wwPDB EM Validation Summary Report

Jun 16, 2025 – 02:58 PM EDT

PDB ID	:	9E1E / pdb_00009e1e
EMDB ID	:	EMD-47391
Title	:	Structure of RyR1 in the primed state in the presence of uracil
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2024-10-21
Resolution	:	2.92 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 ⓘ symbol.

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

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

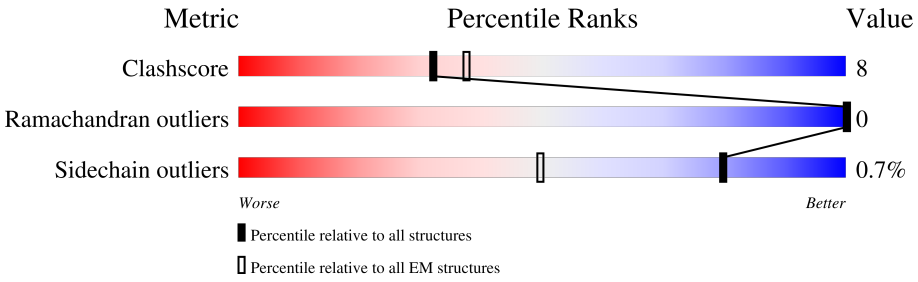
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.92 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	5037	29% 70% 17% 13%
1	B	5037	29% 69% 18% 13%
1	C	5037	29% 69% 18% 13%
1	D	5037	29% 71% 16% 13%
2	E	108	30% 69% 29%
2	F	108	28% 73% 25%
2	G	108	29% 76% 23%
2	H	108	28% 74% 23%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 144088 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.

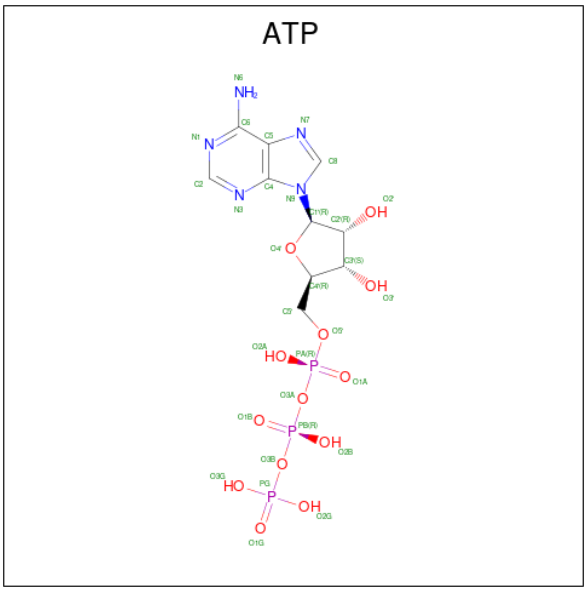
- Molecule 1 is a protein called Ryanodine receptor 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	H	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	G	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	F	107	Total 831	C 527	N 146	O 154	S 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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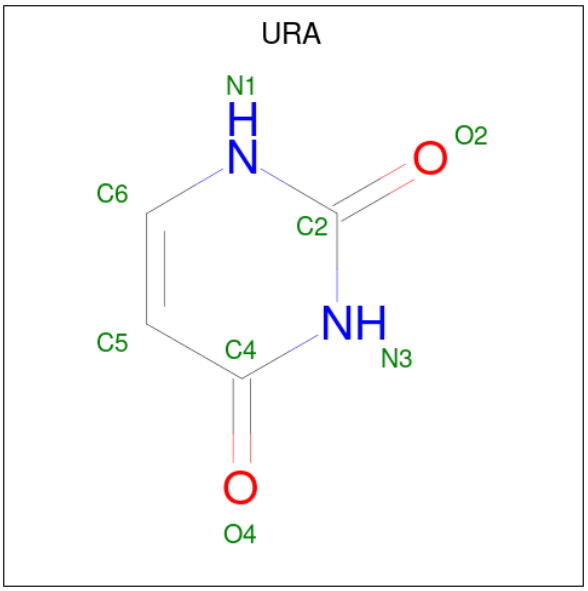
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Zn 1 1	0
5	D	1	Total Zn 1 1	0
5	C	1	Total Zn 1 1	0

- Molecule 6 is URACIL (CCD ID: URA) (formula: $C_4H_4N_2O_2$) (labeled as "Ligand of Interest" by depositor).



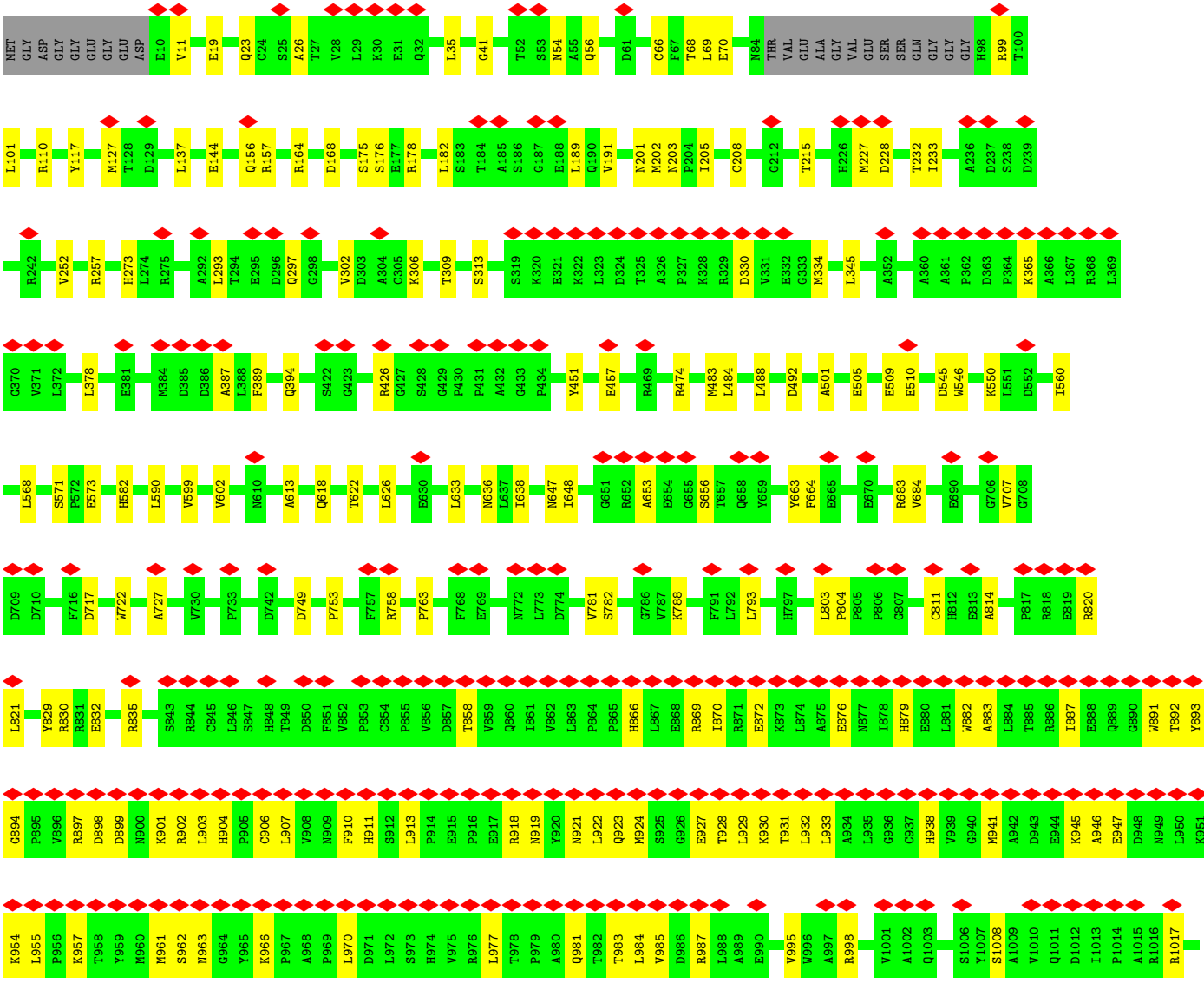
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 8 4 2 2	0
6	B	1	Total C N O 8 4 2 2	0
6	D	1	Total C N O 8 4 2 2	0
6	C	1	Total C N O 8 4 2 2	0

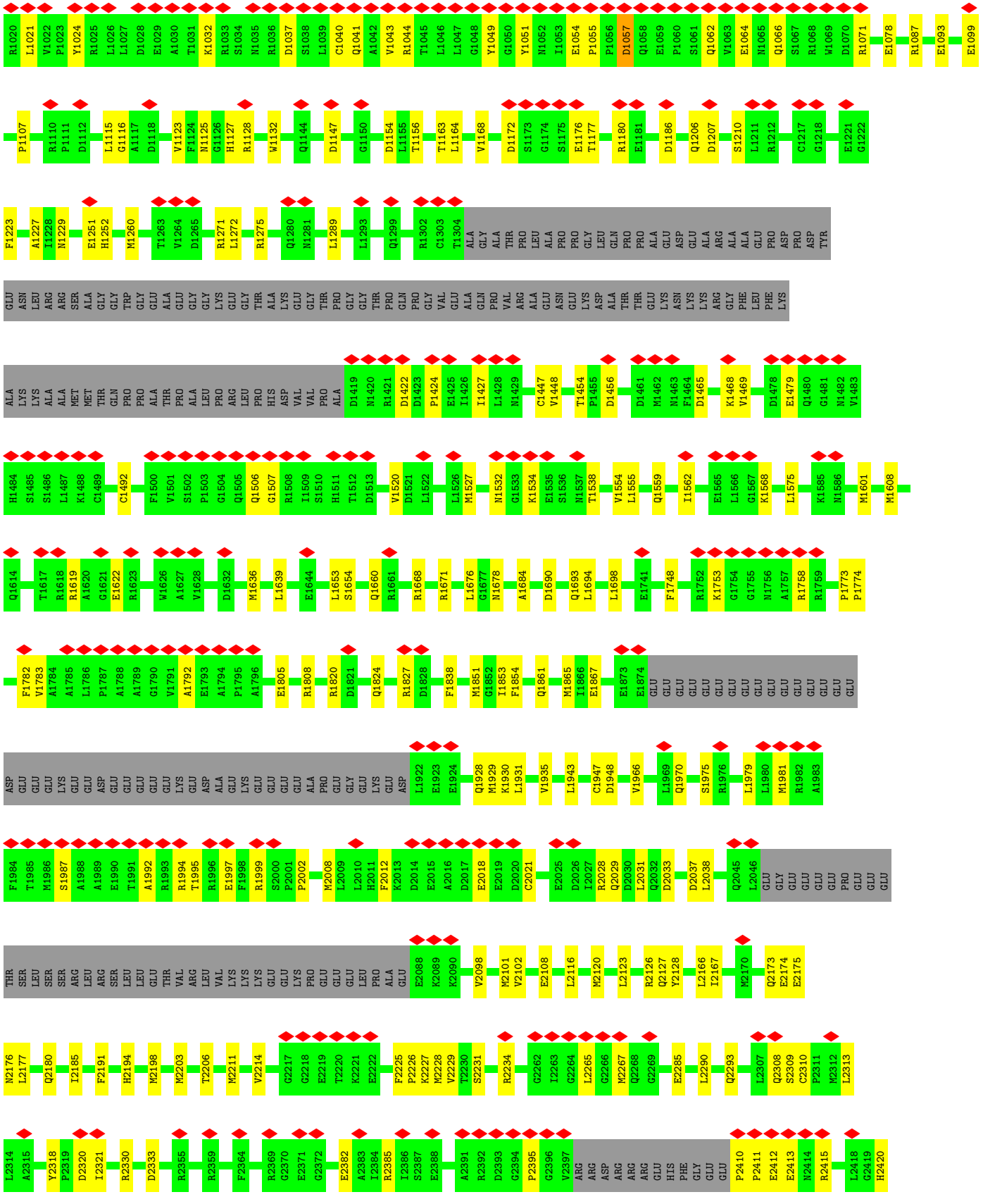
3 Residue-property plots (i)

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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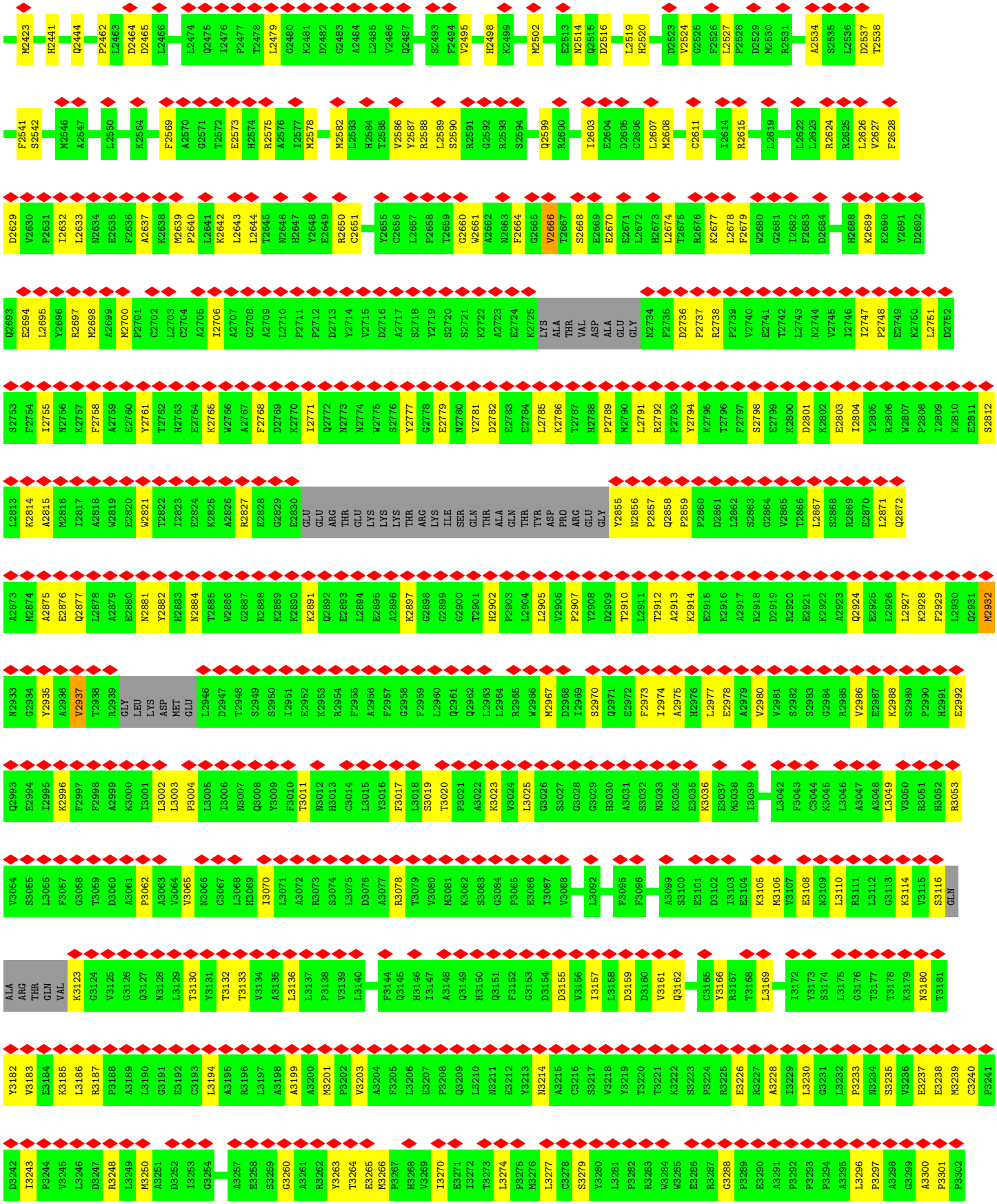
P1107 R1110 P1111 D1112 L1115 G1116 A1117 D1118 V1123 F1124 N1125 G1126 H1127 R1128 W1132 Q1144 D1147 G1150 D1154 L1155 T1156 T1163 L1164 V1168 D1172 S1173 G1174 S1175 E1176 T1177 R1180 E1181 D1186 Q1206 D1207 S1210 L1211 R1212 C1217 G1218 E1221 G1222
F1223 A1227 I1228 N1229 E1251 H1252 M1260 T1263 V1264 D1265 R1271 L1272 R1275 Q1280 N1281 L1289 L1293 Q1299 R1302 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 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 N1429 C1447 V1448 T1454 P1455 D1456 D1461 M1462 N1463 F1464 D1465 K1468 V1469 D1478 E1479 Q1480 G1481 N1482 V1483
H1484 S1485 S1486 L1487 K1488 C1489 C1492 F1500 V1501 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 V1520 D1521 L1522 L1526 M1527 N1532 G1533 K1534 E1535 S1536 N1537 T1538 V1554 L1555 Q1559 I1562 E1565 L1566 G1567 K1568 L1575 K1585 N1586 M1601 M1608
Q1614 T1617 R1618 R1619 A1620 G1621 E1622 R1623 W1626 A1627 V1628 D1632 M1636 L1639 E1644 L1653 S1654 Q1660 R1661 R1668 R1671 L1676 G1677 N1678 A1684 D1690 Q1693 L1694 L1698 E1741 F1748 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 P1773 P1774
F1782 V1783 A1784 A1785 L1786 P1787 A1788 A1789 G1790 V1791 A1792 E1793 A1794 P1795 A1796 E1805 R1808 R1820 D1821 Q1824 R1827 D1828 F1838 M1851 G1852 I1853 F1854 Q1861 M1865 I1866 E1867 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 GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 Q1928 M1929 K1930 L1931 V1935 L1943 C1947 D1948 V1966 L1969 Q1970 S1975 R1976 L1979 L1980 M1981 R1982 A1983
F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 M2008 L2009 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 E2025 D2026 T2027 R2028 Q2029 D2030 L2031 Q2032 D2033 D2037 L2038 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 V2098 M2101 V2102 E2108 L2116 M2120 L2123 R2126 Q2127 Y2128 L2166 I2167 M2170 Q2173 E2174 E2175
N2176 L2177 Q2180 I2185 F2191 H2194 M2198 M2203 T2206 M2211 V2214 G2217 G2218 E2219 T2220 K2221 E2222 F2225 P2226 K2227 M2228 V2229 T2230 S2231 R2234 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 E2285 L2290 Q2293 L2307 Q2308 S2309 C2310 P2311 M2312 L2313
L2314 A2315 Y2318 P2319 D2320 I2321 R2330 D2333 R2355 R2359 F2364 R2369 G2370 E2371 G2372 E2382 A2383 I2384 R2385 I2386 S2387 E2388 A2391 R2392 D2393 G2394 P2395 G2396 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 R2415 L2418 G2419 H2420


M2423 H2441 Q2444 P2462 L2463 D2464 D2465 L2466 L2474 Q2475 I2476 P2477 T2478 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2486 Q2487 S2493 F2494 V2495 H2498 K2499 M2502 E2513 N2514 Q2515 D2516 L2519 H2520 D2523 V2524 G2525 F2526 L2527 P2528 D2529 M2530 R2531 A2534 S2535 L2536 D2537 T2538
F2541 S2542 M2546 A2547 L2550 K2564 F2569 A2570 G2571 T2572 E2573 H2574 R2575 A2576 I2577 M2578 M2582 L2583 H2584 T2585 V2586 Y2587 R2588 L2589 S2590 R2591 G2592 R2593 S2594 Q2599 R2600 I2603 E2604 D2605 C2606 L2607 M2608 C2611 I2614 R2615 L2619 L2622 L2623 R2624 R2625 L2626 V2627 F2628
D2629 V2630 P2631 I2632 L2633 N2634 E2635 F2636 A2637 K2638 M2639 P2640 L2641 K2642 L2643 L2644 T2645 N2646 H2647 Y2648 E2649 R2650 C2651 Y2655 C2656 L2657 P2658 T2659 G2660 W2661 A2662 N2663 F2664 G2665 V2666 T2667 S2668 E2669 E2670 E2671 L2672 H2673 L2674 T2675 R2676 K2677 L2678 F2679 W2680 G2681 I2682 F2683 D2684 H2688 K2689 K2690 Y2691 D2692
Q2693 E2694 L2695 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 Q2961 Q2962 L2963 L2964 R2965 W2966 M2967 D2968 I2969 S2970 Q2971 E2972 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 Y2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992
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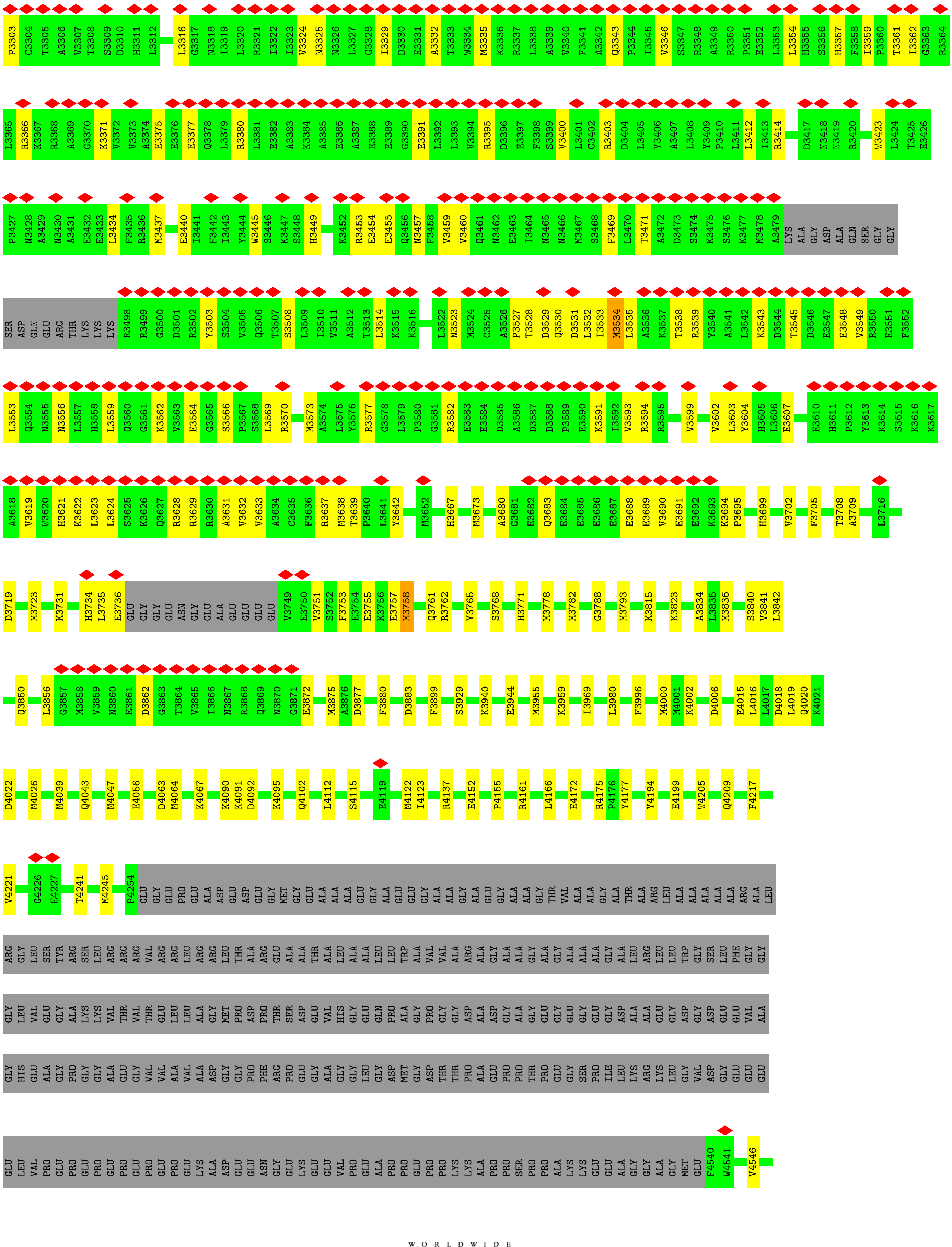
V3054 S3055 L3056 F3057 G3058 T3059 D3060 A3061 P3062 A3063 V3064 V3065 N3066 C3067 L3068 H3069 I3070 L3071 A3072 R3073 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 V3088 L3092 F3095 F3096 A3099 S3100 E3101 D3102 I3103 E3104 K3105 M3106 V3107 E3108 N3109 L3110 R3111 L3112 G3113 K3114 V3115 S3116 GLN
ALA ARG THR GLN VAL K3123 G3124 V3125 G3126 Q3127 N3128 L3129 T3130 Y3131 T3132 T3133 V3134 A3135 L3136 L3137 P3138 V3139 L3140 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Q3162 C3165 Y3166 R3167 T3168 L3169 I3172 Y3173 S3174 L3175 G3176 T3177 T3178 K3179 N3180 T3181
Y3182 V3183 E3184 K3185 L3186 R3187 P3188 A3189 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 N3211 E3212 Y3213 M3214 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 G3254 A3257 E3258 S3259 G3260 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 R3283 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302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L3365 R3366 K3367 R3368 A3369 G3370 K3371 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 D3396 E3397 F3398 S3399 V3400 L3401 C3402 R3403 D3404 L3405 Y3406 A3407 L3408 Y3409 P3410 L3411 L3412 I3413 R3414 D3417 N3418 N3419 R3420 W3423 L3424 T3425 E3426
P3427 N3428 A3429 N3430 A3431 E3432 E3433 L3434 F3435 R3436 M3437 E3440 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 S3448 H3449 K3452 R3453 E3454 E3455 Q3456 N3457 F3458 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 L3522 N3523 M3524 C3525 A3526 P3527 T3528 D3529 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549 R3550 E3551 F3552
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A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 T3639 P3640 L3641 Y3642 M3652 H3667 M3673 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 H3699 V3702 F3705 T3708 A3709 L3716
D3719 M3723 K3731 H3734 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU V3749 E3750 V3751 S3752 F3753 E3754 E3755 K3756 E3757 M3758 Q3761 R3762 Y3765 S3768 H3771 M3778 M3782 G3788 M3793 K3815 K3823 A3834 L3835 M3836 S3840 V3841 L3842
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D4022 M4026 M4039 Q4043 M4047 E4056 D4063 M4064 K4067 K4090 K4091 D4092 K4095 Q4102 L4112 S4115 E4119 M4122 I4123 R4137 E4152 P4155 R4161 L4166 E4172 R4175 P4176 Y4177 Y4194 E4199 W4205 Q4209 F4217
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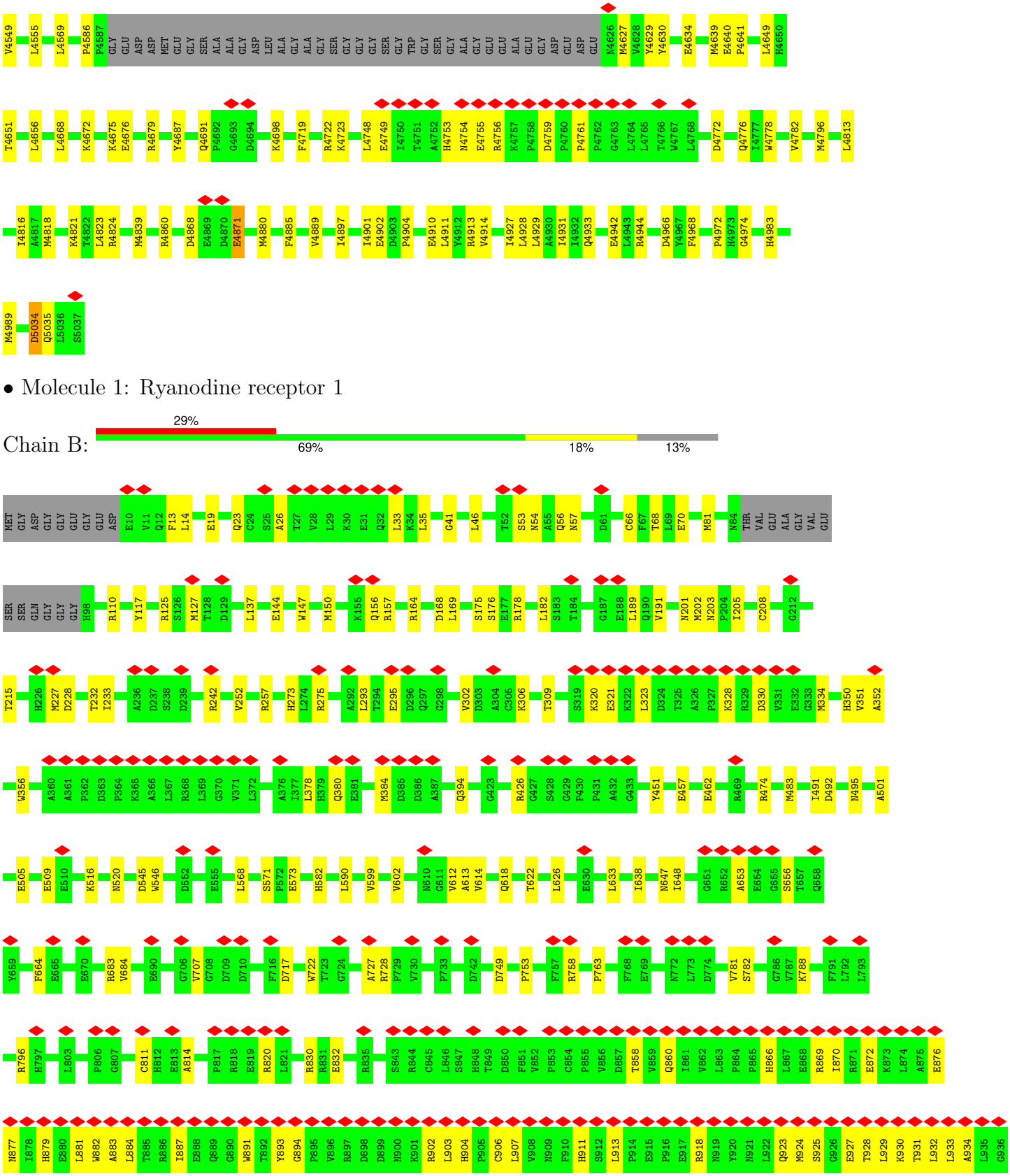
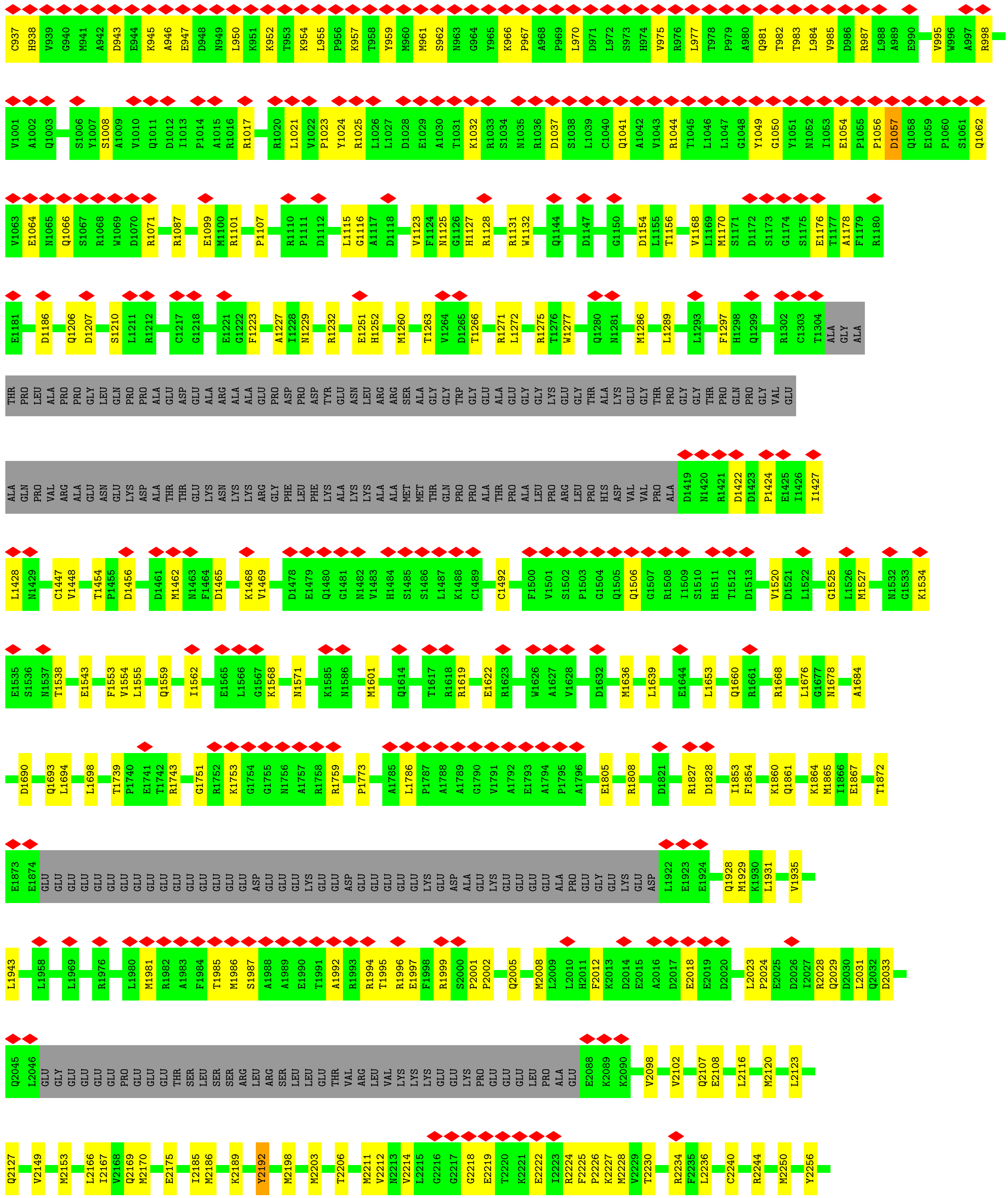
ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY
GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP 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 ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU
GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 V4546



• Molecule 1: Ryanodine receptor 1

Chain B: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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 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
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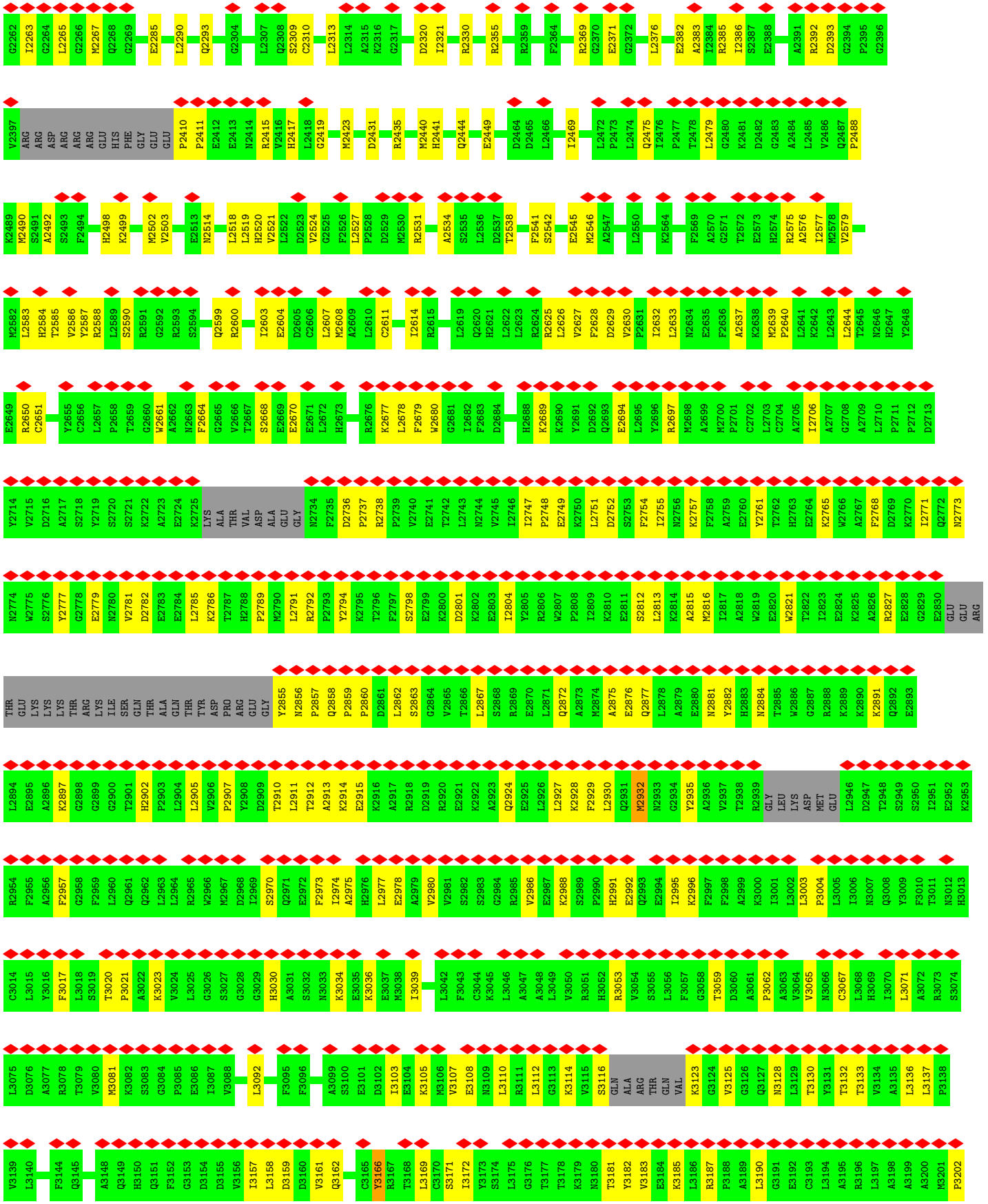
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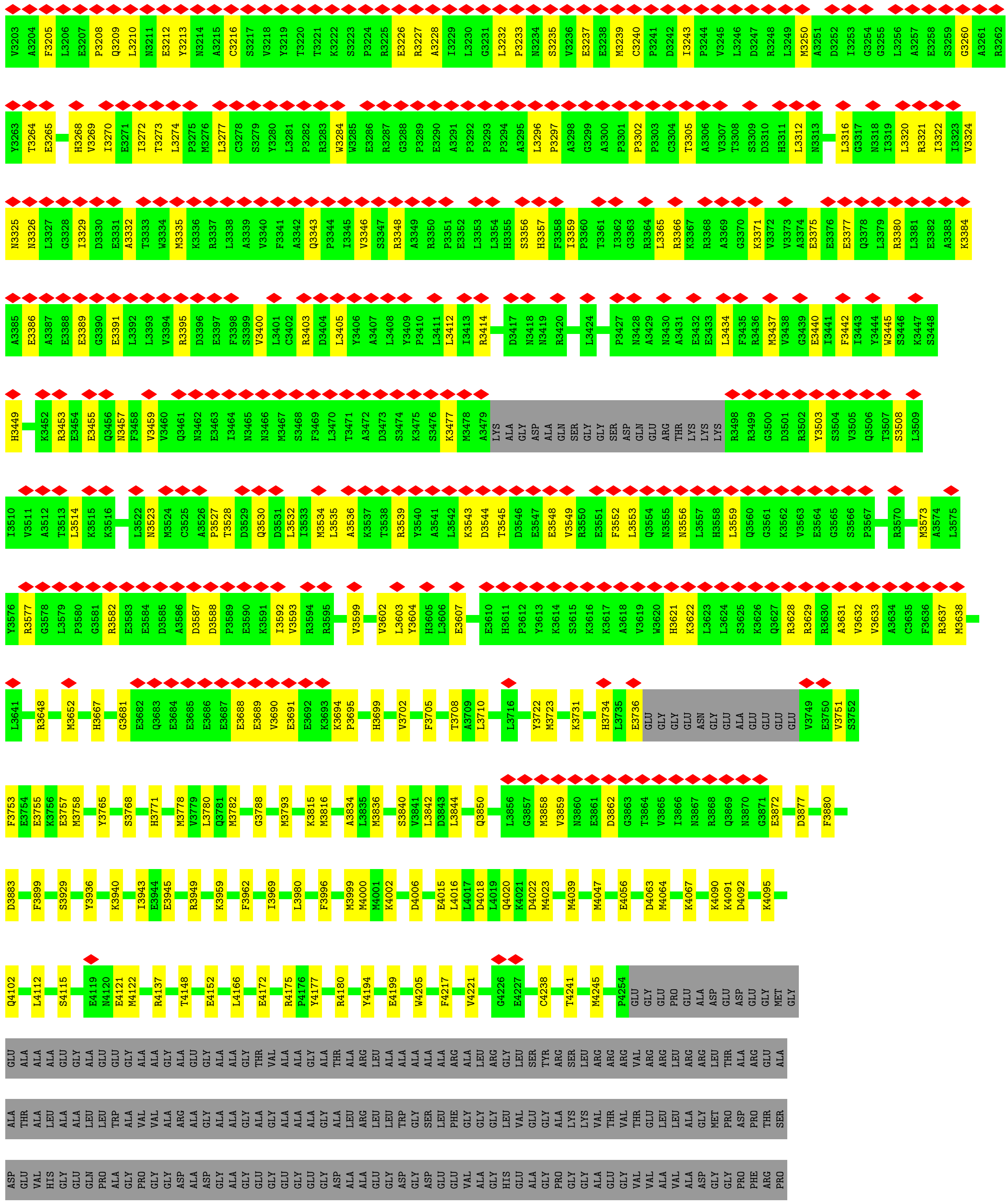
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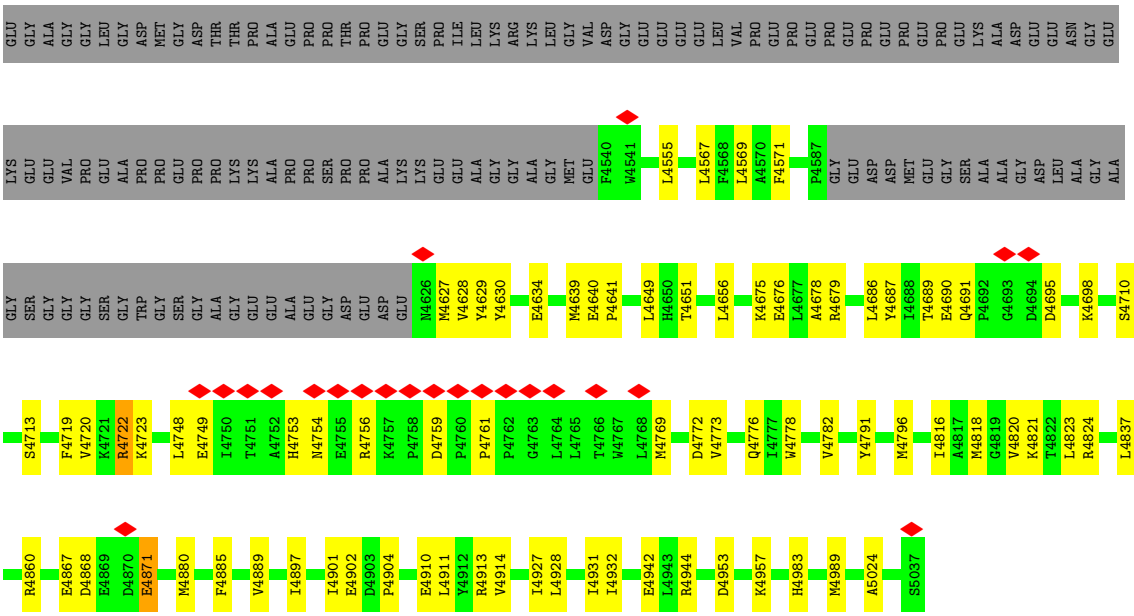
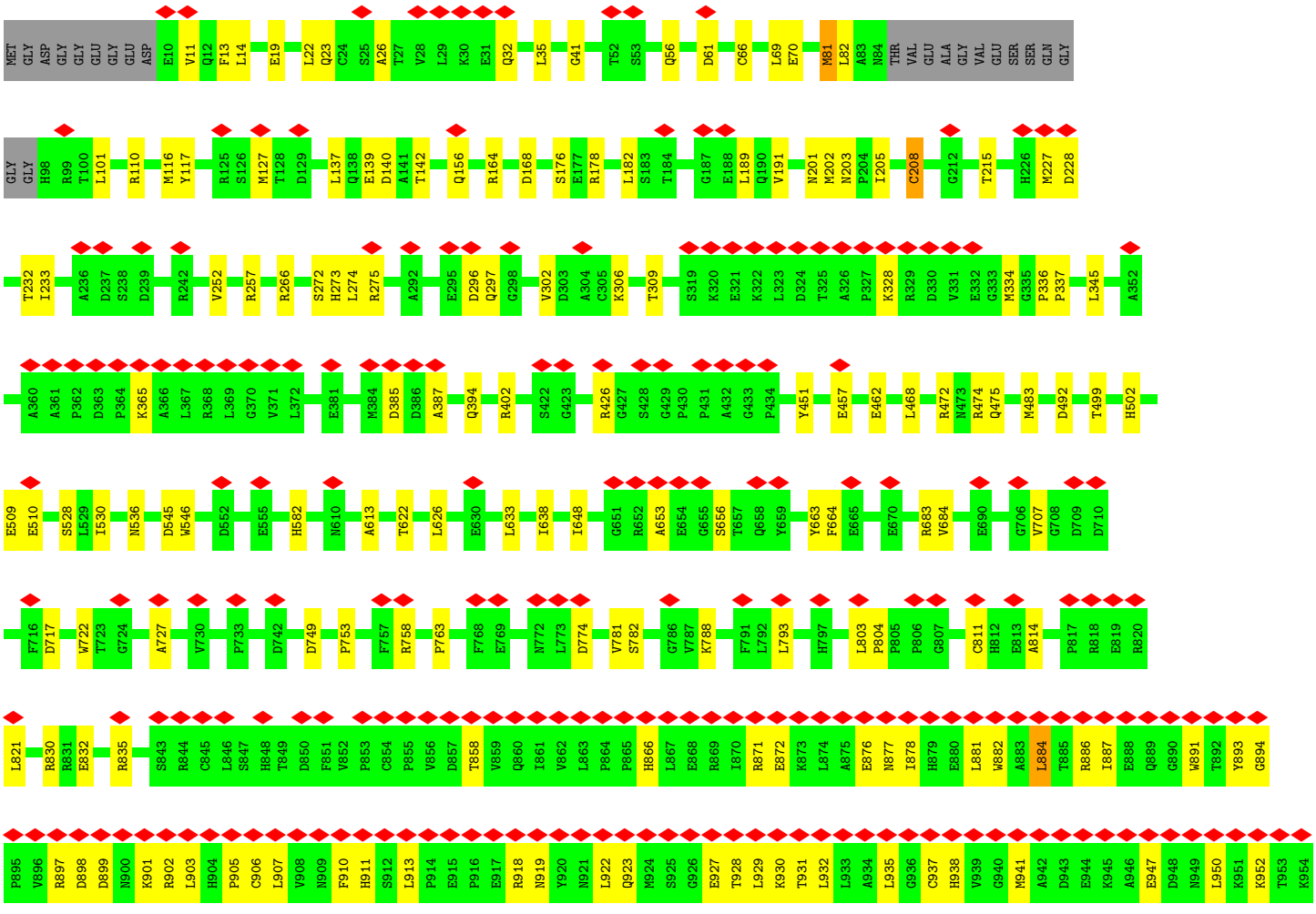
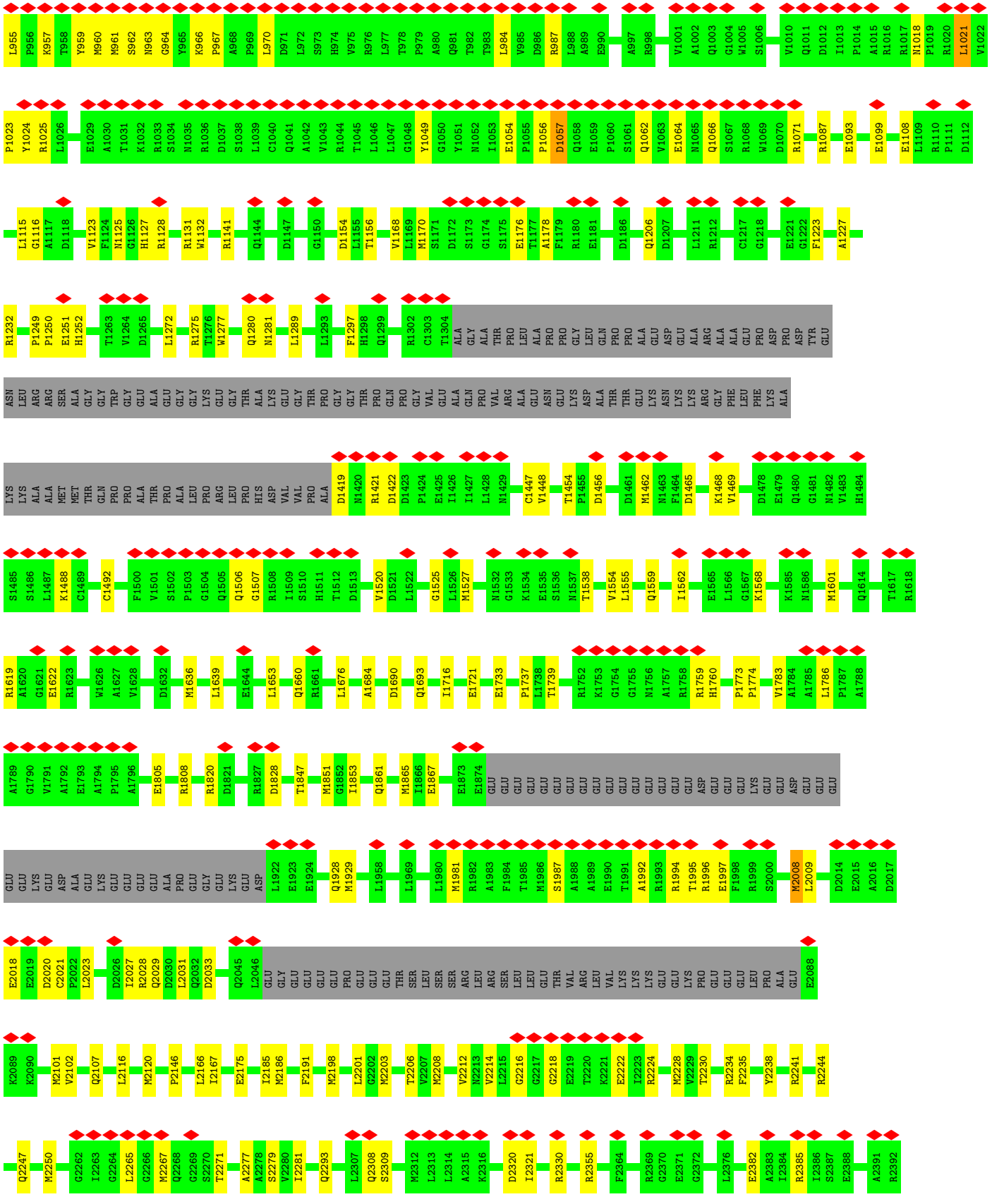
ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO



• Molecule 1: Ryanodine receptor 1

Chain D:

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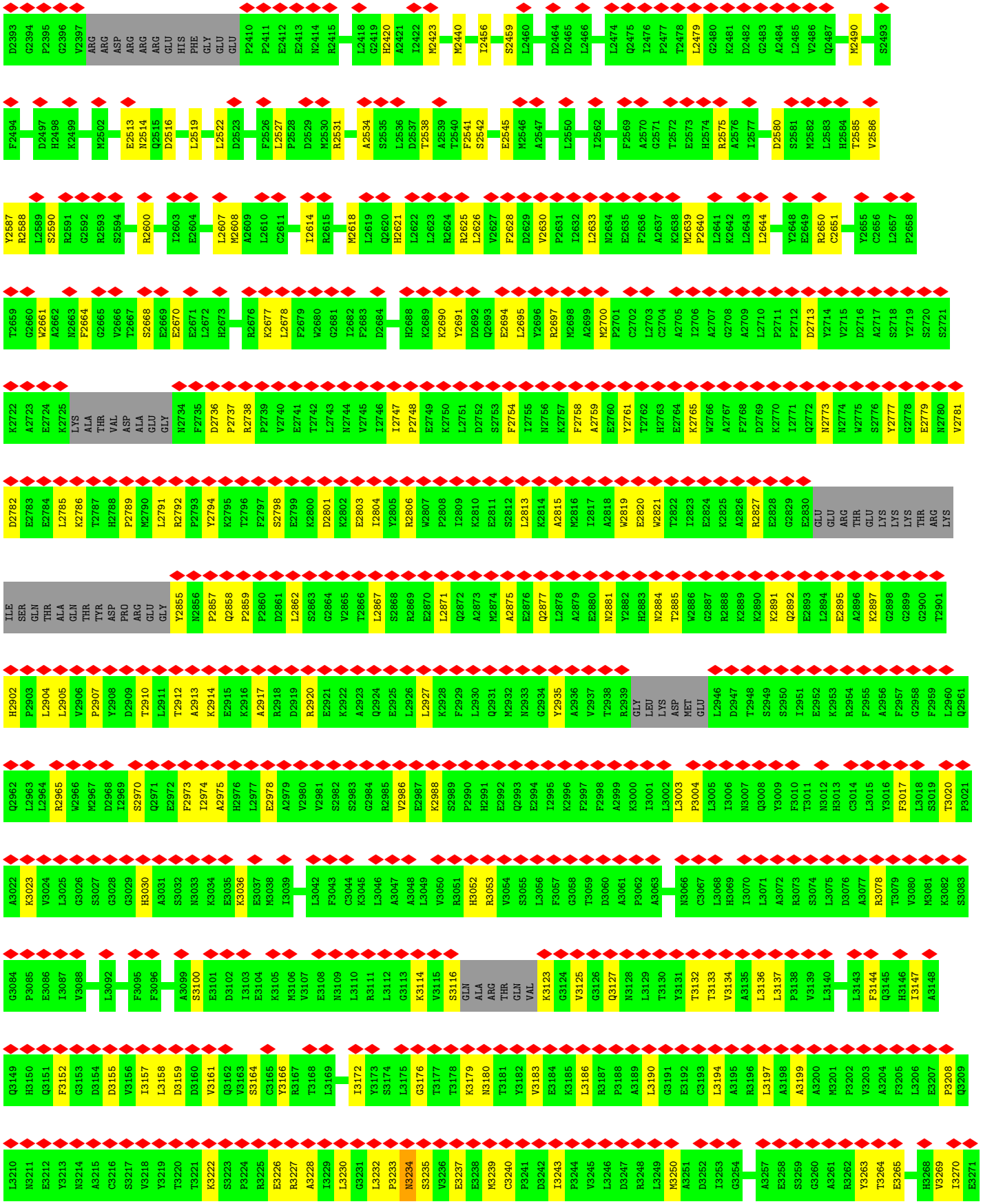
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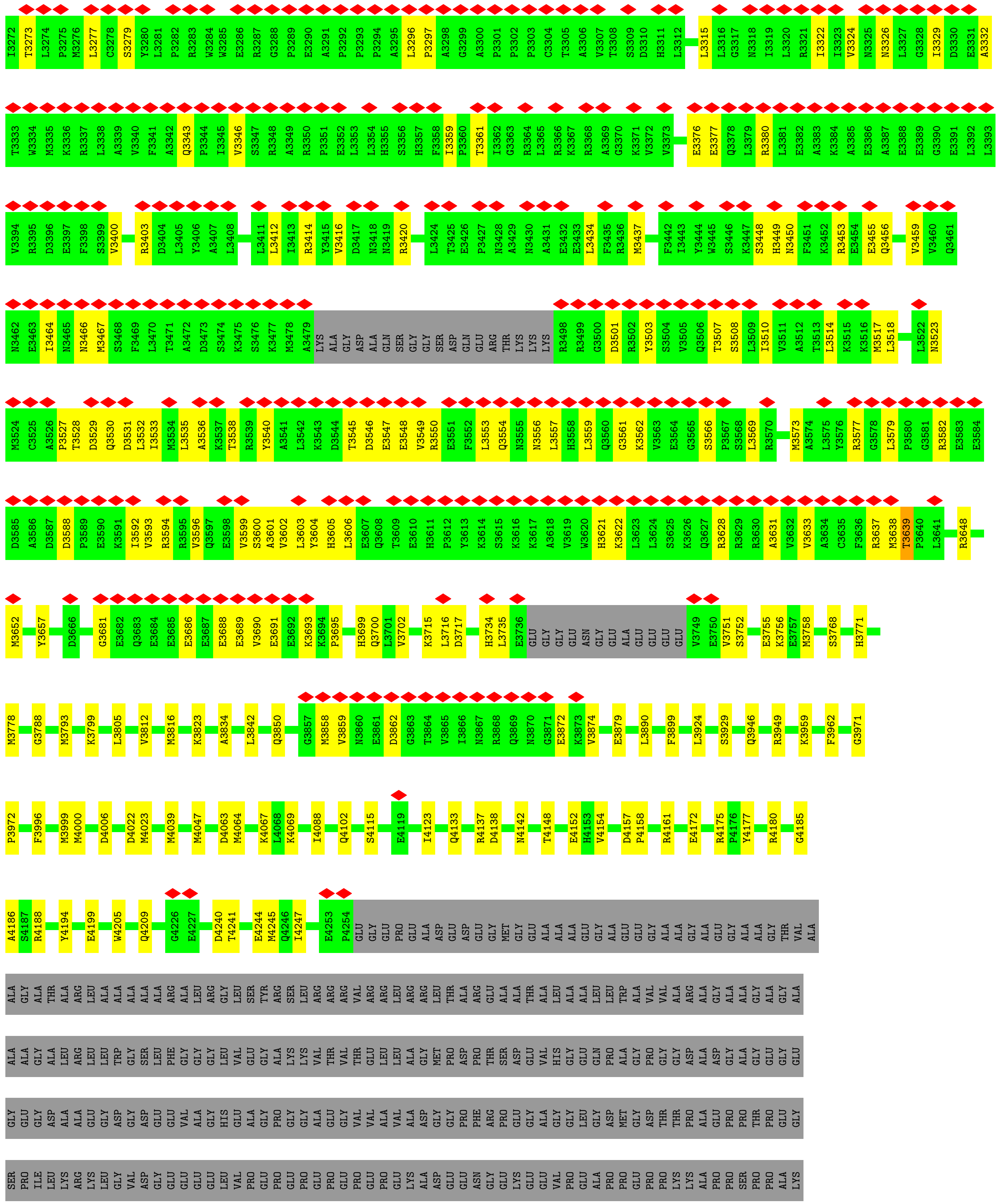
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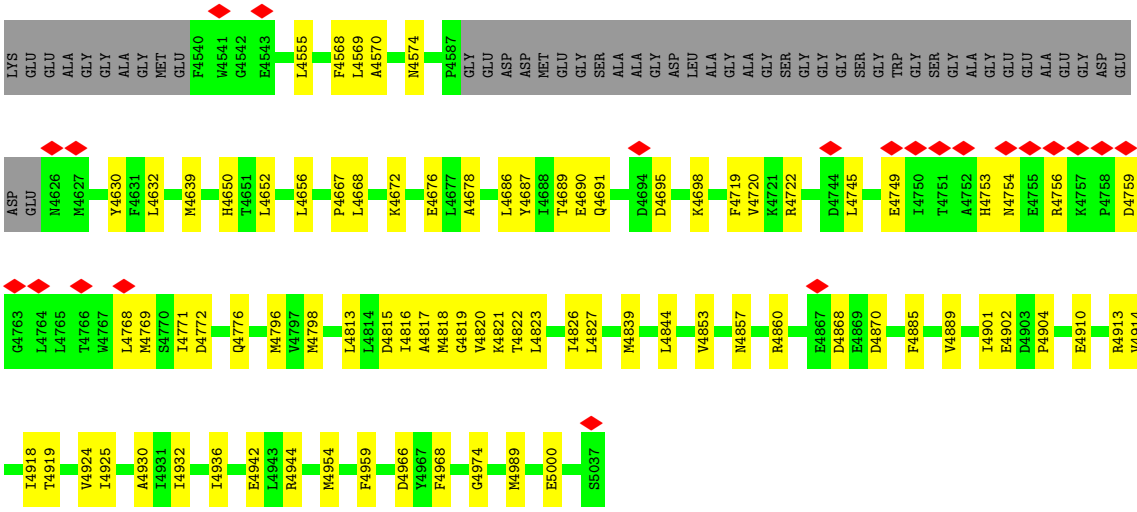
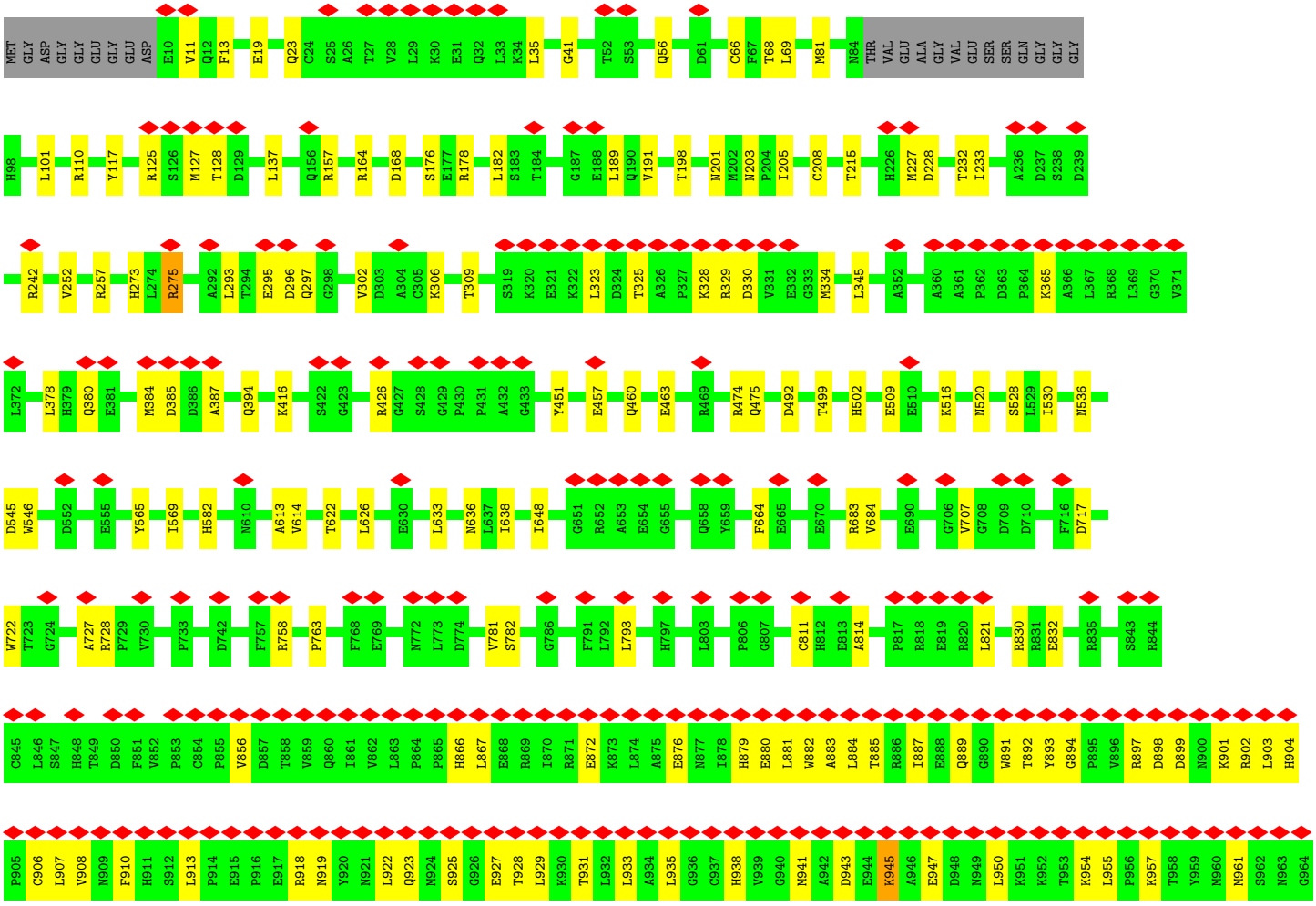
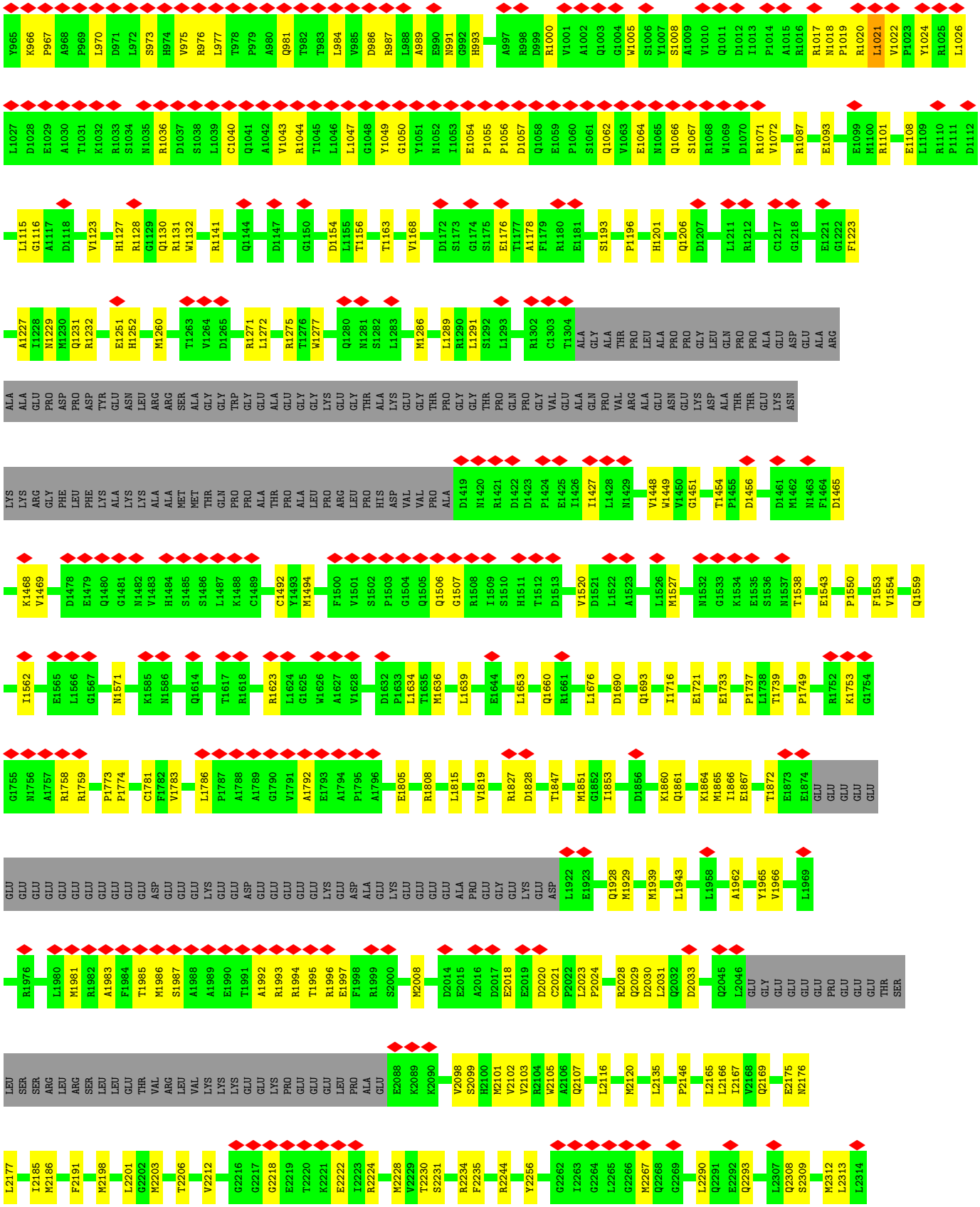


• Molecule 1: Ryanodine receptor 1

Chain C:

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ALA ALA GLU PRO ASP 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
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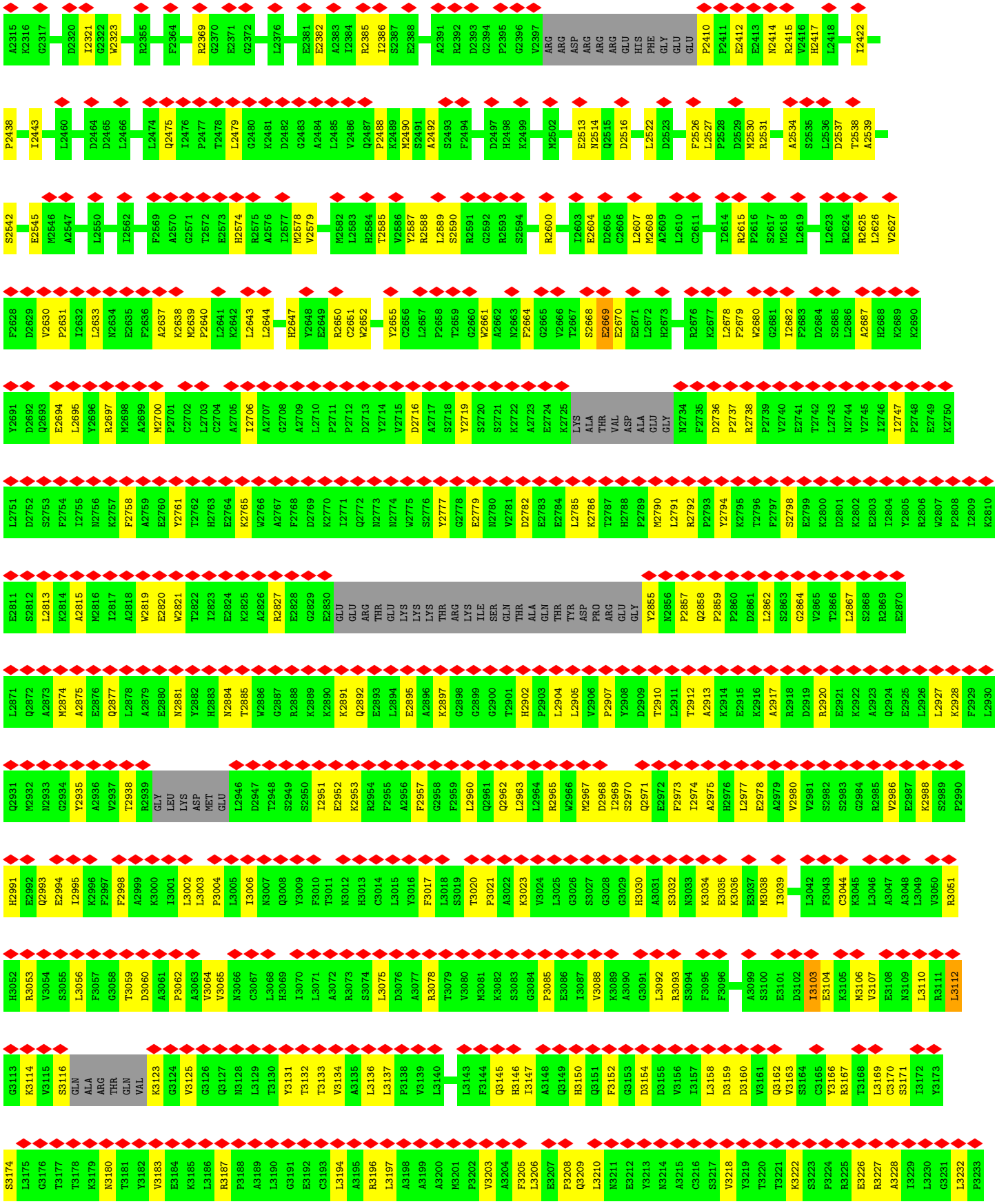
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P2438 I2443 L2460 D2464 D2465 L2466 L2474 Q2475 I2476 P2477 T2478 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2486 Q2487 P2488 K2489 M2490 S2491 A2492 S2493 F2494 D2497 H2498 K2499 M2502 E2513 N2514 Q2515 D2516 L2522 D2523 F2526 L2527 P2528 D2529 M2530 R2531 A2534 S2535 L2536 D2537 T2538 A2539
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F2628 D2629 V2630 P2631 I2632 L2633 N2634 E2635 F2636 A2637 K2638 M2639 P2640 L2641 K2642 L2643 L2644 H2647 Y2648 E2649 R2650 C2651 W2652 Y2655 C2656 L2657 P2658 T2659 G2660 W2661 A2662 N2663 F2664 G2665 V2666 T2667 S2668 E2669 E2670 E2671 L2672 H2673 R2676 K2677 L2678 F2679 W2680 G2681 I2682 F2683 D2684 S2685 L2686 A2687 H2688 K2689 K2690
Y2691 D2692 Q2693 E2694 L2695 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
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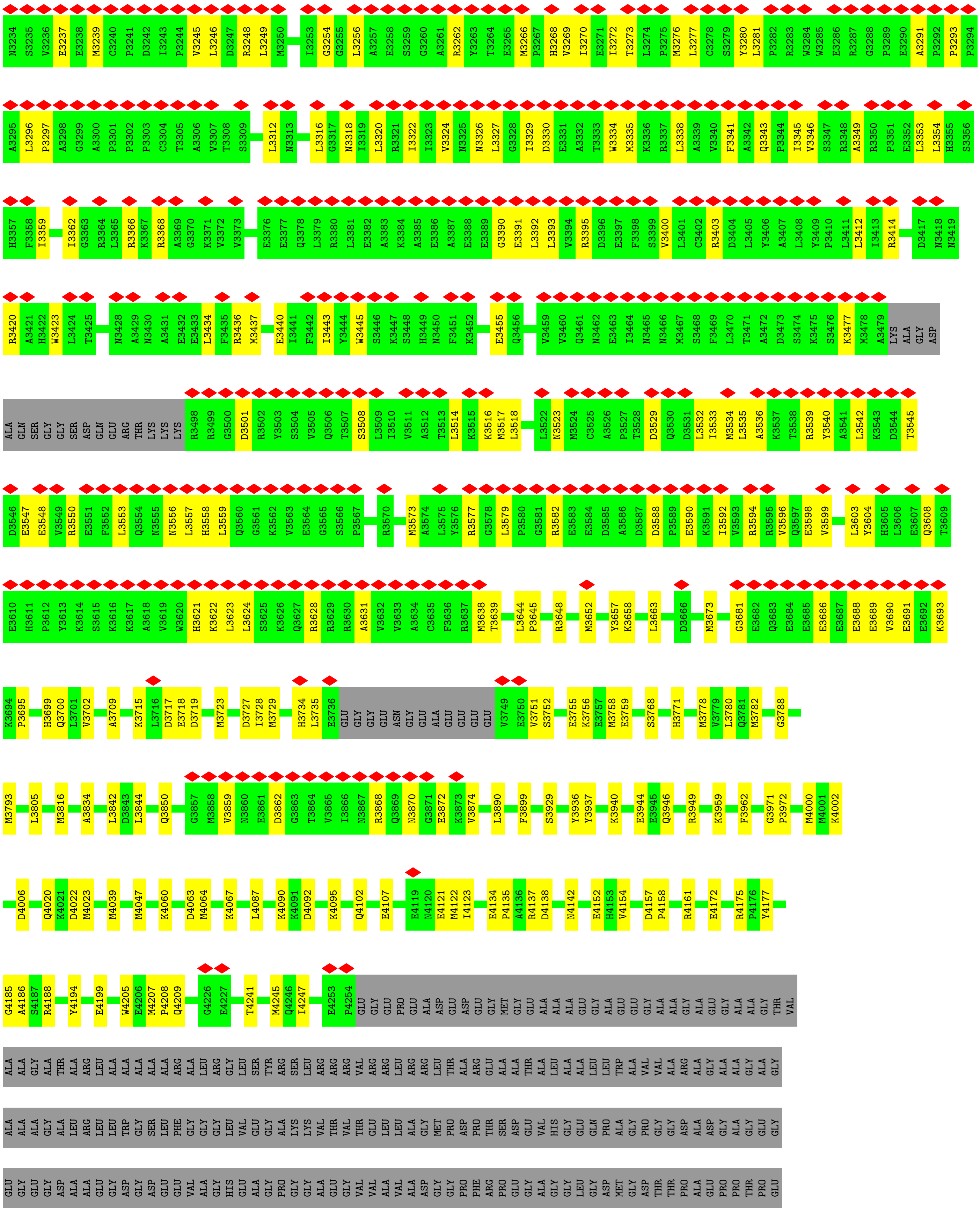
G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 V3125 G3126 Q3127 N3128 L3129 T3130 Y3131 T3132 T3133 V3134 A3135 L3136 L3137 P3138 V3139 L3140 L3143 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 L3169 C3170 S3171 I3172 Y3173
S3174 L3175 G3176 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3186 R3187 P3188 A3189 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233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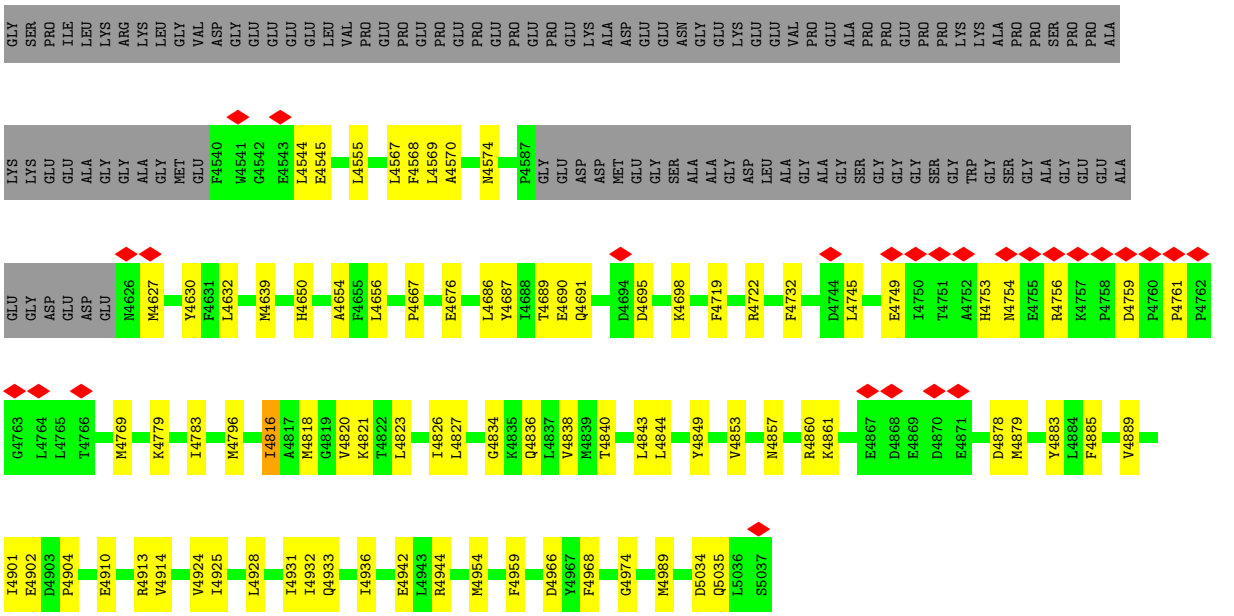
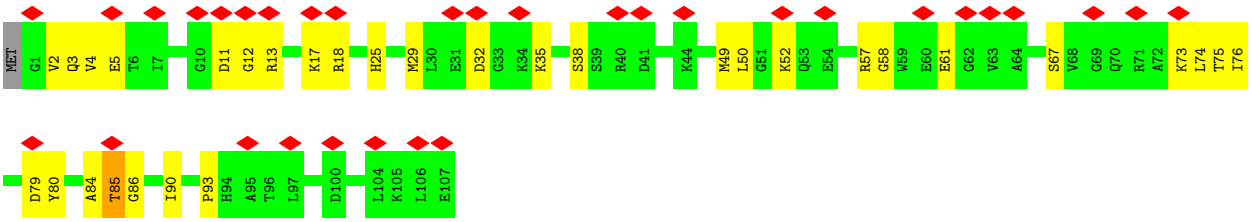
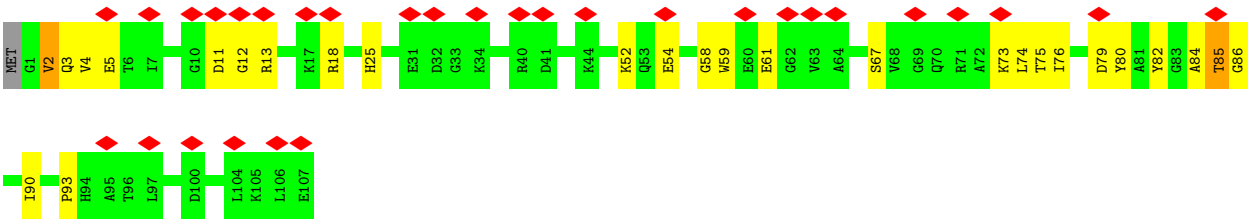
G4185 A4186 S4187 R4188 Y4194 E4199 W4205 E4206 M4207 P4208 Q4209 G4226 E4227 T4241 M4245 Q4246 I4247 E4253 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL
ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA 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 LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY
ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA 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 ALA GLY GLU GLY
GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP 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 ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU



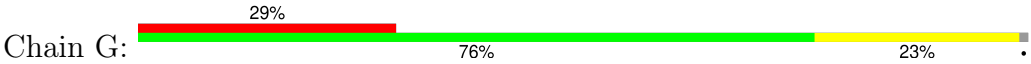
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

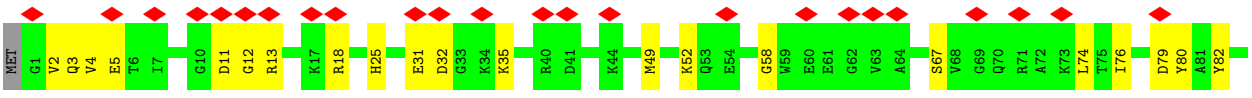


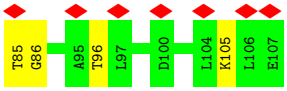
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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

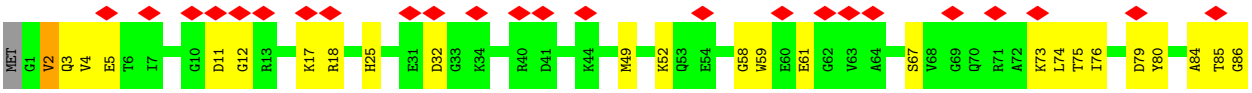


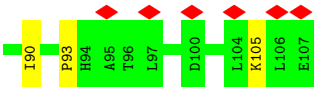




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33584	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	0.482	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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, CA, ZN, URA

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	0.17	0/35977	0.34	2/48726 (0.0%)
1	B	0.17	0/35977	0.34	0/48726
1	C	0.16	0/35977	0.34	2/48726 (0.0%)
1	D	0.15	0/35977	0.31	1/48726 (0.0%)
2	E	0.17	0/850	0.36	0/1146
2	F	0.18	0/850	0.40	0/1146
2	G	0.18	0/850	0.39	0/1146
2	H	0.17	0/850	0.36	0/1146
All	All	0.16	0/147308	0.33	5/199488 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2669	GLU	CA-CB-CG	5.61	125.32	114.10
1	C	2971	GLN	CA-CB-CG	5.30	124.70	114.10
1	D	1783	VAL	N-CA-C	-5.25	108.16	113.20
1	A	1783	VAL	N-CA-C	-5.21	108.20	113.20
1	A	3534	MET	CB-CG-SD	5.12	128.06	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	34797	570	0
1	B	35150	0	34797	609	0
1	C	35150	0	34797	639	0
1	D	35150	0	34797	542	0
2	E	831	0	831	19	0
2	F	831	0	831	18	0
2	G	831	0	831	16	0
2	H	831	0	831	17	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	0	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	8	0	3	0	0
6	B	8	0	3	0	0
6	C	8	0	3	0	0
6	D	8	0	3	0	0
All	All	144088	0	142572	2402	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 8.

The worst 5 of 2402 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:2647:HIS:HE2	1:C:2655:TYR:HH	1.18	0.89
1:C:893:TYR:HB2	1:C:961:MET:HE2	1.53	0.89
1:C:3254:GLY:HA2	1:C:3318:ASN:HD21	1.40	0.86
1:D:957:LYS:H	1:D:957:LYS:HD2	1.41	0.84
1:B:3233:PRO:HD2	1:B:3239:MET:HE1	1.59	0.82

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%)	4260 (97%)	125 (3%)	0	100	100
1	B	4385/5037 (87%)	4251 (97%)	134 (3%)	0	100	100
1	C	4385/5037 (87%)	4264 (97%)	121 (3%)	0	100	100
1	D	4385/5037 (87%)	4272 (97%)	113 (3%)	0	100	100
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	17960/20580 (87%)	17447 (97%)	513 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	3812 (99%)	24 (1%)	84	94
1	B	3836/4276 (90%)	3812 (99%)	24 (1%)	84	94
1	C	3836/4276 (90%)	3817 (100%)	19 (0%)	86	95
1	D	3836/4276 (90%)	3812 (99%)	24 (1%)	84	94
2	E	89/90 (99%)	83 (93%)	6 (7%)	13	37
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	89/90 (99%)	87 (98%)	2 (2%)	47 76
2	H	89/90 (99%)	85 (96%)	4 (4%)	23 54
All	All	15700/17464 (90%)	15594 (99%)	106 (1%)	80 93

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3899	PHE
1	D	1021	LEU
1	C	3103	ILE
1	B	4722	ARG
1	D	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3211	ASN
1	C	2260	ASN
1	D	949	ASN
1	C	2194	HIS
1	C	3734	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
6	URA	A	5304	-	8,8,8	0.59	0	10,10,10	1.08	1 (10%)
6	URA	D	5304	-	8,8,8	0.61	0	10,10,10	1.05	1 (10%)
3	ATP	B	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
3	ATP	C	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
6	URA	B	5304	-	8,8,8	0.60	0	10,10,10	1.12	1 (10%)
3	ATP	D	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
6	URA	C	5304	-	8,8,8	0.62	0	10,10,10	1.06	1 (10%)
3	ATP	A	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)

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
6	URA	A	5304	-	-	-	0/1/1/1
6	URA	D	5304	-	-	-	0/1/1/1
3	ATP	B	5301	-	-	8/18/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/18/38/38	0/3/3/3
6	URA	B	5304	-	-	-	0/1/1/1
3	ATP	D	5301	-	-	6/18/38/38	0/3/3/3
6	URA	C	5304	-	-	-	0/1/1/1
3	ATP	A	5301	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5301	ATP	C4'-O4'-C1'	-4.28	106.00	109.92
3	D	5301	ATP	C4'-O4'-C1'	-4.27	106.02	109.92
3	C	5301	ATP	C4'-O4'-C1'	-4.27	106.02	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5301	ATP	C4'-O4'-C1'	-4.23	106.05	109.92
6	B	5304	URA	C4-N3-C2	2.41	127.88	125.55

There are no chirality outliers.

5 of 26 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-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A

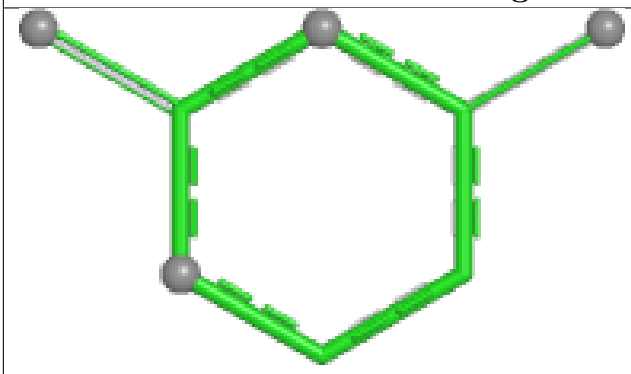
There are no ring outliers.

2 monomers are involved in 2 short contacts:

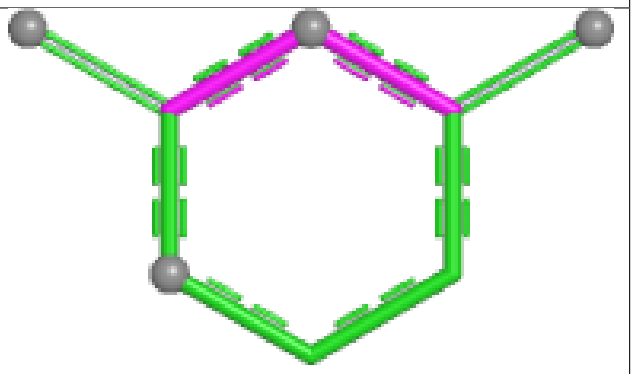
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	1	0
3	A	5301	ATP	1	0

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.

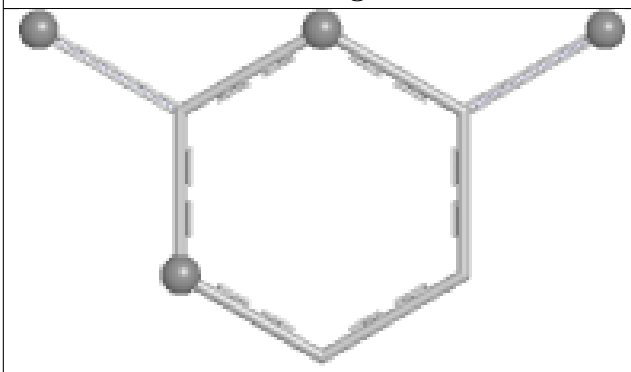
Ligand URA A 5304



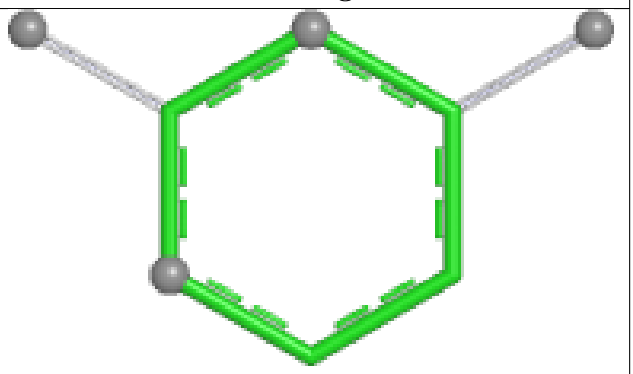
Bond lengths



Bond angles

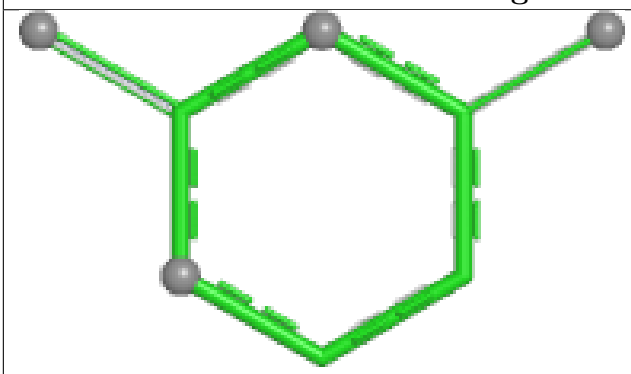


Torsions

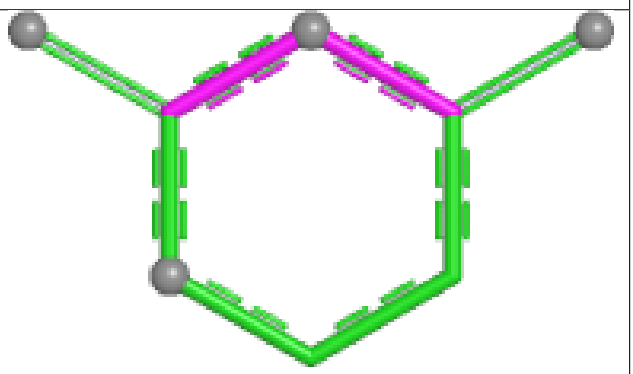


Rings

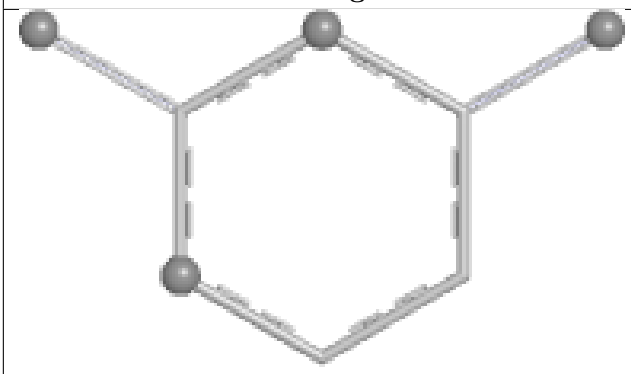
Ligand URA D 5304



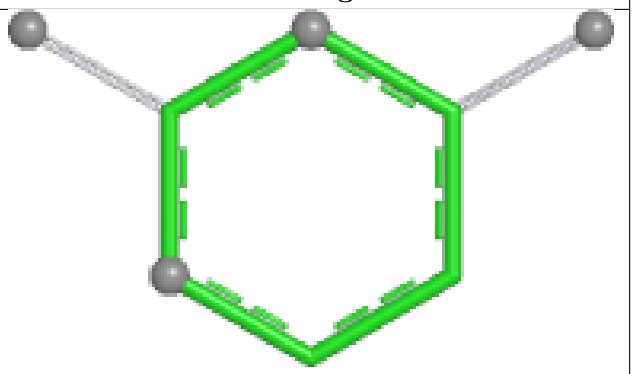
Bond lengths



Bond angles

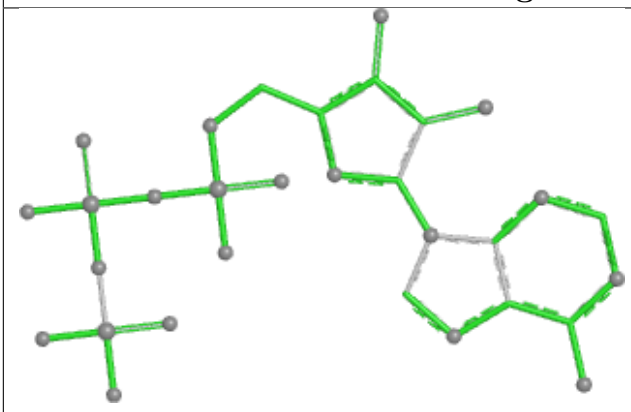


Torsions

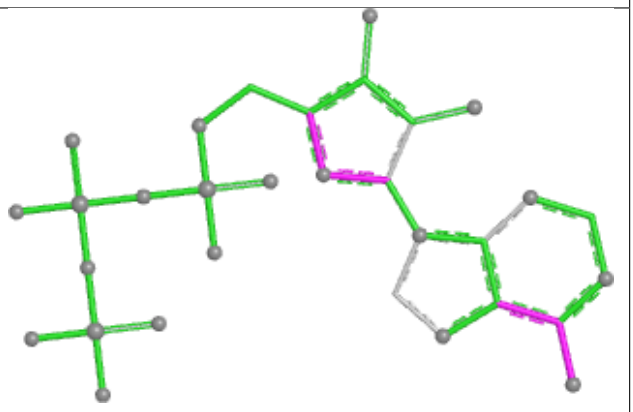


Rings

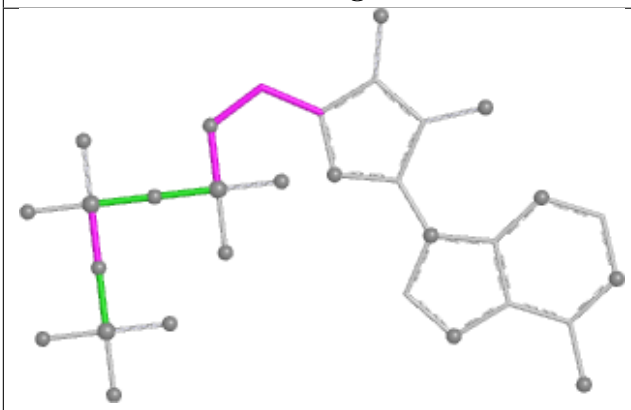
Ligand ATP B 5301



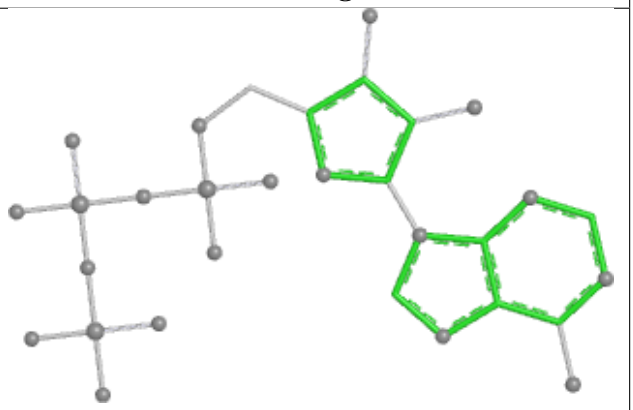
Bond lengths



Bond angles

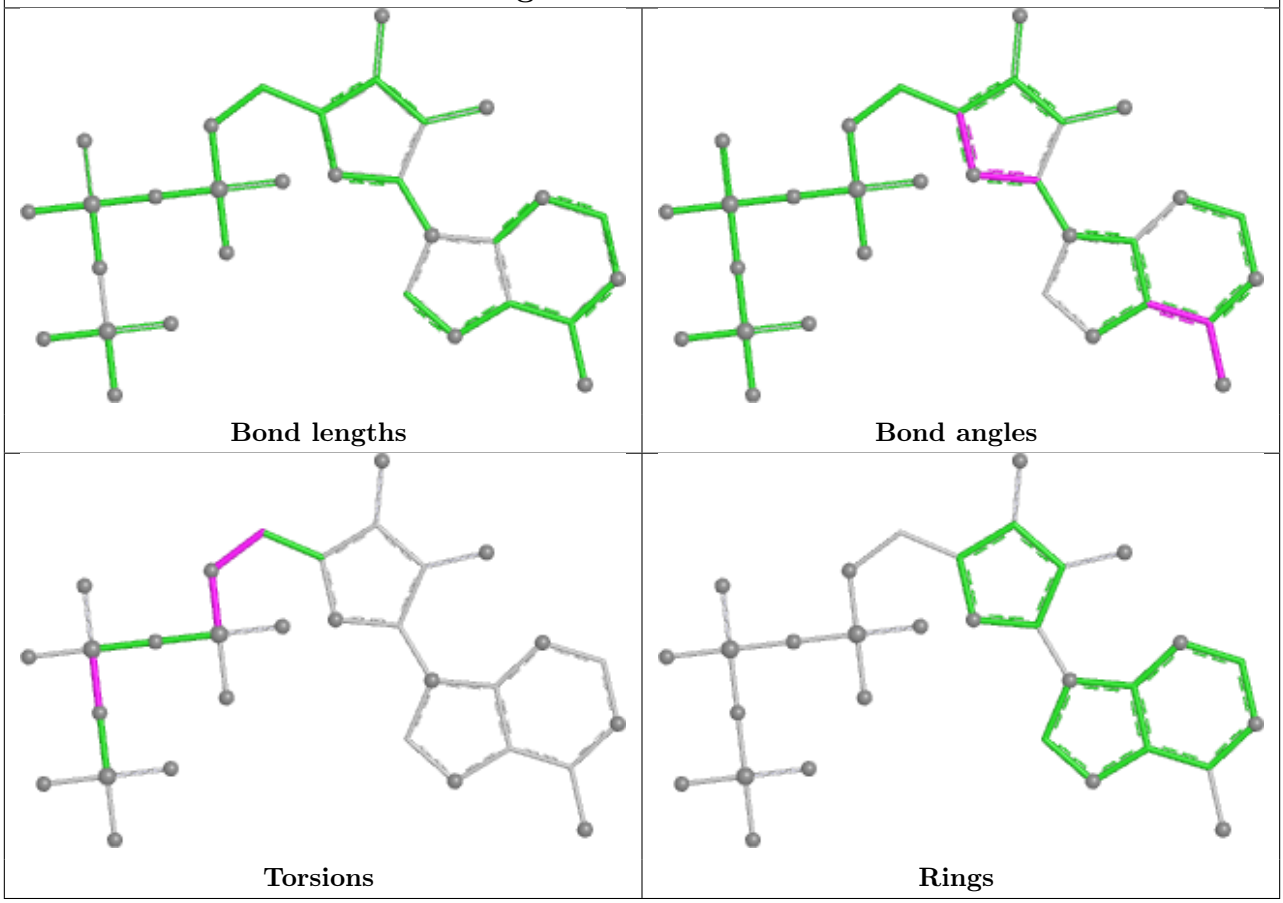


Torsions

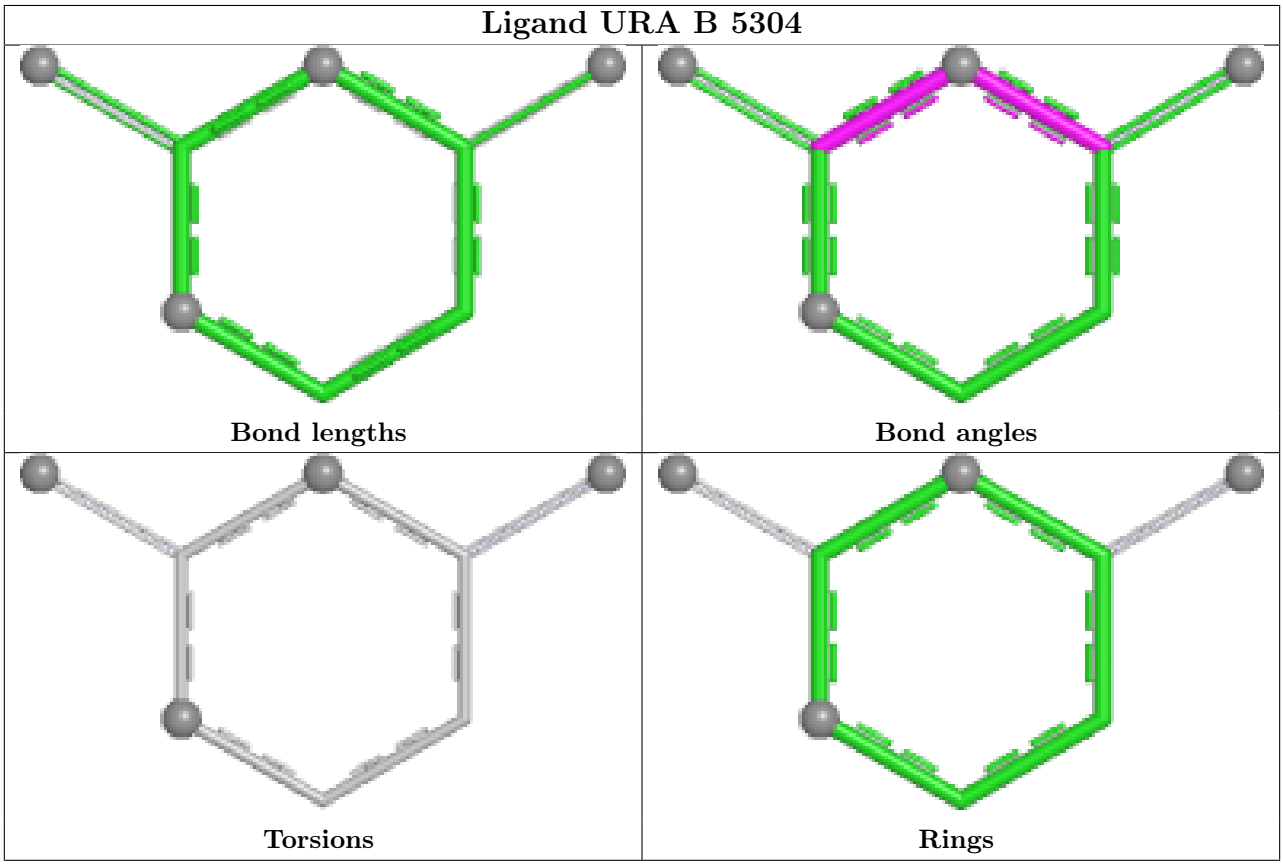


Rings

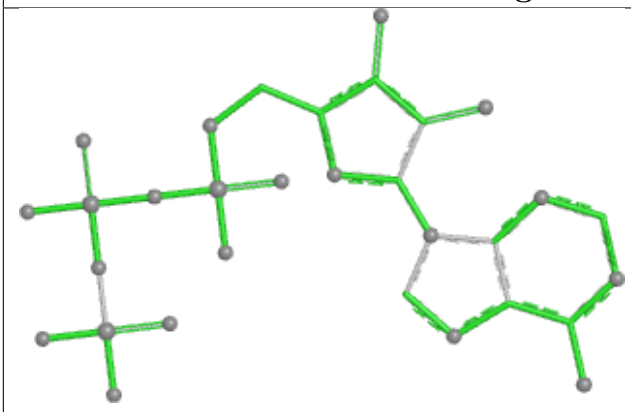
Ligand ATP C 5301



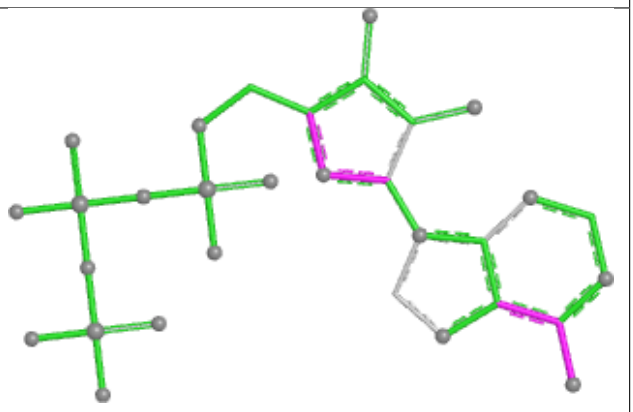
Ligand URA B 5304



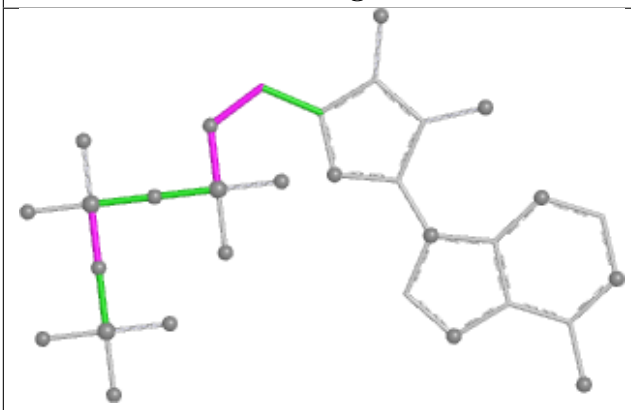
Ligand ATP D 5301



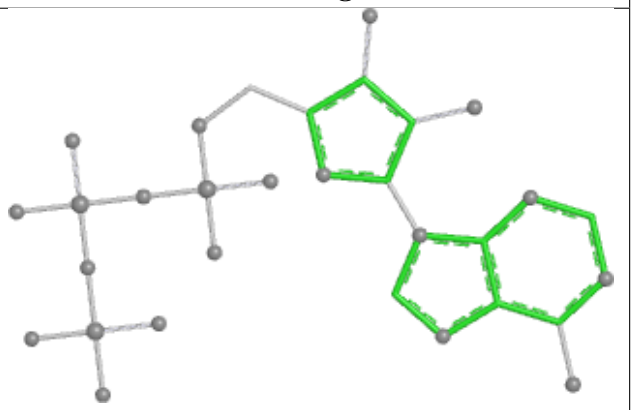
Bond lengths



Bond angles

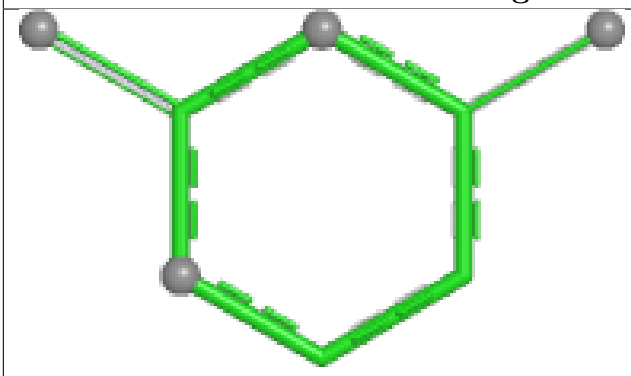


Torsions

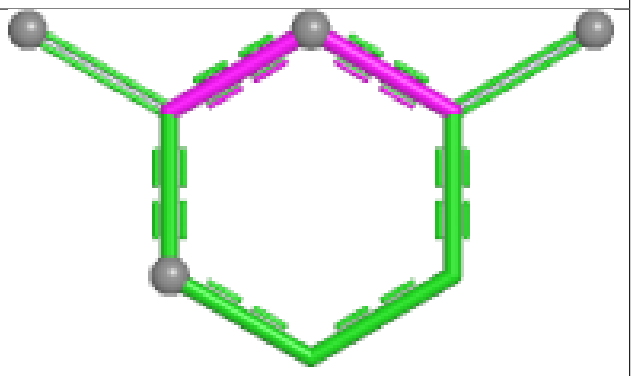


Rings

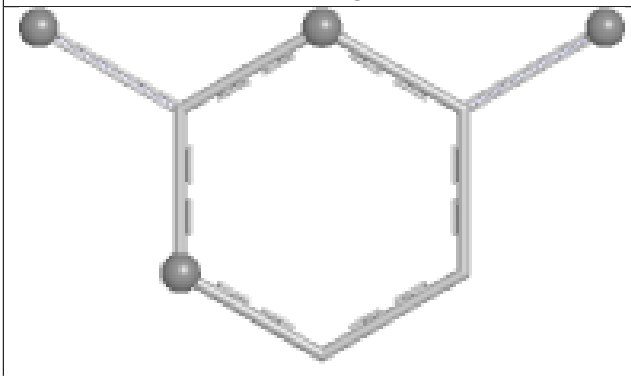
Ligand URA C 5304



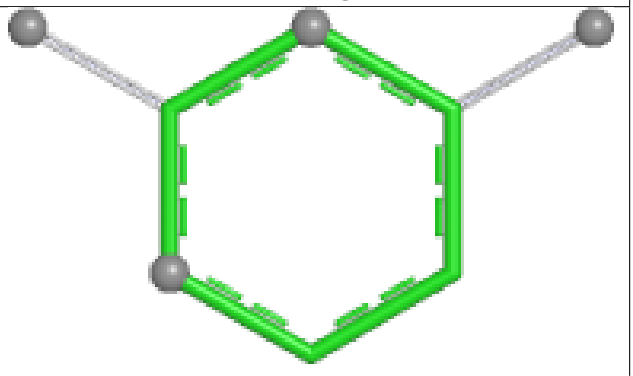
Bond lengths



Bond angles

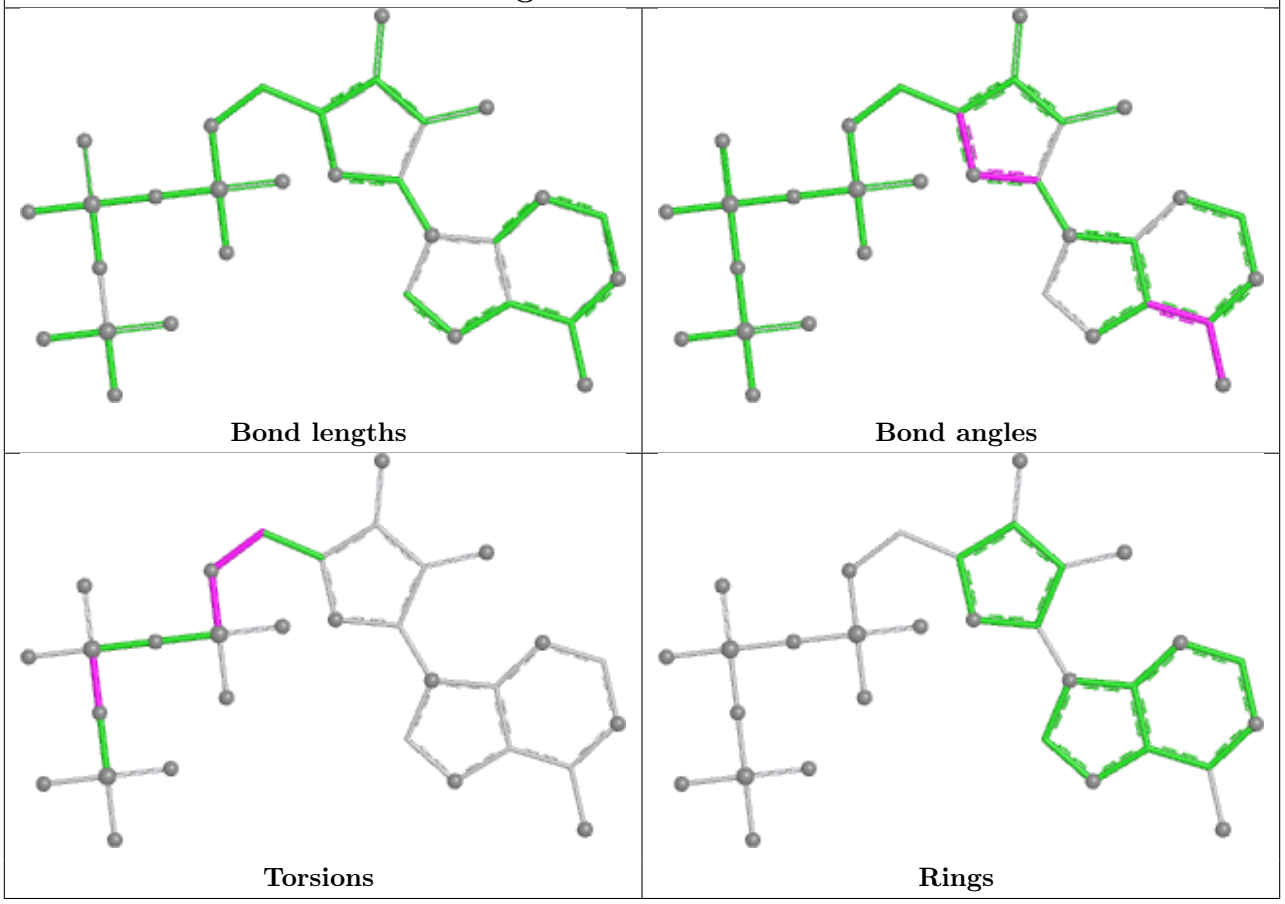


Torsions



Rings

Ligand ATP A 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.

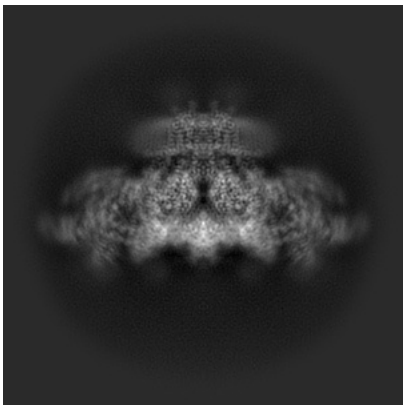
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47391. These allow visual inspection of the internal detail of the map and identification of artifacts.

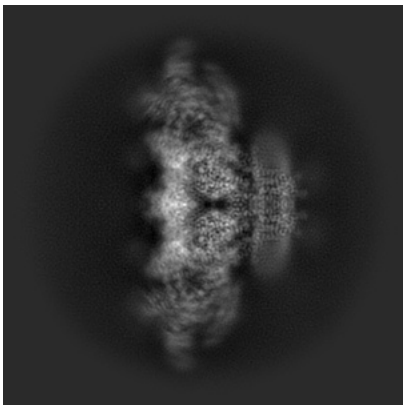
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

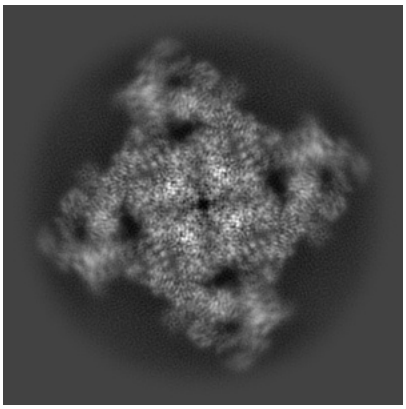
6.1.1 Primary map



X

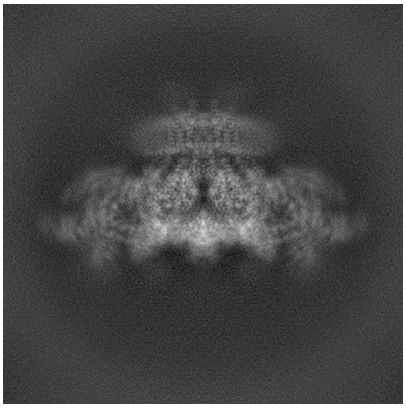


Y

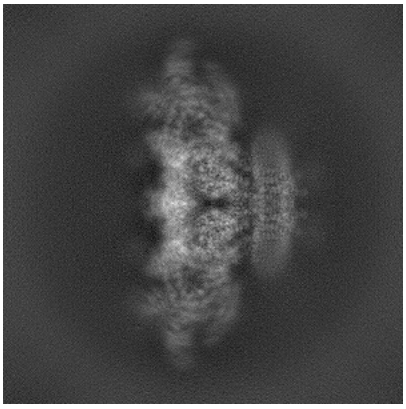


Z

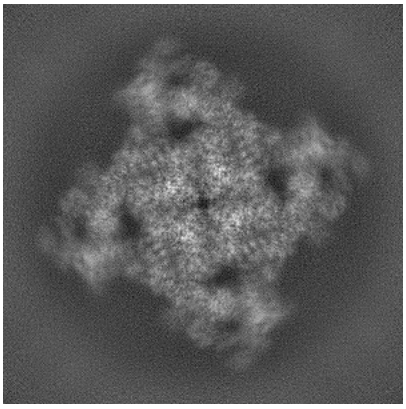
6.1.2 Raw map



X



Y

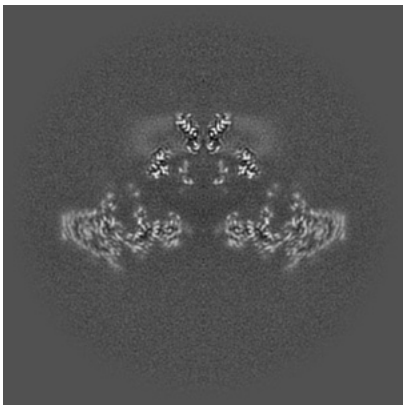


Z

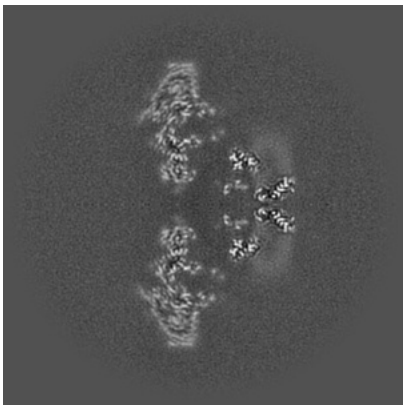
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

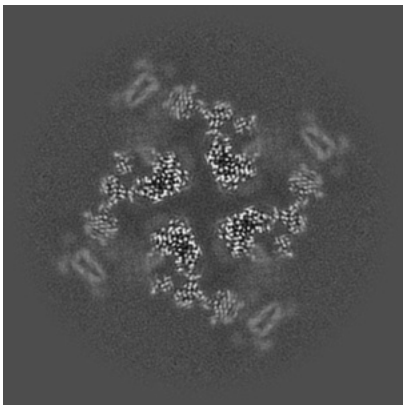
6.2.1 Primary map



X Index: 256

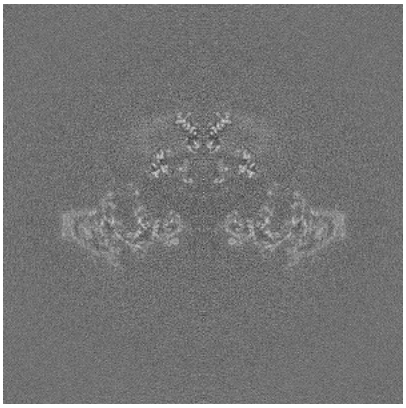


Y Index: 256

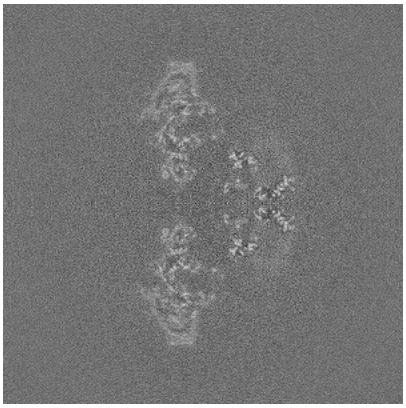


Z Index: 256

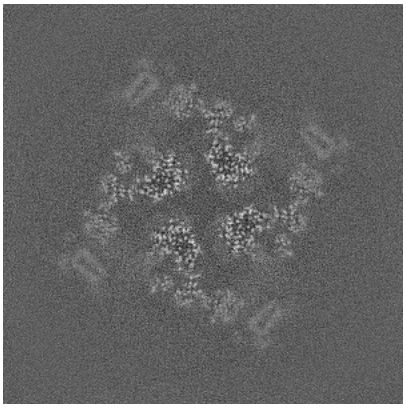
6.2.2 Raw map



X Index: 256



Y Index: 256

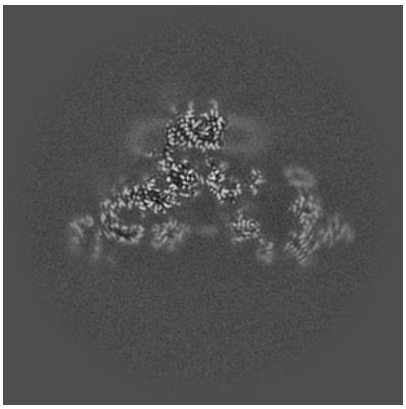


Z Index: 256

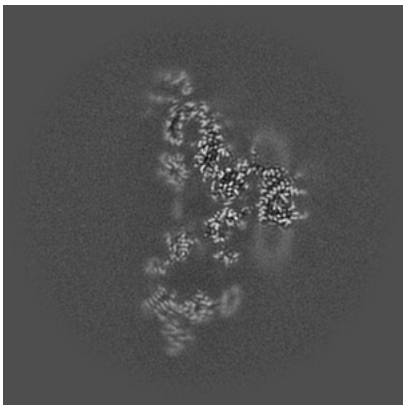
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

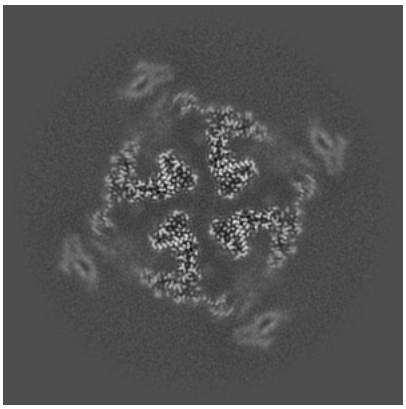
6.3.1 Primary map



X Index: 239

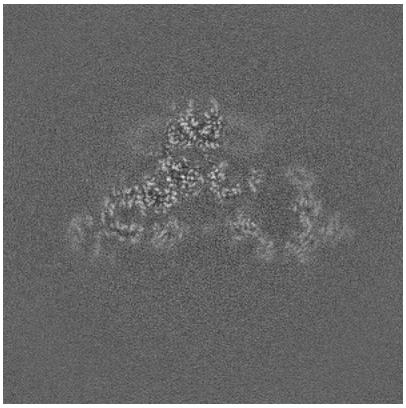


Y Index: 239

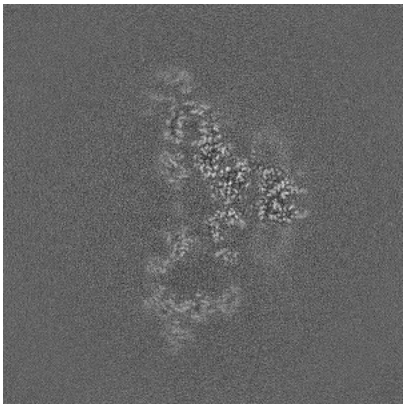


Z Index: 265

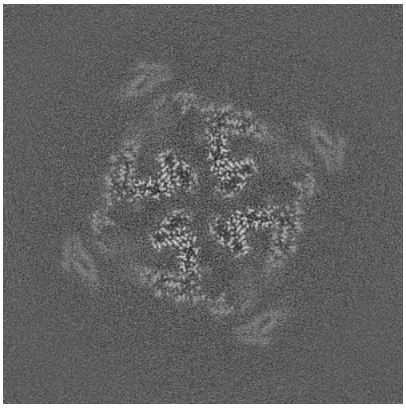
6.3.2 Raw map



X Index: 240



Y Index: 240

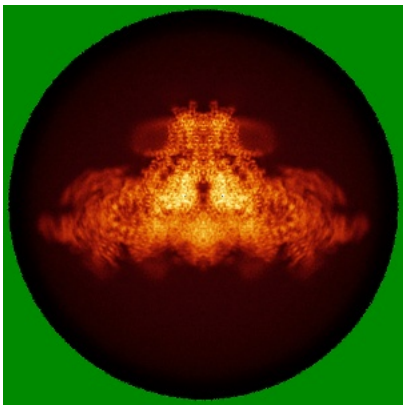


Z Index: 266

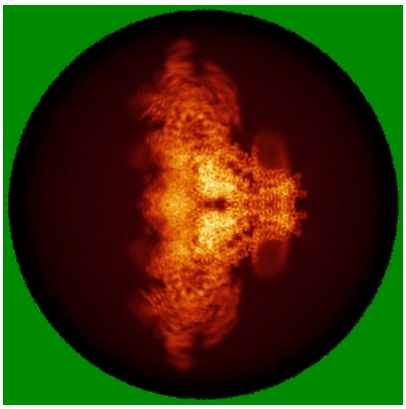
The images above show the largest variance slices of the map in three orthogonal directions.

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

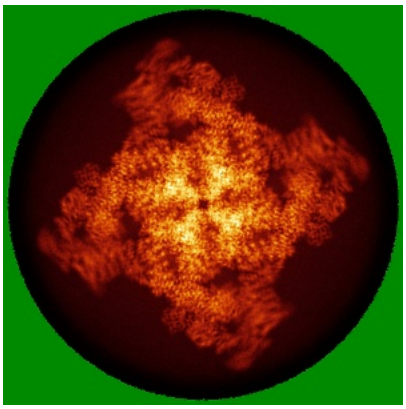
6.4.1 Primary map



X

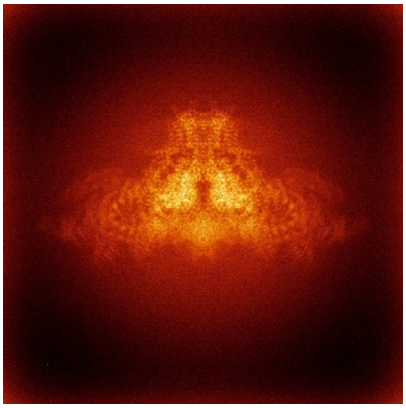


Y

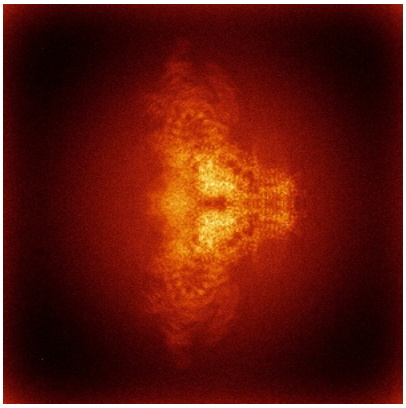


Z

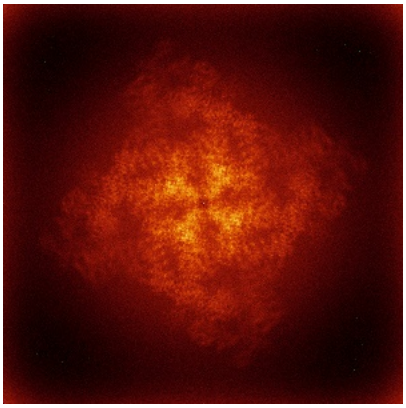
6.4.2 Raw map



X



Y

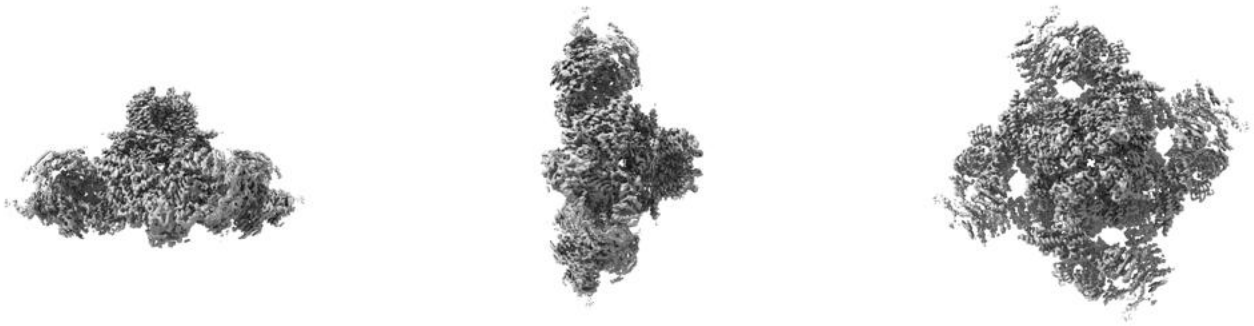


Z

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)

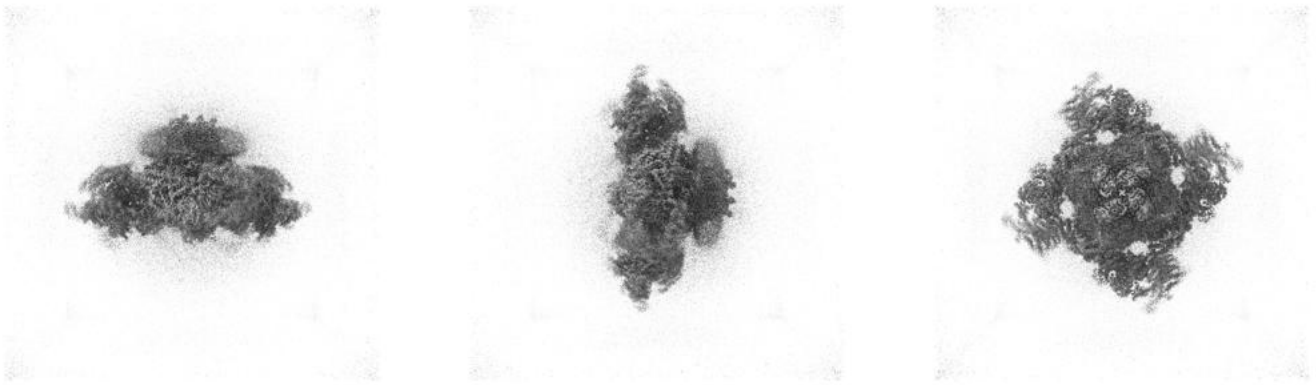
6.5.1 Primary map



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.

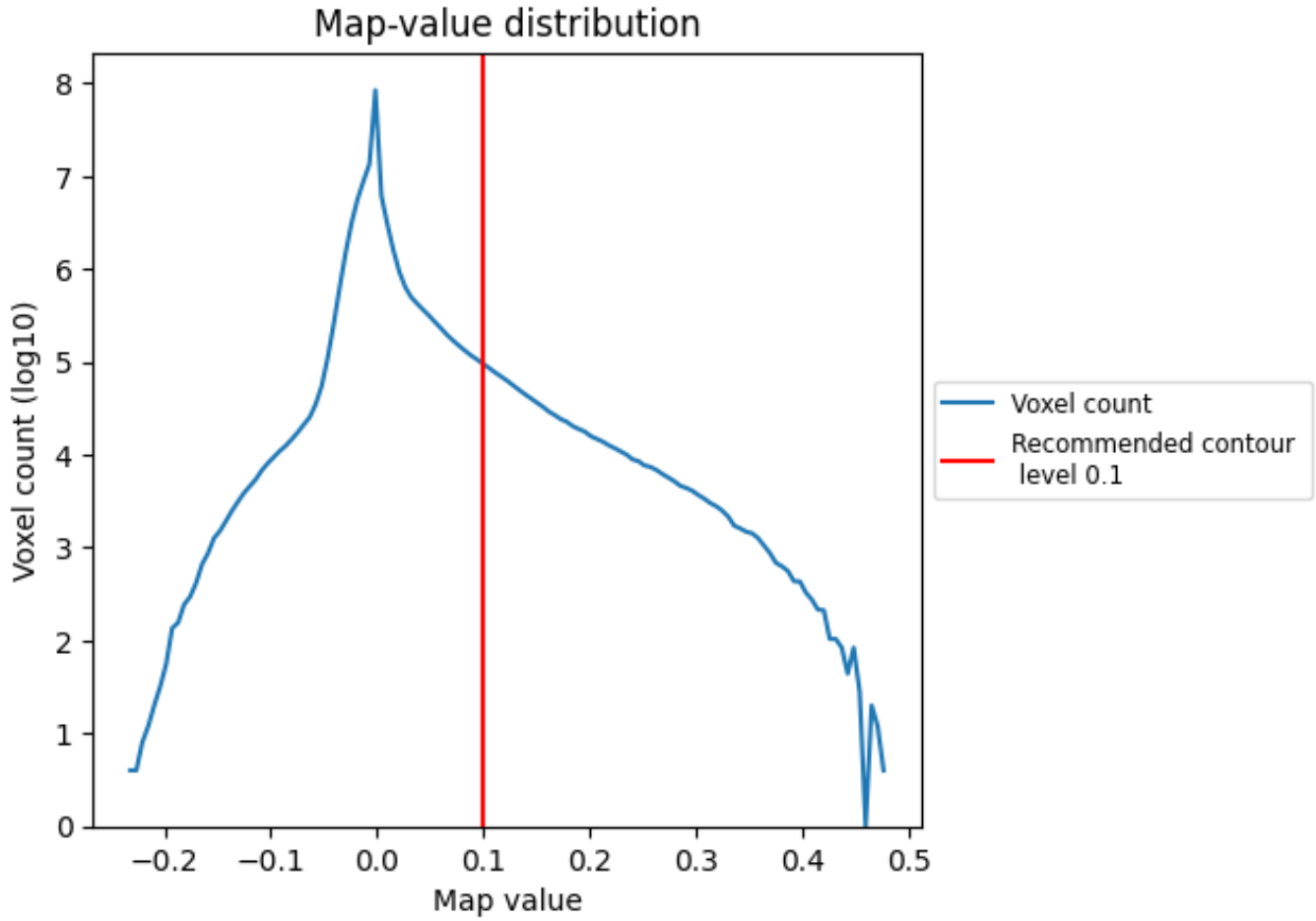
6.6 Mask visualisation (i)

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

7 Map analysis

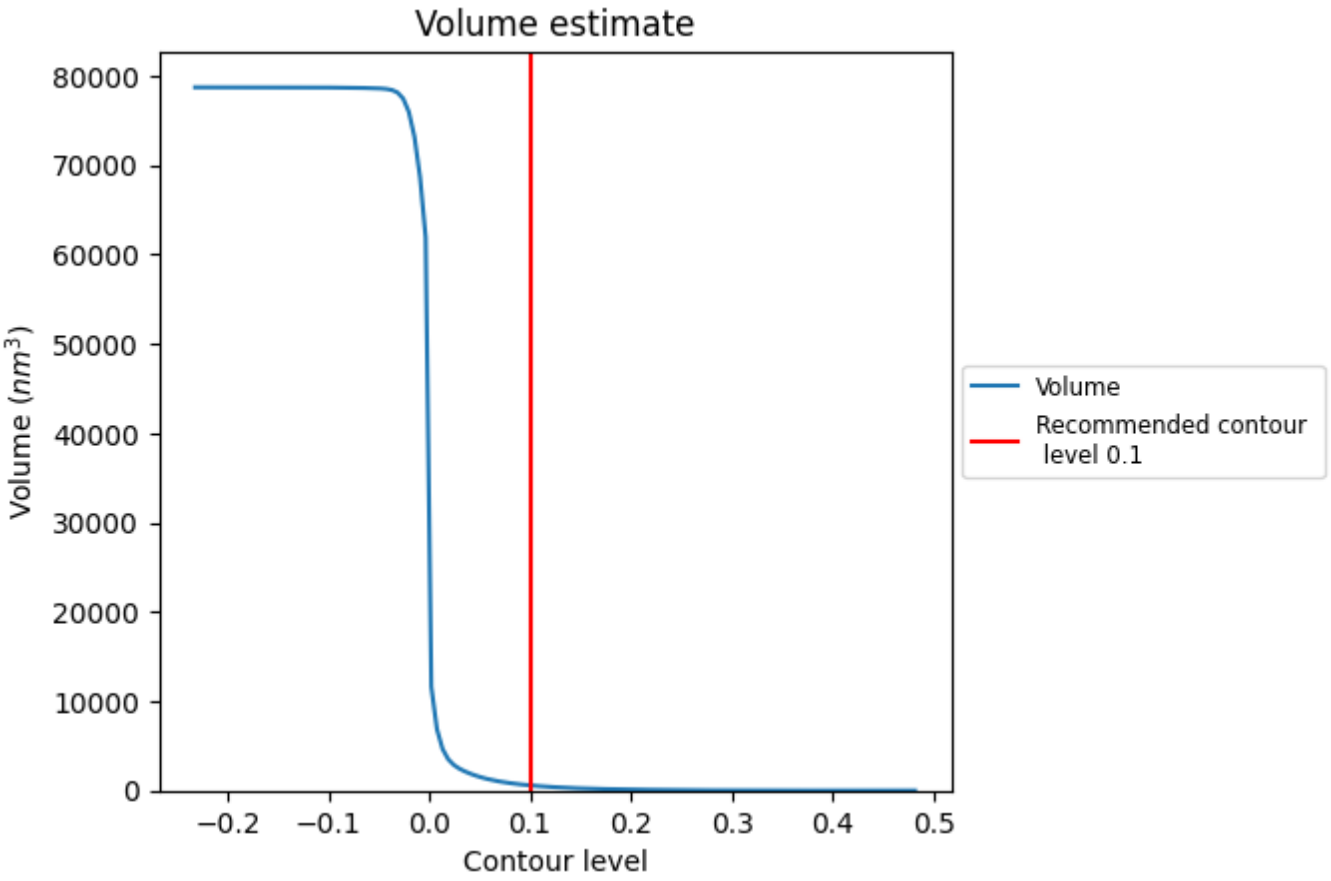
This section contains the results of statistical analysis of the map.

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.

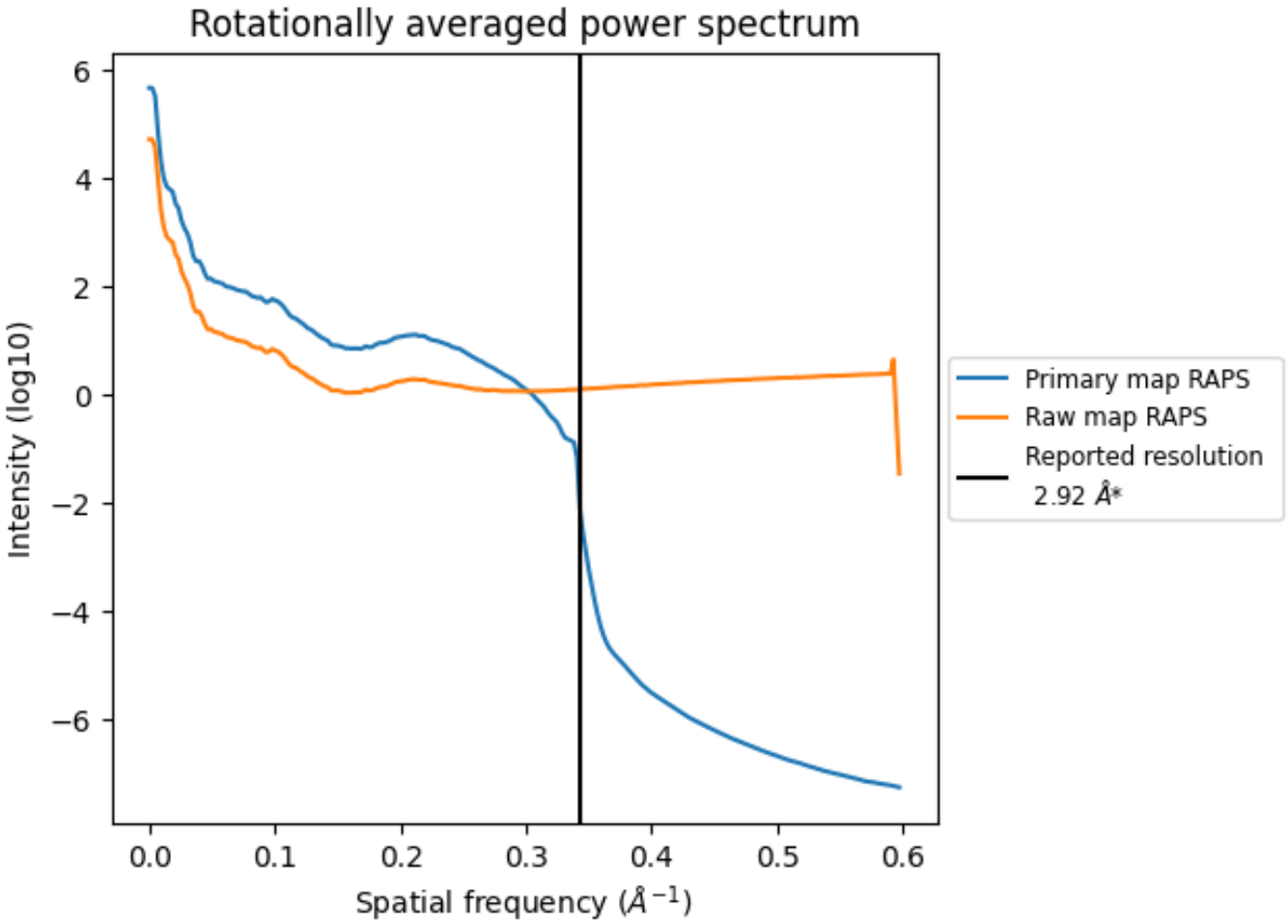
7.2 Volume estimate (i)



The volume at the recommended contour level is 584 nm^3; this corresponds to an approximate mass of 528 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)

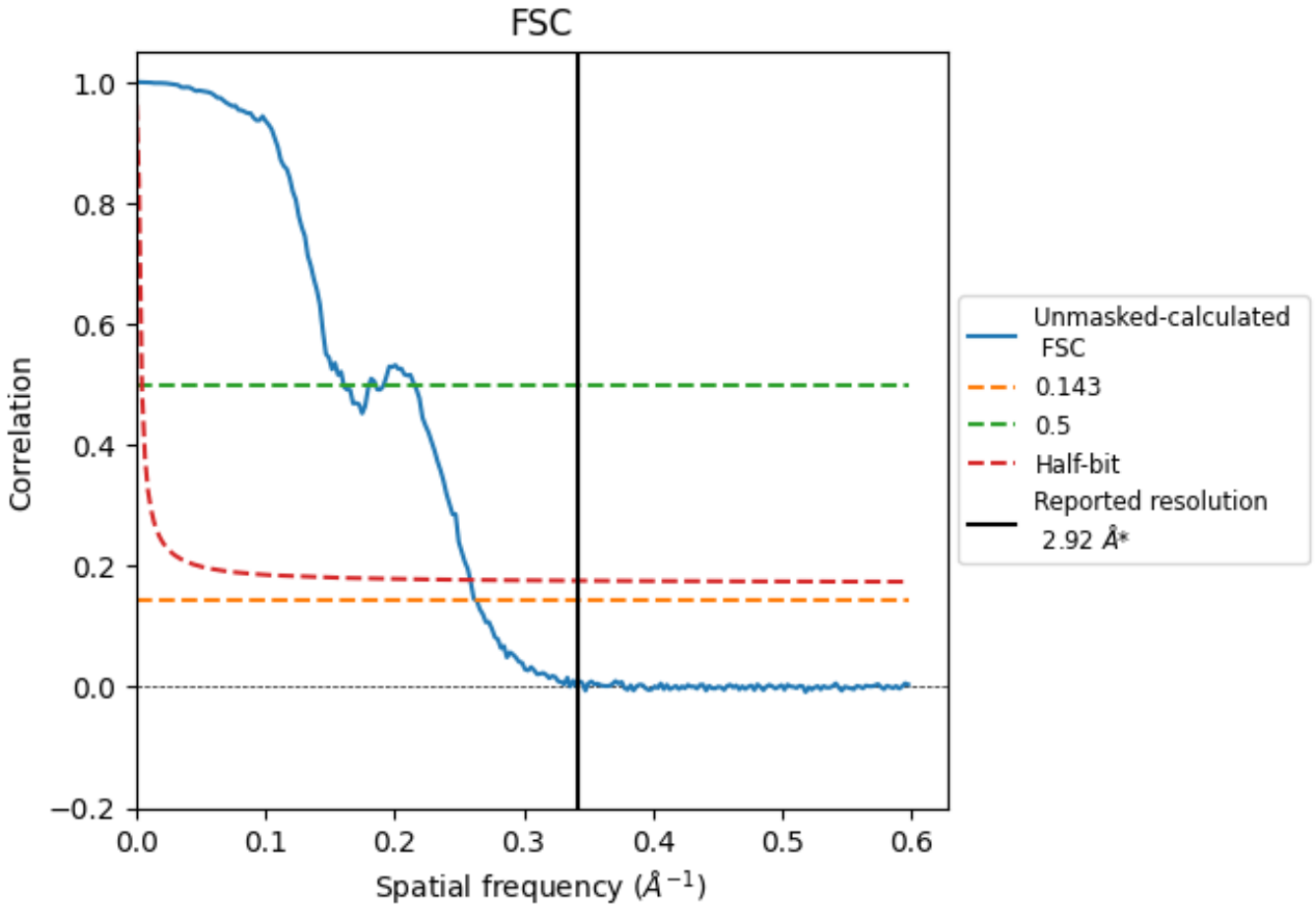


*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8.2 Resolution estimates (i)

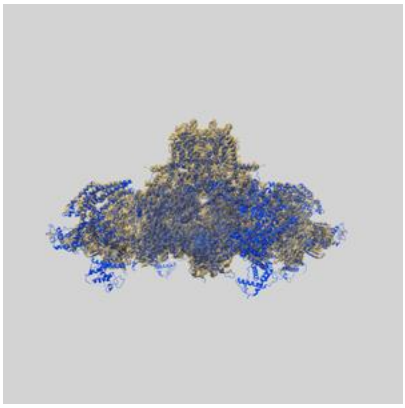
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.23	3.87

*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 3.80 differs from the reported value 2.92 by more than 10 %

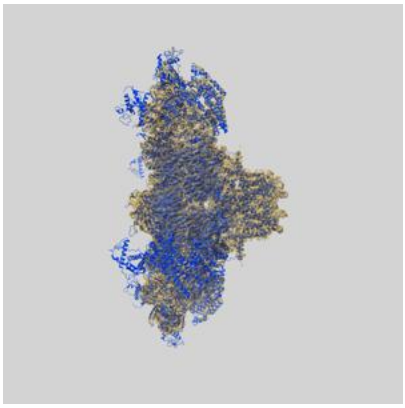
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47391 and PDB model 9E1E. Per-residue inclusion information can be found in section 3 on page 6.

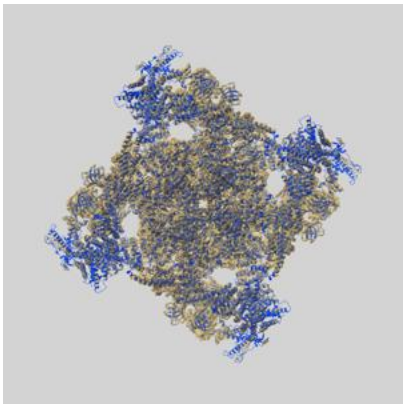
9.1 Map-model overlay



X



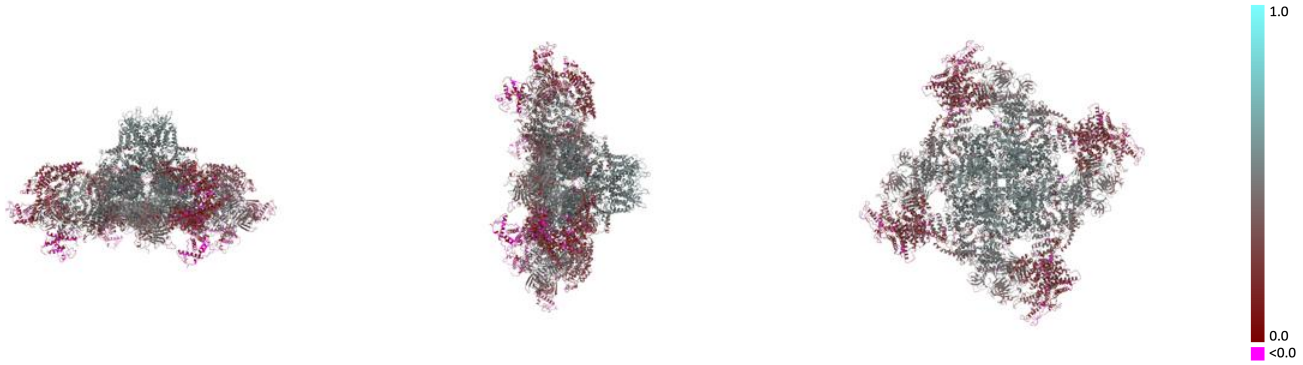
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

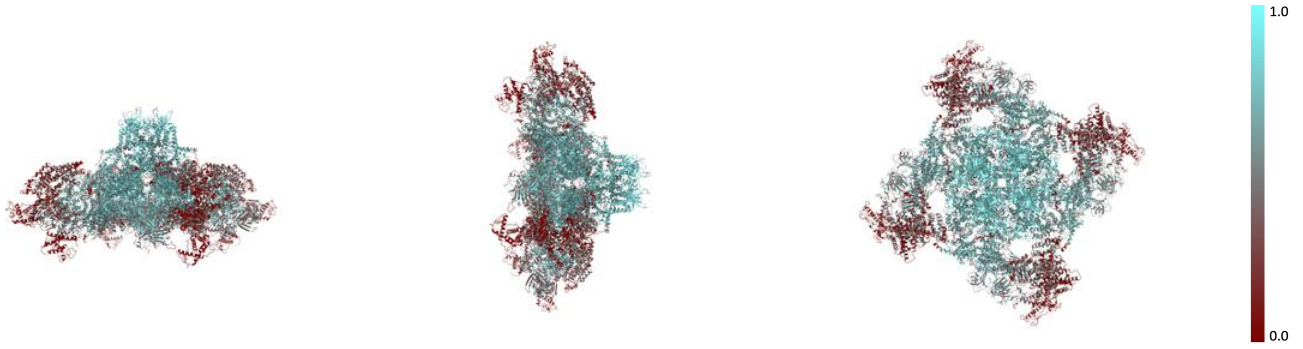
9.2 Q-score mapped to coordinate model



X Y Z

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

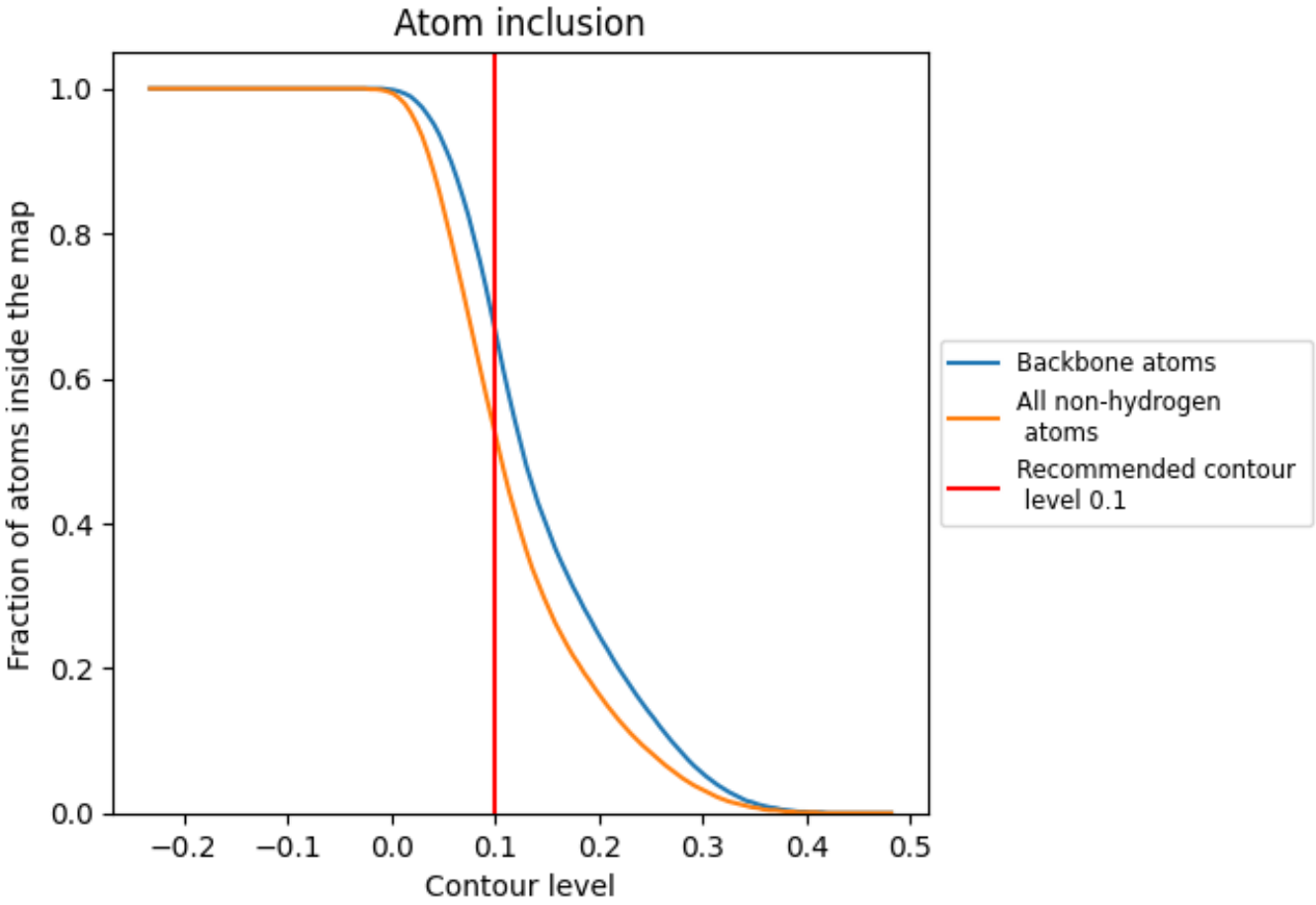
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 52% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5250	0.3760
A	0.5260	0.3740
B	0.5260	0.3740
C	0.5240	0.3730
D	0.5270	0.3750
E	0.4910	0.4340
F	0.4930	0.4290
G	0.4920	0.4280
H	0.4930	0.4300