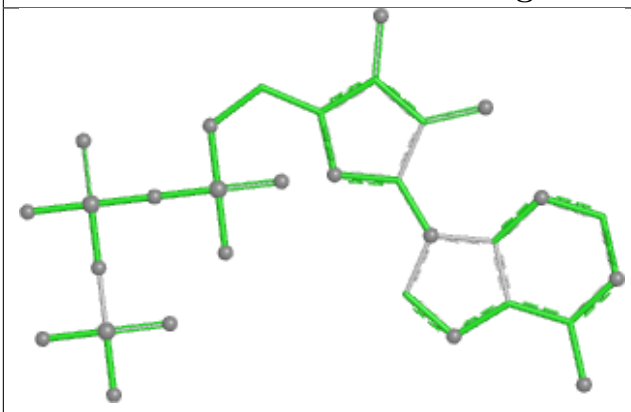
Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	PB-O3A-PA-O5'
5	A	5004	ATP	PB-O3A-PA-O5'
5	B	5002	ATP	PB-O3A-PA-O5'
5	B	5004	ATP	PB-O3A-PA-O5'
5	C	5002	ATP	PB-O3A-PA-O5'

There are no ring outliers.

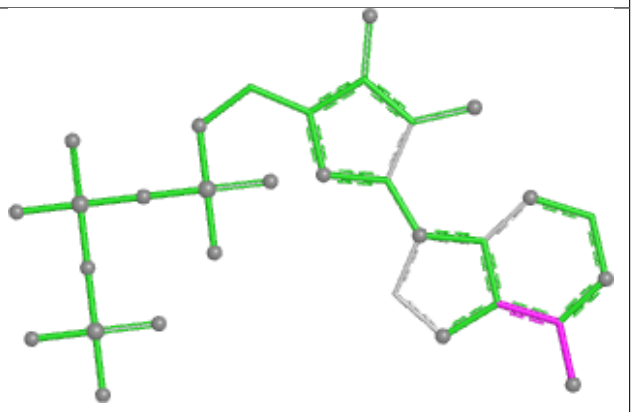
No monomer is involved in short contacts.

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

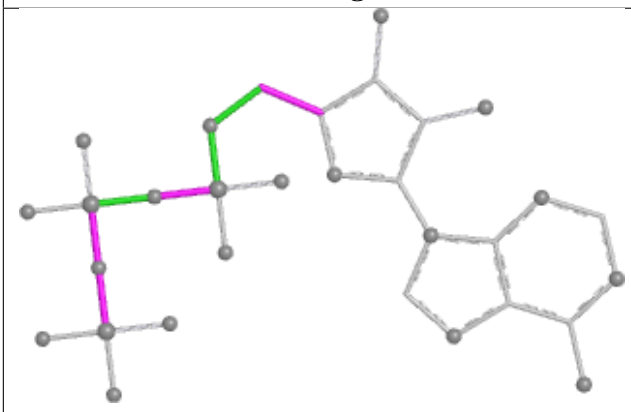
Ligand ATP B 5004



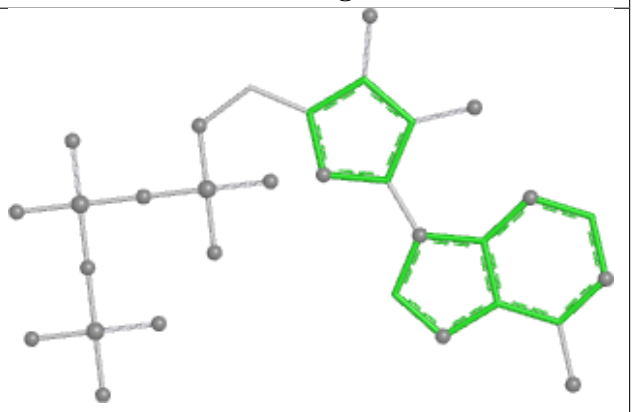
Bond lengths



Bond angles

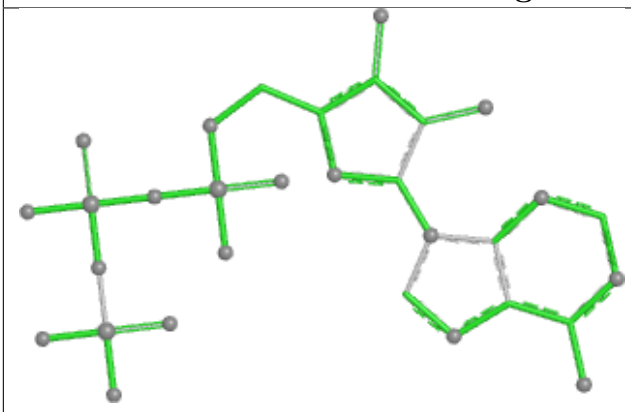


Torsions

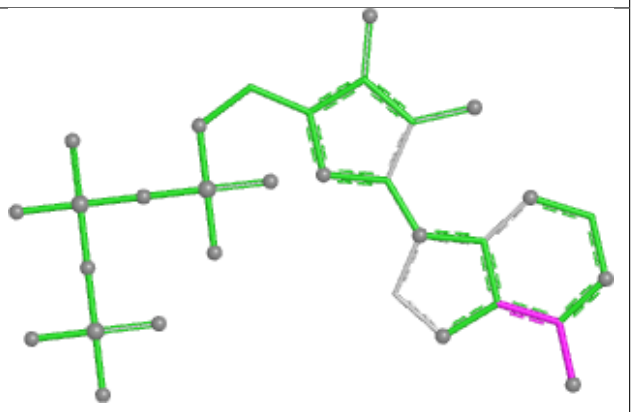


Rings

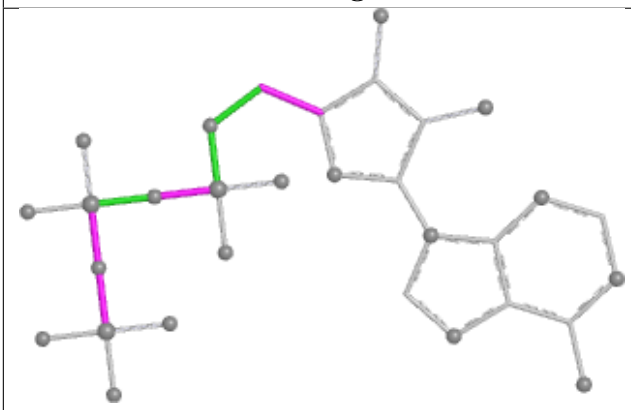
Ligand ATP D 5004



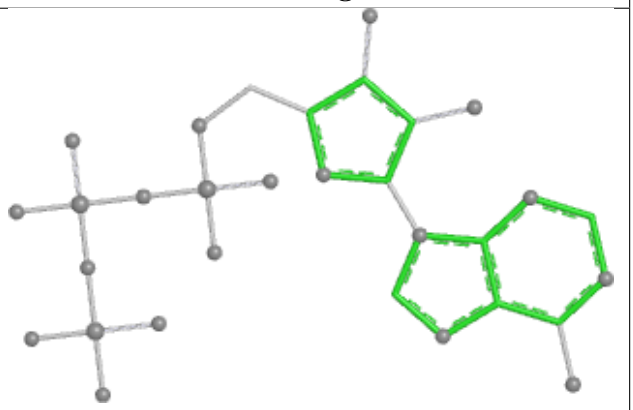
Bond lengths



Bond angles

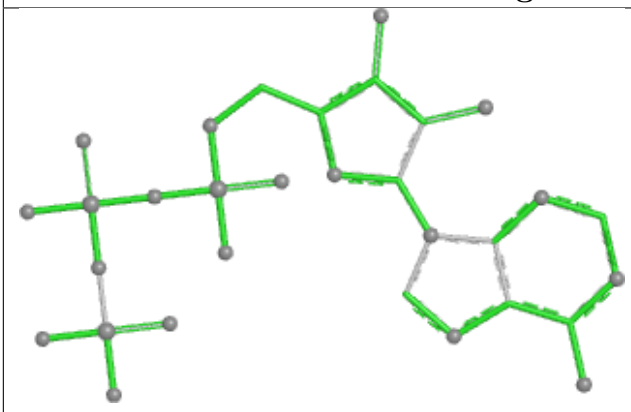


Torsions

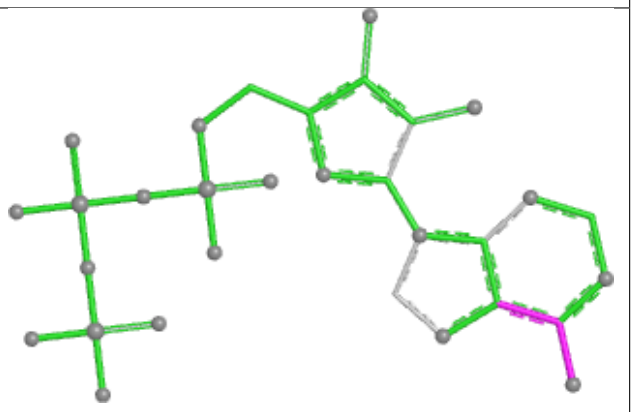


Rings

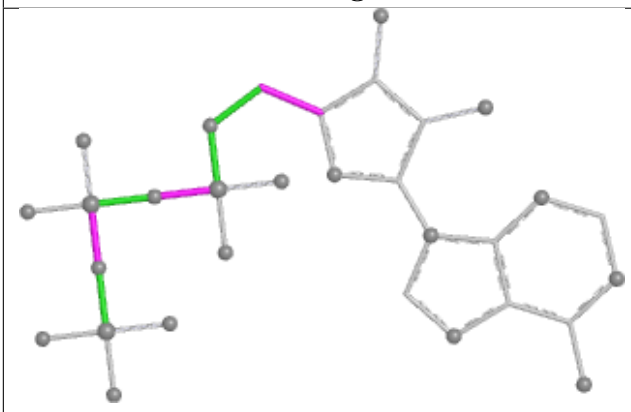
Ligand ATP B 5002



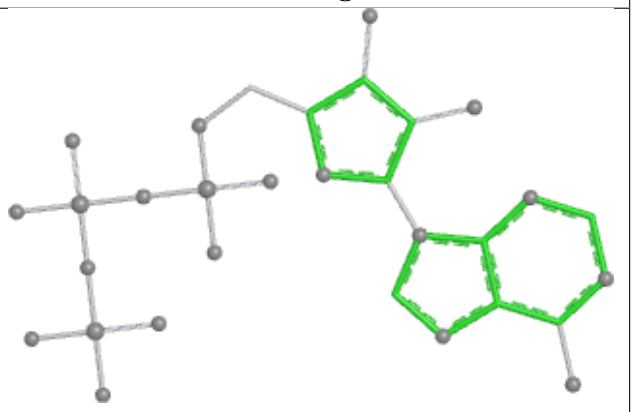
Bond lengths



Bond angles

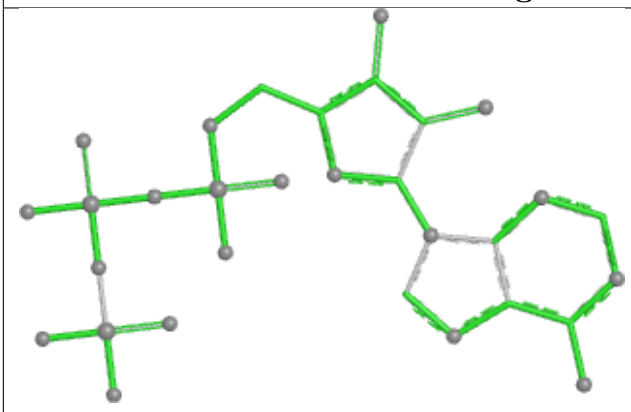


Torsions

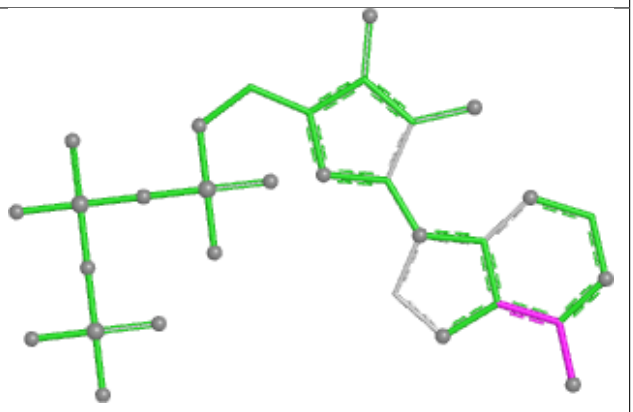


Rings

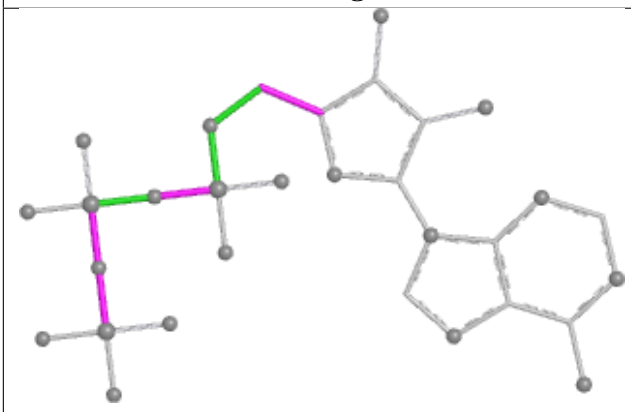
Ligand ATP A 5004



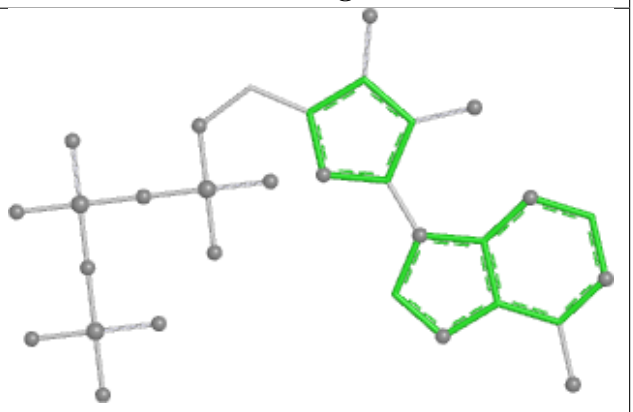
Bond lengths



Bond angles

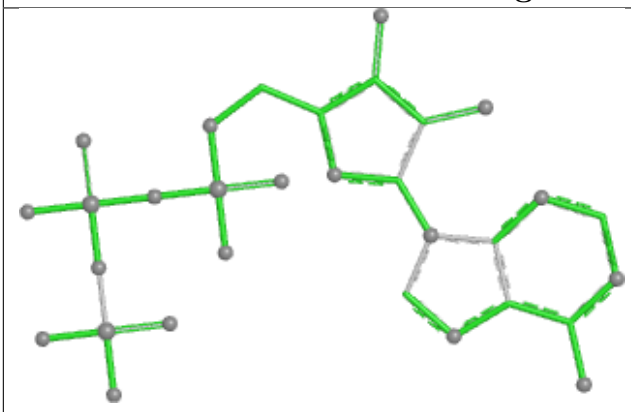


Torsions

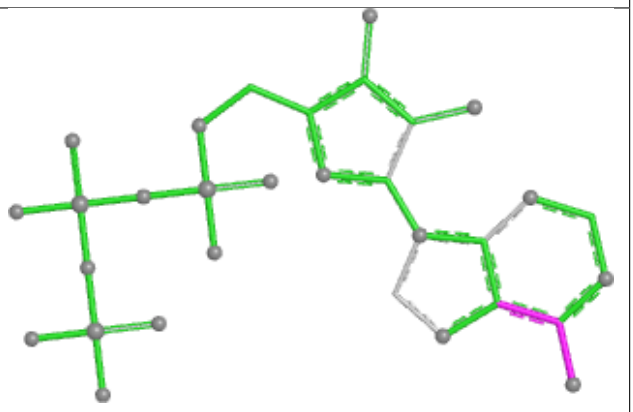


Rings

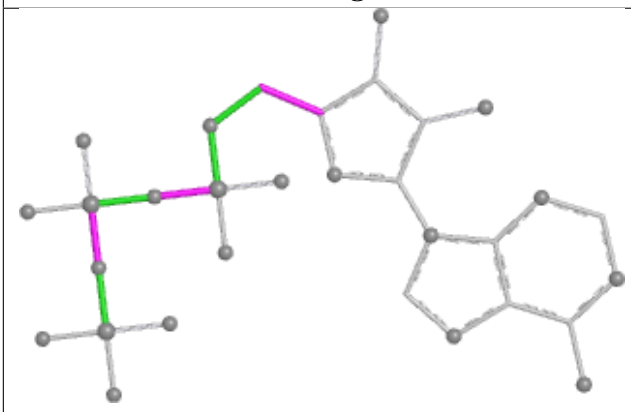
Ligand ATP D 5002



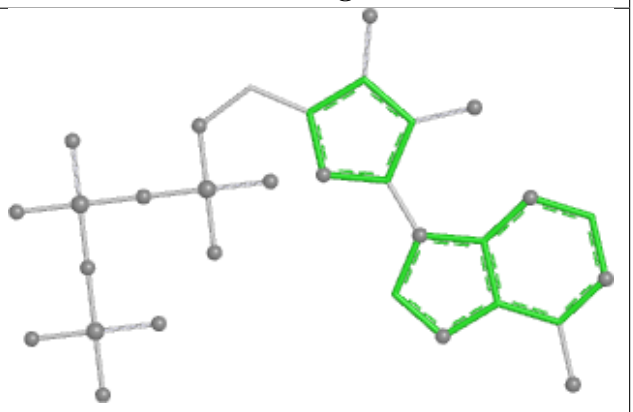
Bond lengths



Bond angles

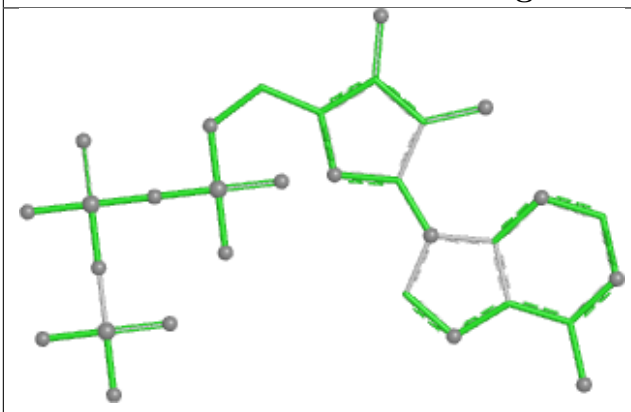


Torsions

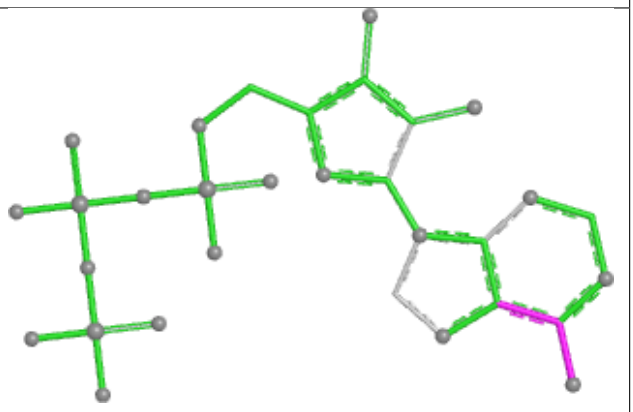


Rings

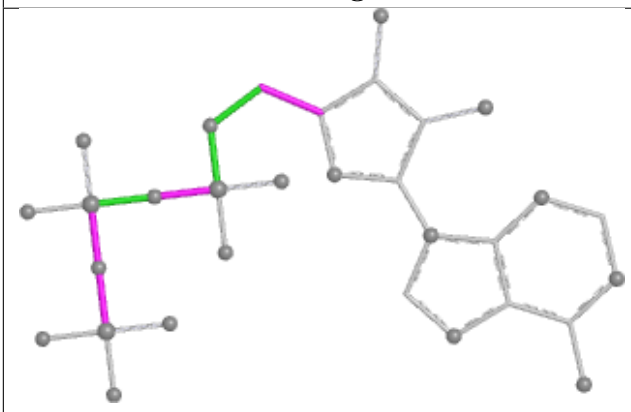
Ligand ATP C 5004



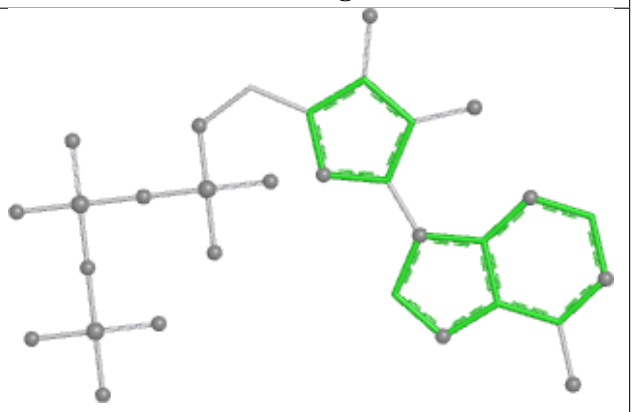
Bond lengths



Bond angles

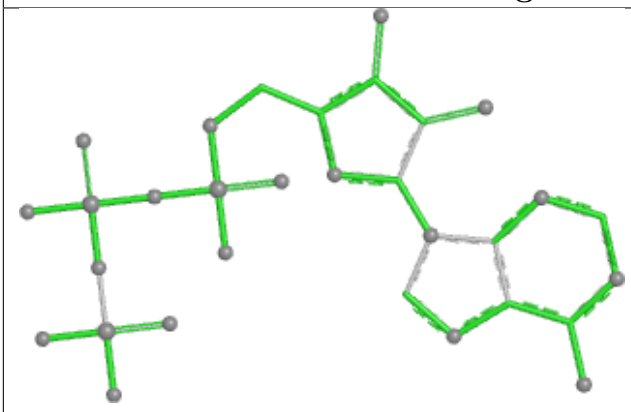


Torsions

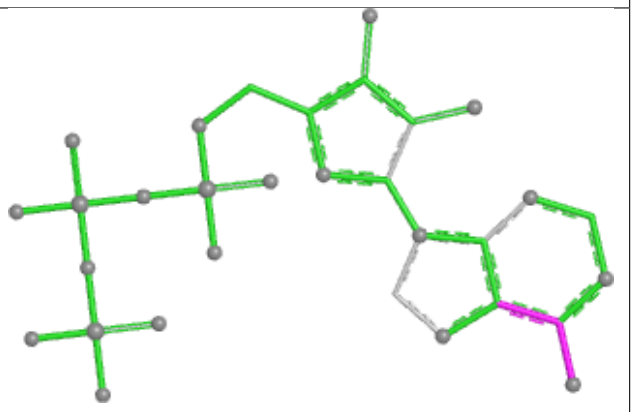


Rings

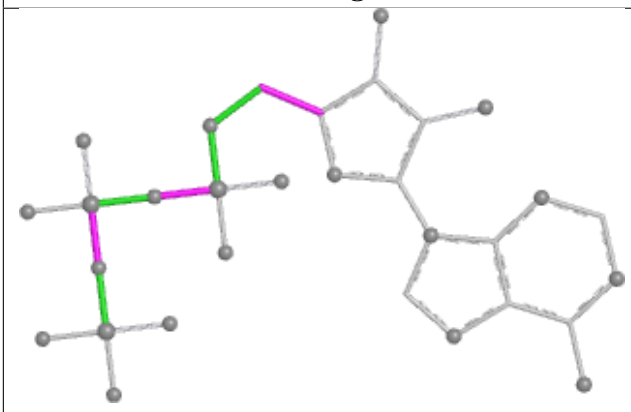
Ligand ATP C 5002



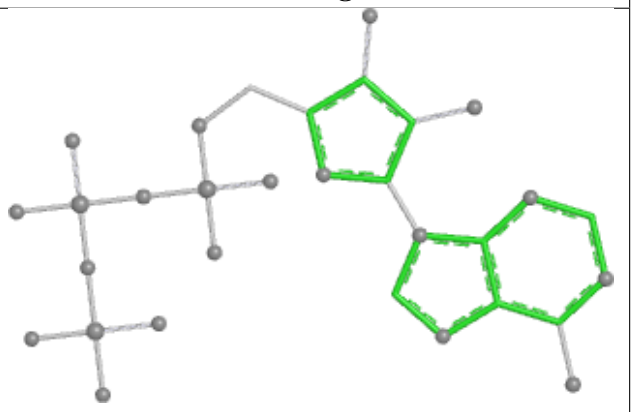
Bond lengths



Bond angles

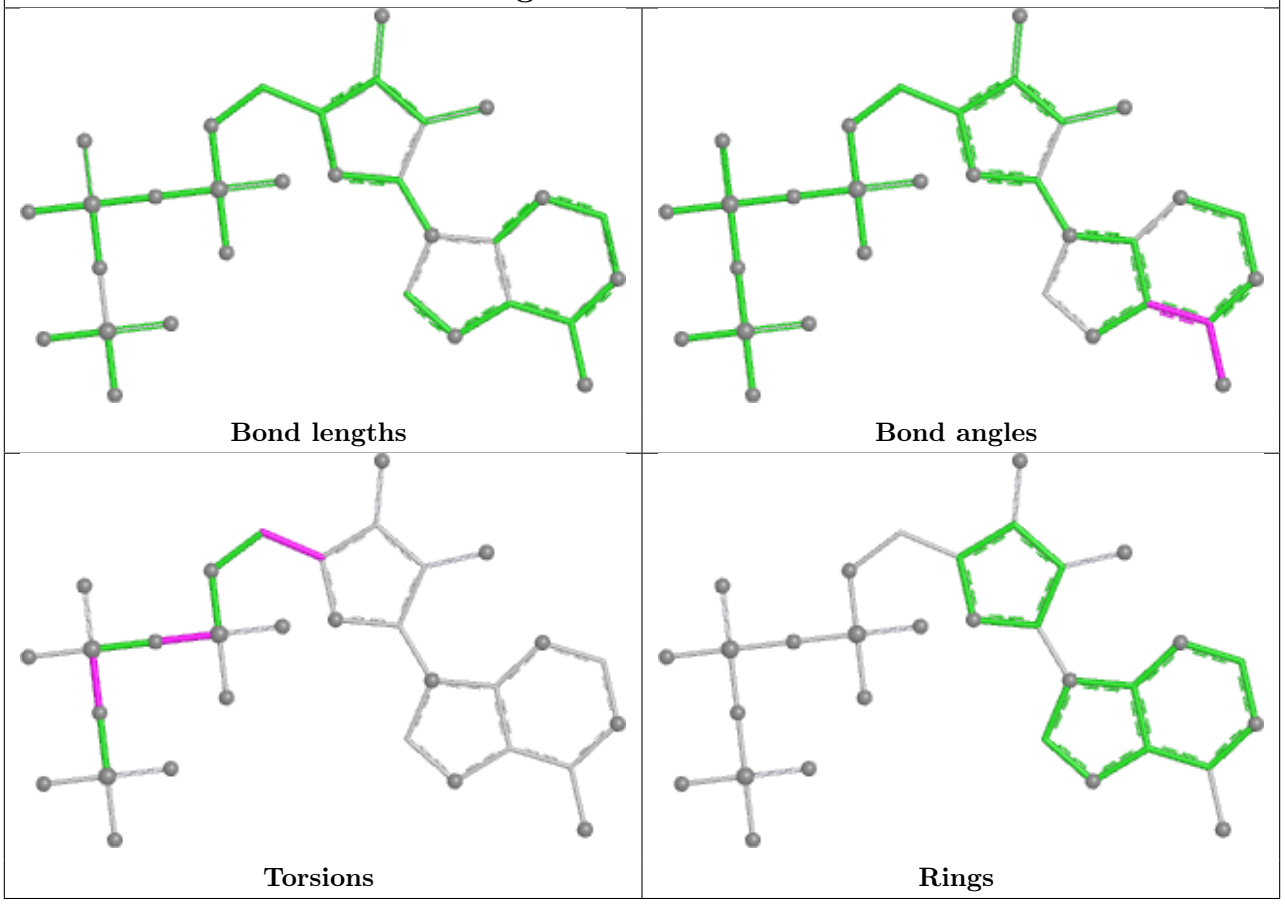


Torsions



Rings

Ligand ATP A 5002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

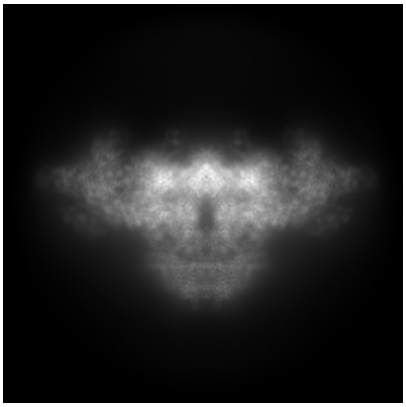
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42768. These allow visual inspection of the internal detail of the map and identification of artifacts.

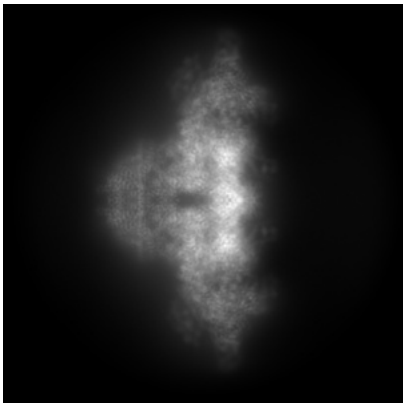
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

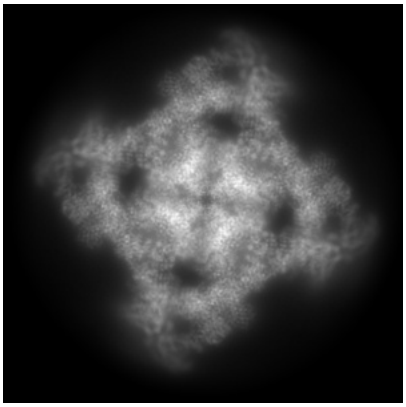
6.1.1 Primary map



X



Y

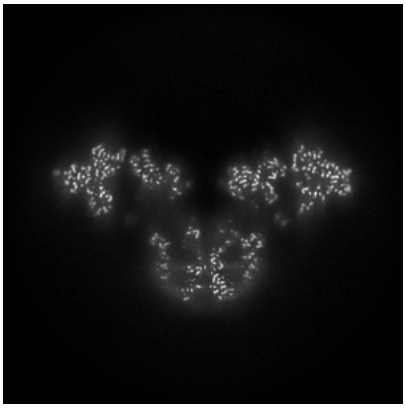


Z

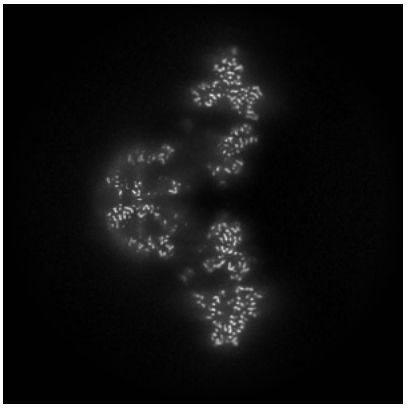
The images above show the map projected in three orthogonal directions.

6.2 Central slices

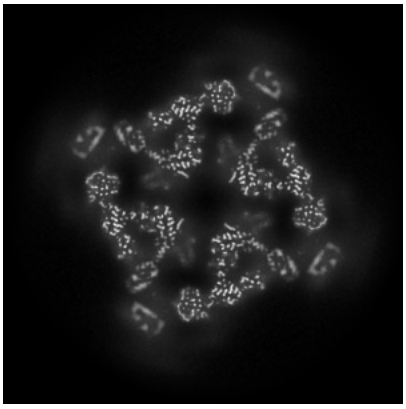
6.2.1 Primary map



X Index: 256



Y Index: 256

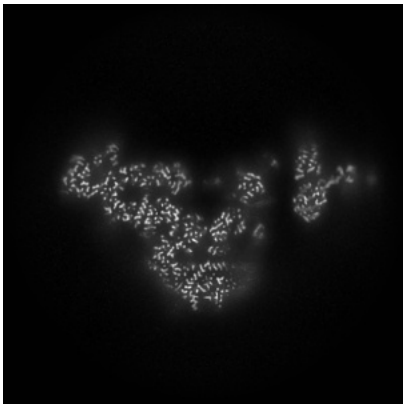


Z Index: 256

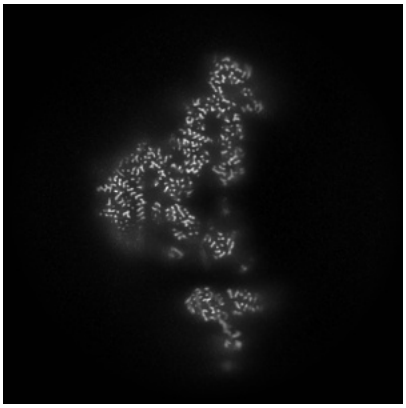
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

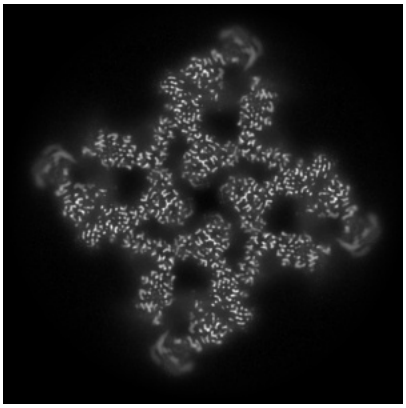
6.3.1 Primary map



X Index: 278



Y Index: 278

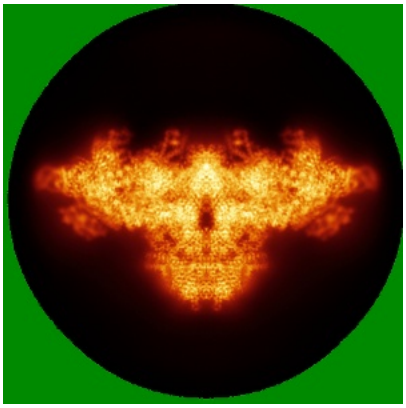


Z Index: 285

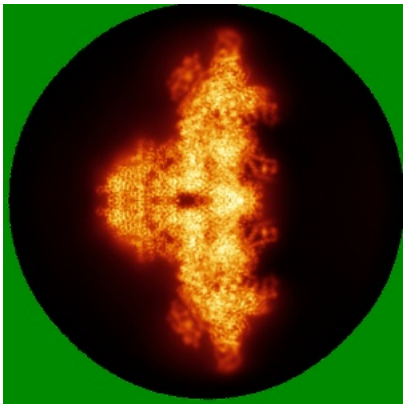
The images above show the largest variance slices of the map in three orthogonal directions.

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

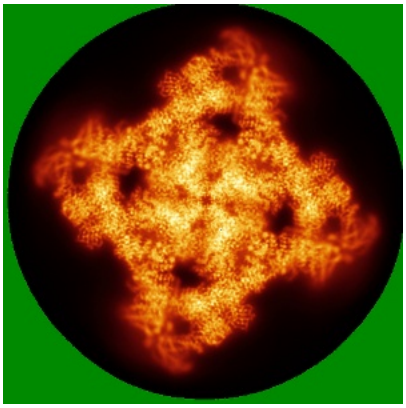
6.4.1 Primary map



X



Y

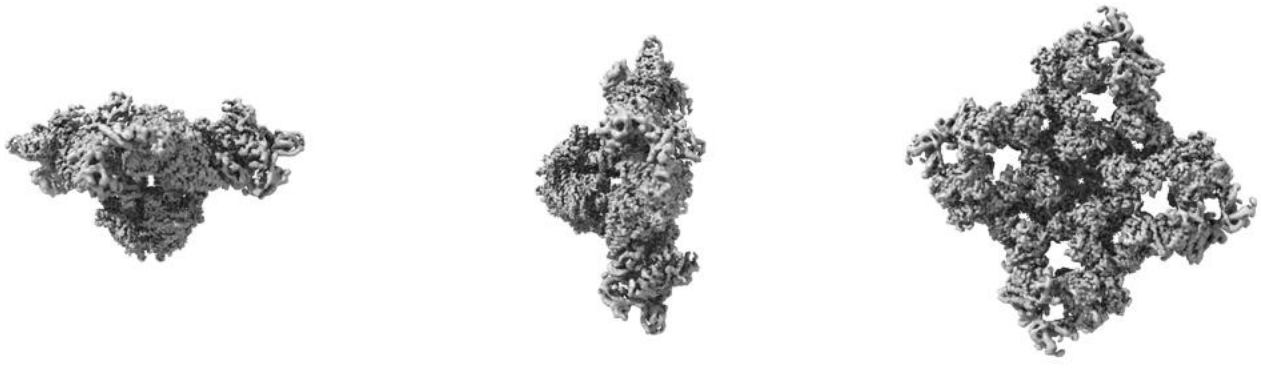


Z

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

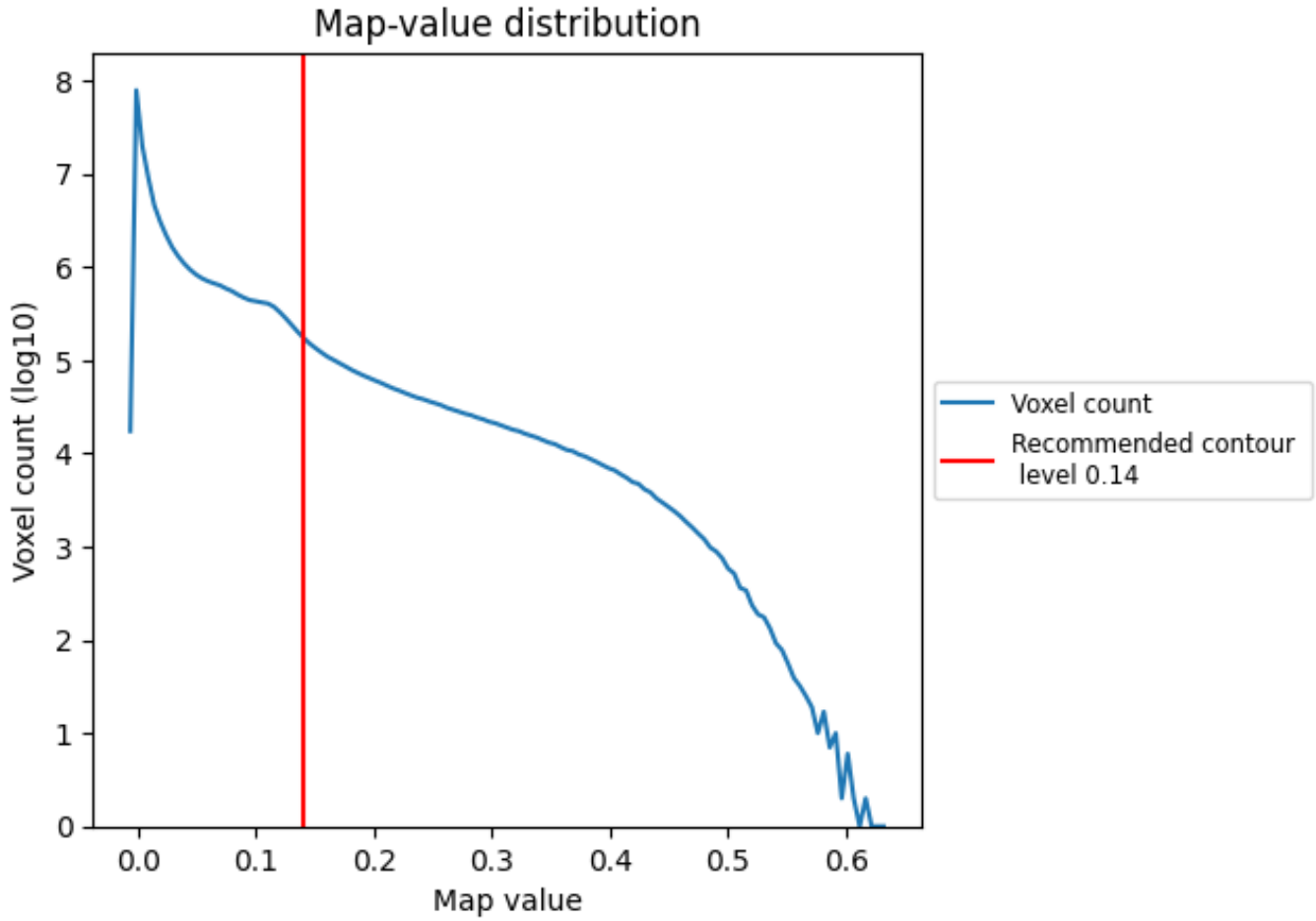
6.6 Mask visualisation (i)

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

7 Map analysis

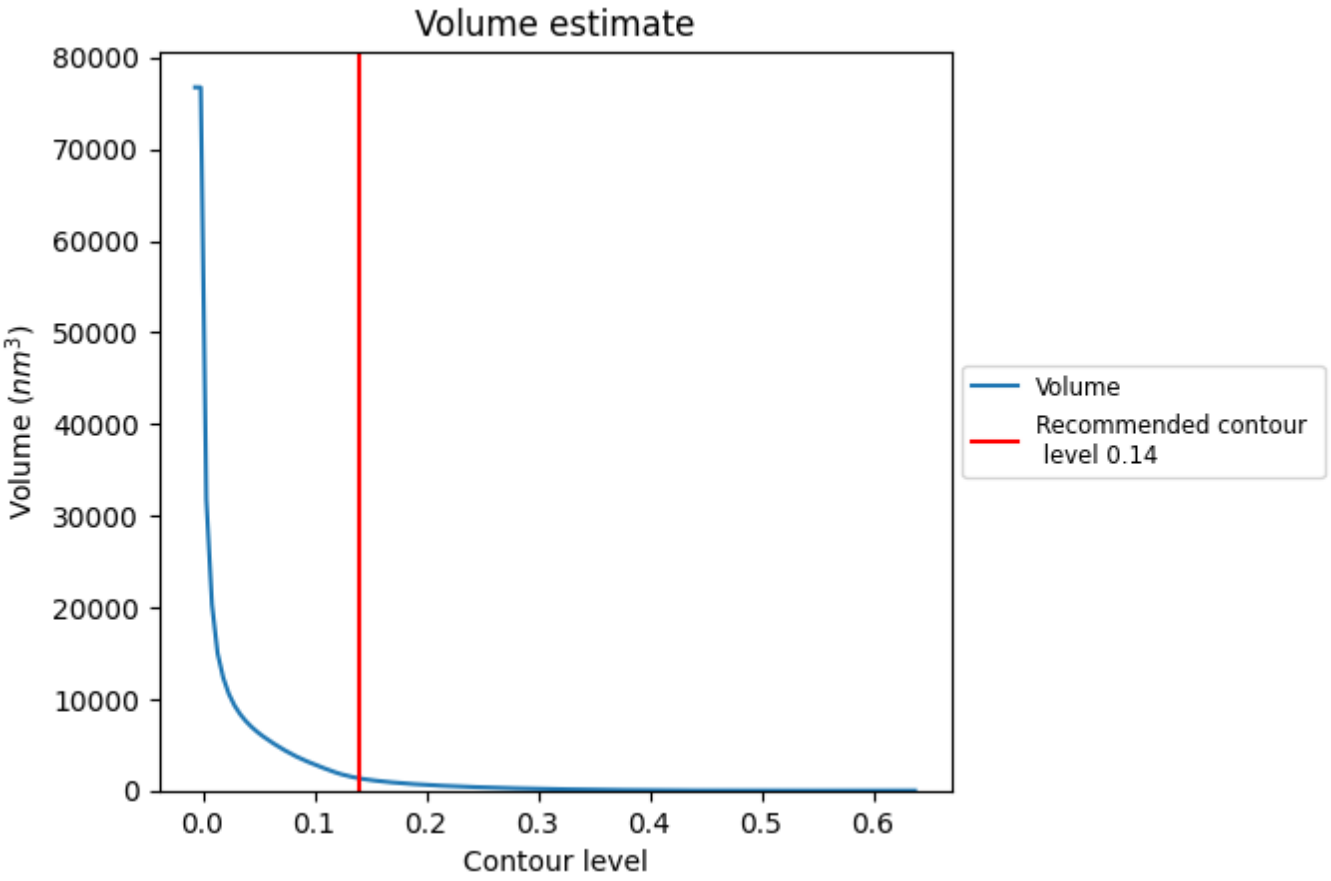
This section contains the results of statistical analysis of the map.

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.

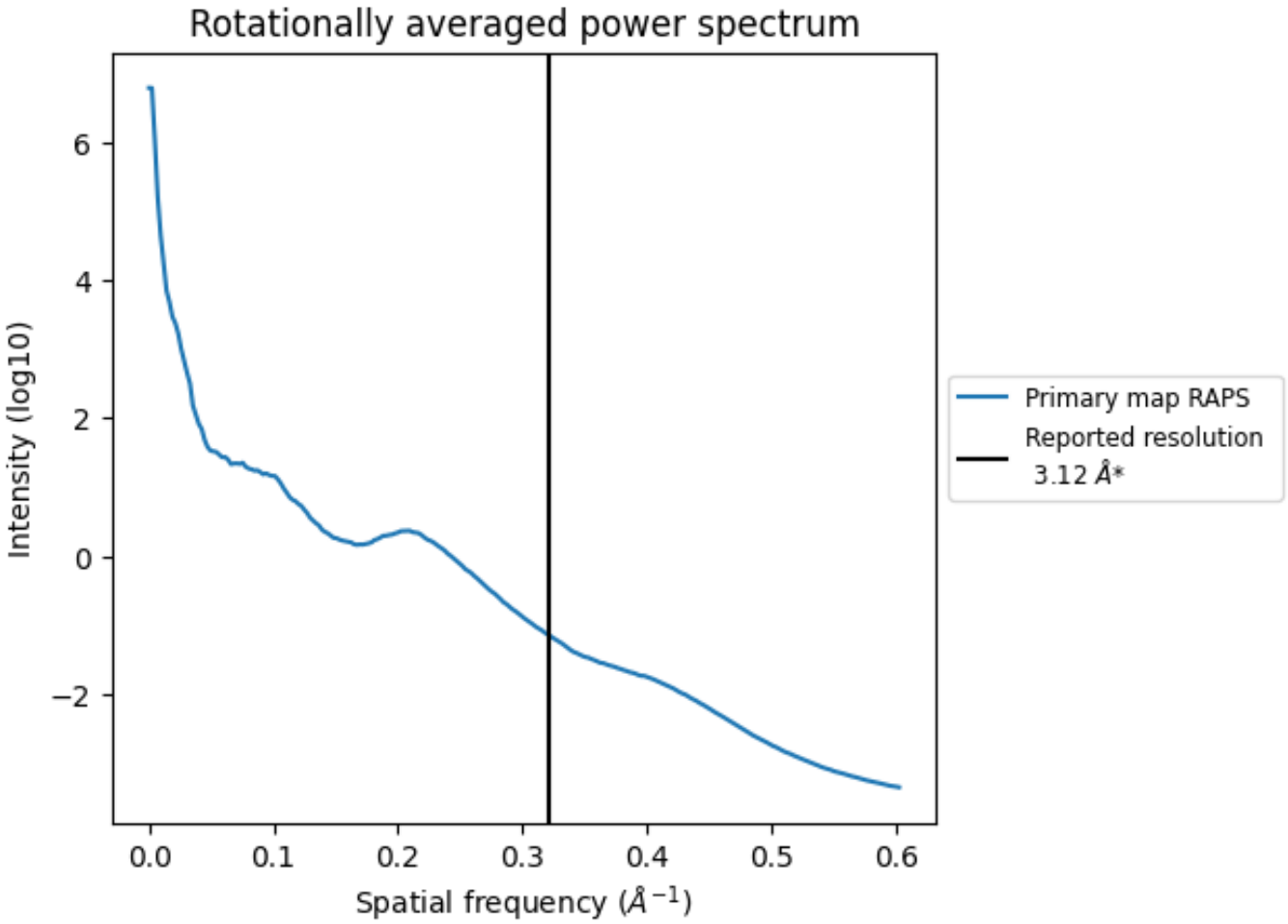
7.2 Volume estimate (i)



The volume at the recommended contour level is 1339 nm^3; this corresponds to an approximate mass of 1210 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 0.321 Å^{-1}

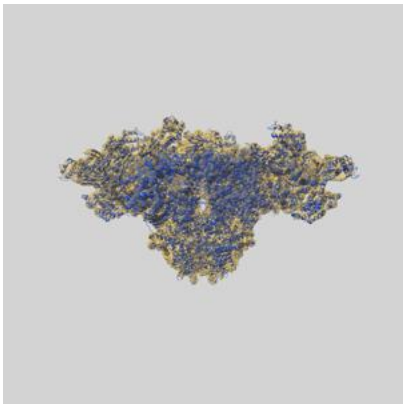
8 Fourier-Shell correlation (i)

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

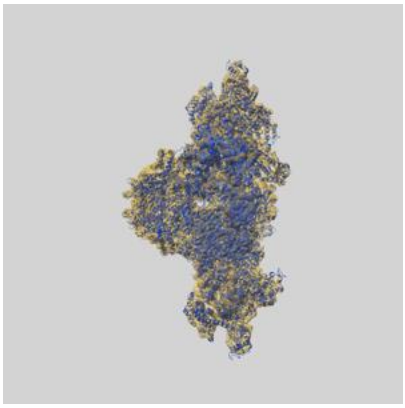
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42768 and PDB model 8UXL. Per-residue inclusion information can be found in section 3 on page 7.

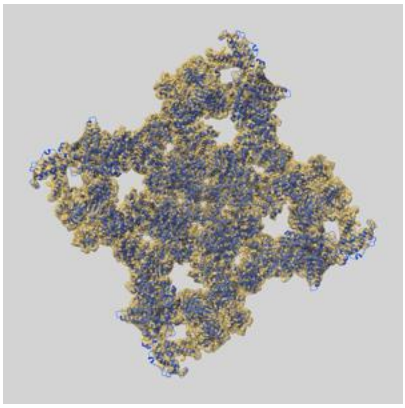
9.1 Map-model overlay



X



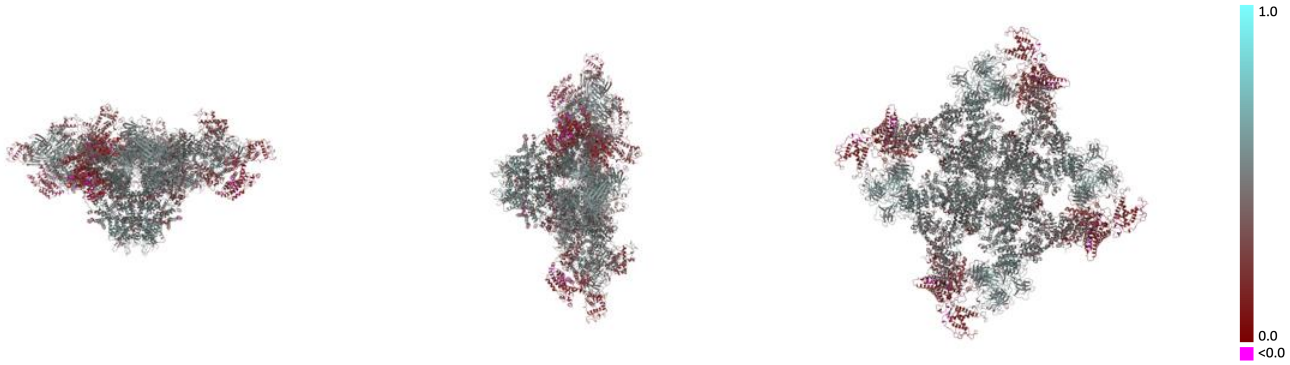
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 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.

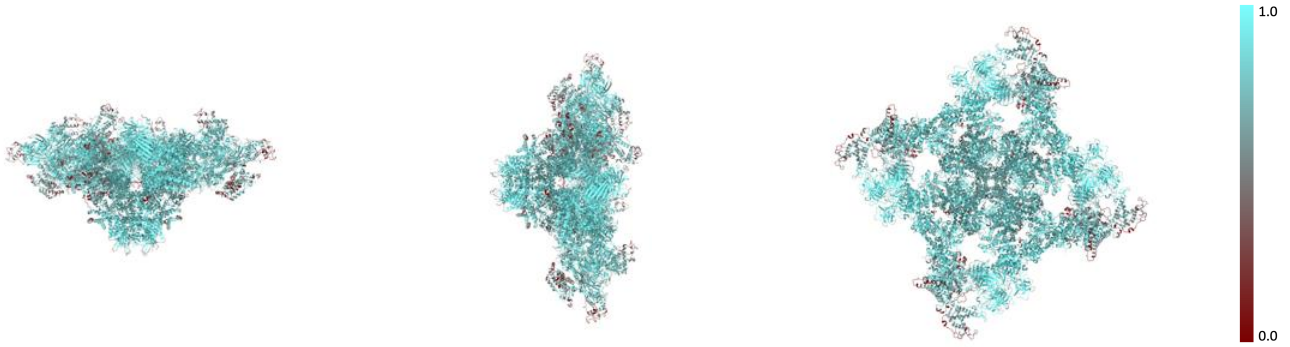
9.2 Q-score mapped to coordinate model (i)



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.

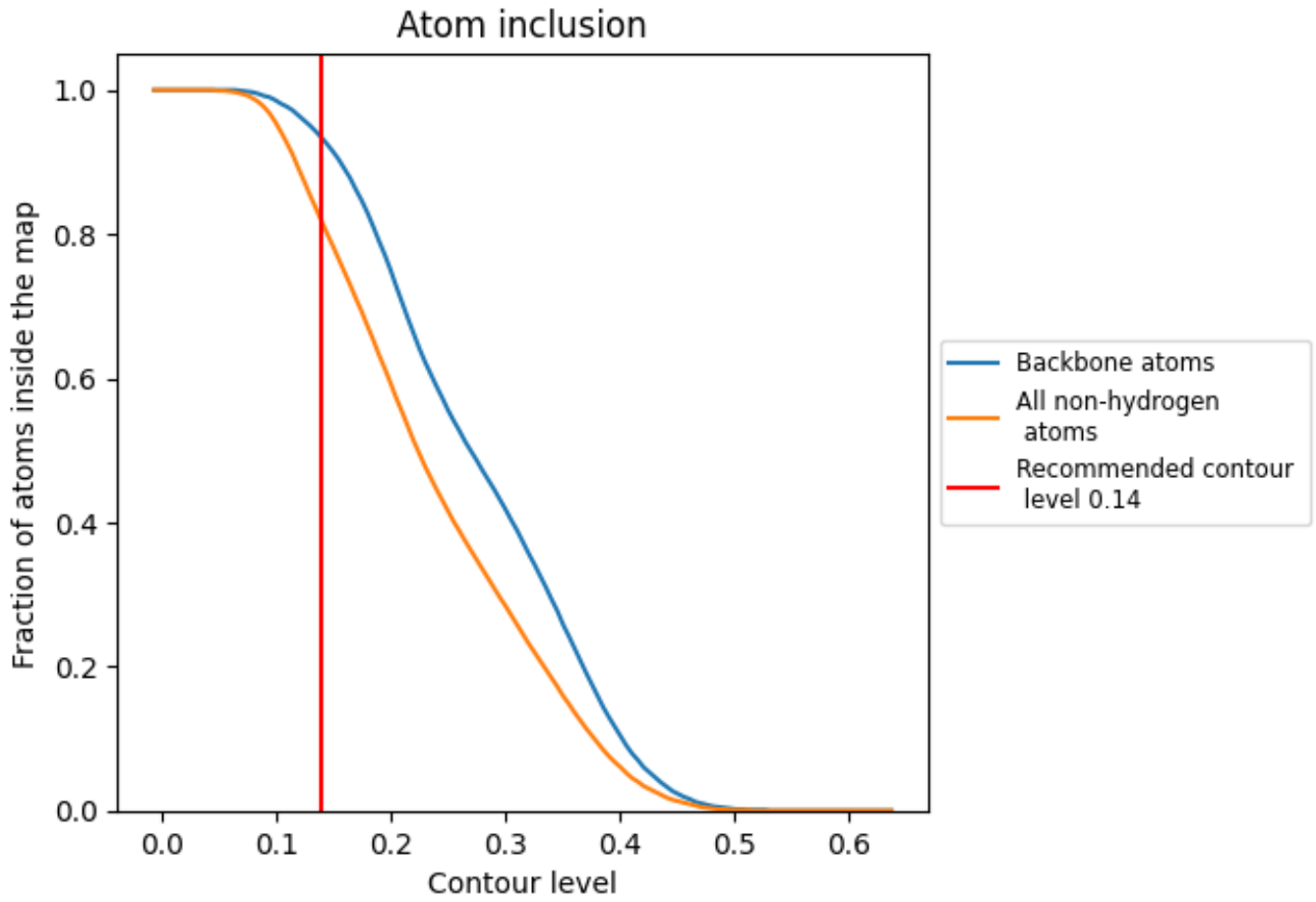
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 82% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.4170
A	0.8150	0.4190
B	0.8170	0.4250
C	0.8150	0.4210
D	0.8110	0.4130
E	0.9130	0.5170
F	0.9130	0.5160
G	0.9130	0.5190
H	0.9160	0.5180
I	0.7920	0.2590
J	0.7920	0.2600
K	0.7950	0.2600
L	0.7890	0.2530