wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 03:23 PM UTC

PDB ID	:	9E1D / pdb_00009e1d
EMDB ID	:	EMD-47390
Title	:	Structure of RyR1 in the primed state in the presence of enprofylline
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2024-10-21
Resolution	:	2.76 Å(reported)
Based on initial model	:	7TZC

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:

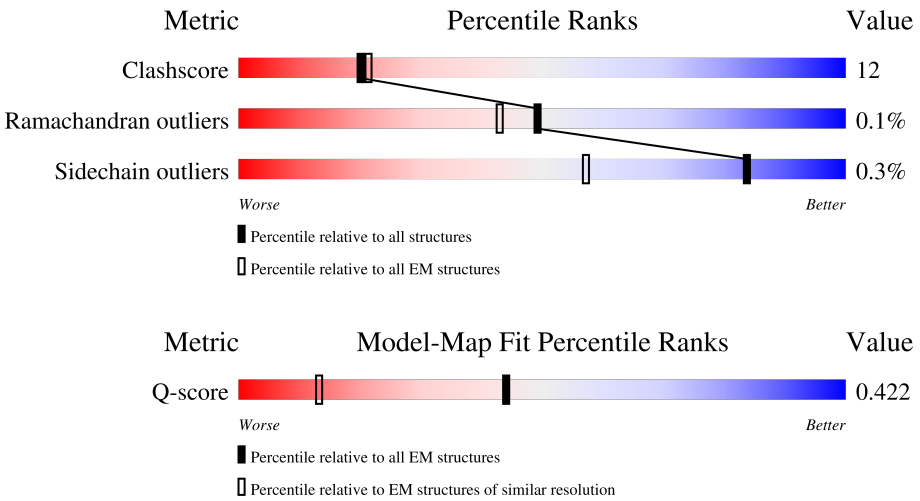
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.76 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10642 (2.26 - 3.26)

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	5037	20% 65% 22% 13%
1	B	5037	20% 66% 21% 13%
1	C	5037	20% 65% 21% 13%
1	D	5037	20% 65% 21% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	5% 71% 26% ...
2	F	108	5% 71% 26% ...
2	G	108	70% 27% ...
2	H	108	5% 70% 27% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	A1BD3	A	5304	-	X	-	-
6	A1BD3	B	5304	-	X	-	-
6	A1BD3	C	5304	-	X	-	-
6	A1BD3	D	5304	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 144112 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.

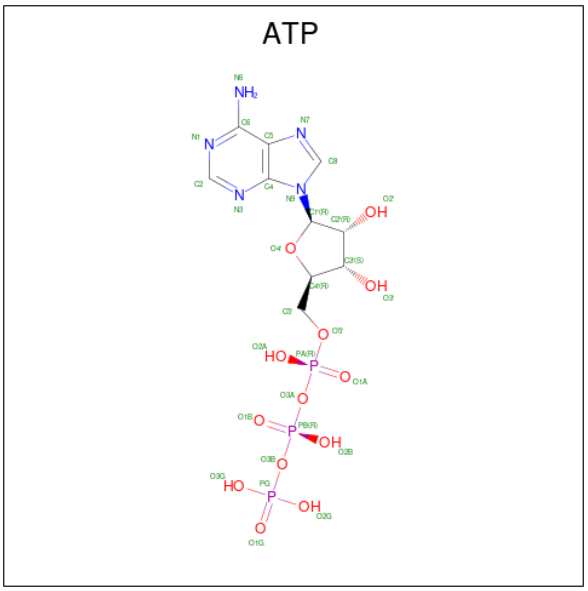
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4404	35150	22365	6063	6485	237	9	0
1	B	4404	35150	22365	6063	6485	237	9	0
1	D	4404	35150	22365	6063	6485	237	9	0
1	C	4404	35150	22365	6063	6485	237	9	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	831	527	146	154	4	0	0
2	H	107	831	527	146	154	4	0	0
2	G	107	831	527	146	154	4	0	0
2	F	107	831	527	146	154	4	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
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	D	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	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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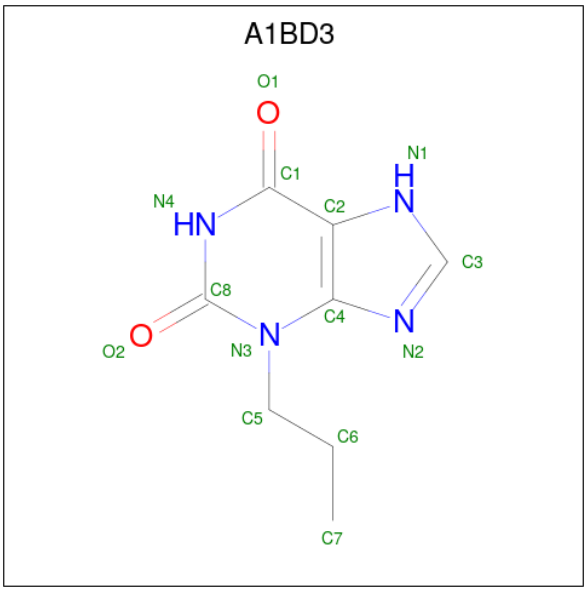
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	B	1	1	1	0
5	D	1	1	1	0
5	C	1	1	1	0

- Molecule 6 is enprofylline (CCD ID: A1BD3) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



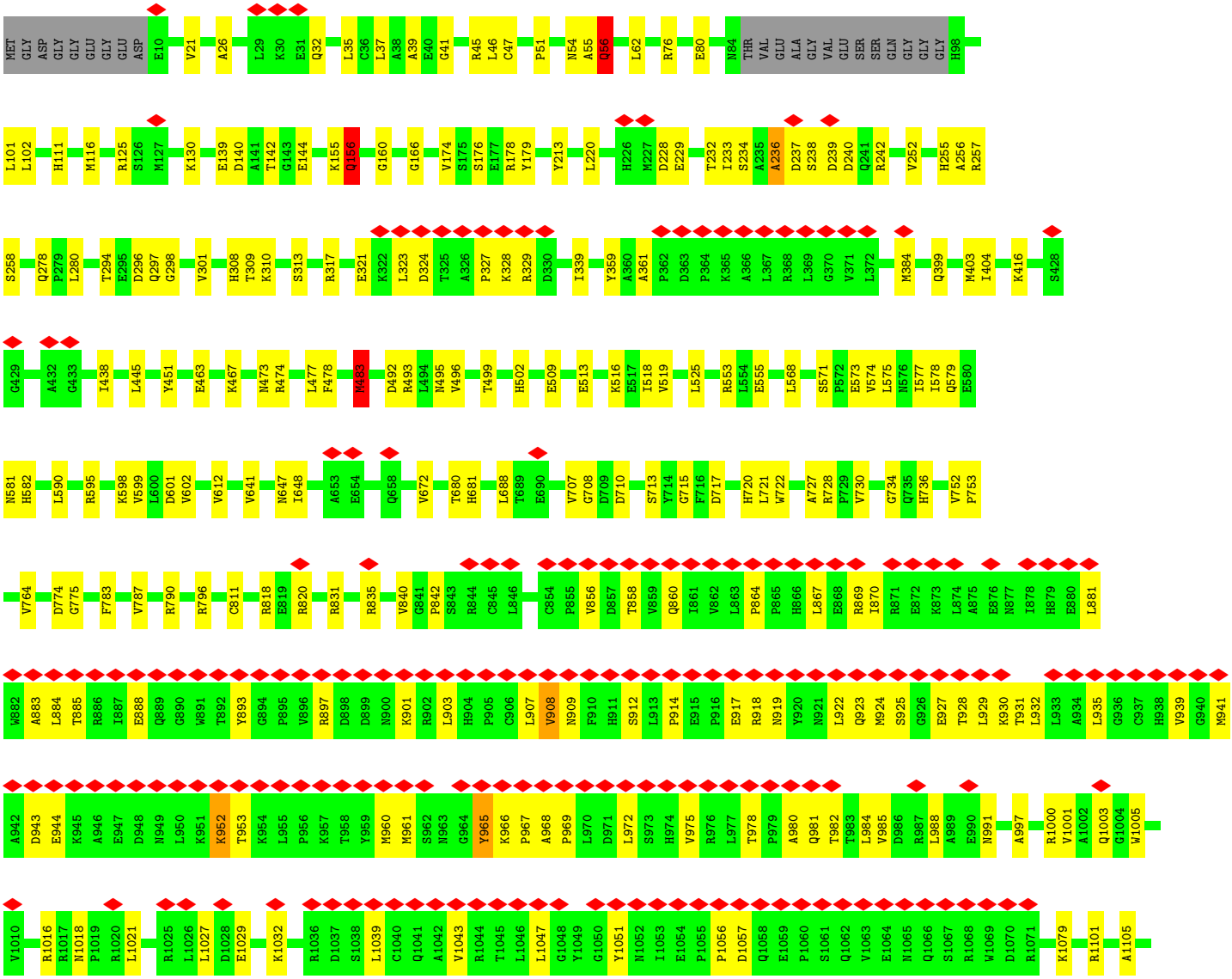
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	4	2	0
6	B	1	14	8	4	2	0
6	D	1	14	8	4	2	0
6	C	1	14	8	4	2	0

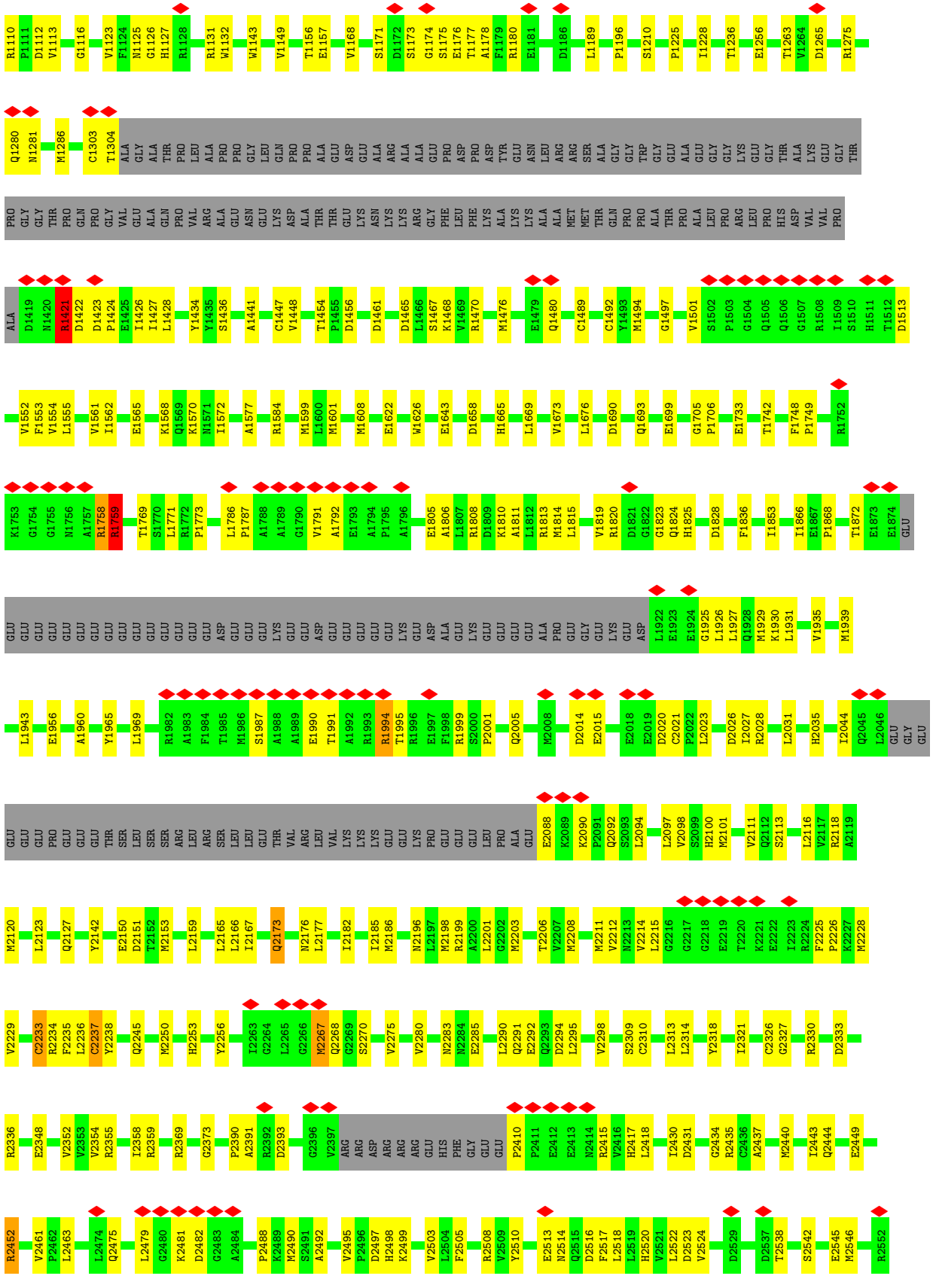
3 Residue-property plots (i)

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 1

Chain A:

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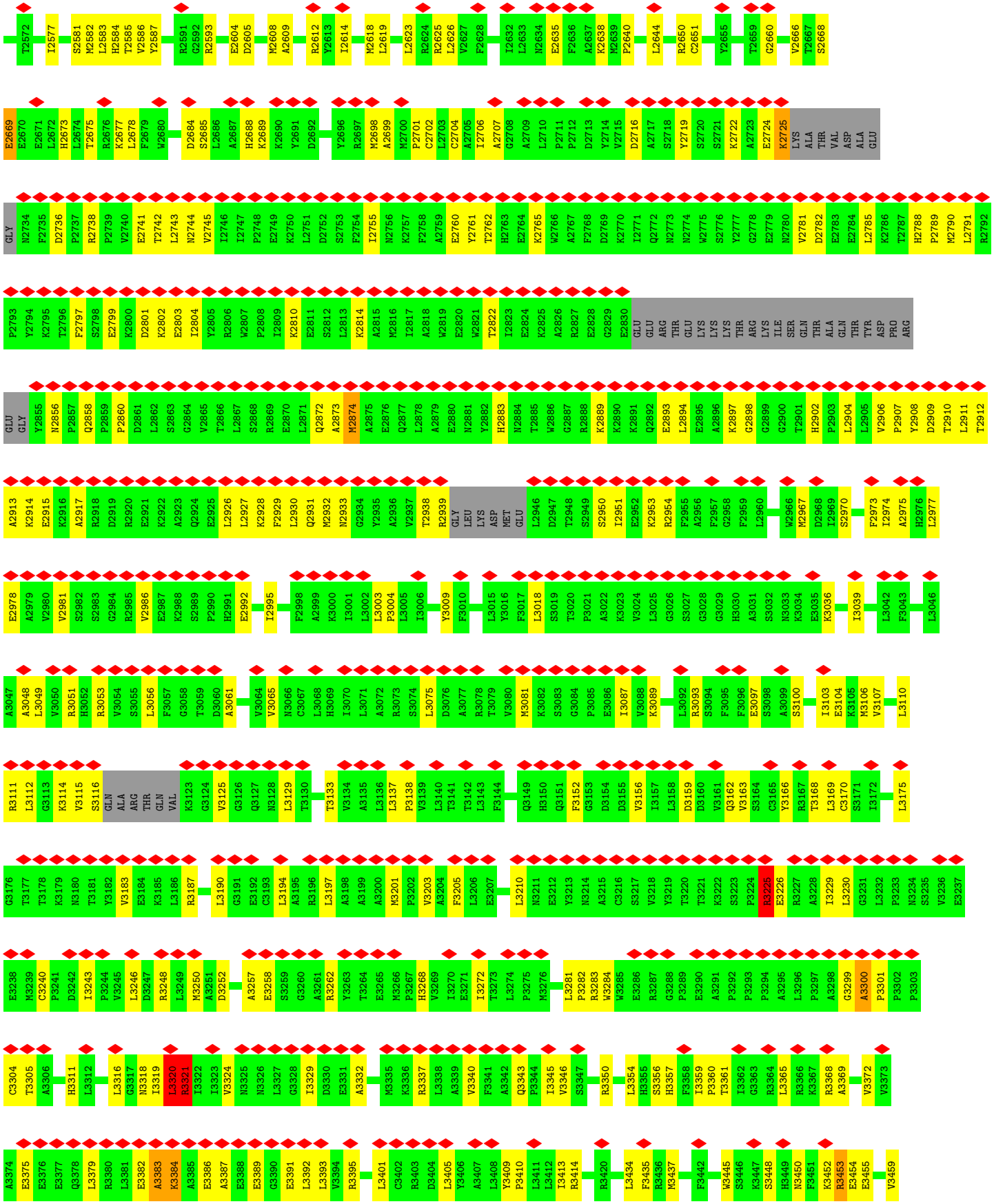
Q1280 N1281 M1286 C1303 T1304 ALA GLY ALA ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR
PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO
ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 L1428 Y1434 Y1435 S1436 A1441 C1447 V1448 T1454 P1455 D1456 D1461 D1465 L1466 S1467 K1468 V1469 R1470 M1476 E1479 Q1480 C1489 C1492 Y1493 M1494 G1497 V1501 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513
V1552 F1553 V1554 L1555 V1561 I1562 E1565 K1568 Q1569 K1570 N1571 I1572 A1577 R1584 M1599 L1600 M1601 M1608 E1622 W1626 E1643 D1658 H1665 L1669 V1673 L1676 D1690 Q1693 E1699 G1705 P1706 E1733 T1742 F1748 P1749 R1752
K1753 G1754 G1755 N1756 A1757 R1758 R1759 T1769 S1770 L1771 R1772 P1773 L1786 P1787 A1788 A1789 G1790 V1791 A1792 E1793 A1794 P1795 A1796 E1805 A1806 L1807 R1808 D1809 K1810 A1811 L1812 R1813 M1814 L1815 V1819 R1820 D1821 G1822 G1823 Q1824 H1825 D1828 F1836 I1853 I1866 E1867 P1868 T1872 E1873 E1874 GLU
GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 M1939
L1943 E1956 A1960 Y1965 L1969 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 Q2005 M2008 D2014 E2015 E2018 E2019 D2020 C2021 P2022 L2023 D2026 I2027 R2028 L2031 H2035 I2044 Q2045 L2046 GLU GLY GLU
GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 P2091 Q2092 S2093 L2094 L2097 V2098 S2099 H2100 M2101 V2111 Q2112 S2113 L2116 V2117 R2118 A2119
M2120 L2123 Q2127 Y2142 E2150 D2151 T2152 M2153 L2159 L2165 L2166 I2167 Q2173 N2176 L2177 I2182 I2185 M2186 N2196 L2197 M2198 R2199 A2200 L2201 G2202 M2203 T2206 V2207 M2208 M2211 V2212 W2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 F2225 P2226 K2227 M2228
V2229 C2233 R2234 F2235 L2236 C2237 Y2238 Q2245 M2250 H2253 Y2256 I2253 G2264 L2265 G2266 M2267 Q2268 G2269 S2270 V2275 V2280 N2283 W2284 E2285 L2290 Q2291 E2292 Q2293 D2294 L2295 V2298 S2309 C2310 L2313 L2314 Y2318 I2321 C2326 G2327 R2330 D2333
R2336 E2348 V2352 V2353 V2354 R2355 I2358 R2359 R2369 G2373 P2390 A2391 R2392 D2393 G2396 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 R2415 V2416 H2417 L2418 I2430 D2431 G2434 R2435 C2436 A2437 M2440 I2443 Q2444 E2449
R2452 V2461 P2462 L2463 L2474 Q2475 L2479 G2480 K2481 D2482 G2483 A2484 P2488 K2489 M2490 S2491 A2492 V2495 P2496 D2497 H2498 K2499 V2503 L2504 F2505 R2508 V2509 Y2510 E2513 N2514 Q2515 D2516 F2517 L2518 L2519 H2520 V2521 L2522 D2523 V2524 D2529 D2537 T2538 S2542 E2545 M2546 R2552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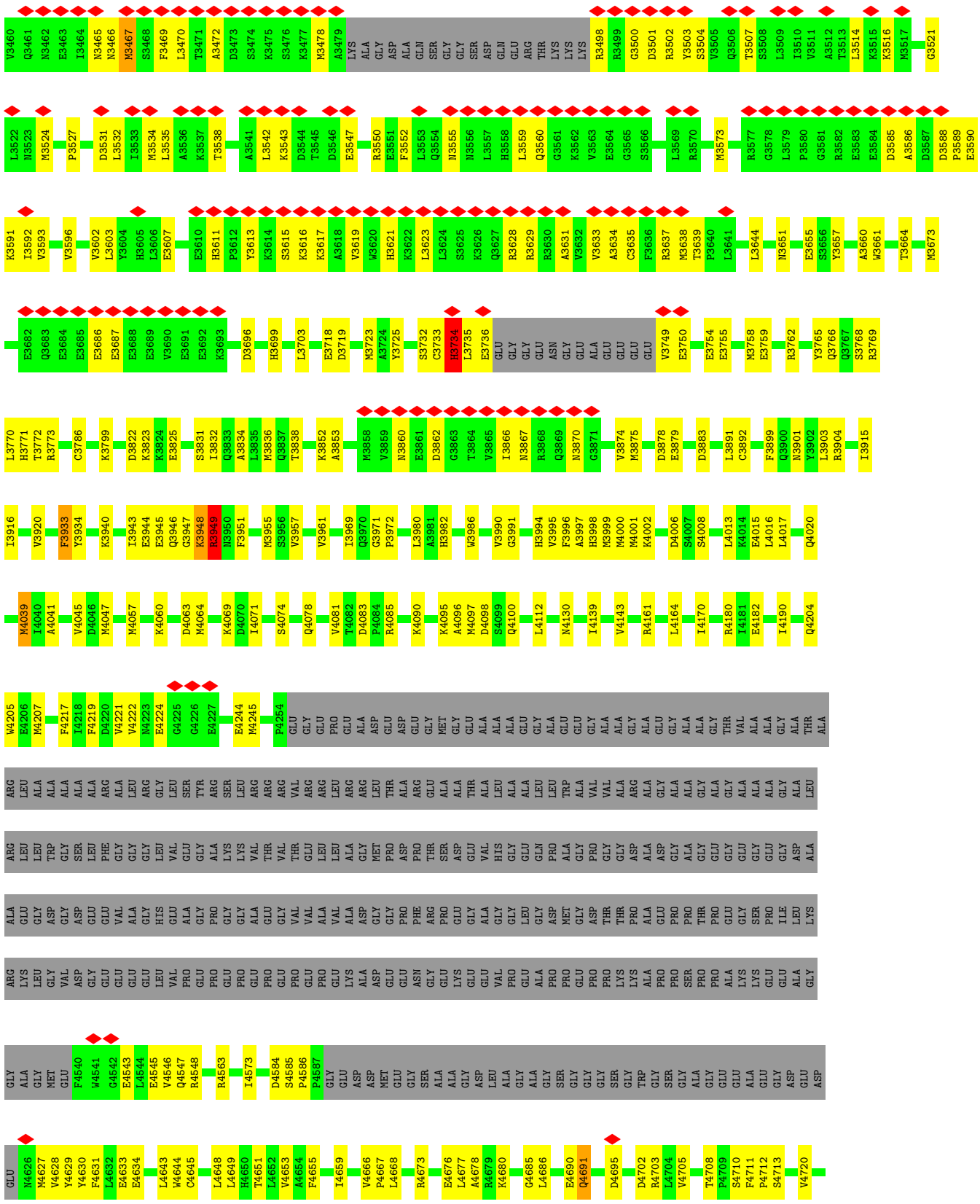
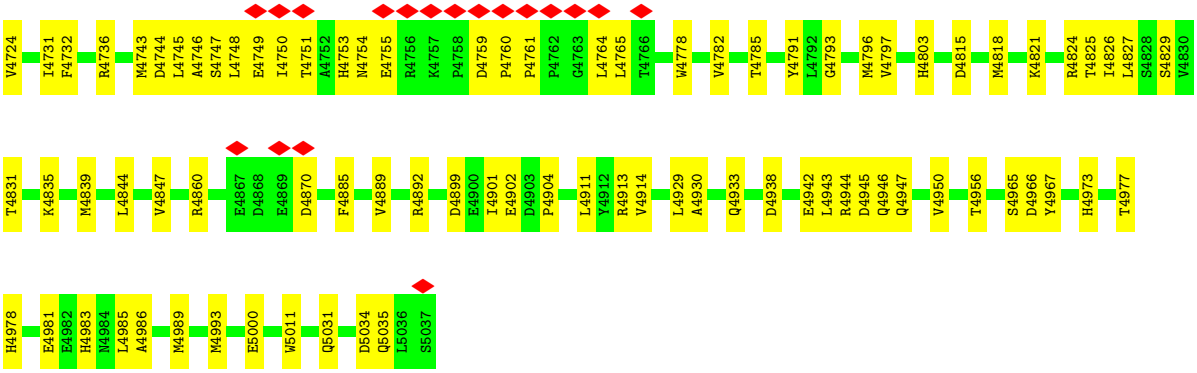
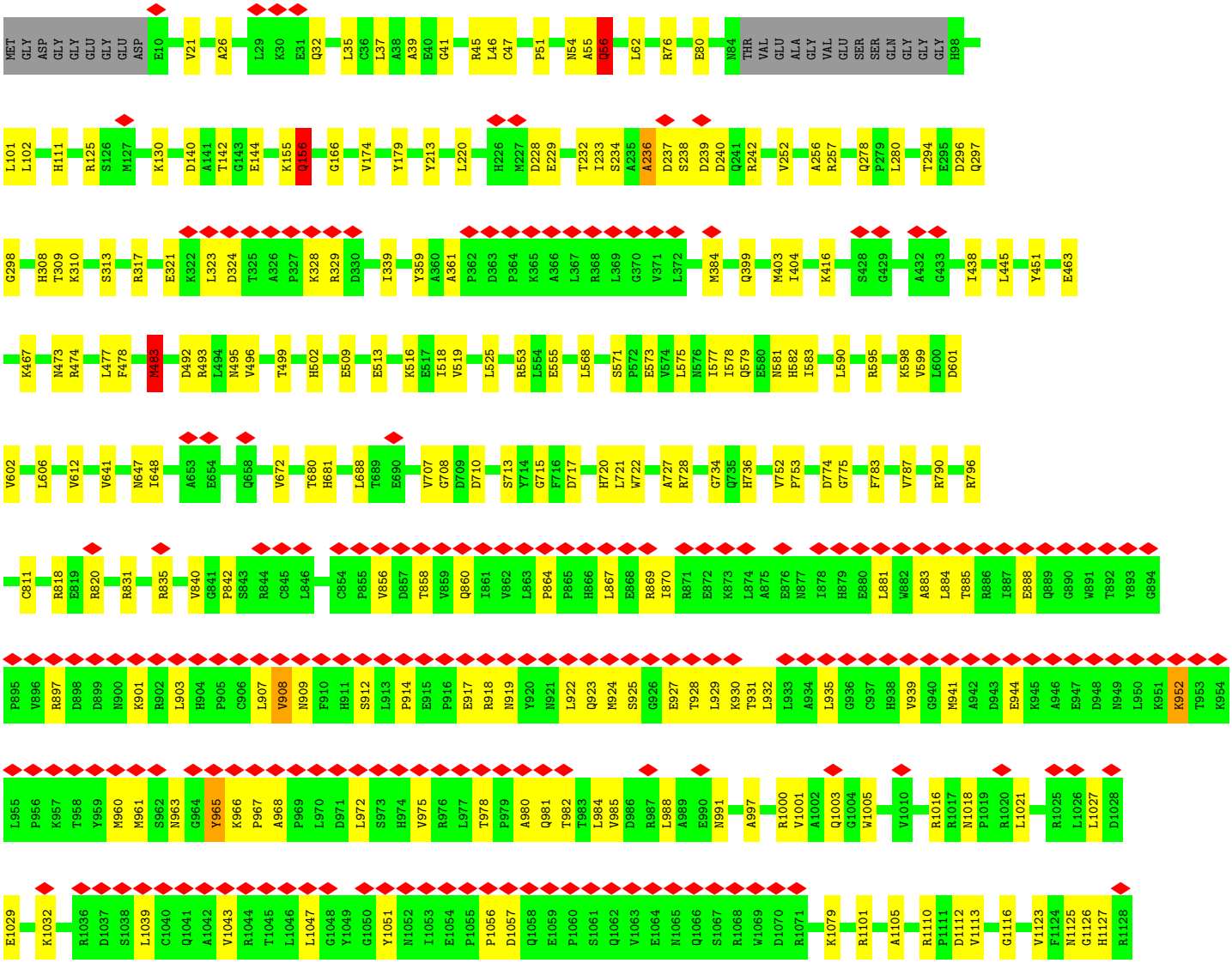
E2669 E2670 E2671 L2672 H2673 L2674 T2675 R2676 K2677 L2678 F2679 V2680 D2684 S2685 L2686 A2687 H2688 K2689 K2690 Y2691 D2692 Y2696 R2697 M2698 A2699 M2700 P2701 C2702 L2703 C2704 A2705 I2706 A2707 G2708 A2709 L2710 P2711 P2712 D2713 Y2714 V2715 D2716 A2717 S2718 Y2719 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU
GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792
P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG
GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912
A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU L2946 D2947 T2948 S2949 S2950 I2951 E2952 K2953 R2954 F2955 A2956 F2957 G2958 F2959 L2960 W2966 M2967 D2968 I2969 S2970 F2973 I2974 A2975 H2976 L2977
E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 I2995 F2998 A2999 K3000 I3001 L3002 L3003 P3004 L3005 I3006 Y3009 F3010 L3015 Y3016 F3017 L3018 S3019 T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 A3031 S3032 N3033 K3034 E3035 K3036 I3039 L3042 F3043 L3046
A3047 A3048 L3049 V3050 R3051 H3052 R3053 V3054 S3055 L3056 F3057 G3058 T3059 D3060 A3061 V3064 V3065 N3066 C3067 L3068 H3069 I3070 L3071 A3072 R3073 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 V3088 K3089 L3092 R3093 S3094 F3095 F3096 E3097 S3098 A3099 S3100 I3103 E3104 K3105 M3106 V3107 L3110
R3111 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 V3125 G3126 Q3127 N3128 L3129 T3130 T3133 V3134 A3135 L3136 L3137 P3138 V3139 L3140 T3141 T3142 L3143 F3144 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 L3169 C3170 S3171 I3172 L3175
G3176 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3186 R3187 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237
E3238 M3239 C3240 P3241 D3242 I3243 P3244 V3245 L3246 D3247 R3248 L3249 M3250 A3251 D3252 A3257 E3258 S3259 G3260 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 L3281 P3282 R3283 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303
C3304 T3305 A3306 H3311 L3312 L3316 G3317 N3318 I3319 L3320 R3321 I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 M3335 K3336 R3337 L3338 A3339 V3340 F3341 A3342 Q3343 P3344 I3345 V3346 S3347 R3350 L3354 H3355 S3356 H3357 F3358 I3359 P3360 T3361 I3362 G3363 R3364 L3365 R3366 K3367 R3368 A3369 V3372 V3373
A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 L3401 C3402 R3403 D3404 L3405 Y3406 A3407 L3408 Y3409 P3410 L3411 L3412 I3413 R3414 R3420 L3434 F3435 R3436 M3437 F3442 W3445 S3446 K3447 S3448 H3449 N3450 F3451 K3452 R3453 E3454 E3455 V3459

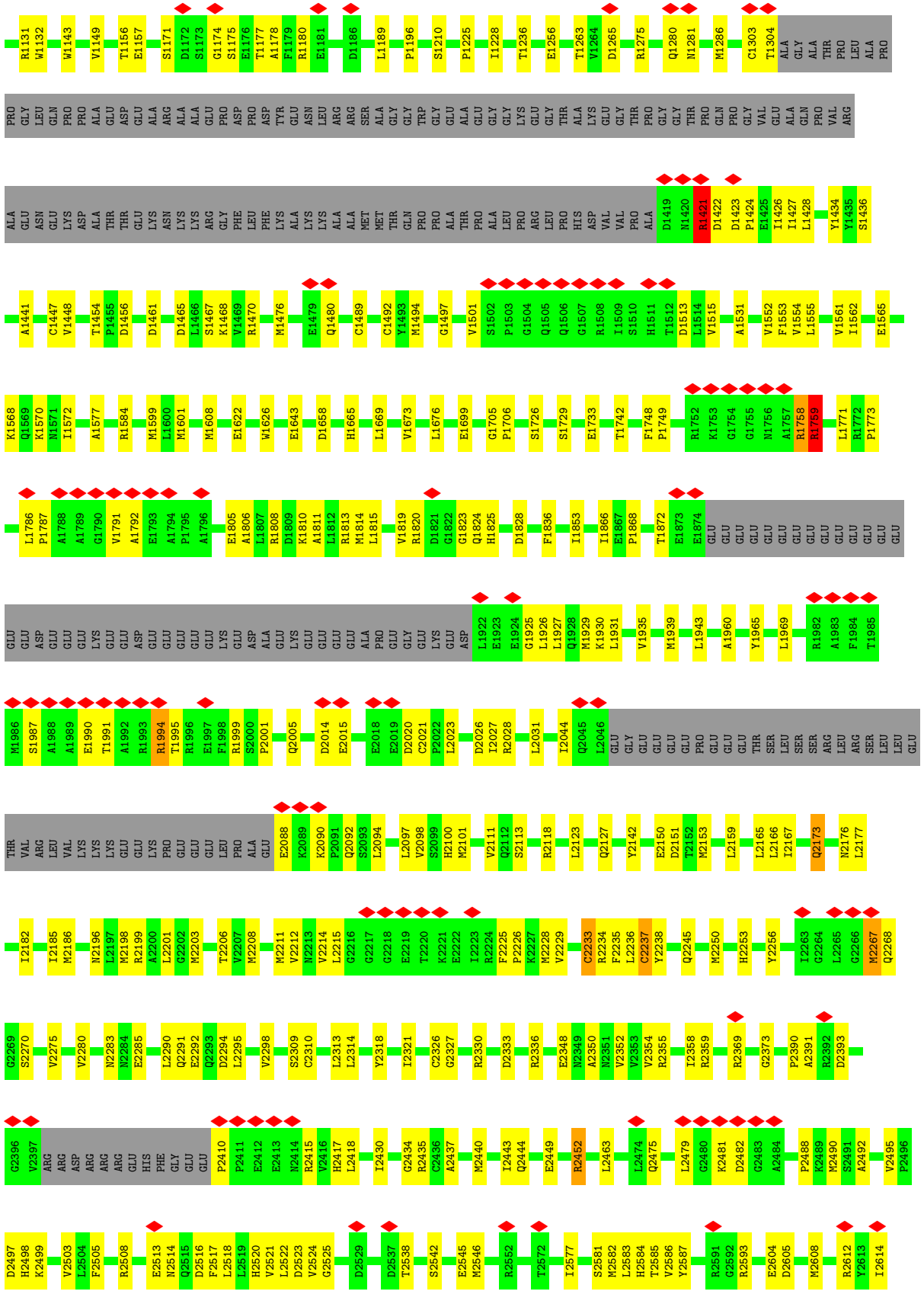




- Molecule 1: Ryanodine receptor 1

Chain B:

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PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG
ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 L1428 Y1434 Y1435 S1436
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L1786 P1787 A1788 A1789 G1790 V1791 A1792 E1793 A1794 P1795 A1796 E1805 A1806 L1807 R1808 D1809 K1810 A1811 L1812 R1813 M1814 L1815 V1819 R1820 D1821 G1822 G1823 Q1824 H1825 D1828 F1836 I1853 I1866 E1867 P1868 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 M1939 L1943 A1960 Y1965 L1969 R1982 A1983 F1984 T1985
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THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 P2091 Q2092 S2093 L2094 L2097 V2098 S2099 H2100 M2101 V2111 Q2112 S2113 R2118 L2123 Q2127 Y2142 E2150 D2151 T2152 M2153 L2159 L2165 L2166 I2167 Q2173 M2176 L2177
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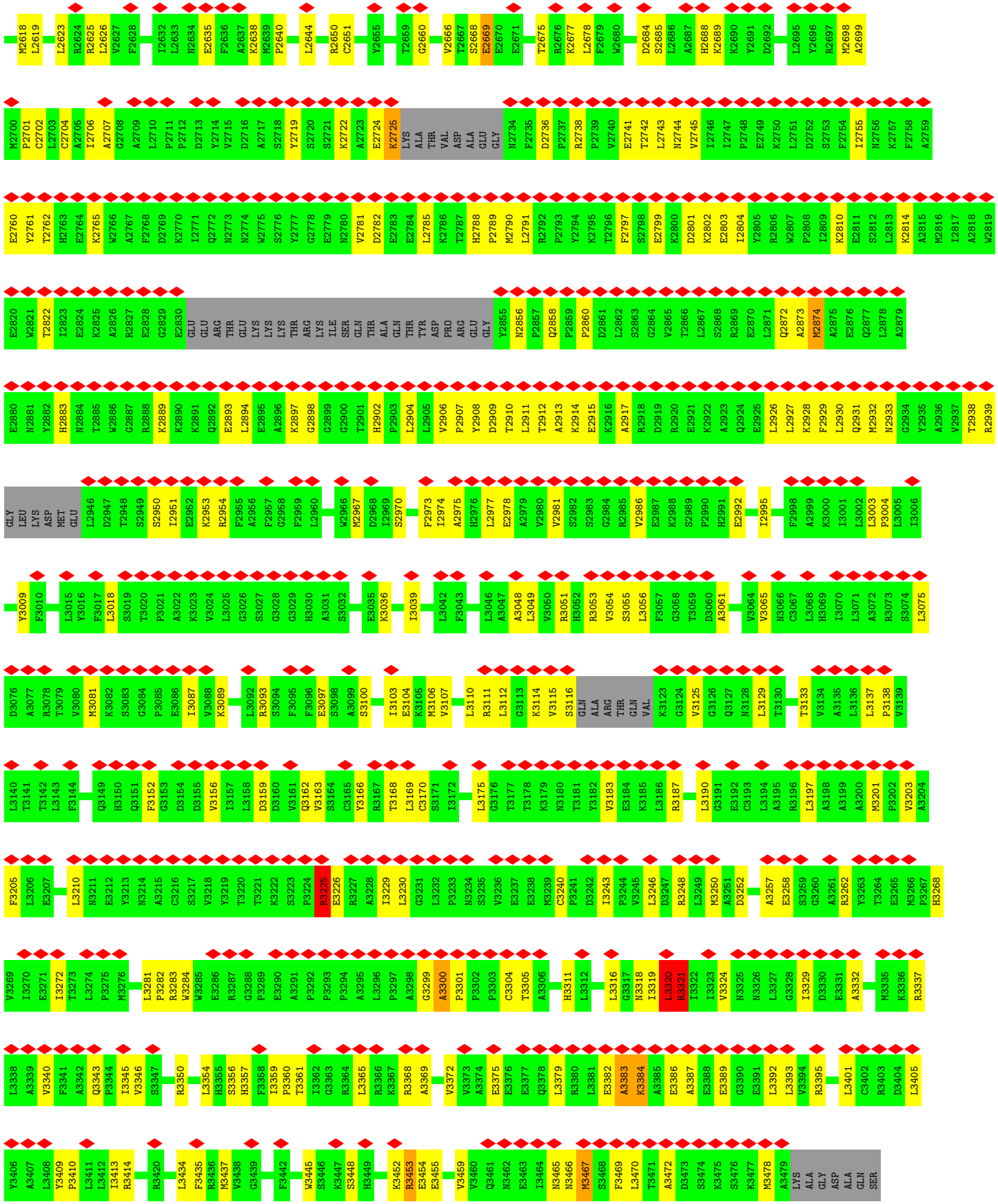
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L3140 T3141 T3142 L3143 F3144 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 L3169 C3170 S3171 I3172 L3175 G3176 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3186 R3187 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 P3202 V3203 A3204
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L3338 A3339 V3340 F3341 A3342 Q3343 P3344 I3345 V3346 S3347 R3350 L3354 H3355 S3356 H3357 F3358 I3359 P3360 T3361 I3362 G3363 R3364 L3365 R3366 K3367 R3368 A3369 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 L3401 C3402 R3403 D3404 L3405
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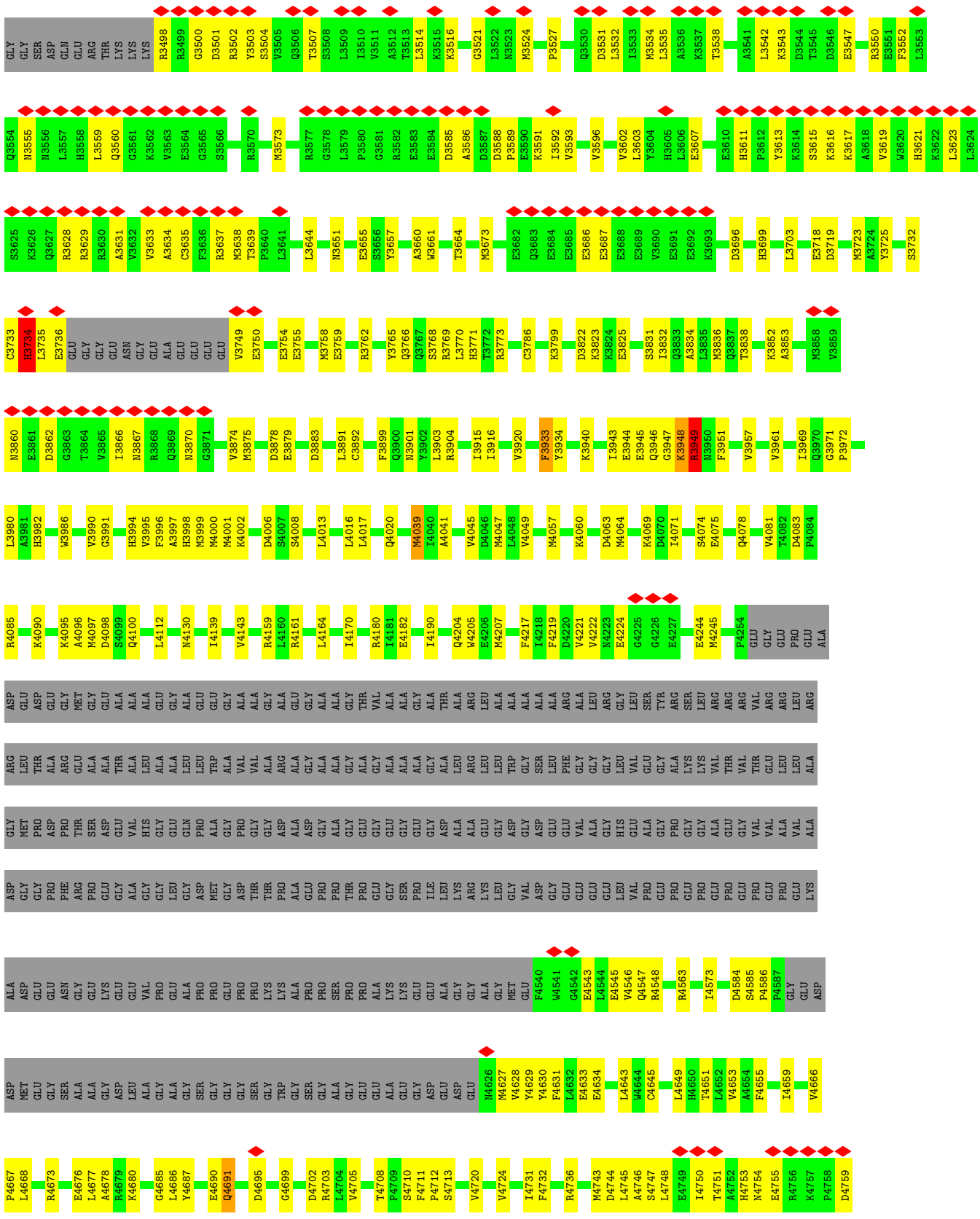
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ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG
ARG LEU THR ALA ARG GLU ALA THR ALA ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA
GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY GLU GLU GLY GLU GLU GLY ASP ALA ARG GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU GLU ALA GLY PRO GLY GLY GLY ALA GLU GLY VAL VAL ALA VAL
ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY LEU GLY ALA ASP MET GLY ASP THR THR PRO ALA GLU PRO GLU PRO PRO GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU GLU PRO GLU PRO PRO GLU PRO GLU PRO GLU GLU LYS
ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO PRO SER PRO PRO PRO ALA ALA LYS LYS GLU GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 R4548 R4563 I4573 D4584 S4585 P4586 P4587 GLY GLU ASP
ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY ALA GLY GLU GLU ASP GLU GLU GLY ASP GLU ASP GLU M4626 M4627 V4628 Y4629 Y4630 F4631 L4632 E4633 E4634 L4643 W4644 C4645 L4649 H4650 T4651 L4652 V4653 A4654 F4655 I4659 V4666
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S5037

- Molecule 1: Ryanodine receptor 1

Chain D: 20% 65% 21% 13%

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P279 L280 T294 E295 D296 Q297 G298 V301 H308 T309 K310 S313 R317 E321 K322 L323 D324 T325 A326 P327 K328 R329 D330 I339 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 M384 Q399 M403 I404 K416 S428 G429 A432

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F1124 N1125 G1126 H1127 R1128 R1131 W1132 W1143 V1149 T1156 E1157 V1168 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 D1186 L1189 P1196 S1210 P1225 I1228 T1236 E1256 T1263 V1264 D1265 R1275 Q1280 N1281 M1286 C1303 T1304 ALA GLY

ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY GLY THR PRO GLN PRO GLY VAL

GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 I1426

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GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 M1939 L1943 E1956 A1960 Y1965 L1969

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SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 P2091 Q2092 S2093 L2094 L2097 V2098 S2099 H2100 M2101 V2111 Q2112 S2113 V2117 R2118 A2119 M2120 Y2142 E2150 D2151 T2152 M2153 L2159 L2165 L2166 I2167 Q2173

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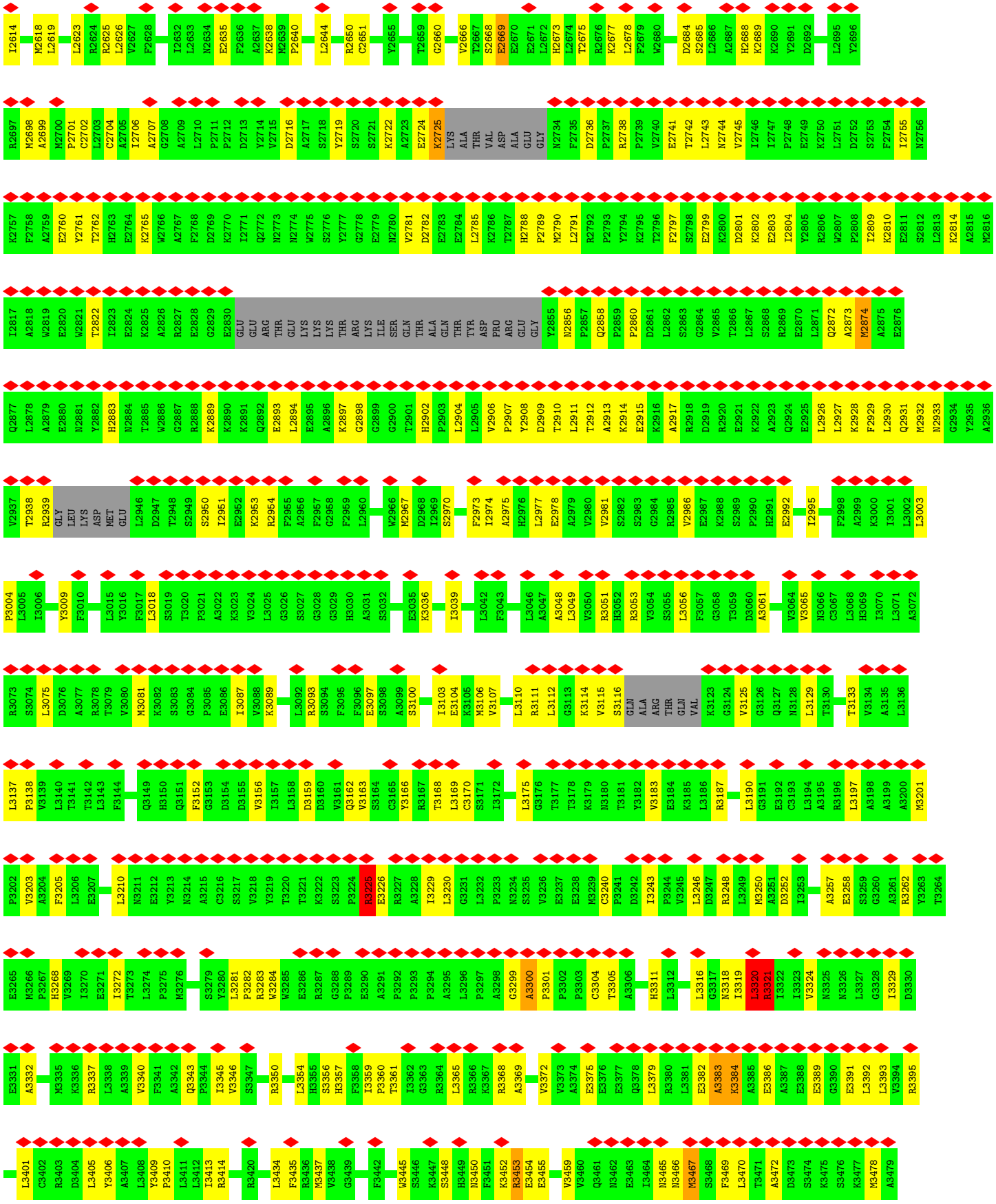
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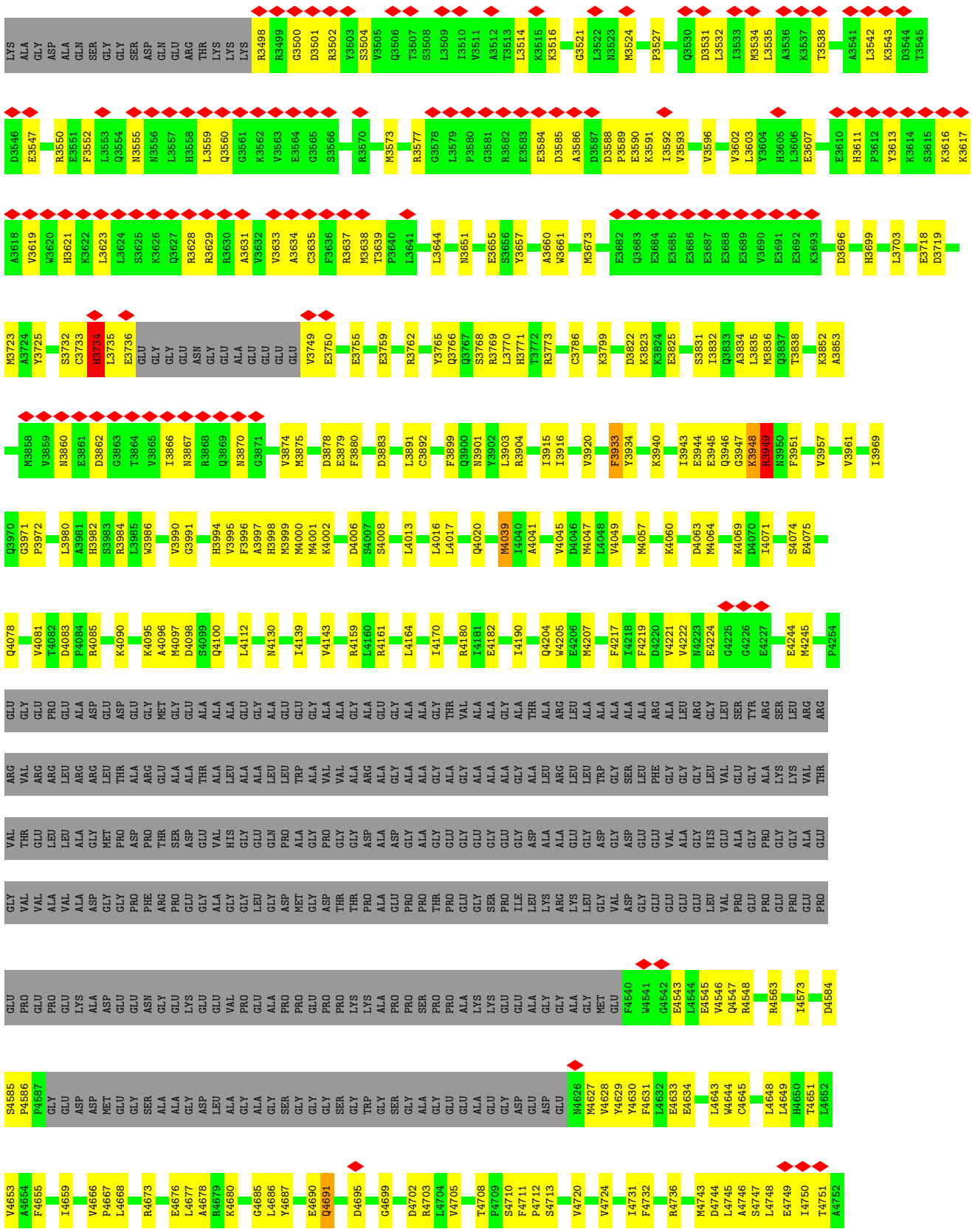
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GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO PRO PRO PRO LYS LYS ALA PRO PRO SER PRO PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 R4548 R4563 I4573 D4584
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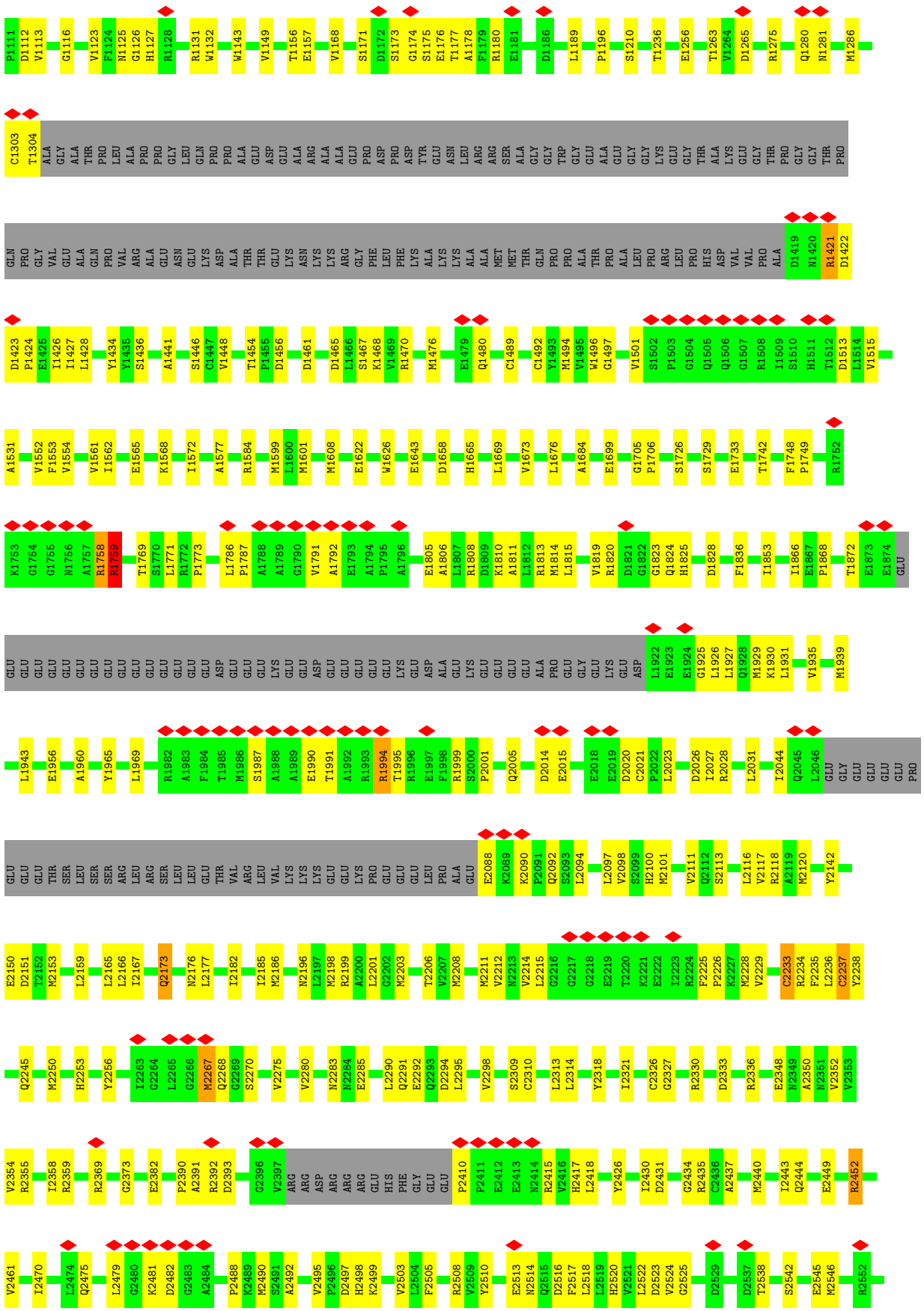
• Molecule 1: Ryanodine receptor 1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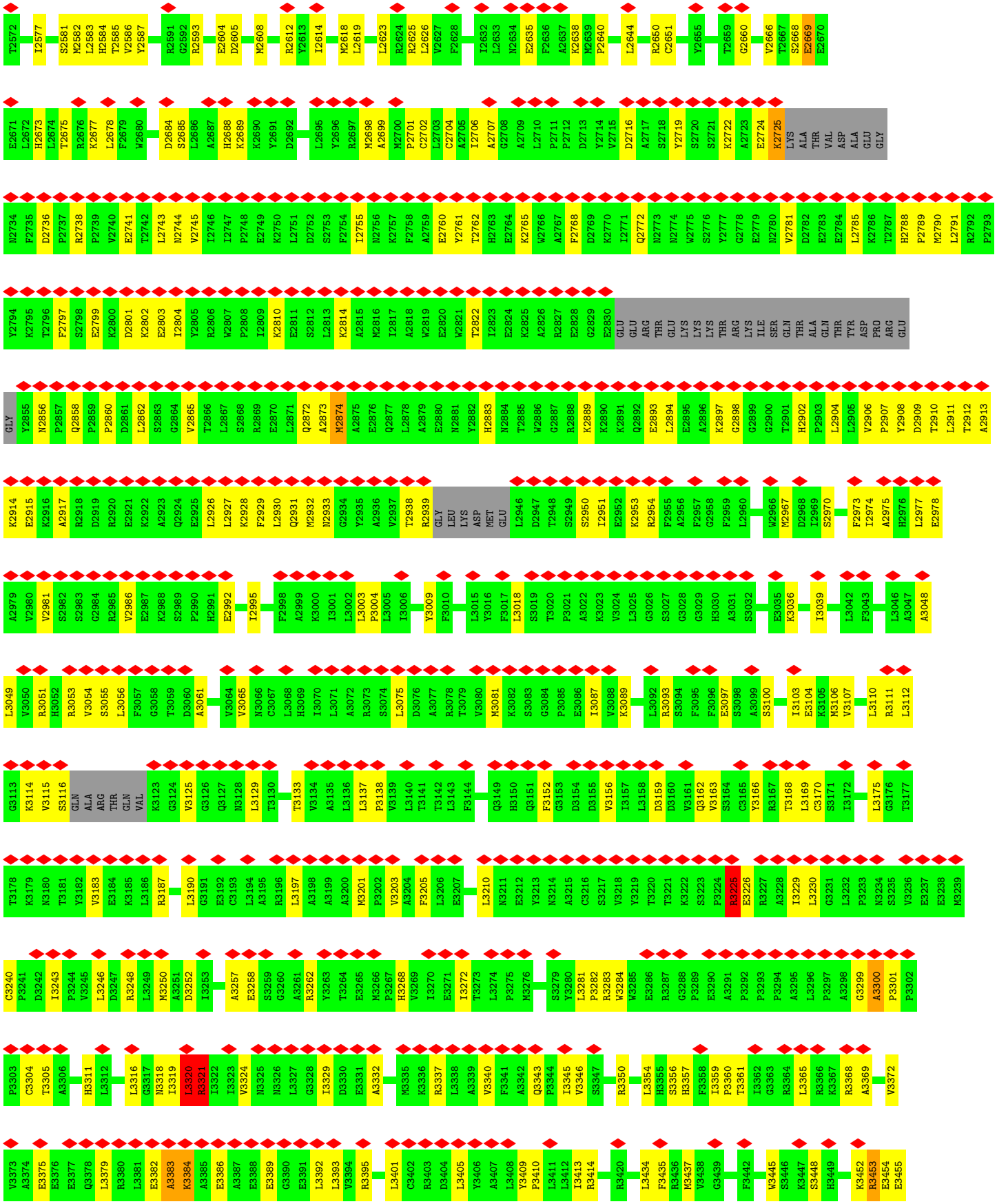
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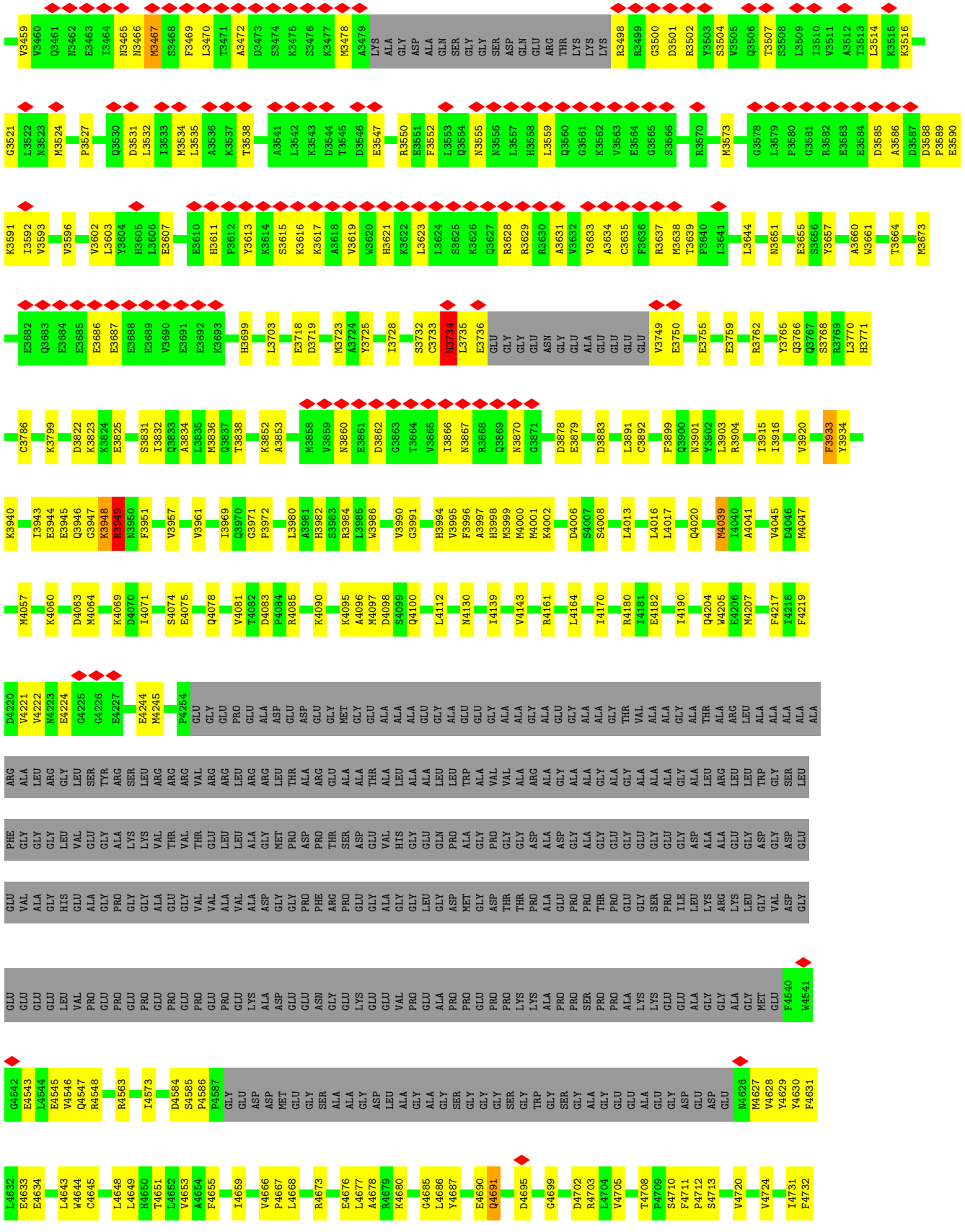
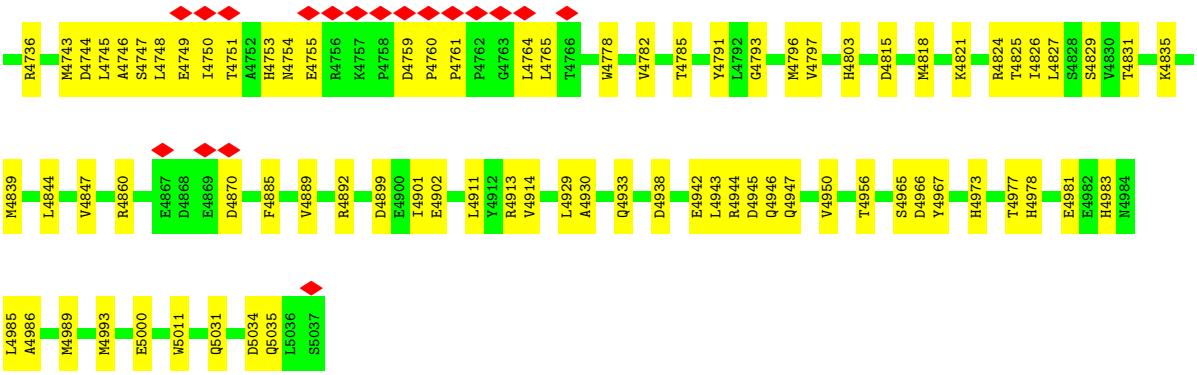
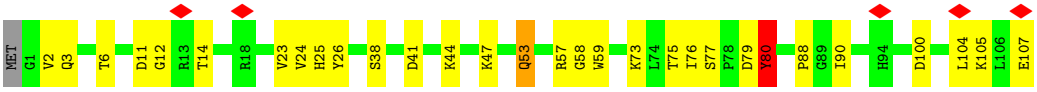
G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 V3125 G3126 Q3127 N3128 L3129 T3130 T3133 V3134 A3135 L3136 L3137 P3138 V3139 L3140 T3141 T3142 L3143 F3144 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 L3169 C3170 S3171 I3172 L3175 G3176 T3177
T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3186 R3187 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239
C3240 P3241 D3242 I3243 P3244 V3245 L3246 D3247 R3248 L3249 M3250 A3251 D3252 I3253 A3257 E3258 S3259 G3260 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 S3279 Y3280 I3281 P3282 R3283 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302
P3303 C3304 T3305 A3306 H3311 L3312 L3316 G3317 N3318 I3319 L3320 R3321 I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 M3335 K3336 R3337 L3338 A3339 V3340 F3341 A3342 Q3343 P3344 I3345 V3346 S3347 R3350 L3354 H3355 S3356 H3357 F3358 I3359 P3360 T3361 I3362 G3363 R3364 L3365 R3366 K3367 R3368 A3369 V3372
V3373 A3374 E3375 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 L3401 C3402 R3403 D3404 L3405 Y3406 A3407 L3408 Y3409 P3410 L3411 I3412 I3413 R3414 R3420 L3434 F3435 R3436 M3437 Y3438 G3439 F3442 W3445 S3446 K3447 S3448 H3449 K3452 R3453 E3454 E3455


V3459 V3460 Q3461 N3462 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 R3502 Y3503 S3504 V3505 Q3506 T3507 S3508 L3509 I3510 V3511 A3512 T3513 L3514 K3515 K3516
G3521 L3522 N3523 M3524 P3527 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 A3541 L3542 K3543 D3544 T3545 D3546 E3547 R3550 E3551 F3552 L3553 Q3554 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 S3566 R3570 M3573 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590
K3591 I3592 V3593 V3596 V3602 L3603 Y3604 H3605 L3606 E3607 E3610 H3611 P3612 Y3613 K3614 S3615 K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 T3639 P3640 L3641 L3644 N3651 E3655 S3656 Y3657 A3660 W3661 T3664 M3673
E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 H3699 L3703 E3718 D3719 M3723 A3724 Y3725 I3728 S3732 C3733 H3734 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU V3749 E3750 E3755 E3759 R3762 Y3765 Q3766 Q3767 S3768 R3769 L3770 H3771
C3786 K3799 D3822 K3823 K3824 E3825 S3831 I3832 Q3833 A3834 L3835 M3836 Q3837 T3838 K3852 A3853 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 D3878 E3879 D3883 L3891 C3892 F3899 Q3900 N3901 Y3902 L3903 R3904 I3915 I3916 V3920 F3933 Y3934
K3940 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 N3950 F3951 V3957 V3961 I3969 Q3970 G3971 P3972 L3980 A3981 H3982 S3983 R3984 L3985 W3986 V3990 G3991 H3994 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002 D4006 S4007 S4008 L4013 L4016 L4017 Q4020 M4039 I4040 A4041 V4045 D4046 M4047
M4057 K4060 D4063 M4064 K4069 D4070 I4071 S4074 E4075 Q4078 V4081 T4082 D4083 P4084 R4085 K4090 K4095 A4096 M4097 D4098 S4099 Q4100 L4112 N4130 I4139 V4143 R4161 L4164 I4170 R4180 I4181 E4182 I4190 Q4204 W4205 E4206 M4207 F4217 I4218 F4219
D4220 V4221 V4222 N4223 E4224 G4225 G4226 E4227 E4244 M4245 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA ALA GLU GLU GLY GLY ALA GLY ALA GLU GLY ALA ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU LEU ALA ALA
ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA ALA LEU LEU LEU TRP GLY SER LEU
PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN GLN PRO ALA GLY PRO GLY GLY GLY ASP ALA ASP GLY ALA GLY GLU GLU GLU GLY GLY ASP GLU
GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY GLY ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER ILE LEU LEU GLY VAL ASP GLY
GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS LYS GLU GLU PRO GLU GLU ASP GLU GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO PRO ALA LYS LYS GLU GLU ALA ALA GLY GLY ALA GLY MET GLU F4540 W4541
G4542 E4543 L4544 E4545 V4546 Q4547 R4548 R4563 I4573 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY ASP VAL PRO GLU GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU GLU M4626 M4627 V4628 Y4629 Y4630 F4631
L4632 E4633 E4634 L4643 W4644 C4645 L4648 L4649 H4650 T4651 L4652 V4653 A4654 F4655 I4659 V4666 P4667 L4668 R4673 E4676 L4677 A4678 R4679 K4680 G4685 L4686 Y4687 E4690 Q4691 D4695 G4699 D4702 R4703 L4704 V4705 T4708 P4709 S4710 F4711 P4712 S4713 V4720 V4724 I4731 F4732



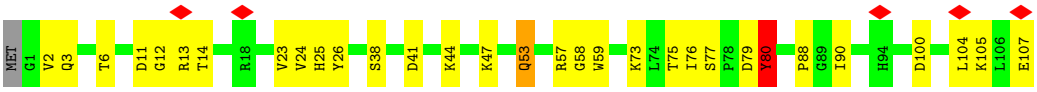
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E:



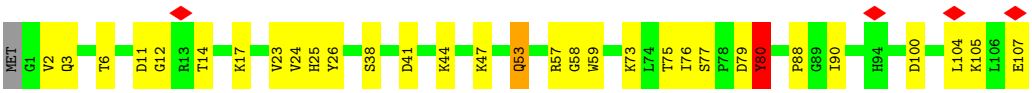
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:



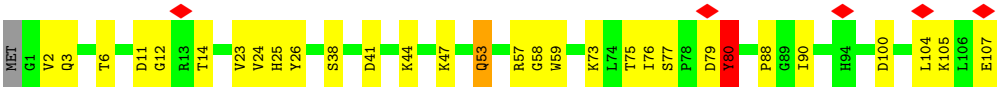
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94090	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.513	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, A1BD3, CA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	29/35977 (0.1%)	0.61	57/48726 (0.1%)
1	B	0.37	29/35977 (0.1%)	0.61	57/48726 (0.1%)
1	C	0.37	29/35977 (0.1%)	0.61	57/48726 (0.1%)
1	D	0.37	29/35977 (0.1%)	0.61	57/48726 (0.1%)
2	E	1.03	9/850 (1.1%)	1.42	11/1146 (1.0%)
2	F	1.03	9/850 (1.1%)	1.42	11/1146 (1.0%)
2	G	1.04	9/850 (1.1%)	1.42	11/1146 (1.0%)
2	H	1.03	9/850 (1.1%)	1.42	11/1146 (1.0%)
All	All	0.39	152/147308 (0.1%)	0.64	272/199488 (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	1	11
1	B	1	11
1	C	1	11
1	D	1	11
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	4	48

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3949	ARG	NE-CZ	-19.60	1.11	1.33
1	B	3949	ARG	NE-CZ	-19.60	1.11	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3949	ARG	NE-CZ	-19.60	1.11	1.33
1	D	3949	ARG	NE-CZ	-19.59	1.11	1.33
1	D	3321	ARG	CG-CD	-19.16	0.94	1.52

The worst 5 of 272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3321	ARG	N-CA-CB	36.30	164.29	110.20
1	D	3321	ARG	N-CA-CB	36.30	164.29	110.20
1	A	3321	ARG	N-CA-CB	36.29	164.28	110.20
1	C	3321	ARG	N-CA-CB	36.29	164.28	110.20
1	D	3949	ARG	NE-CZ-NH1	-34.53	86.97	121.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	3321	ARG	CA
1	B	3321	ARG	CA
1	D	3321	ARG	CA
1	C	3321	ARG	CA

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1421	ARG	Sidechain
1	A	156	GLN	Sidechain
1	A	1758	ARG	Sidechain
1	A	2173	GLN	Sidechain
1	A	3320	LEU	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	35150	0	34794	881	0
1	B	35150	0	34794	863	0
1	C	35150	0	34794	863	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	35150	0	34794	869	0
2	E	831	0	829	25	0
2	F	831	0	829	25	0
2	G	831	0	829	28	0
2	H	831	0	829	26	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	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	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	14	0	0	0	0
6	B	14	0	0	0	0
6	C	14	0	0	0	0
6	D	14	0	0	0	0
All	All	144112	0	142540	3523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 3523 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:2237:CYS:SG	1:B:2237:CYS:CB	2.11	1.39
1:A:2237:CYS:CB	1:A:2237:CYS:SG	2.11	1.38
1:D:2237:CYS:CB	1:D:2237:CYS:SG	2.11	1.37
1:C:2237:CYS:SG	1:C:2237:CYS:CB	2.11	1.37
1:C:2229:VAL:HG11	1:C:2267:MET:HE1	1.26	1.18

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	4385/5037 (87%)	4256 (97%)	123 (3%)	6 (0%)	48	71
1	B	4385/5037 (87%)	4256 (97%)	123 (3%)	6 (0%)	48	71
1	C	4385/5037 (87%)	4256 (97%)	123 (3%)	6 (0%)	48	71
1	D	4385/5037 (87%)	4256 (97%)	123 (3%)	6 (0%)	48	71
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
All	All	17960/20580 (87%)	17432 (97%)	504 (3%)	24 (0%)	49	71

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	908	VAL
1	A	3300	ALA
1	A	3949	ARG
1	B	55	ALA

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	3836/4276 (90%)	3826 (100%)	10 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	3836/4276 (90%)	3826 (100%)	10 (0%)	86 93
1	C	3836/4276 (90%)	3826 (100%)	10 (0%)	86 93
1	D	3836/4276 (90%)	3826 (100%)	10 (0%)	86 93
2	E	89/90 (99%)	88 (99%)	1 (1%)	65 79
2	F	89/90 (99%)	88 (99%)	1 (1%)	65 79
2	G	89/90 (99%)	88 (99%)	1 (1%)	65 79
2	H	89/90 (99%)	88 (99%)	1 (1%)	65 79
All	All	15700/17464 (90%)	15656 (100%)	44 (0%)	84 93

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1759	ARG
1	C	156	GLN
1	D	2268[A]	GLN
1	D	3321	ARG
1	C	960	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4034	ASN
1	C	2856	ASN
1	D	4946	GLN
1	C	725	HIS
1	C	3850	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	5301	-	32,33,33	0.28	0	48,52,52	0.70	0
6	A1BD3	A	5304	-	15,15,15	4.96	9 (60%)	19,21,21	5.14	9 (47%)
6	A1BD3	C	5304	-	15,15,15	4.96	9 (60%)	19,21,21	5.15	9 (47%)
3	ATP	B	5301	-	32,33,33	0.28	0	48,52,52	0.70	0
3	ATP	D	5301	-	32,33,33	0.27	0	48,52,52	0.70	0
6	A1BD3	B	5304	-	15,15,15	4.95	9 (60%)	19,21,21	5.15	9 (47%)
6	A1BD3	D	5304	-	15,15,15	4.96	9 (60%)	19,21,21	5.14	9 (47%)
3	ATP	C	5301	-	32,33,33	0.28	0	48,52,52	0.70	0

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	A	5301	-	-	12/22/38/38	0/3/3/3
6	A1BD3	A	5304	-	-	1/3/3/3	0/2/2/2
6	A1BD3	C	5304	-	-	1/3/3/3	0/2/2/2
3	ATP	B	5301	-	-	12/22/38/38	0/3/3/3
3	ATP	D	5301	-	-	12/22/38/38	0/3/3/3
6	A1BD3	B	5304	-	-	1/3/3/3	0/2/2/2
6	A1BD3	D	5304	-	-	1/3/3/3	0/2/2/2
3	ATP	C	5301	-	-	12/22/38/38	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5304	A1BD3	O2-C8	9.75	1.40	1.23
6	B	5304	A1BD3	O2-C8	9.75	1.40	1.23
6	C	5304	A1BD3	O2-C8	9.75	1.40	1.23
6	D	5304	A1BD3	O2-C8	9.74	1.40	1.23
6	A	5304	A1BD3	O1-C1	8.86	1.40	1.23

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	5304	A1BD3	C3-N2-C4	15.90	114.09	103.45
6	B	5304	A1BD3	C3-N2-C4	15.89	114.09	103.45
6	D	5304	A1BD3	C3-N2-C4	15.89	114.08	103.45
6	A	5304	A1BD3	C3-N2-C4	15.87	114.07	103.45
6	B	5304	A1BD3	C2-C4-N2	-11.85	103.33	111.63

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O1A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	D	5301	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

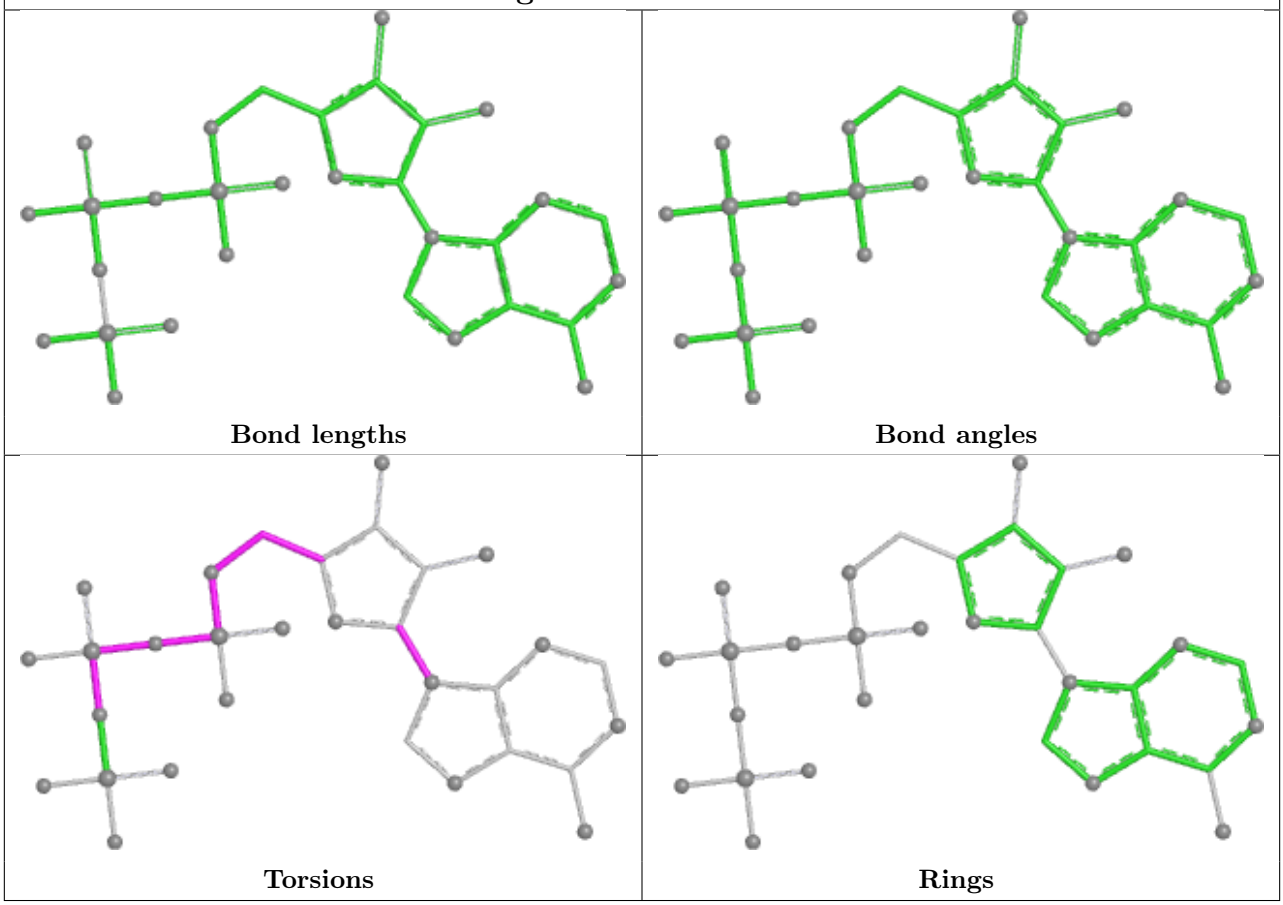
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	ATP	1	0
3	B	5301	ATP	1	0
3	D	5301	ATP	1	0
3	C	5301	ATP	1	0

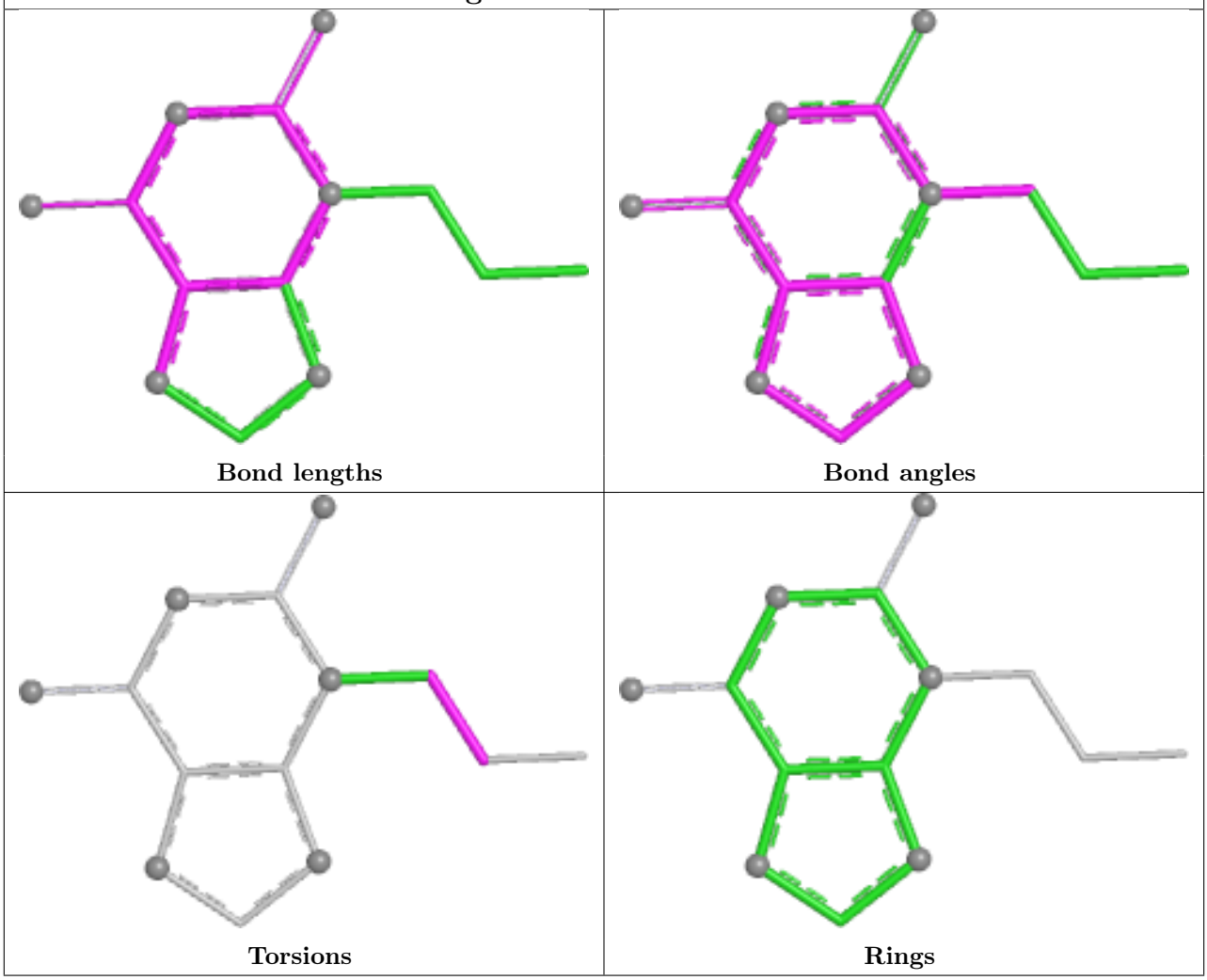
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

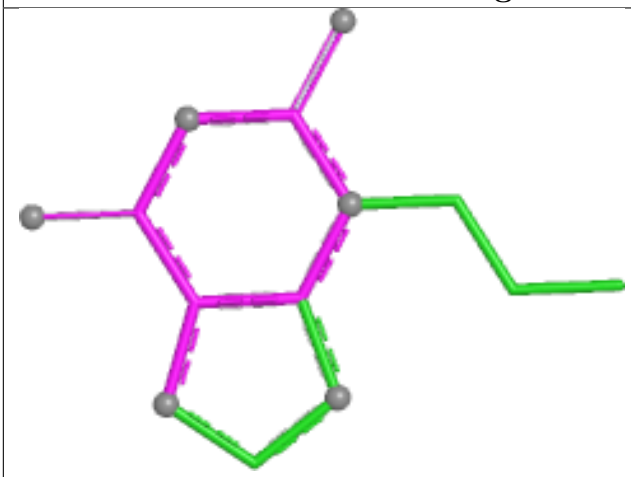
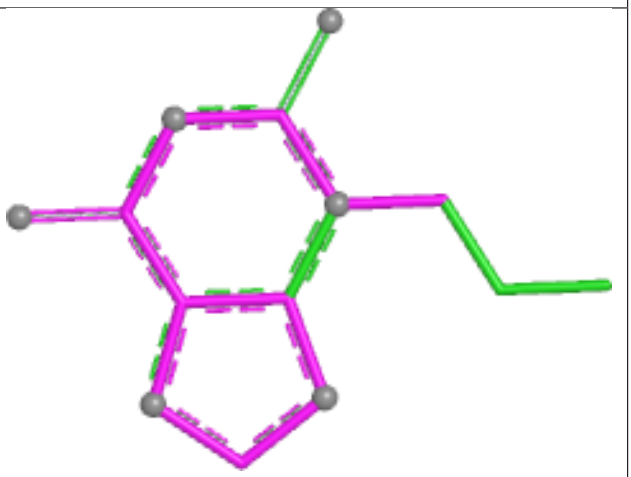
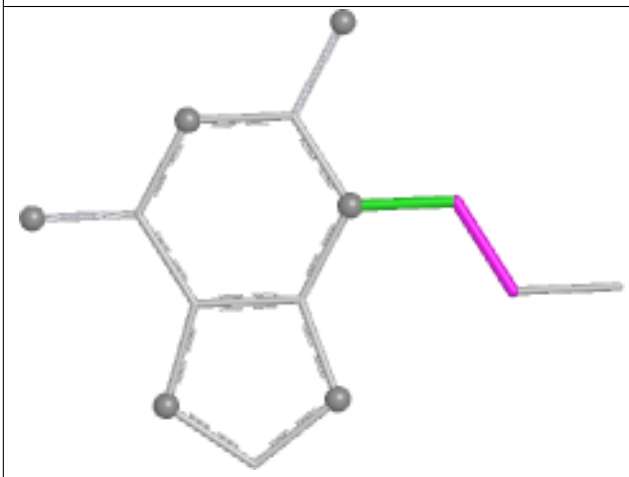
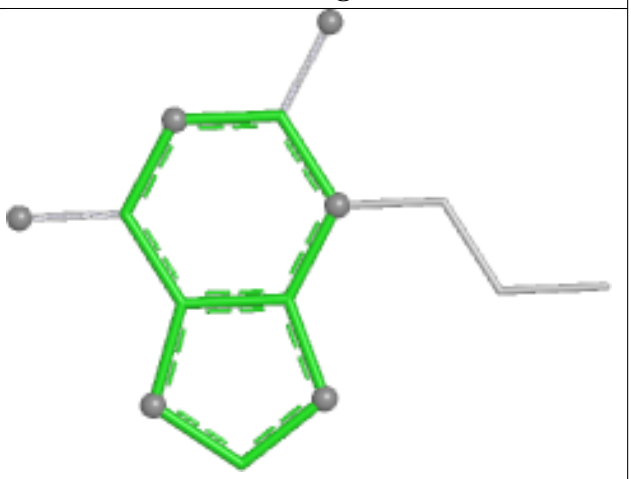
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 5301

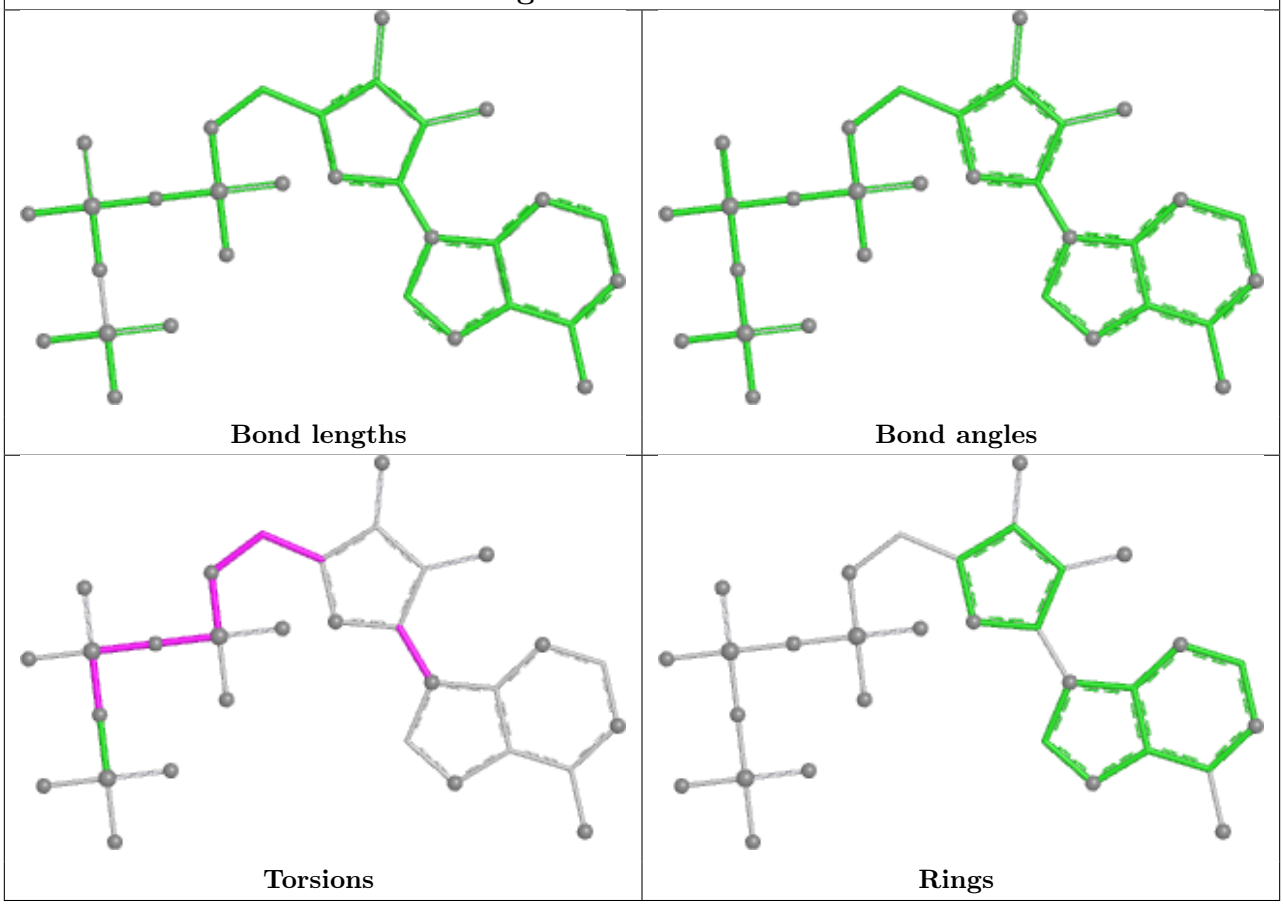


Ligand A1BD3 A 5304

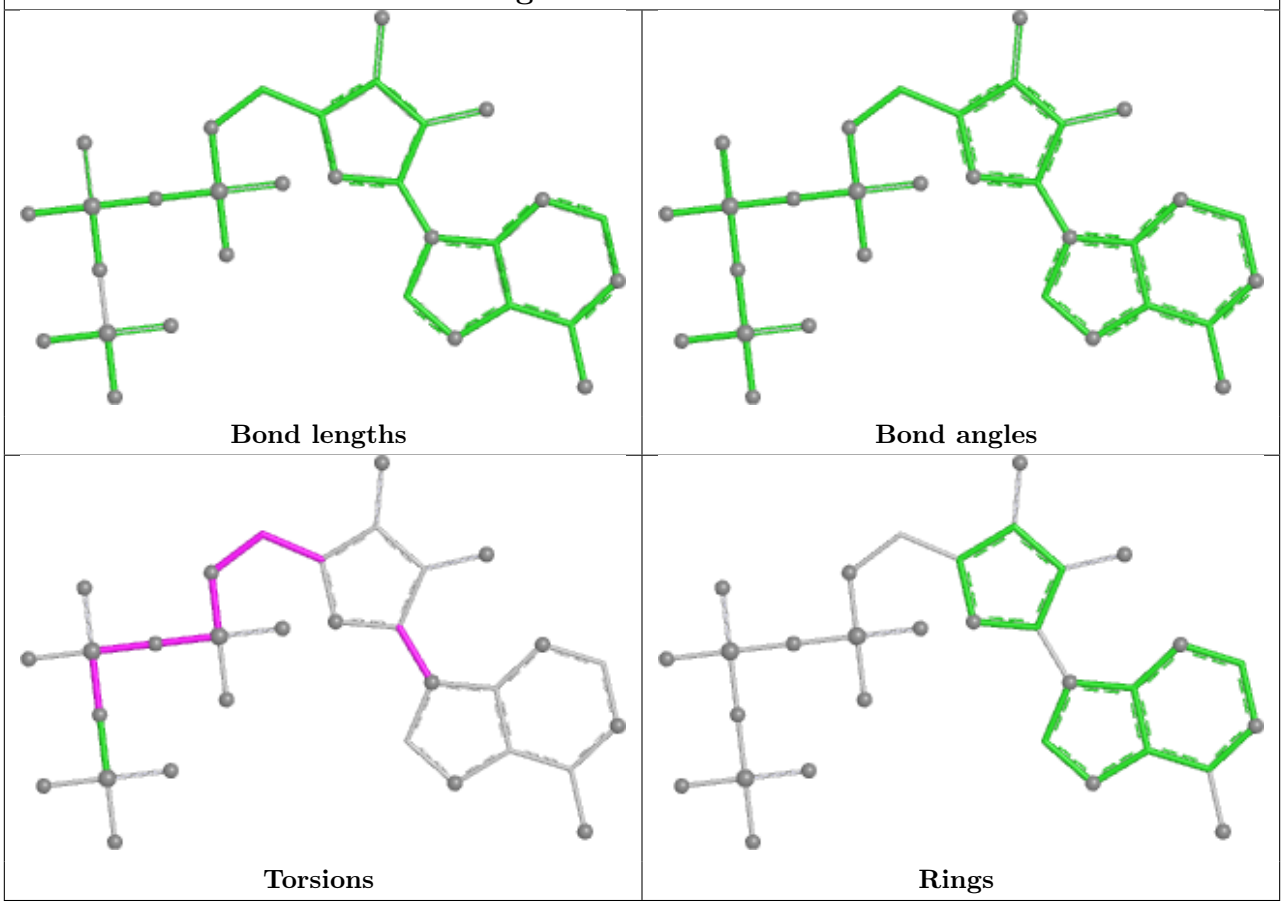


Ligand A1BD3 C 5304	
 Bond lengths	 Bond angles
 Torsions	 Rings

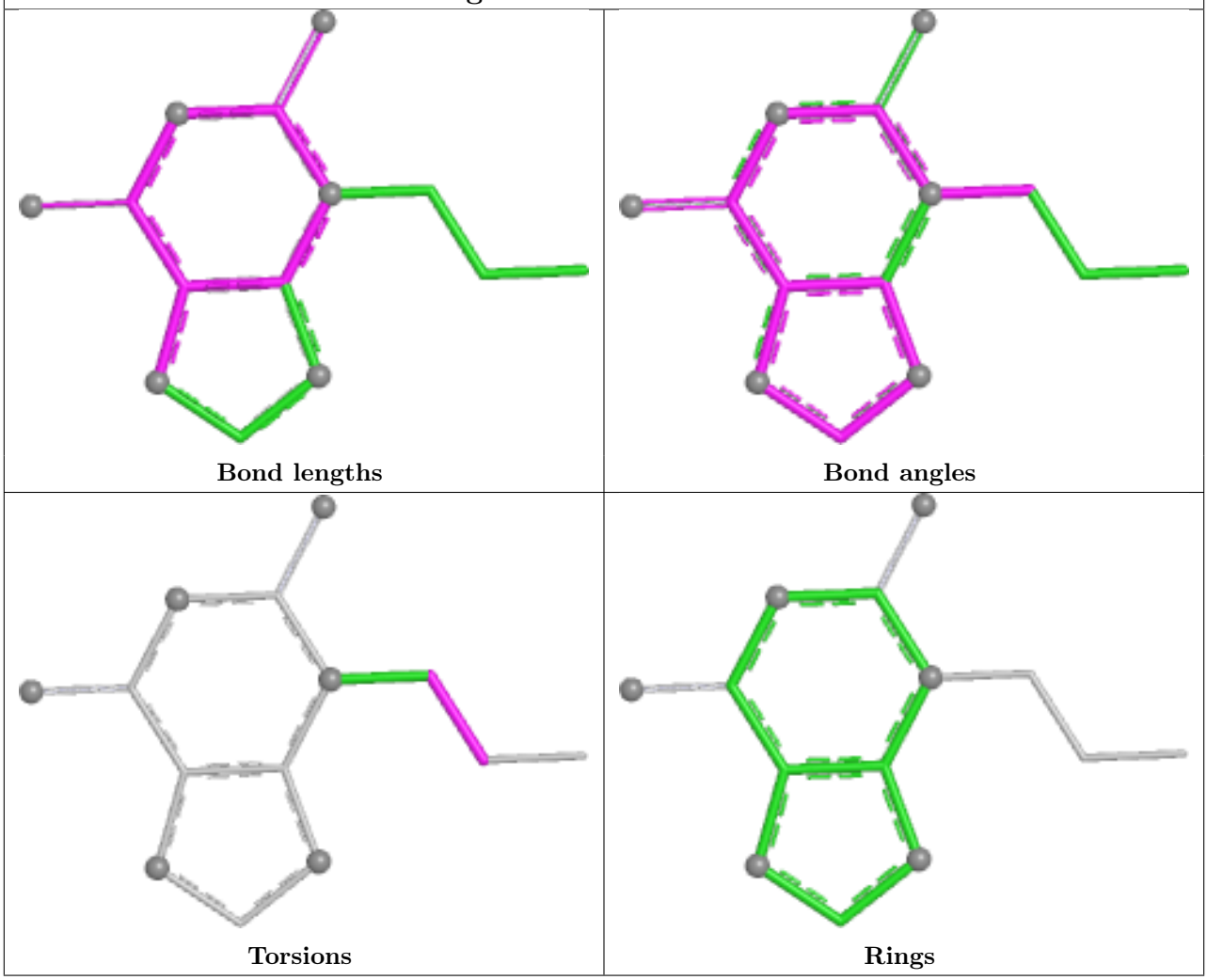
Ligand ATP B 5301



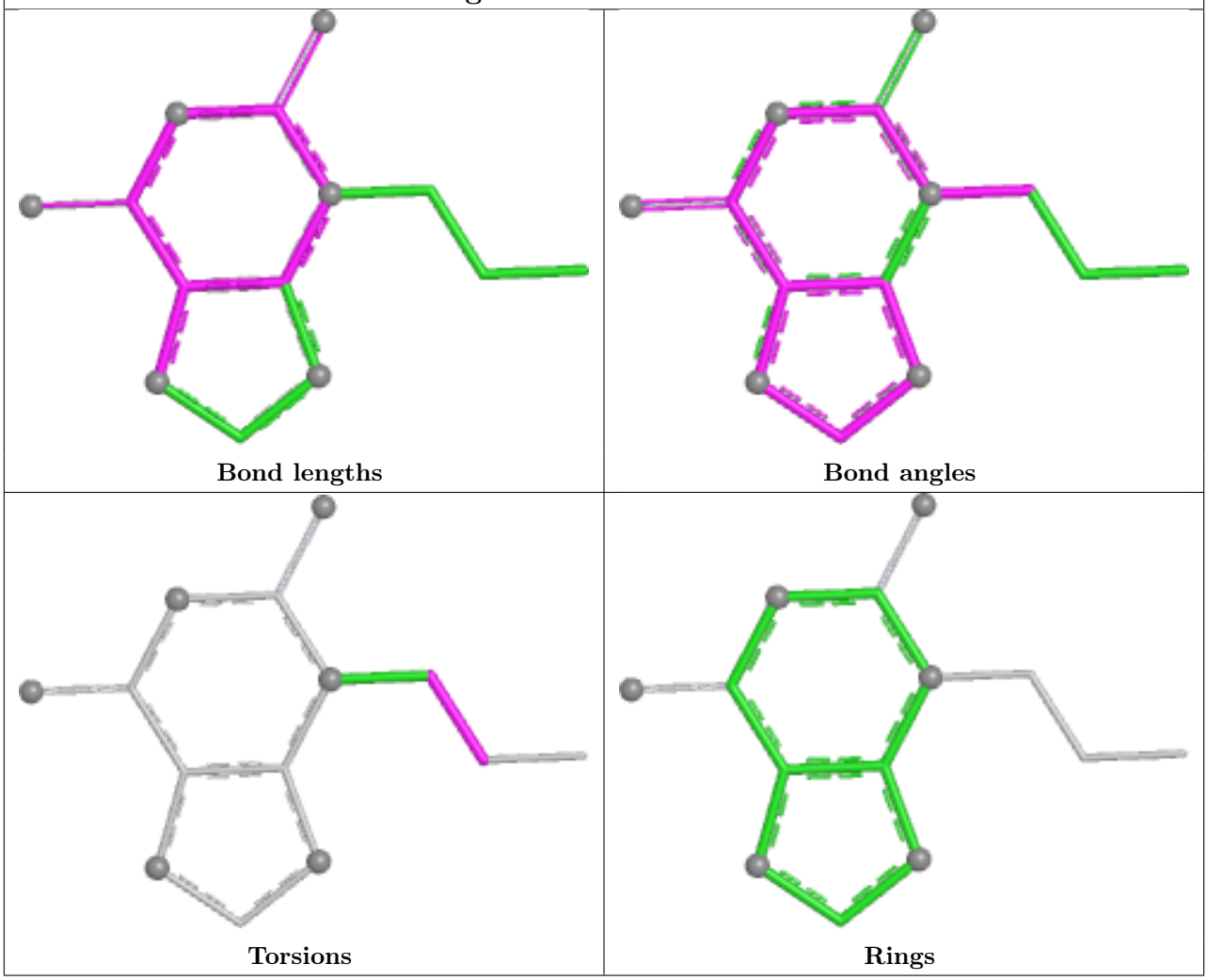
Ligand ATP D 5301



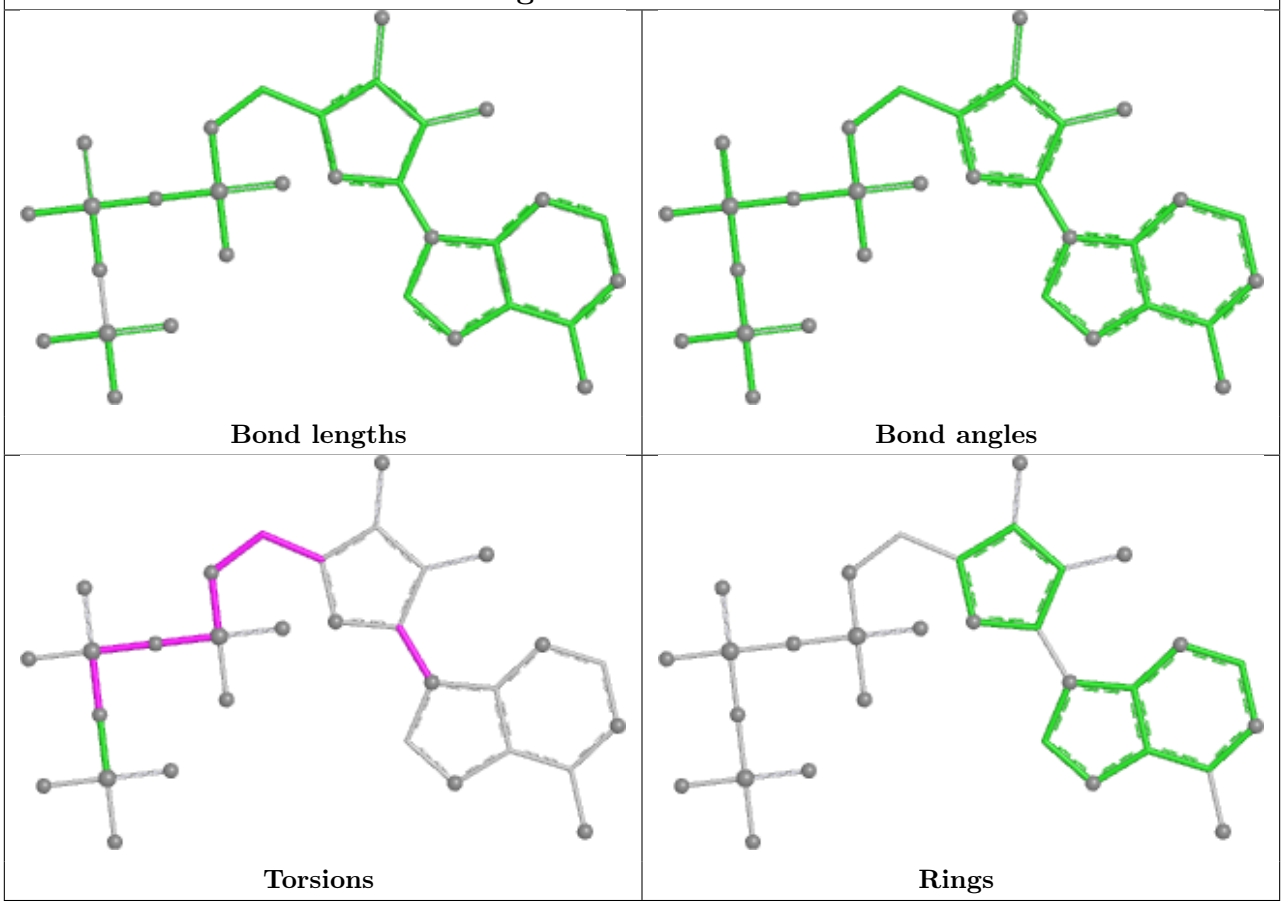
Ligand A1BD3 B 5304



Ligand A1BD3 D 5304



Ligand ATP C 5301



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.

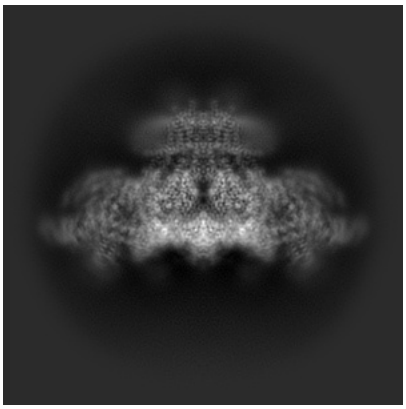
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-47390. These allow visual inspection of the internal detail of the map and identification of artifacts.

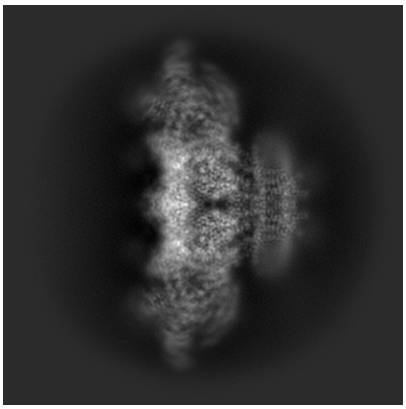
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

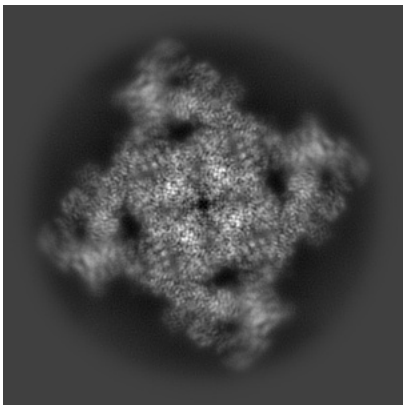
6.1.1 Primary map



X

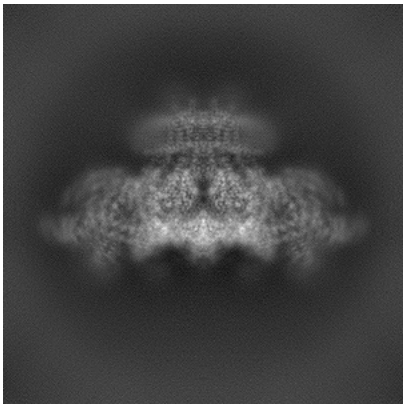


Y

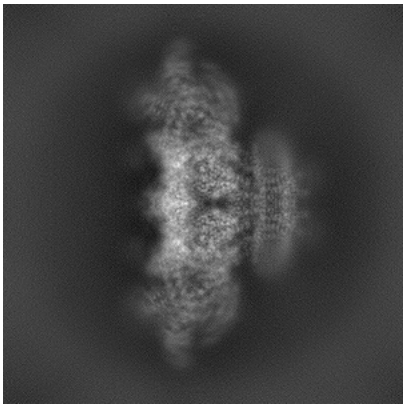


Z

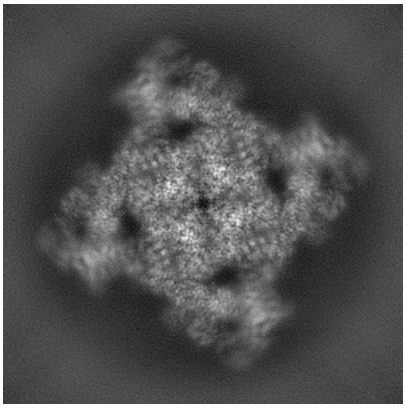
6.1.2 Raw map



X



Y

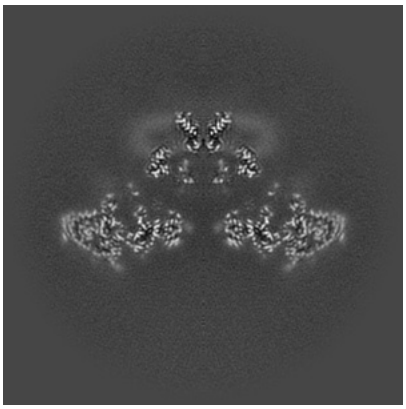


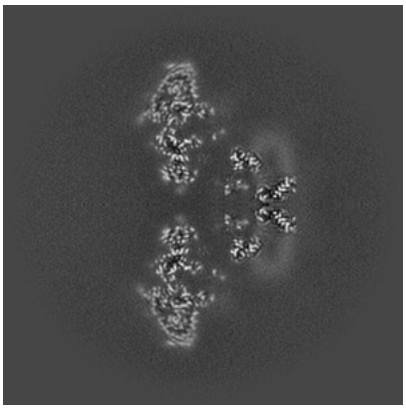
Z

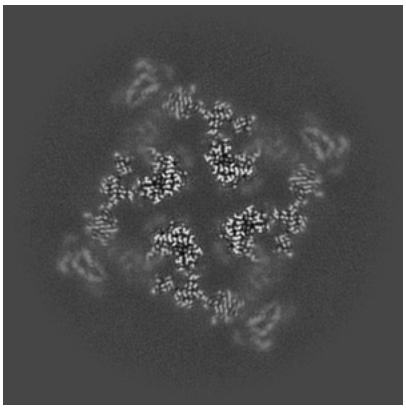
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

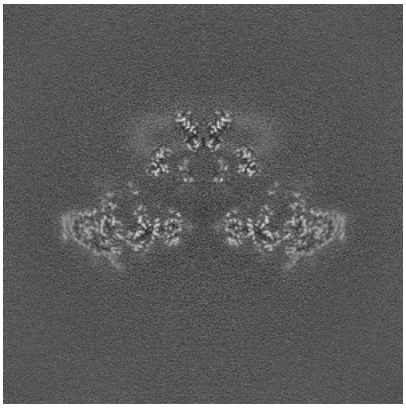
6.2.1 Primary map

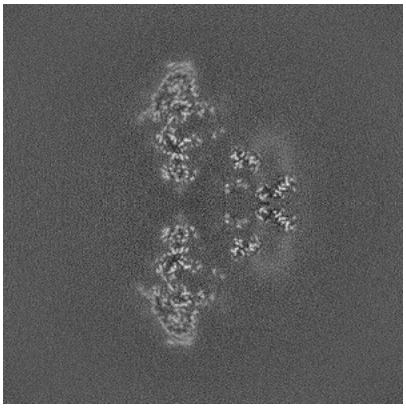

X Index: 256

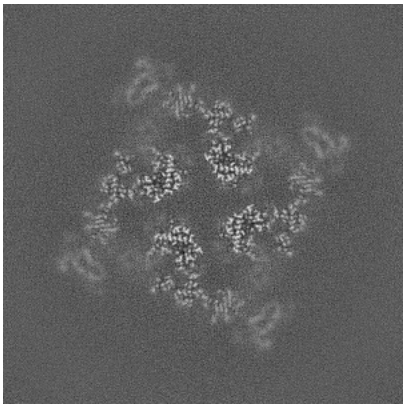

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

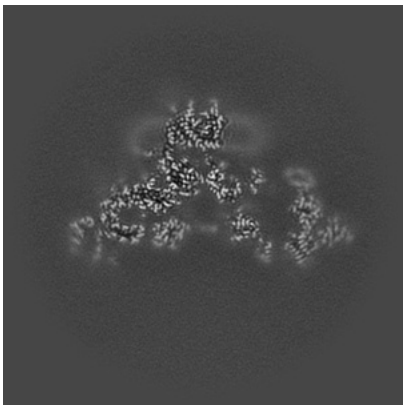

Y Index: 256


Z Index: 256

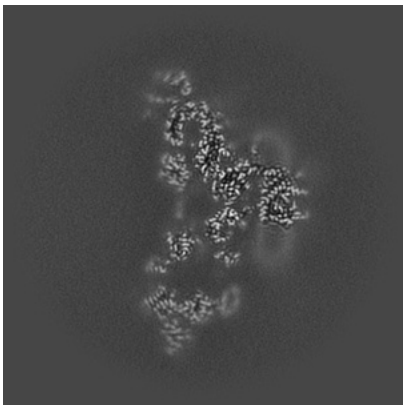
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

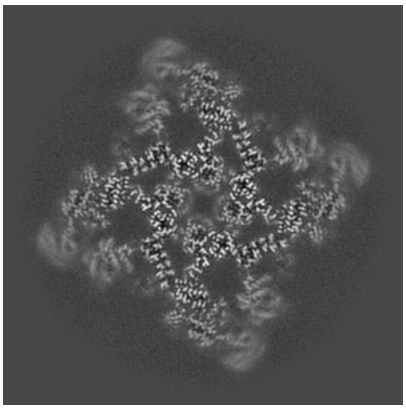
6.3.1 Primary map



X Index: 239

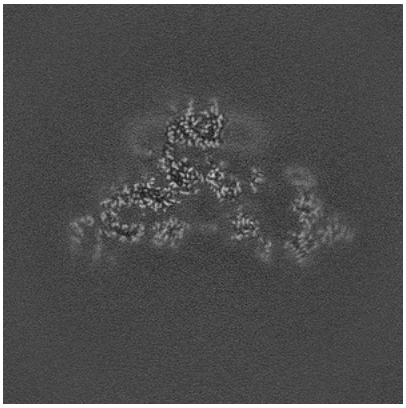


Y Index: 239

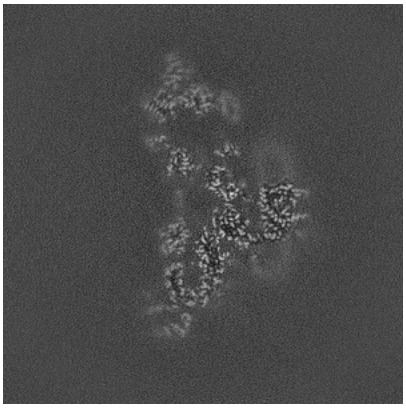


Z Index: 229

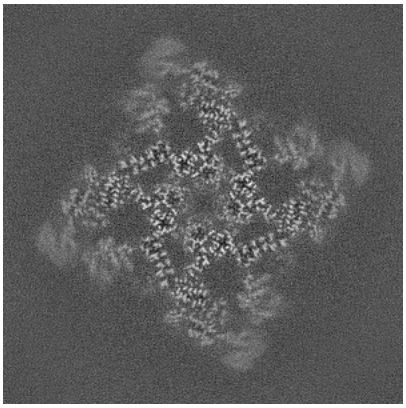
6.3.2 Raw map



X Index: 239



Y Index: 273

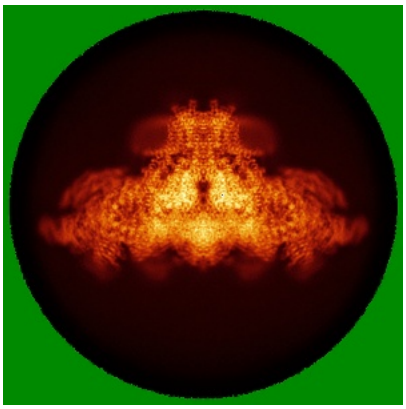


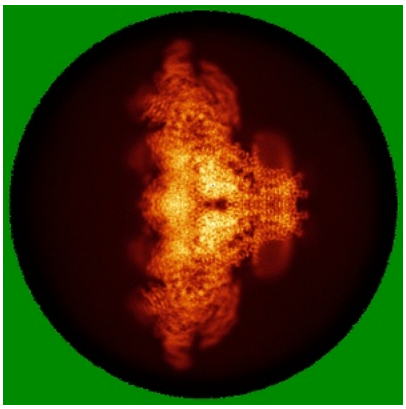
Z Index: 229

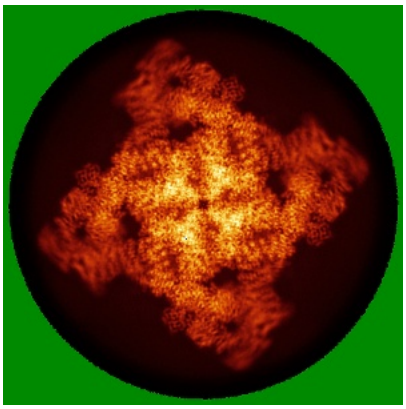
The images above show the largest variance slices of the map in three orthogonal directions.

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

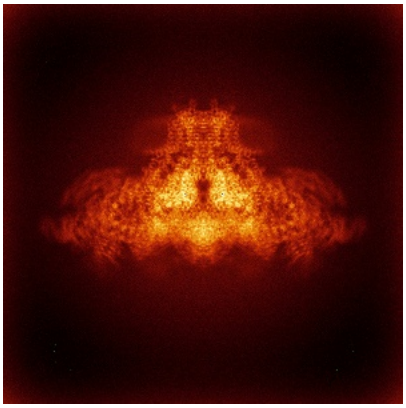
6.4.1 Primary map

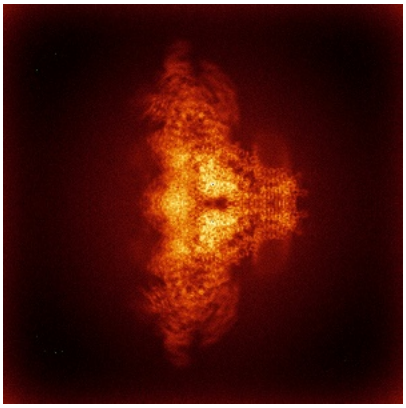

X

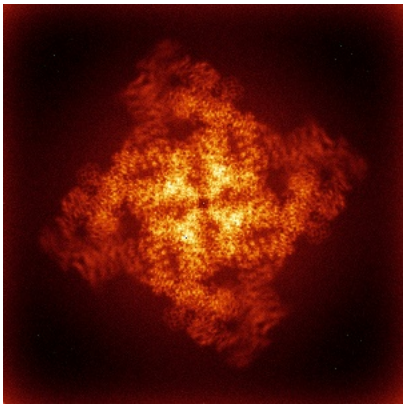

Y


Z

6.4.2 Raw map


X

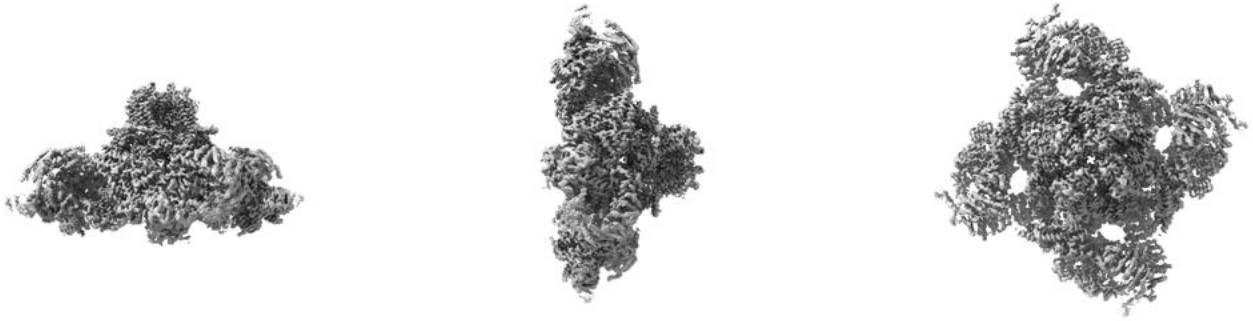

Y


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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

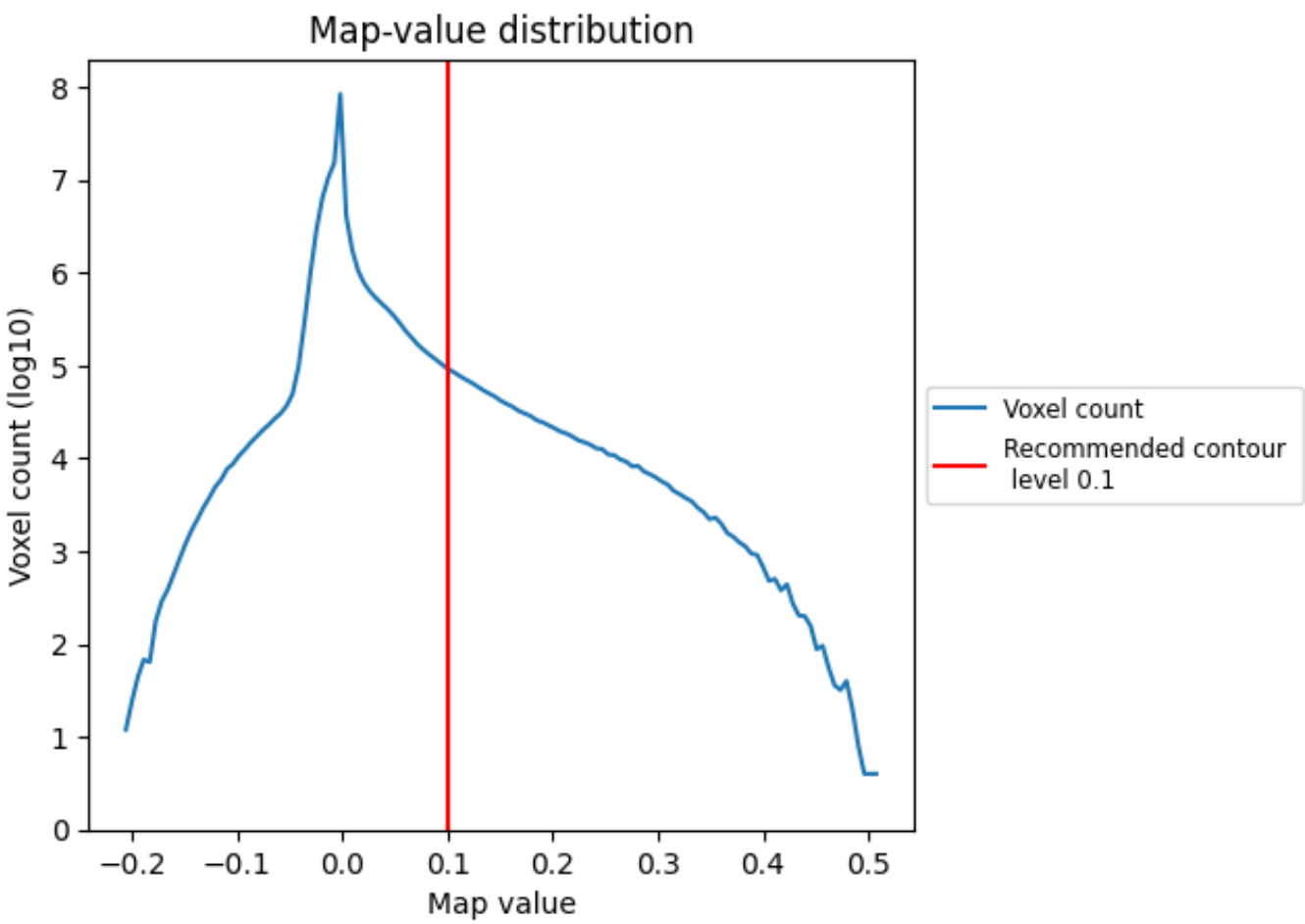
6.6 Mask visualisation (i)

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

7 Map analysis (i)

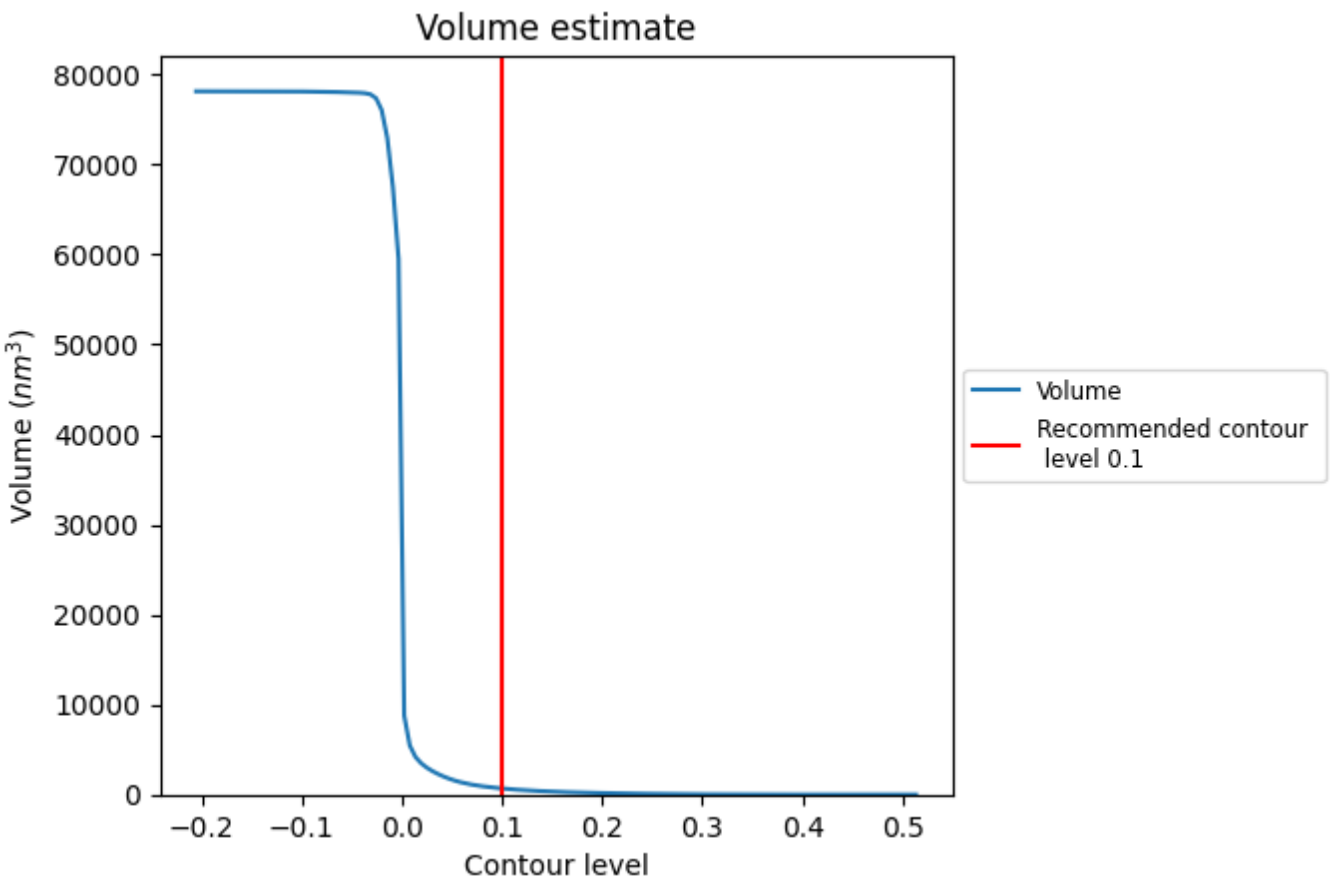
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

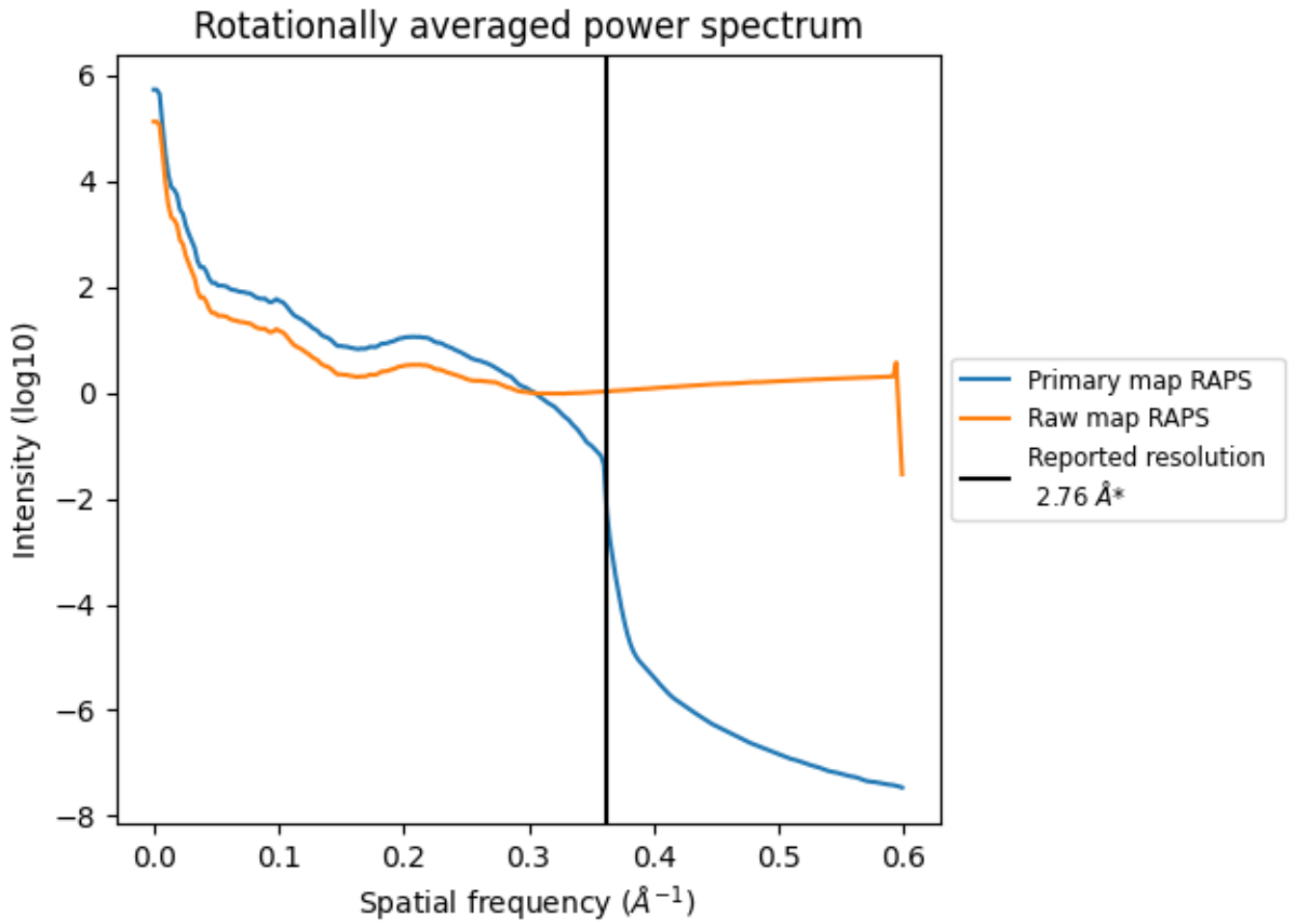
7.2 Volume estimate (i)



The volume at the recommended contour level is 676 nm^3; this corresponds to an approximate mass of 611 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)

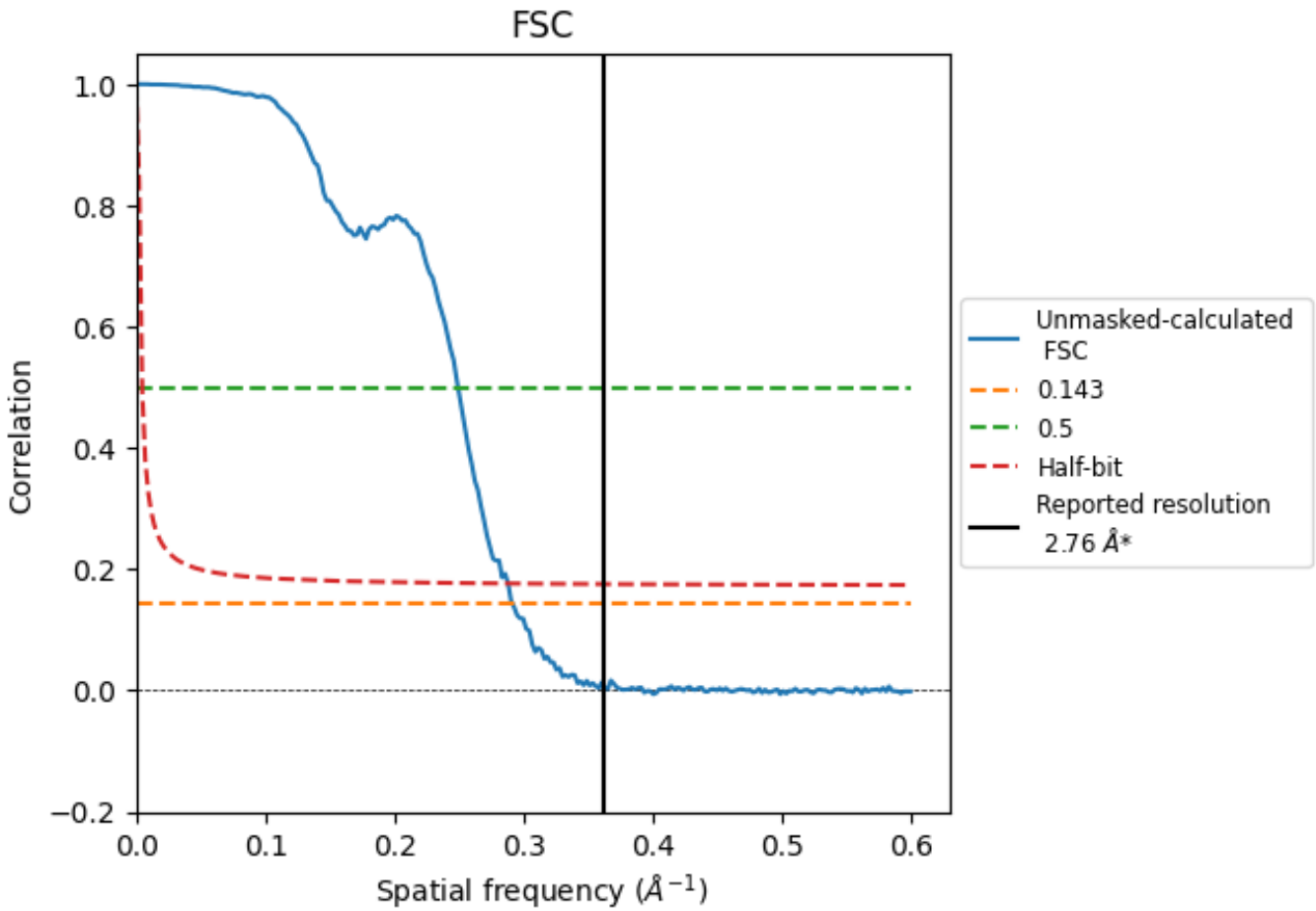


*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.02	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.76 by more than 10 %

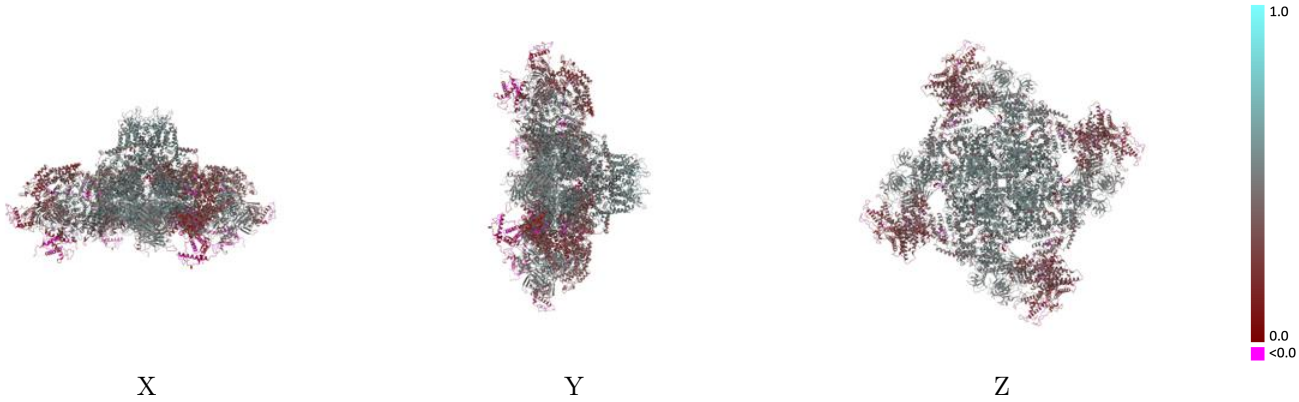
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-47390 and PDB model 9E1D. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)

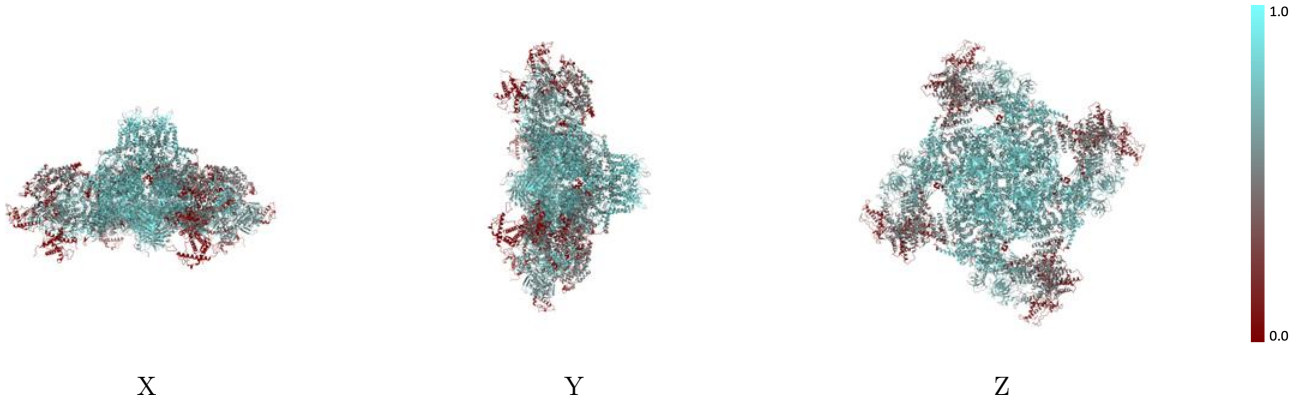
This section was not generated.

9.2 Q-score mapped to coordinate model (i)



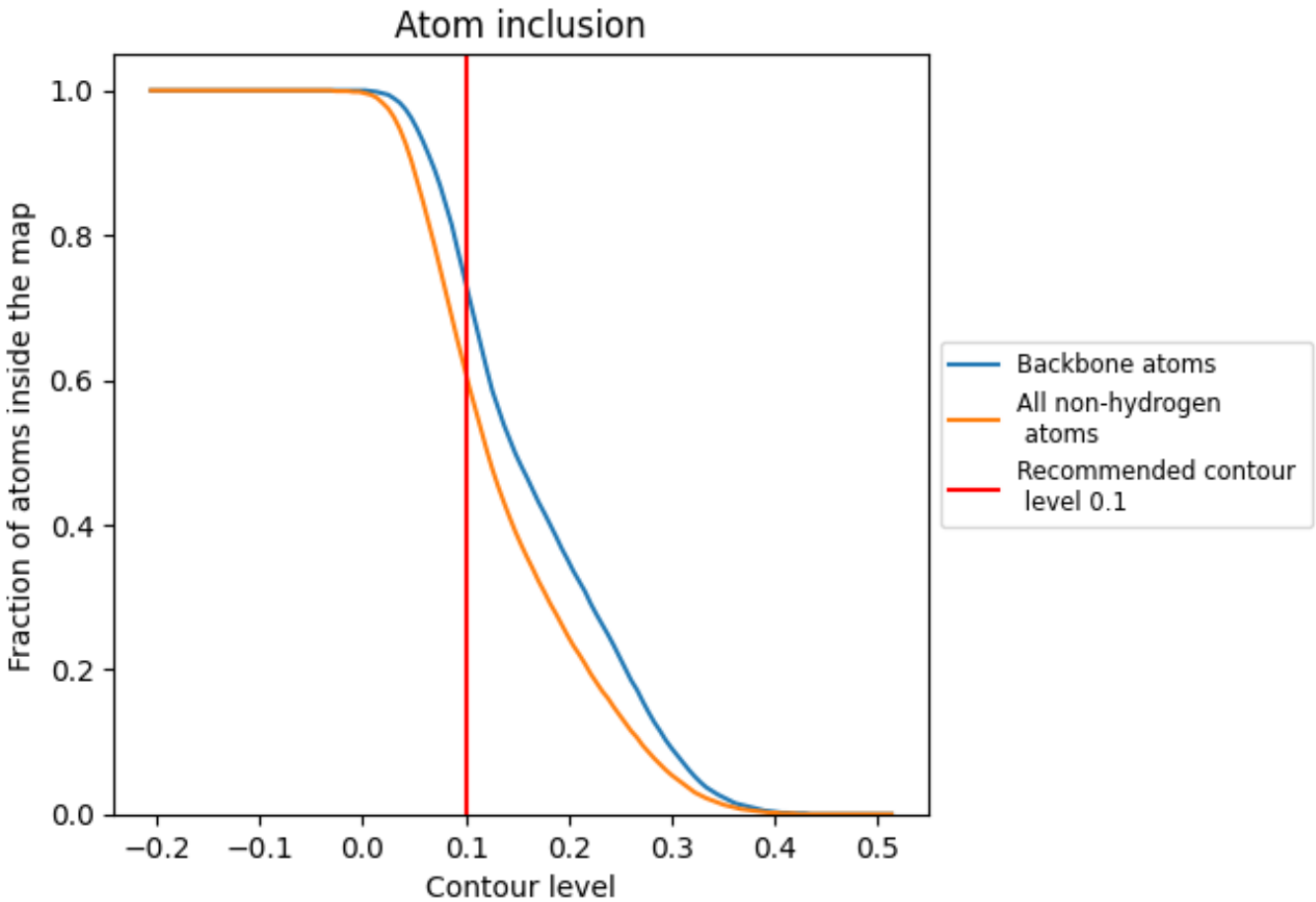
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6090	0.4220
A	0.6100	0.4200
B	0.6090	0.4200
C	0.6090	0.4200
D	0.6090	0.4200
E	0.6110	0.4940
F	0.6140	0.4920
G	0.6100	0.4900
H	0.6090	0.4920