wwPDB EM Validation Summary Report (i)

Mar 19, 2024 – 02:28 PM JST

PDB ID	:	5GL0
EMDB ID	:	EMD-9520
Title	:	Structure of RyR1 in a closed state (C4 conformer)
Authors	:	Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on	:	2016-07-07
Resolution	:	4.20 Å(reported)

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

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

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

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

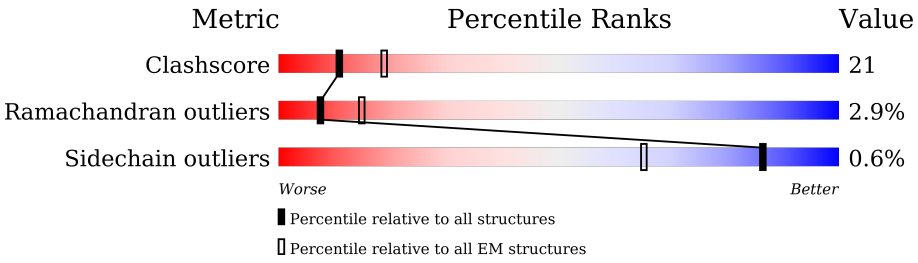
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	5037	24% 44% 26% · 27%
1	C	5037	24% 44% 26% · 27%
1	E	5037	24% 44% 26% · 27%
1	G	5037	24% 44% 27% · 27%
2	B	108	36% 60% 38% ··
2	D	108	36% 61% 37% ··
2	F	108	36% 63% 35% ··
2	H	108	31% 64% 34% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 111000 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	3660	Total 26917	C 17107	N 4682	O 4971	S 157	0	0
1	C	3660	Total 26917	C 17107	N 4682	O 4971	S 157	0	0
1	E	3660	Total 26917	C 17107	N 4682	O 4971	S 157	0	0
1	G	3660	Total 26917	C 17107	N 4682	O 4971	S 157	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total 832	C 527	N 146	O 155	S 4	0	0
2	D	107	Total 832	C 527	N 146	O 155	S 4	0	0
2	F	107	Total 832	C 527	N 146	O 155	S 4	0	0
2	H	107	Total 832	C 527	N 146	O 155	S 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

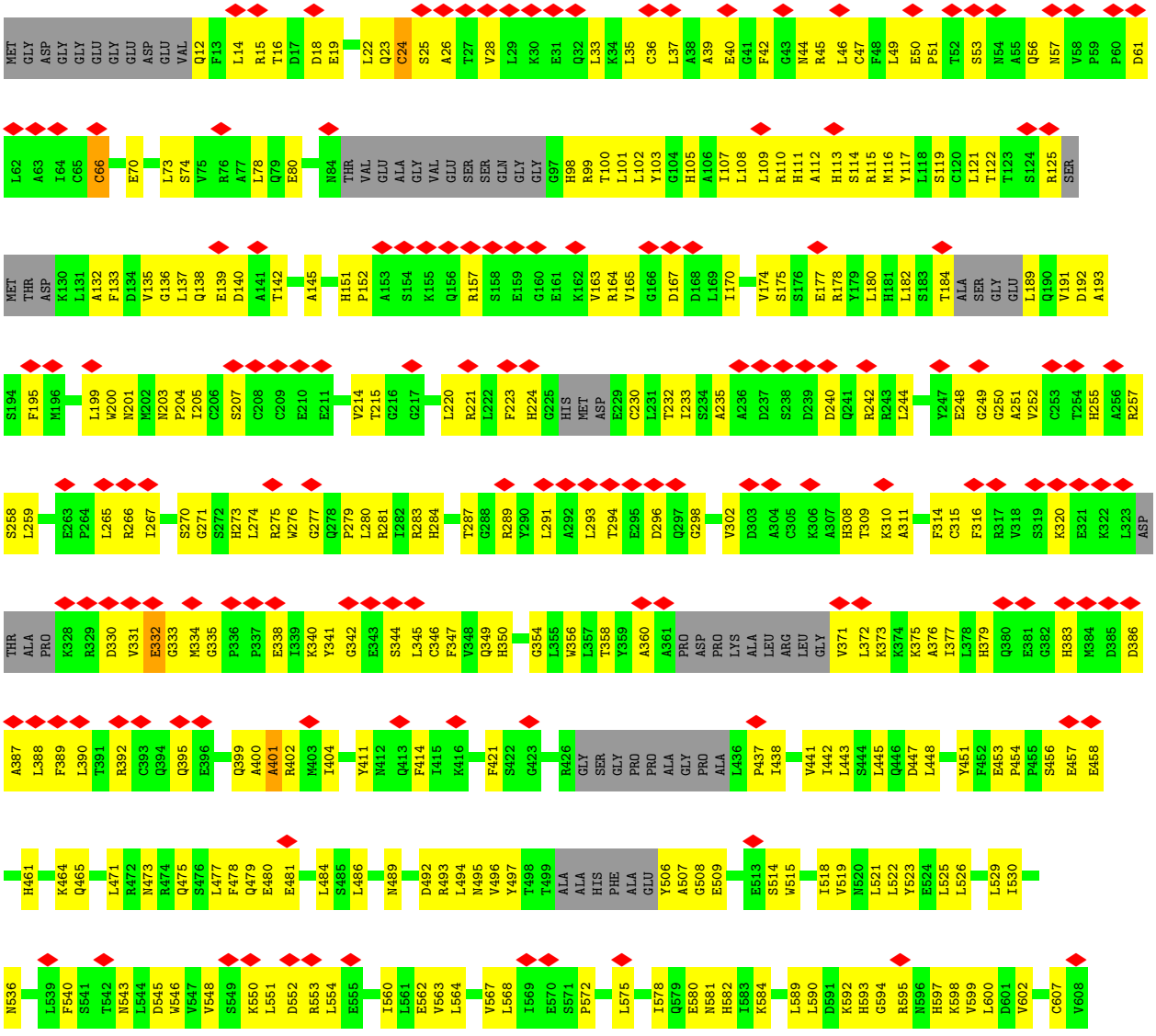
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	E	1	Total 1	Zn 1	0
3	G	1	Total 1	Zn 1	0

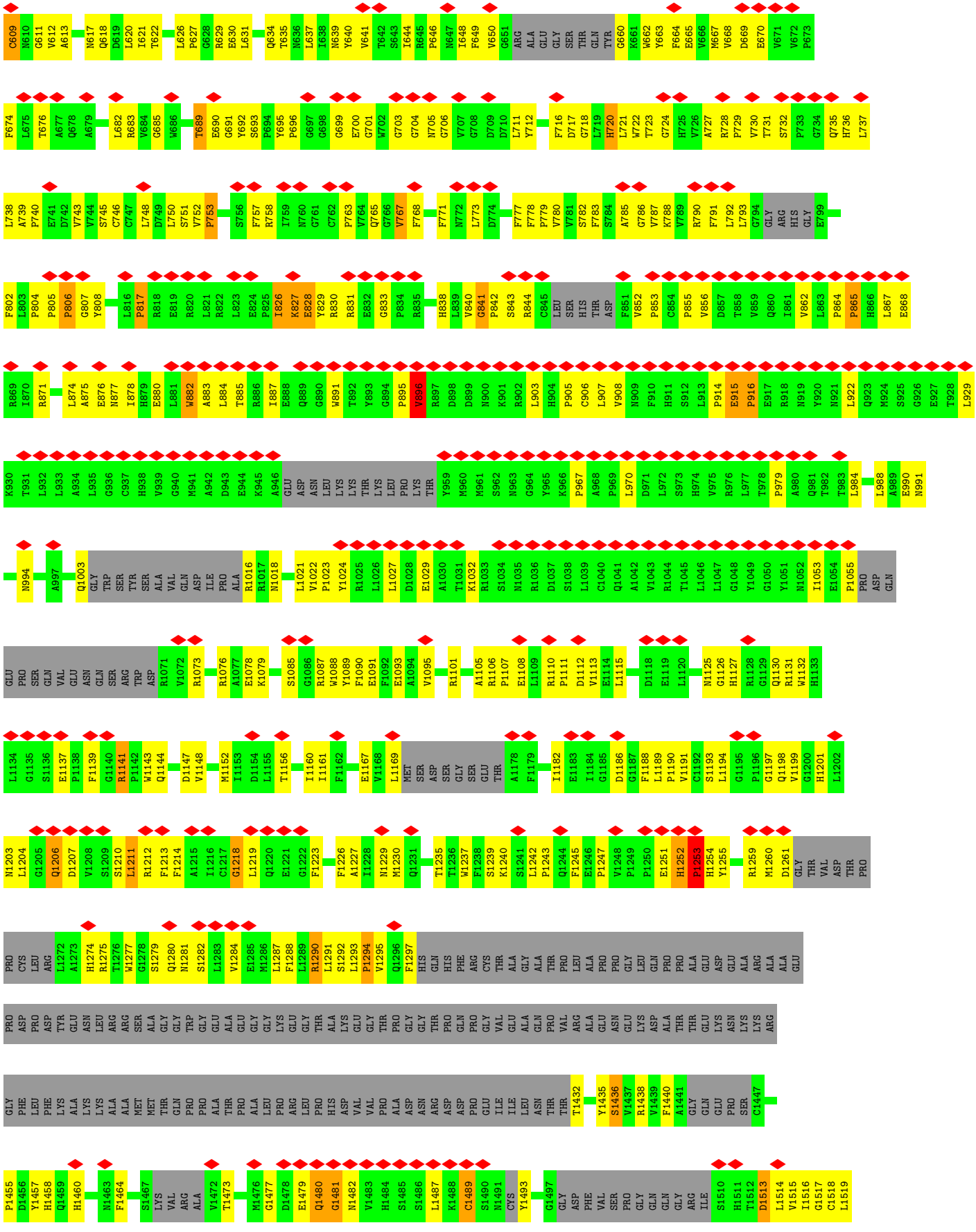
3 Residue-property plots (i)

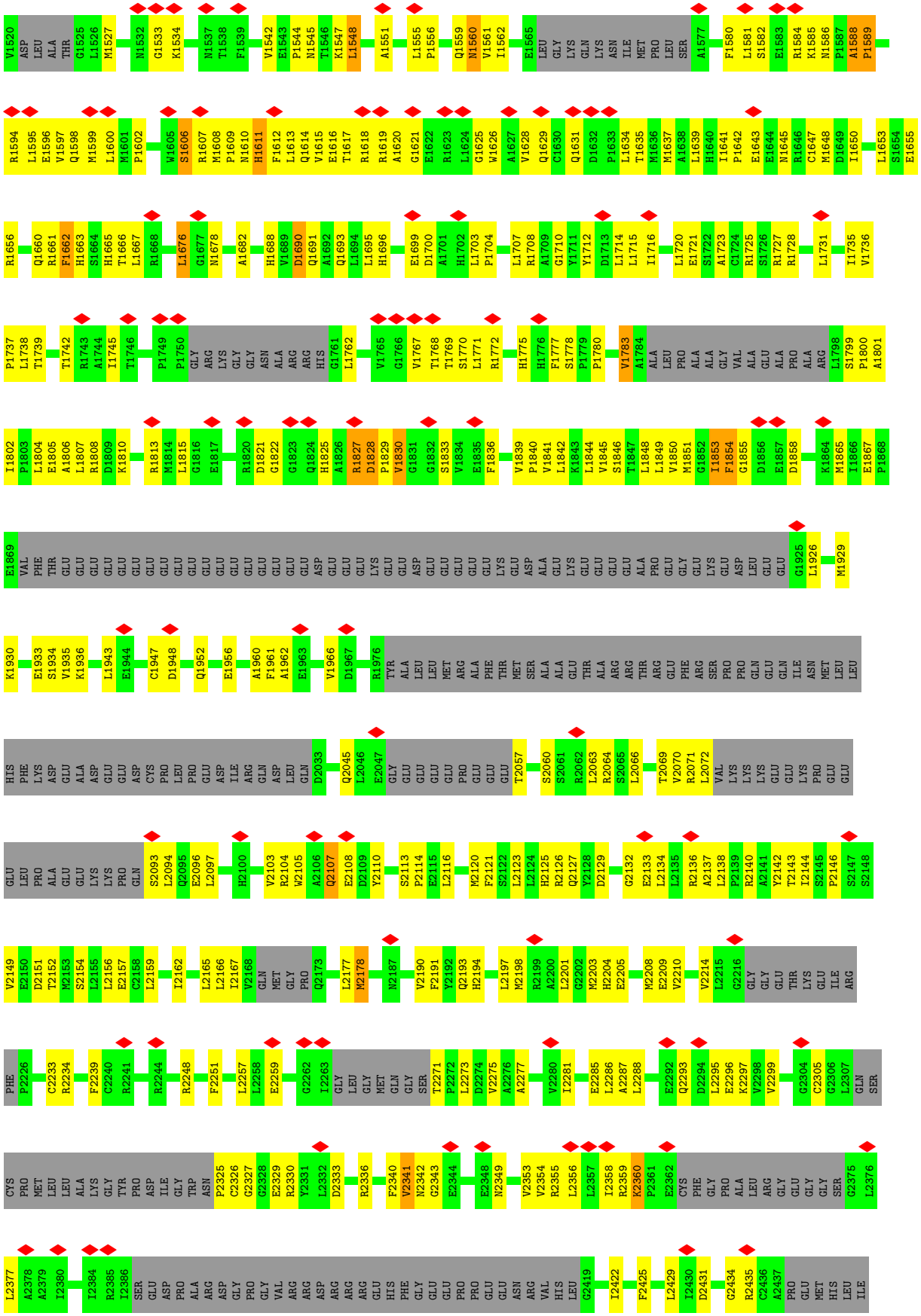
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

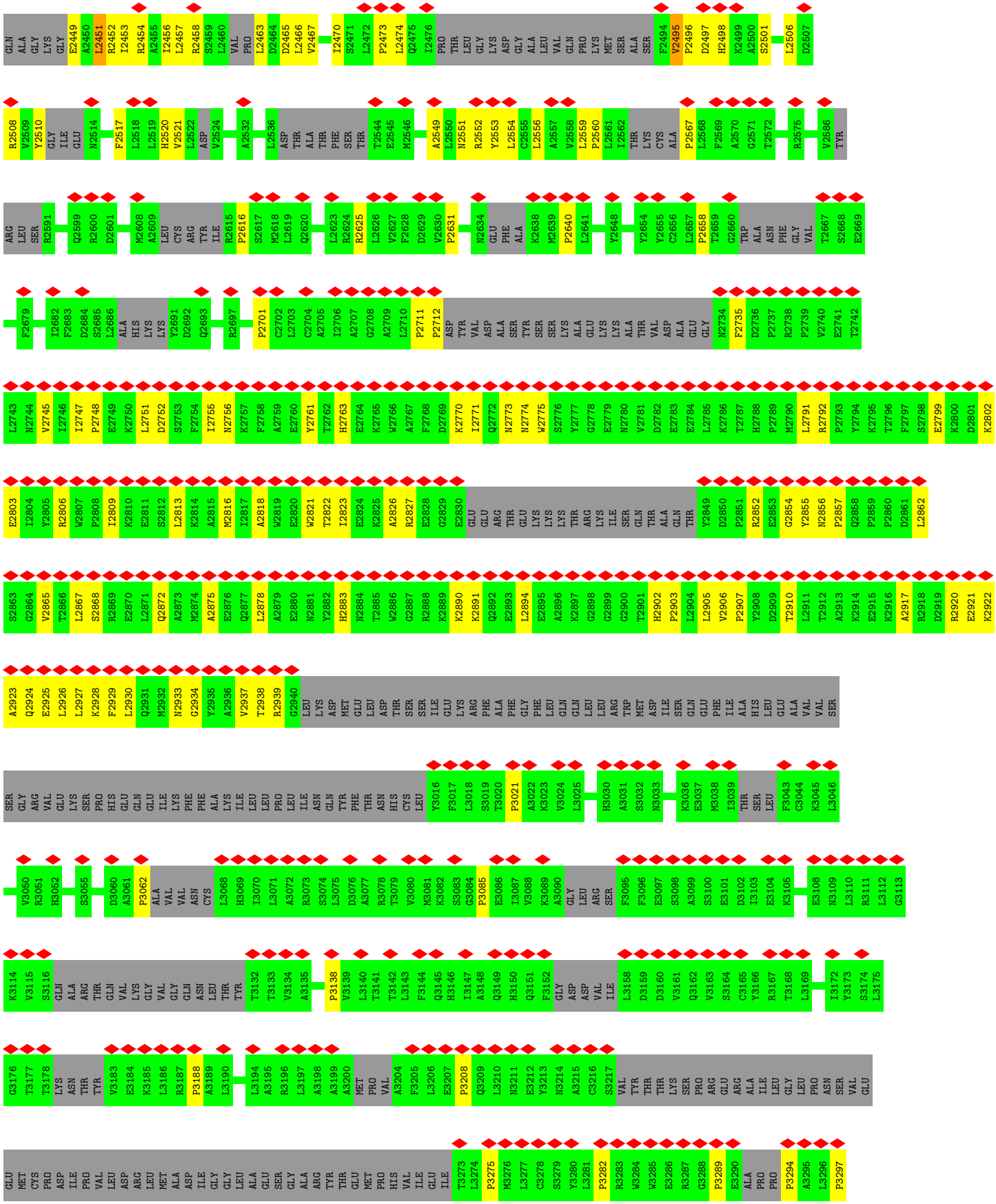
- Molecule 1: Ryanodine receptor 1

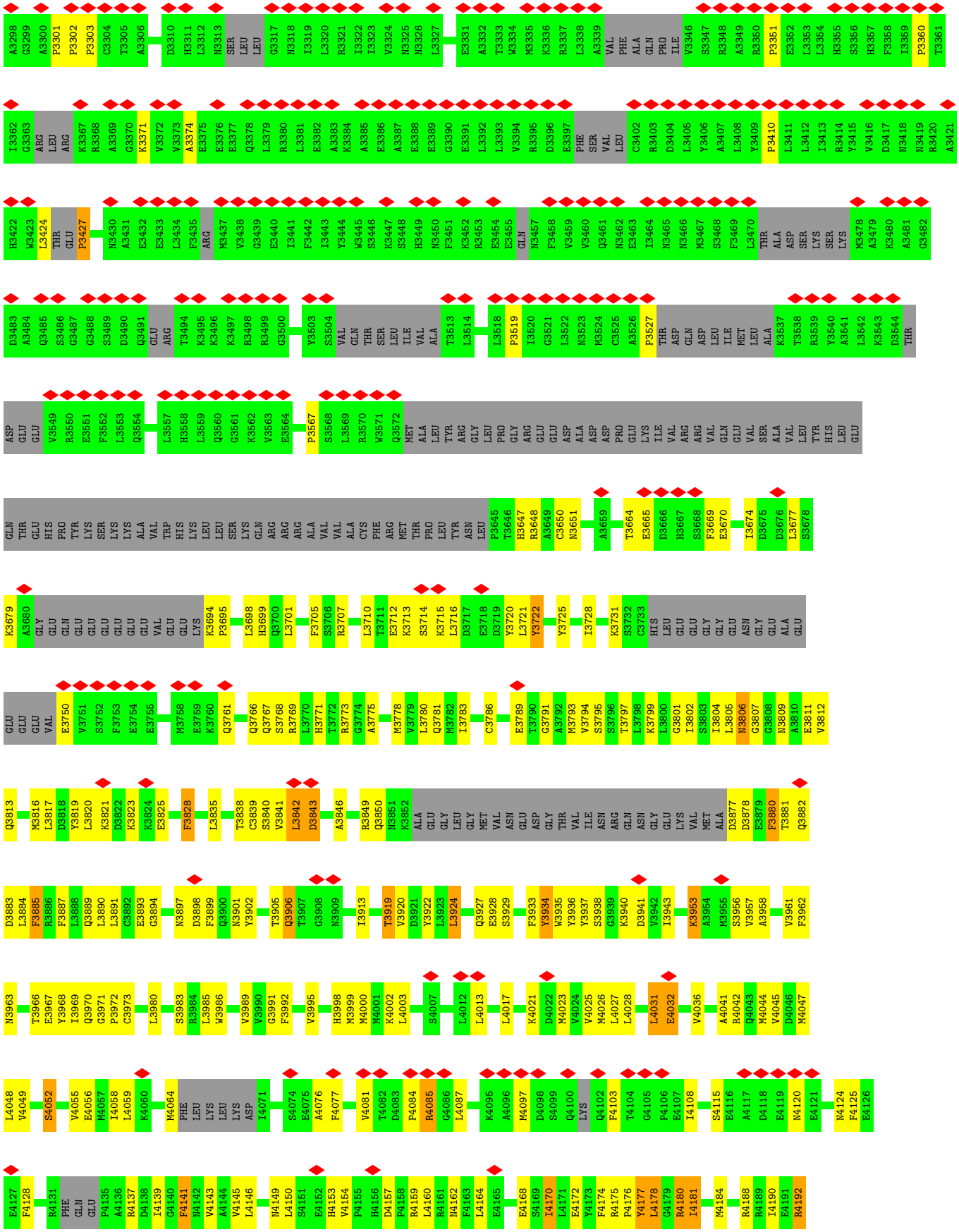
Chain A:








GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU VAL GLN PRO LYS MET SER ALA SER F2494 V2495 P2496 D2497 H2498 K2499 A2500 S2501 L2506 D2507
R2508 V2509 Y2510 GLY ILE GLU N2514 F2517 L2518 L2519 H2520 V2521 L2522 ASP V2524 A2532 L2536 ASP THR ALA THR PHE SER THR T2544 E2545 M2546 A2549 L2550 N2551 R2552 Y2553 L2554 G2555 L2556 A2557 V2558 L2559 P2560 L2561 I2562 THR LYS CYS ALA P2567 L2568 F2569 A2570 G2571 T2572 R2575 V2586 TYR
ARG LEU SER R2591 Q2599 R2600 D2601 M2608 A2609 LEU CYS ARG TYR ILE R2615 P2616 S2617 M2618 L2619 Q2620 L2623 R2624 R2625 L2626 V2627 F2628 D2629 V2630 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 L2641 Y2648 Y2654 Y2655 C2656 L2657 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 S2668 E2669
F2679 I2682 F2683 D2684 S2685 L2686 ALA HIS LYS LYS Y2691 D2692 Q2693 R2697 P2701 C2702 L2703 C2704 A2705 I2706 A2707 G2708 A2709 L2710 P2711 P2712 ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS 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 Y2849 D2850 P2851 R2852 E2853 G2854 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 G2940 LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER
SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS ILE LEU LEU PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 F3017 L3018 S3019 T3020 P3021 A3022 K3023 V3024 L3025 H3030 A3031 S3032 N3033 K3036 E3037 M3038 I3039 THR SER LEU F3043 C3044 K3045 L3046
V3050 R3051 H3052 S3055 D3060 A3061 P3062 ALA VAL VAL ASN CYS L3068 H3069 I3070 L3071 A3072 R3073 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 V3088 K3089 A3090 GLY LEU ARG SER F3095 F3096 E3097 S3098 A3099 S3100 E3101 D3102 I3103 E3104 K3105 E3108 N3109 L3110 R3111 L3112 G3113
K3114 V3115 S3116 GLN ALA ARG THR GLN VAL LYS GLY VAL GLY GLN ASN LEU THR TYR T3132 T3133 V3134 A3135 P3138 V3139 L3140 T3141 T3142 L3143 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 GLY ASP ASP VAL ILE L3158 D3159 D3160 V3161 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 L3169 I3172 Y3173 S3174 L3175
G3176 T3177 T3178 LYS ASN THR TYR V3183 E3184 K3185 L3186 R3187 P3188 A3189 L3190 L3194 A3195 R3196 L3197 A3198 A3199 A3200 MET PRO VAL A3204 F3205 L3206 E3207 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 VAL TYR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU
GLU MET CYS PRO ASP ILE PRO VAL LEU ASP ARG LEU MET ALA ASP ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 R3283 W3284 W3285 E3286 R3287 G3288 P3289 E3290 ALA PRO PRO P3294 A3295 L3296 P3297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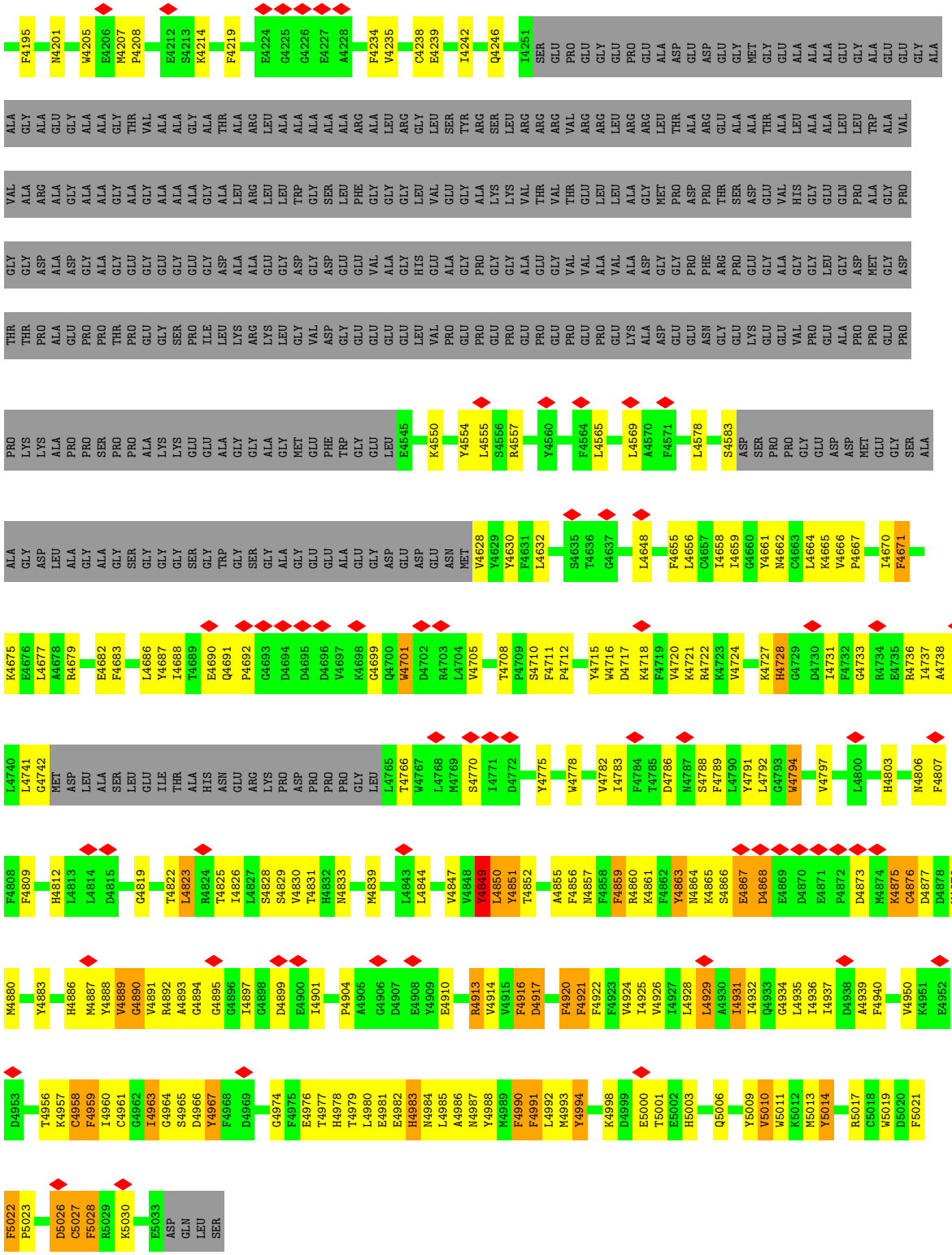
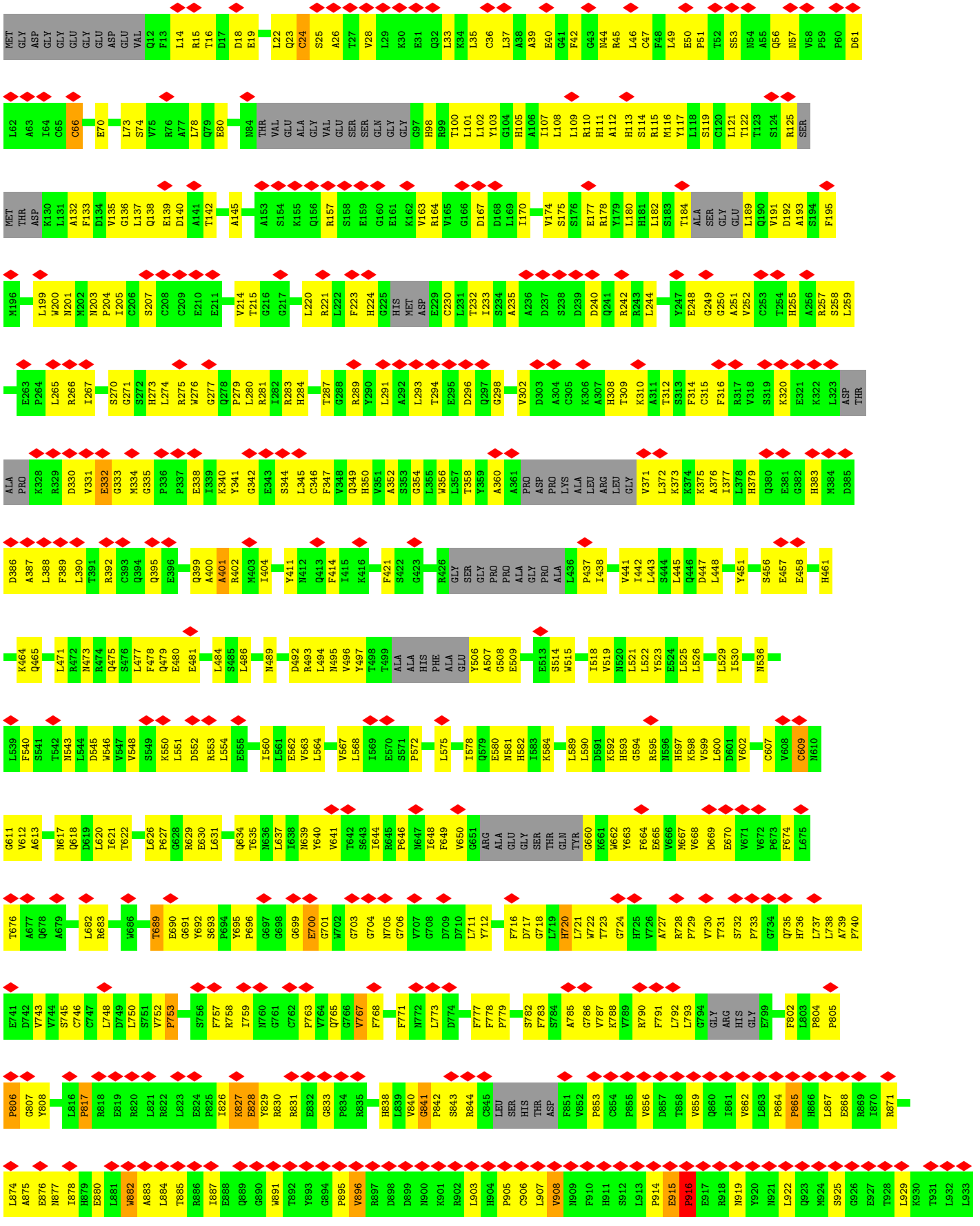
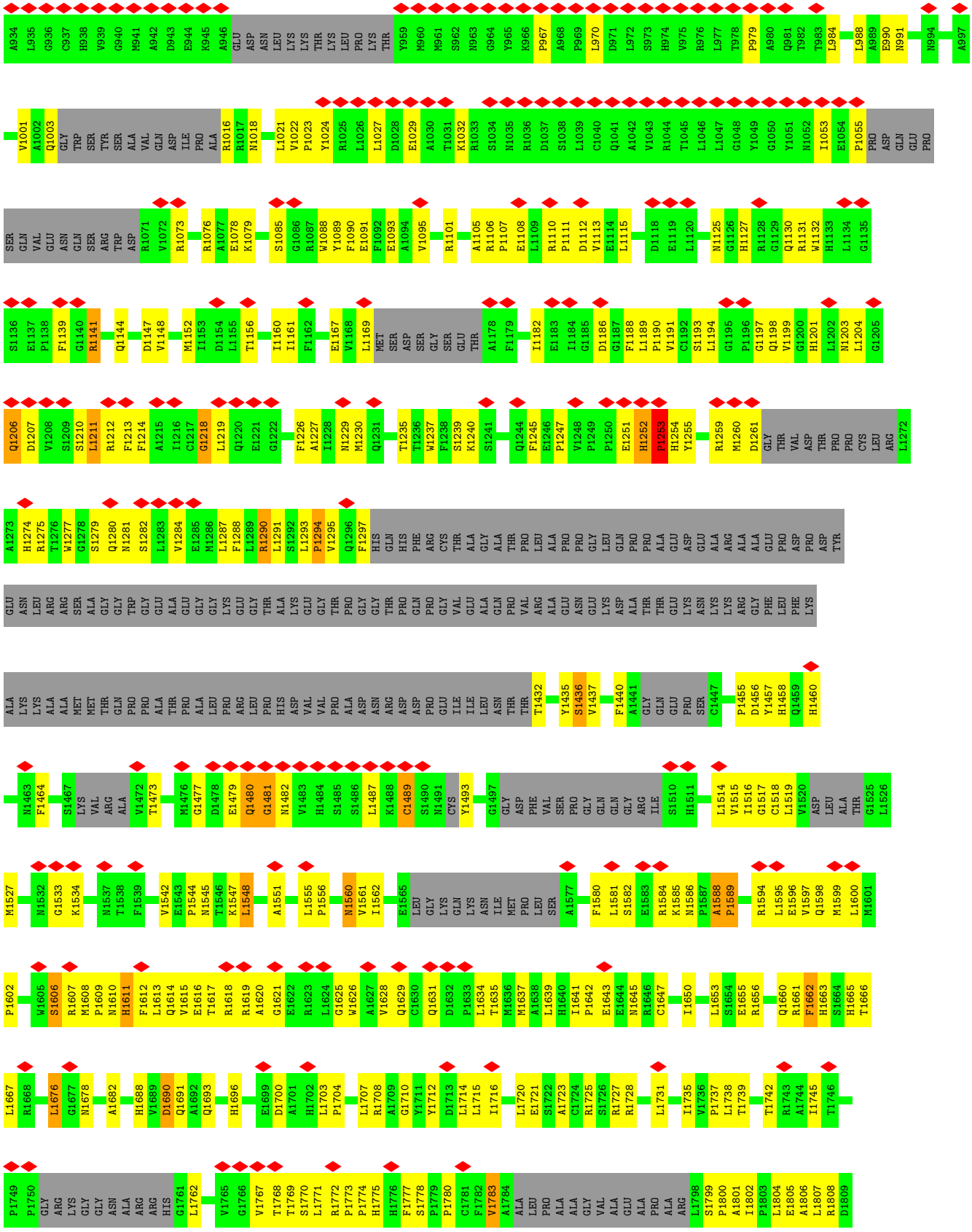
E3331 A3332 T3333 W3334 M3335 K3336 R3337 L3338 A3339 VAL PHE ALA GLN PRO ILE V3346 S3347 R3348 A3349 R3350 P3351 E3352 L3353 L3354 H3355 S3356 H3357 F3358 I3359 P3360 T3361
I3362 G3363 ARG LEU ARG K3367 R3368 A3369 G3370 K3371 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 D3396 E3397 PHE SER VAL LEU C3402 R3403 D3404 L3405 Y3406 A3407 L3408 Y3409 P3410 L3411 L3412 I3413 R3414 Y3415 V3416 D3417 N3418 N3419 R3420 A3421
H3422 W3423 L3424 THR GLU P3427 N3430 A3431 E3432 E3433 L3434 F3435 ARG M3437 V3438 G3439 E3440 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 S3448 H3449 N3450 F3451 K3452 R3453 E3454 E3455 GLN N3457 F3458 V3459 V3460 Q3461 N3462 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 THR ALA ASP SER LYS SER LYS M3478 A3479 K3480 A3481 G3482
D3483 A3484 Q3485 S3486 G3487 G3488 S3489 D3490 Q3491 GLU ARG T3494 K3495 K3496 K3497 R3498 R3499 G3500 Y3503 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513 L3514 L3518 P3519 I3520 G3521 L3522 N3523 M3524 C3525 A3526 P3527 THR ASP GLN ASP LEU ILE MET LEU ALA K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 THR
ASP GLU GLU V3549 R3550 E3551 F3552 L3553 Q3554 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 P3567 S3568 L3569 R3570 W3571 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP ASP PRO GLU LYS ILE VAL ARG ARG VAL GLN GLU VAL SER ALA VAL LEU TYR HIS LEU GLU
GLN THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 R3648 A3649 C3650 N3651 A3659 T3664 E3665 D3666 H3667 S3668 F3669 E3670 I3674 D3675 D3676 L3677 S3678
K3679 A3680 GLY GLU GLN GLU GLU GLU GLU VAL VAL GLU LYS K3694 P3695 L3698 H3699 Q3700 L3701 F3705 S3706 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 L3721 Y3722 Y3725 I3728 K3731 S3732 C3733 HIS LEU GLU GLU GLN GLY GLY GLU ASN GLY GLU ALA GLU
GLU GLU GLU VAL E3750 V3751 S3752 F3753 E3754 E3755 M3758 E3759 K3760 Q3761 Q3766 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 M3778 Y3779 L3780 Q3781 M3782 I3783 C3786 E3789 T3790 G3791 A3792 M3793 V3794 S3795 S3796 T3797 L3798 K3799 L3800 G3801 I3802 S3803 I3804 L3805 N3806 G3807 G3808 N3809 A3810 E3811 V3812
Q3813 M3816 L3817 D3818 Y3819 L3820 K3821 D3822 K3823 K3824 E3825 F3828 L3835 T3838 C3839 S3840 V3841 L3842 D3843 A3846 R3849 Q3850 N3851 K3852 ALA GLU GLY LEU GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL MET ALA D3877 D3878 E3879 F3880 T3881 Q3882
D3883 L3884 F3885 R3886 F3887 L3888 Q3889 L3890 L3891 C3892 E3893 G3894 N3897 D3898 F3899 Q3900 N3901 Y3902 T3905 Q3906 T3907 G3908 N3909 I3913 T3919 V3920 D3921 Y3922 L3923 L3924 Q3927 E3928 S3929 F3933 Y3934 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 K3953 A3954 M3955 S3956 V3957 A3958 V3961 F3962
N3963 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 L3980 S3983 R3984 L3985 W3986 V3989 V3990 G3991 F3992 V3995 H3998 M3999 M4000 M4001 K4002 L4003 S4007 L4012 L4013 L4017 K4021 D4022 M4023 V4024 V4025 M4026 L4027 L4028 L4031 E4032 V4036 A4041 R4042 Q4043 M4044 V4045 D4046 M4047
L4048 V4049 S4062 V4055 E4056 M4057 I4058 L4059 K4060 M4064 PHE LEU LYS LEU LYS ASP I4071 S4074 E4075 A4076 F4077 V4081 T4082 D4083 P4084 R4085 G4086 L4087 K4095 A4096 M4097 D4098 S4099 Q4100 LYS Q4102 F4103 T4104 G4105 P4106 E4107 I4108 S4115 E4116 A4117 D4118 E4119 N4120 E4121 N4124 F4125 E4126
E4127 F4128 R4131 PHE GLN GLU P4135 A4136 R4137 D4138 I4139 G4140 F4141 N4142 V4143 A4144 V4145 L4146 N4149 L4150 S4151 E4152 H4153 V4154 P4155 H4156 D4157 P4158 R4159 L4160 R4161 N4162 F4163 L4164 E4165 E4168 S4169 I4170 L4171 E4172 Y4173 F4174 R4175 P4176 Y4177 L4178 G4179 R4180 I4181 M4184 R4188 R4189 I4190 E4191 R4192



• Molecule 1: Ryanodine receptor 1

Chain C:

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V1001 A1002 Q1003 GLY TRP SER TYR SER ALA VAL GLN ASP ILE PRO ALA R1016 R1017 N1018 L1021 V1022 P1023 Y1024 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 P1055 PRO ASP GLN GLU PRO
SER GLN VAL GLU ASN GLN SER ARG TRP ASP R1071 V1072 R1073 R1076 A1077 E1078 K1079 S1085 C1086 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 A1094 V1095 R1101 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 D1118 E1119 L1120 N1125 G1126 H1127 R1128 G1129 Q1130 R1131 W1132 H1133 L1134 G1135
S1136 E1137 P1138 F1139 G1140 R1141 Q1144 D1147 V1148 M1152 I1153 D1154 L1155 T1156 I1160 I1161 F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 F1179 I1182 E1183 I1184 G1185 D1186 G1187 F1188 L1189 P1190 V1191 C1192 S1193 L1194 G1195 P1196 G1197 G1198 V1199 G1200 H1201 L1202 N1203 L1204 G1205
Q1206 D1207 V1208 S1209 S1210 L1211 R1212 F1213 F1214 A1215 I1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1226 A1227 I1228 N1229 M1230 Q1231 T1235 T1236 W1237 F1238 S1239 K1240 S1241 Q1244 F1245 E1246 P1247 V1248 P1249 P1250 E1251 H1252 P1253 H1254 Y1255 R1259 M1260 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272
A1273 H1274 R1275 T1276 W1277 G1278 S1279 Q1280 N1281 S1282 L1283 V1284 E1285 M1286 L1287 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR 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 GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY GLY THR PRO GLY GLY THR PRO GLN PRO GLY GLY VAL GLU GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU 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 PRO ARG LEU PRO HIS ASP VAL VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO PRO GLU ILE ILE LEU ASN THR THR T1432 Y1435 S1436 V1437 F1440 A1441 GLY GLN GLU PRO SER C1447 P1455 D1456 Y1457 H1458 Q1459 H1460
N1463 F1464 S1467 LYS VAL ARG ALA V1472 T1473 M1476 G1477 D1478 E1479 Q1480 G1481 N1482 V1483 H1484 S1485 S1486 L1487 K1488 C1489 S1490 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 H1511 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP LEU ALA THR G1525 L1526
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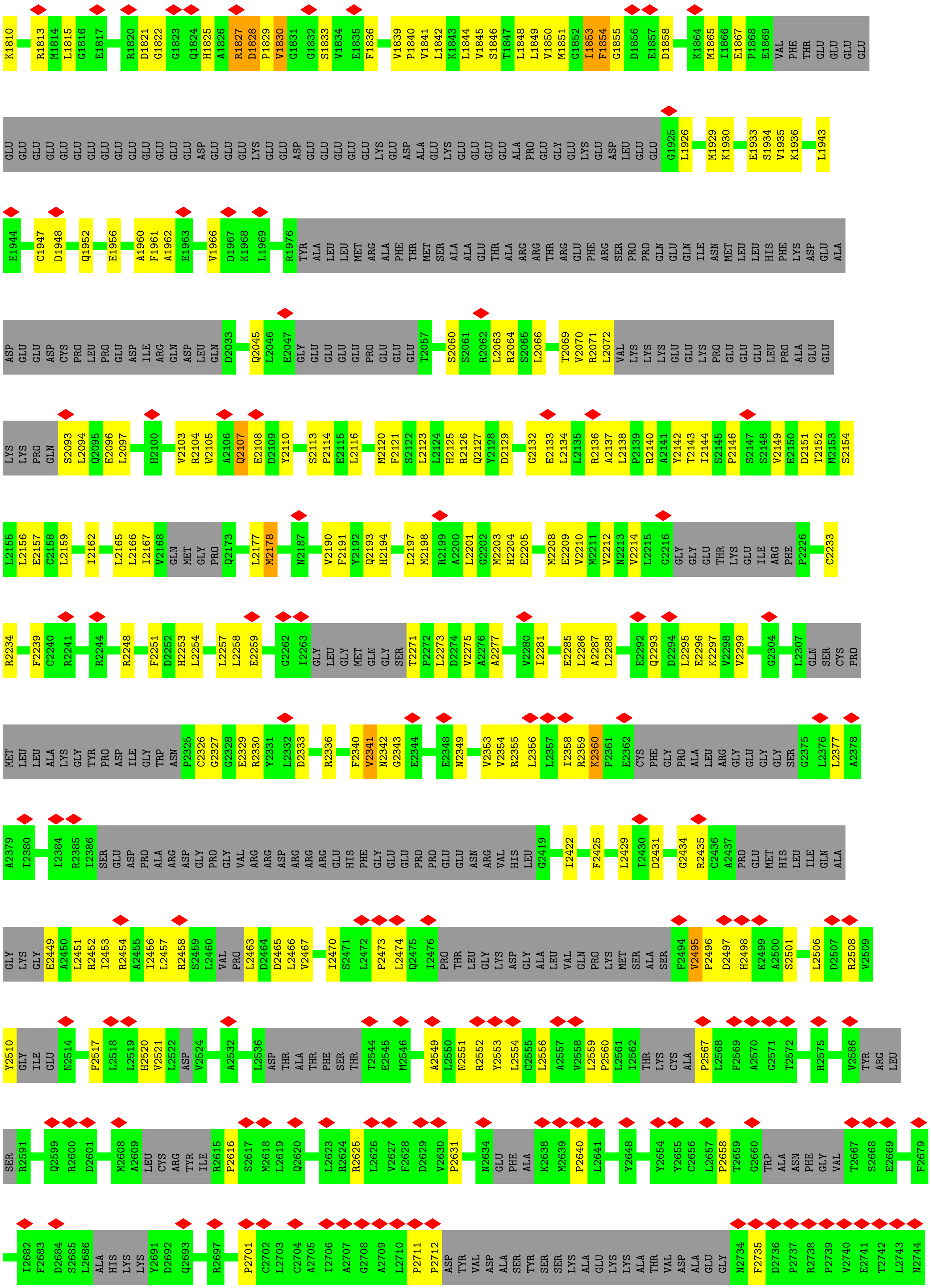
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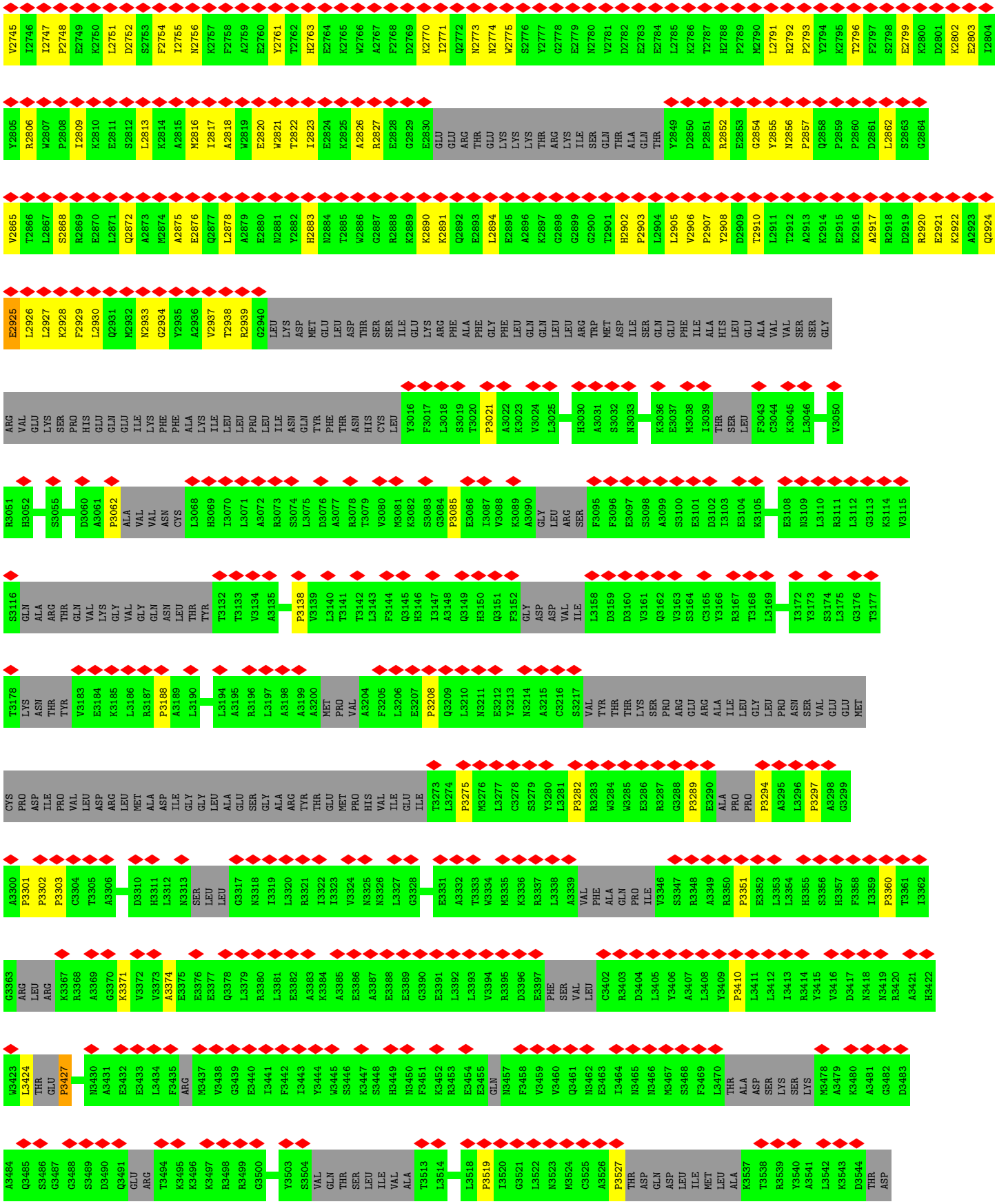
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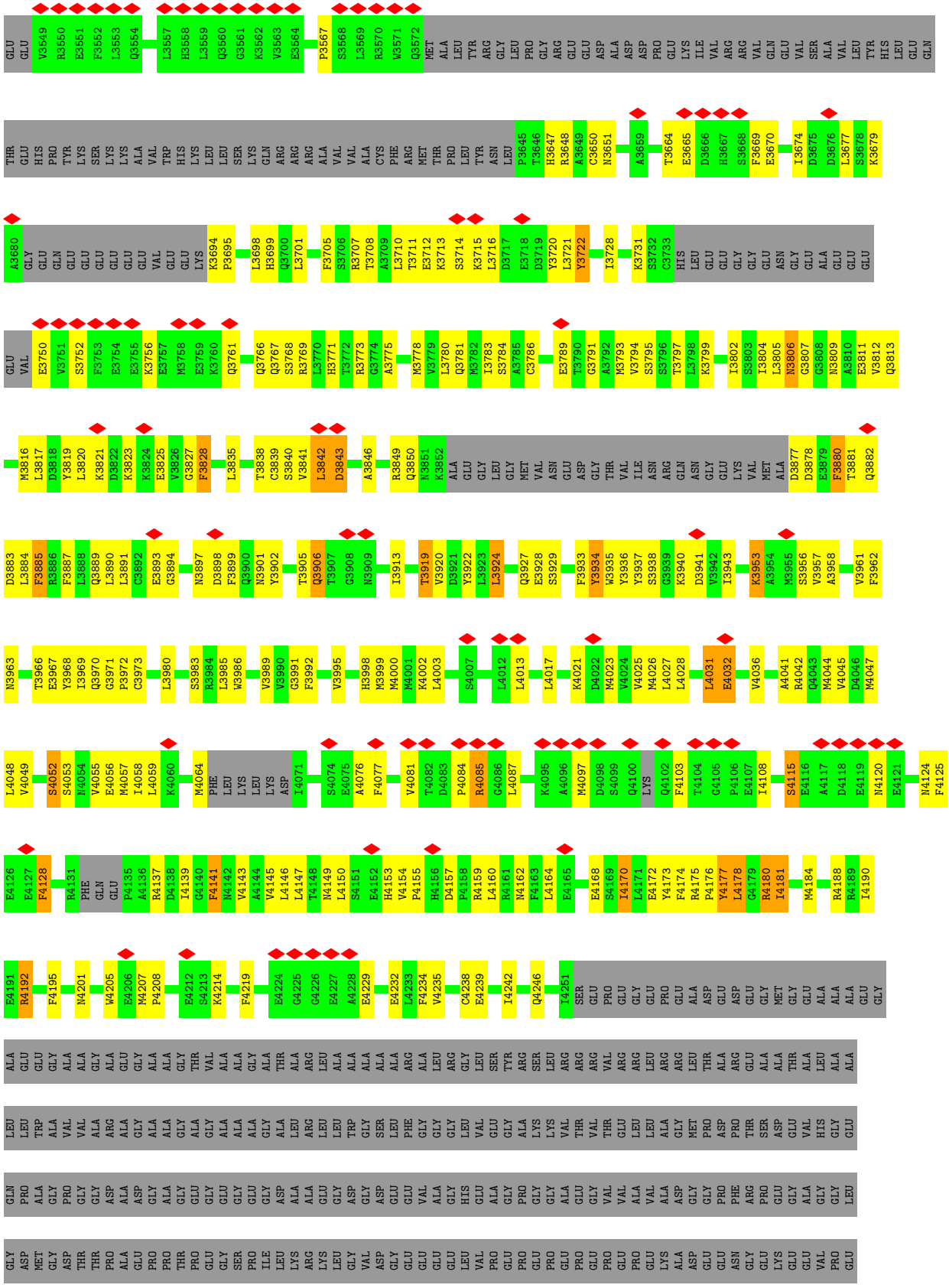
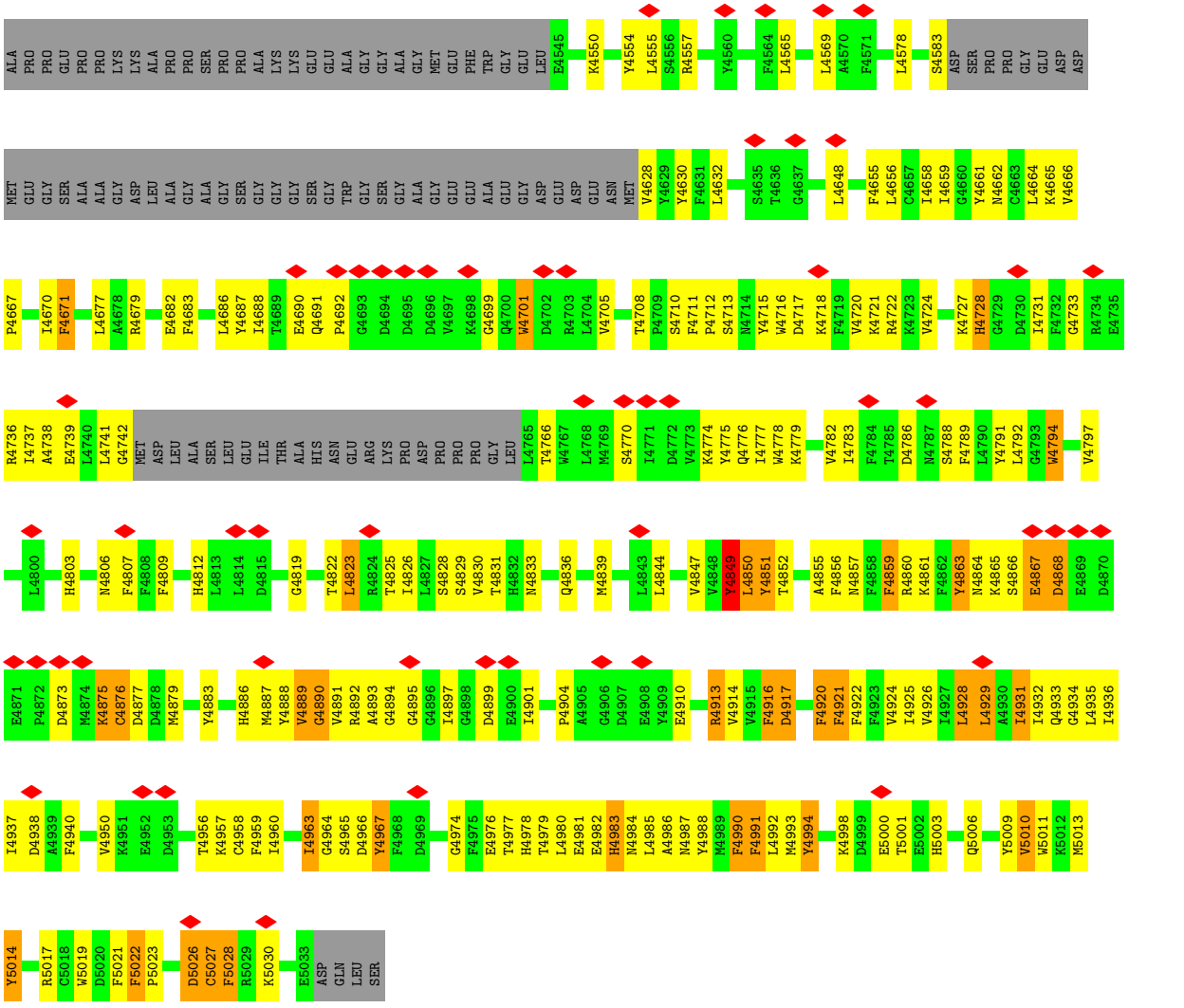
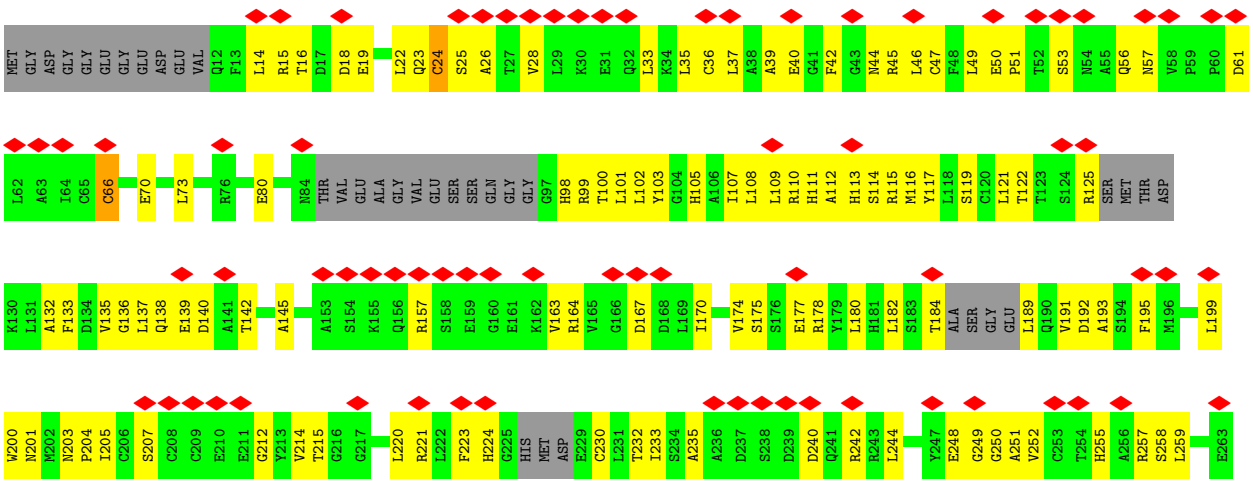
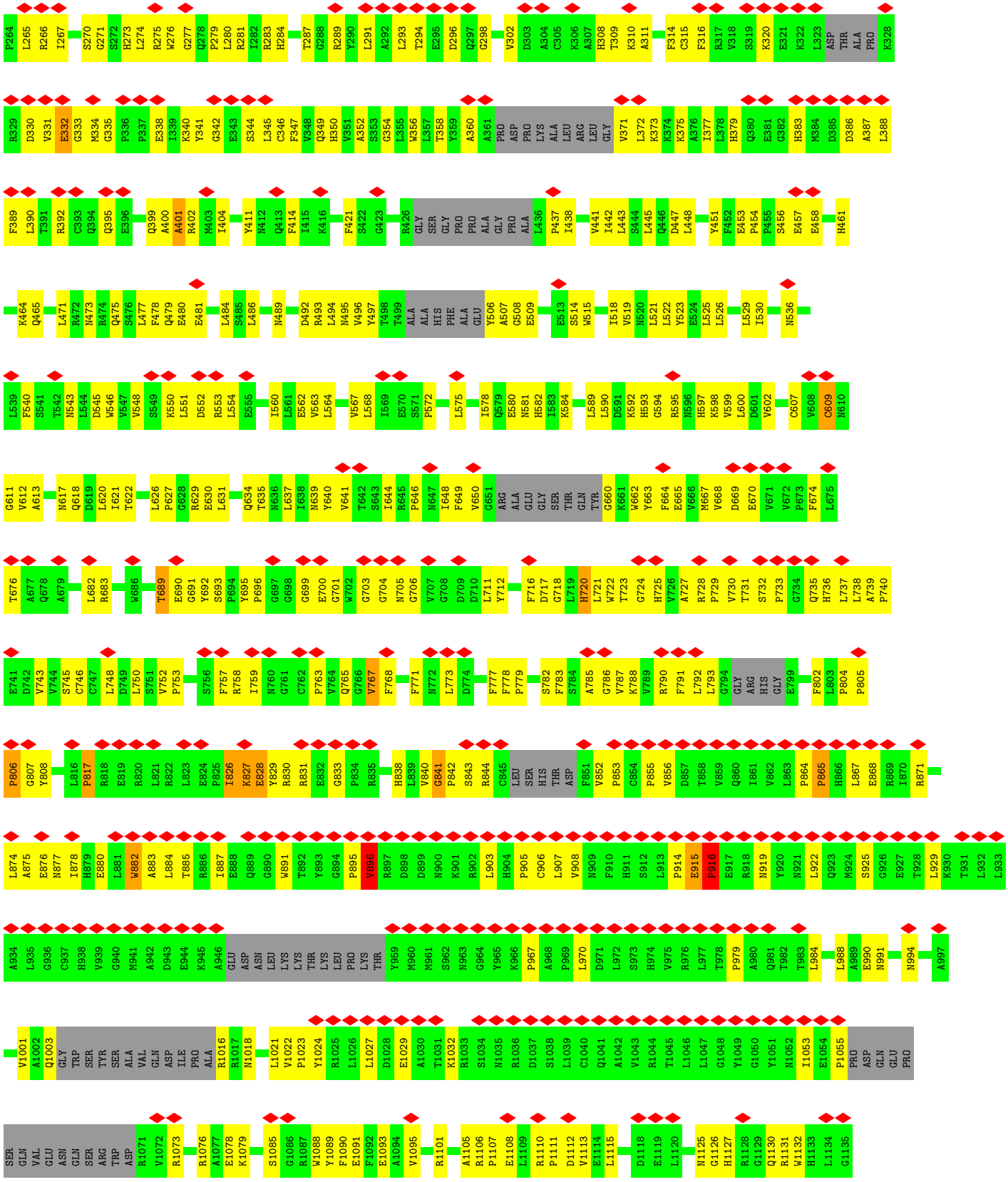




• Molecule 1: Ryanodine receptor 1

Chain E:

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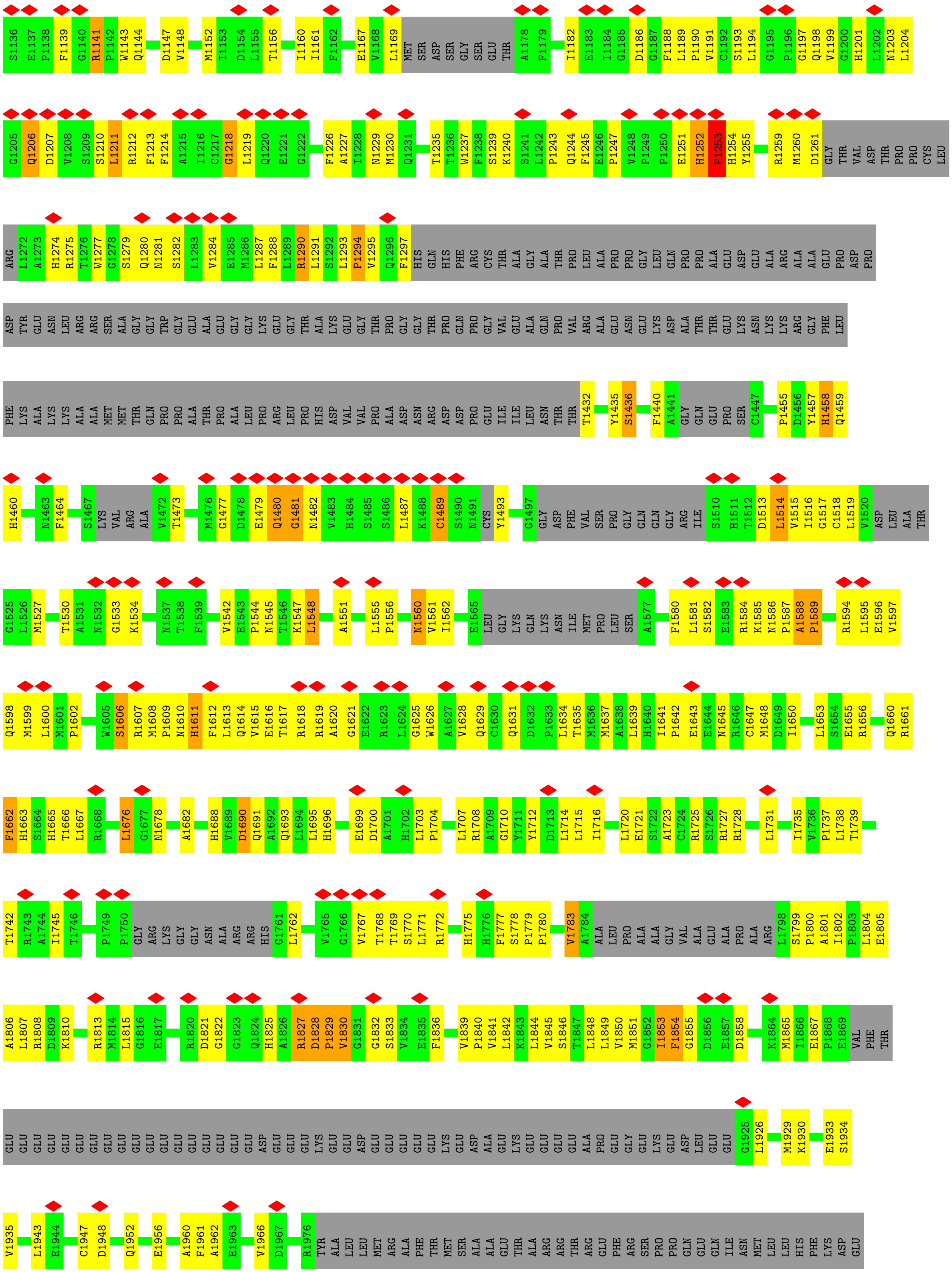
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T1742 R1743 A1744 I1745 T1746 P1749 P1750 GLY ARG LYS GLY GLY ASN ALA ARG ARG HIS G1761 L1762 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 H1775 H1776 F1777 S1778 P1779 P1780 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 S1799 P1800 A1801 I1802 P1803 L1804 E1805
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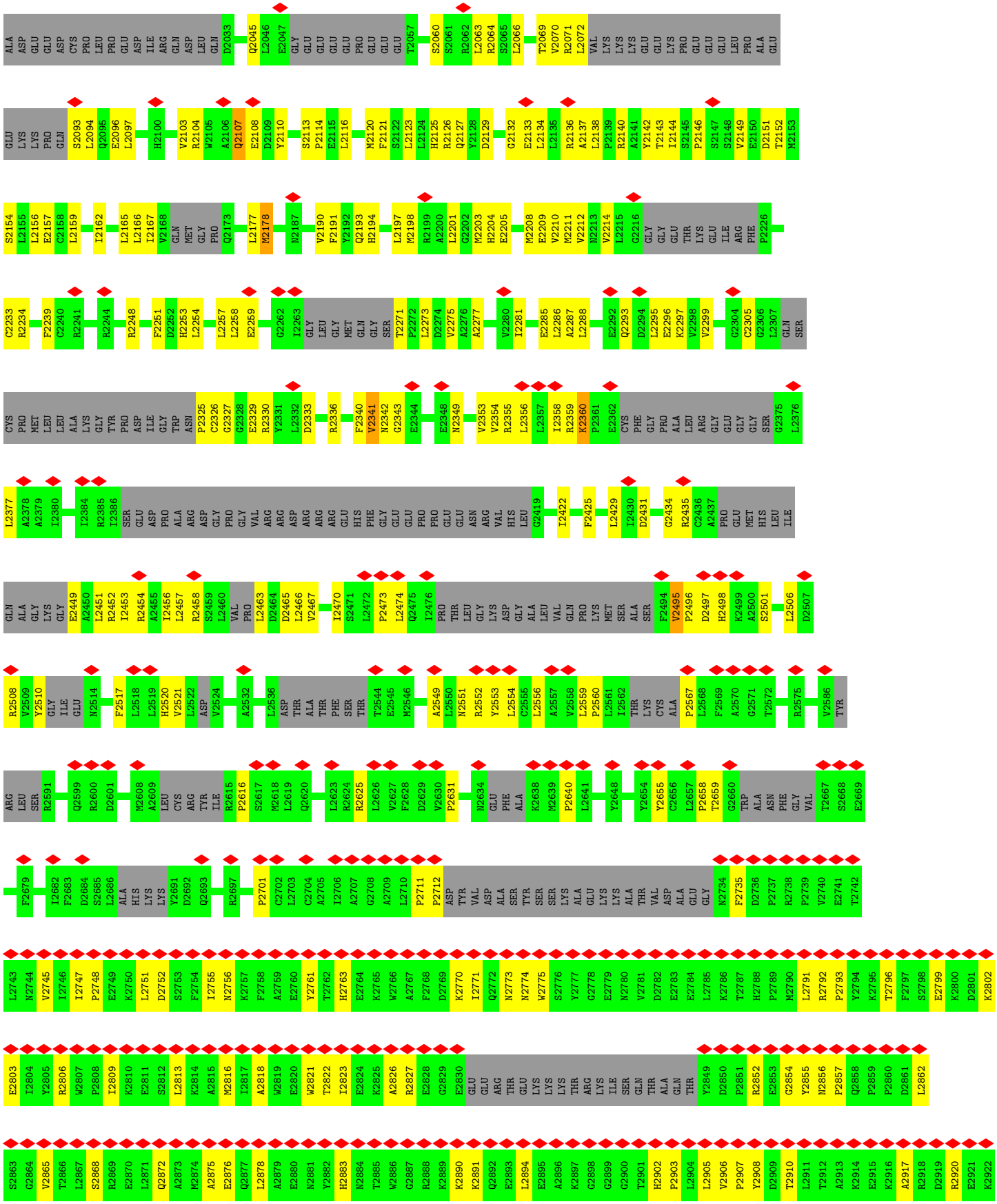
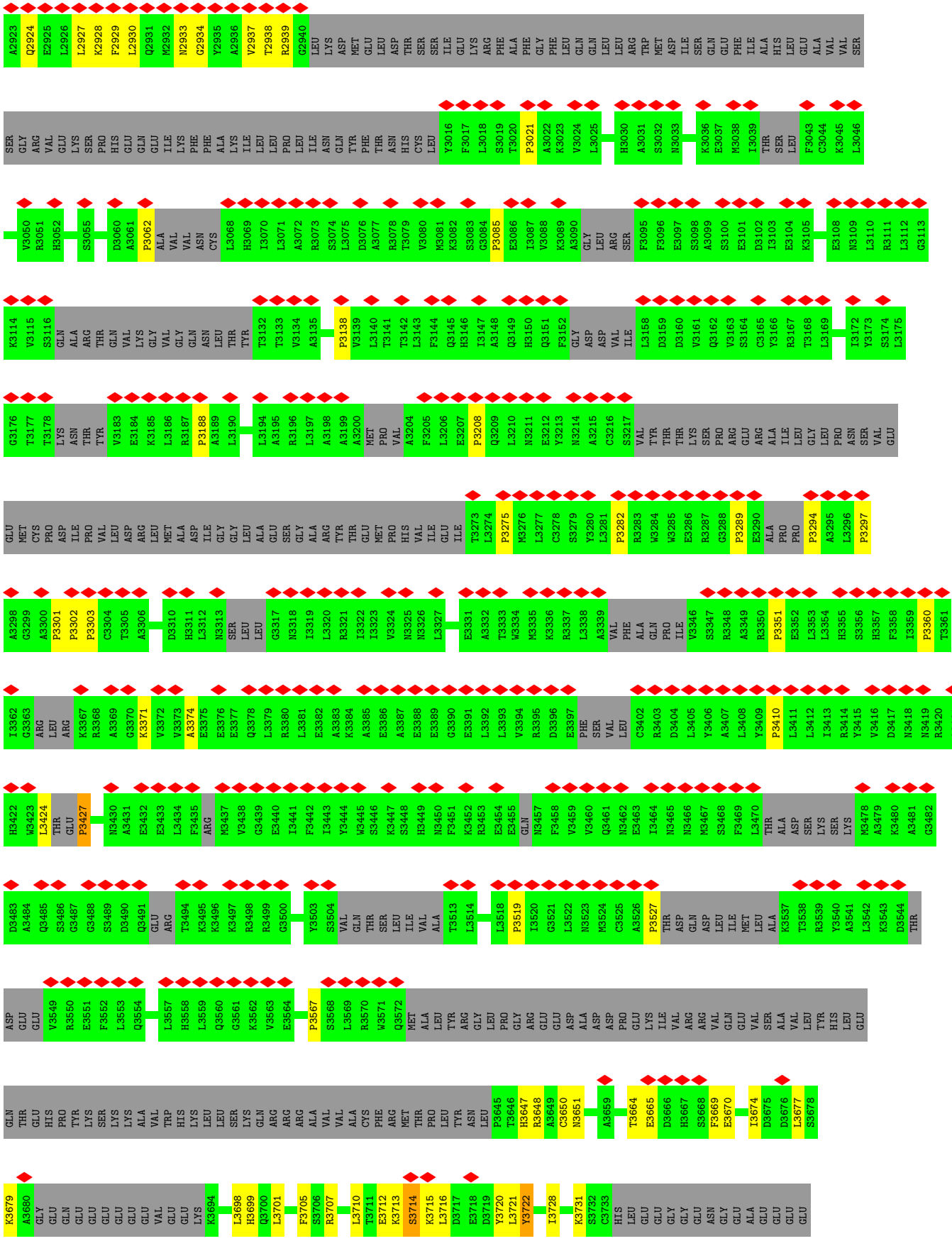
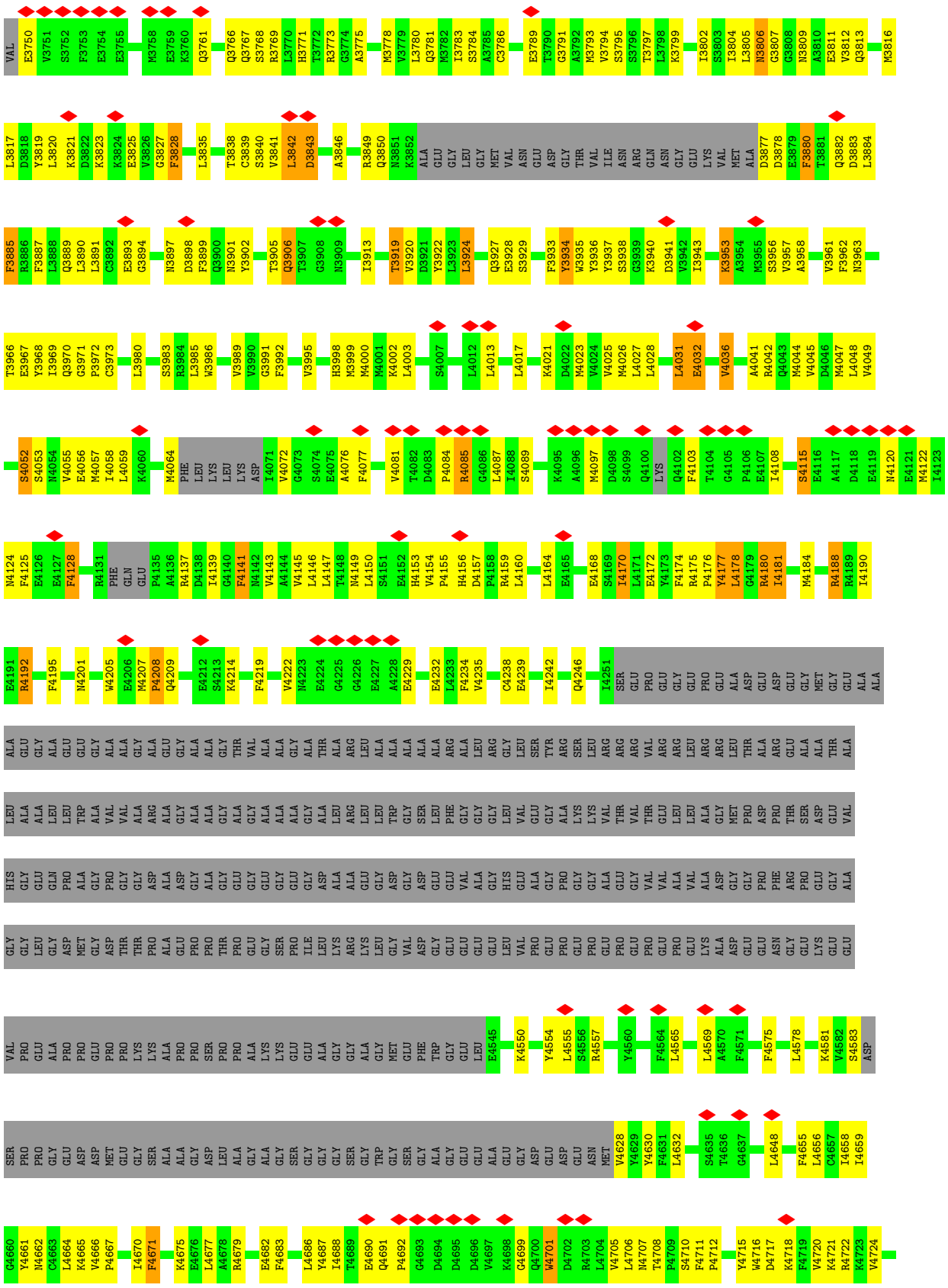
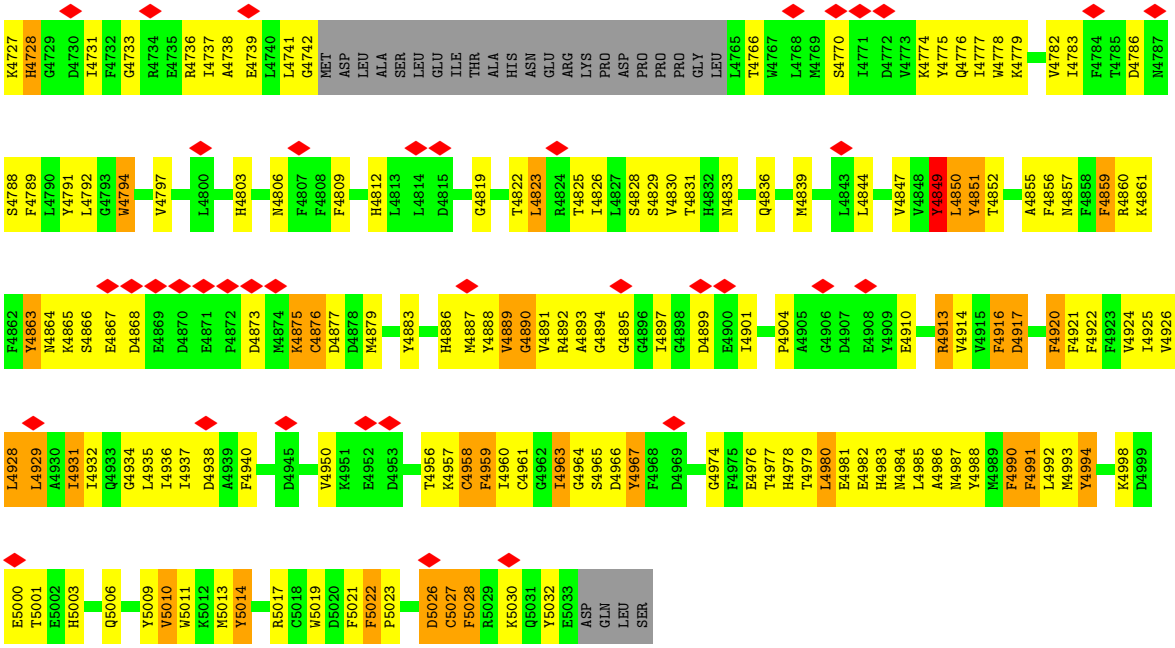
GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU GLU G1925 L1926 M1929 K1930 E1933 S1934
V1935 L1943 E1944 C1947 D1948 Q1952 E1956 A1960 F1961 A1962 E1963 V1966 D1967 R1976 TYR ALA LEU LEU MET ARG ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU



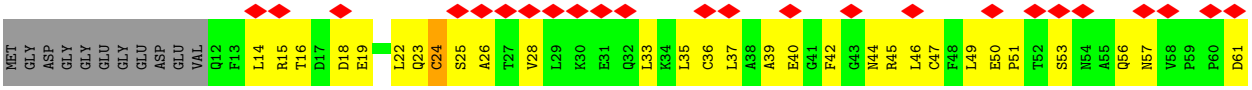


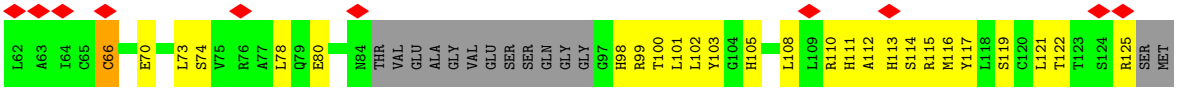


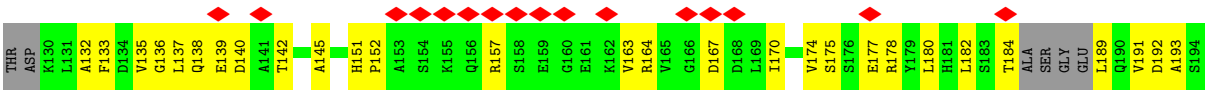


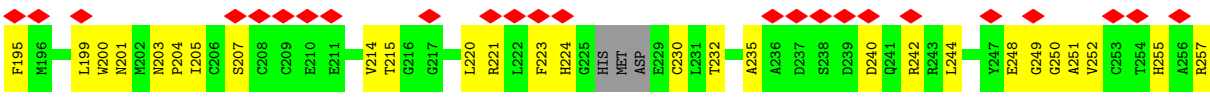
• Molecule 1: Ryanodine receptor 1

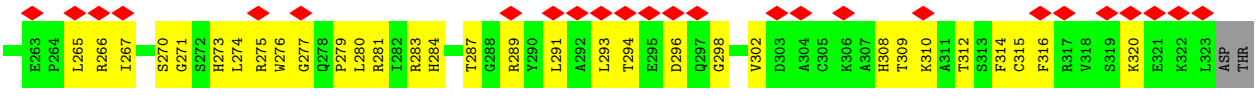
Chain G:

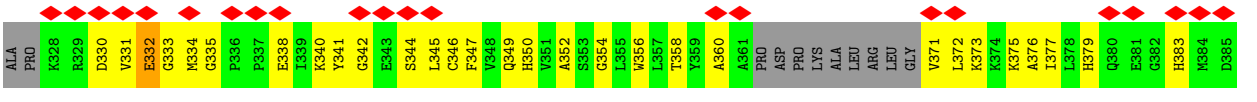


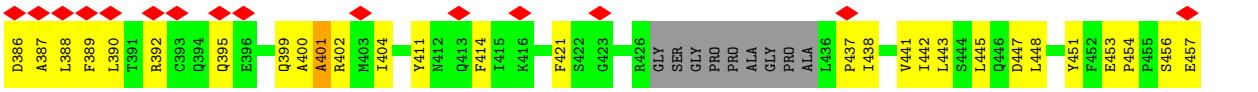


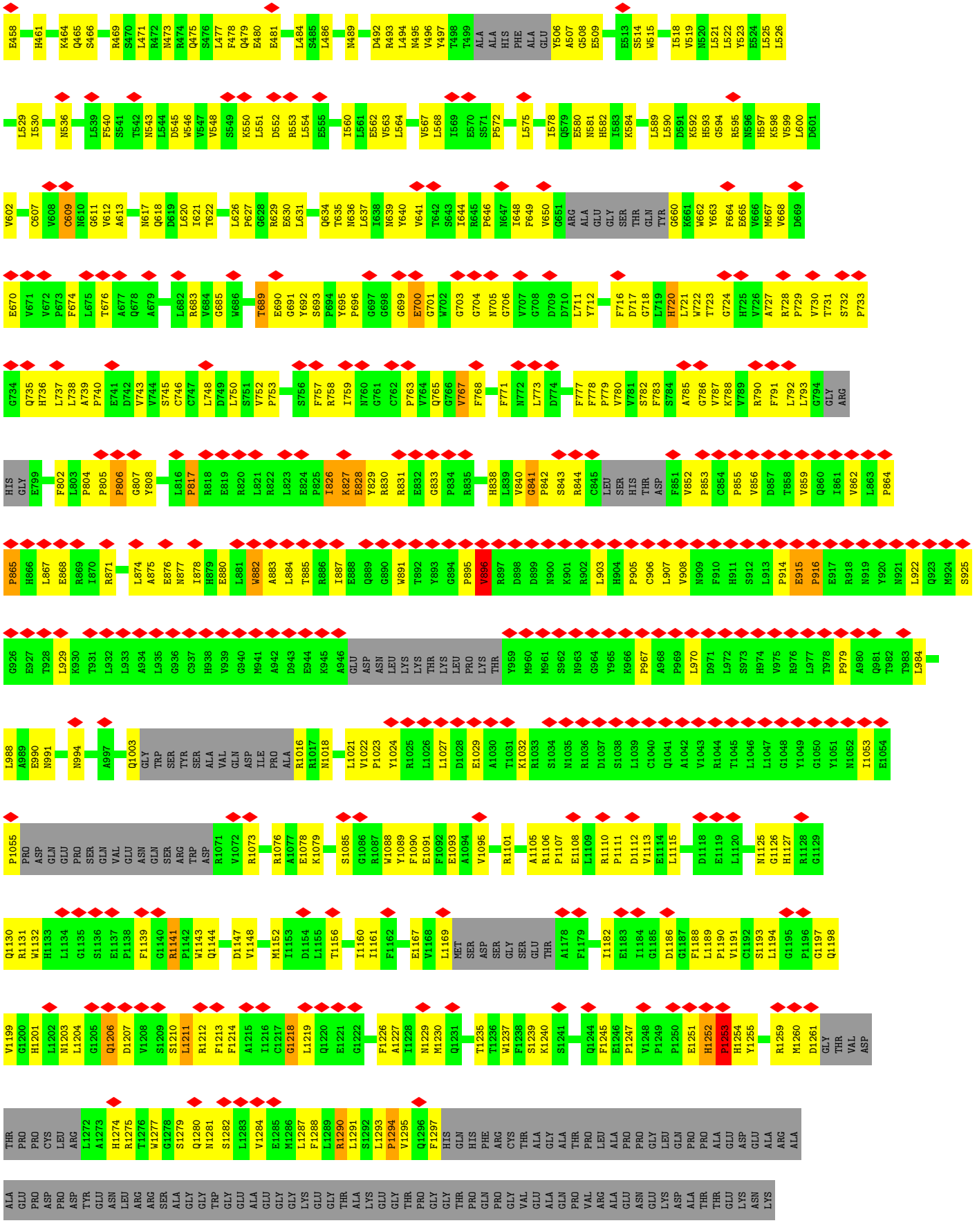








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L529 T530 N536 L539 F540 S541 T542 N543 L544 D545 W546 V547 V548 S549 K550 L551 D552 R553 L554 E555 I560 L561 E562 V563 L564 V567 L568 I569 E570 S571 P572 L575 I578 Q579 E580 N581 H582 I583 K584 L589 L590 D591 K592 H593 G594 R595 N596 H597 K598 V599 L600 D601
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E670 V671 V672 P673 F674 L675 T676 A677 Q678 A679 L682 R683 V684 G685 W686 T689 E690 G691 Y692 S693 P694 Y695 P696 G697 G698 G699 E700 G701 W702 G703 G704 N705 G706 V707 G708 D709 D710 L711 Y712 F716 D717 G718 L719 H720 L721 W722 T723 G724 H725 V726 A727 R728 P729 V730 T731 S732 P733
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HIS GLY E799 F802 L803 P804 P805 P806 G807 Y808 L816 P817 R818 E819 R820 L821 R822 L823 E824 P825 I826 K827 E828 Y829 R830 R831 E832 G833 P834 R835 H838 L839 V840 G841 P842 S843 R844 C845 LEU SER HIS THR ASP F851 V852 P853 C854 P855 V856 D857 T858 V859 Q860 I861 V862 L863 P864
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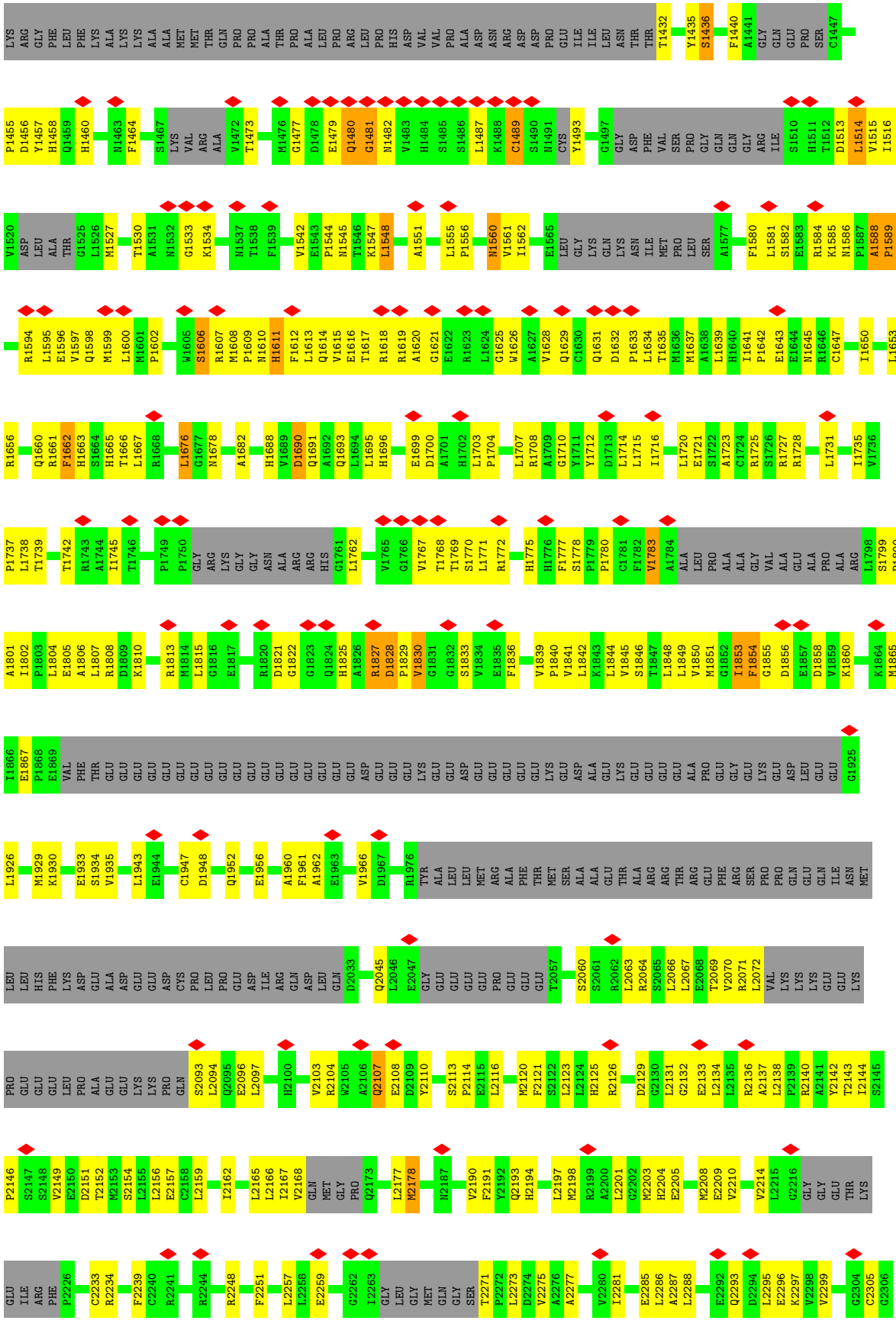
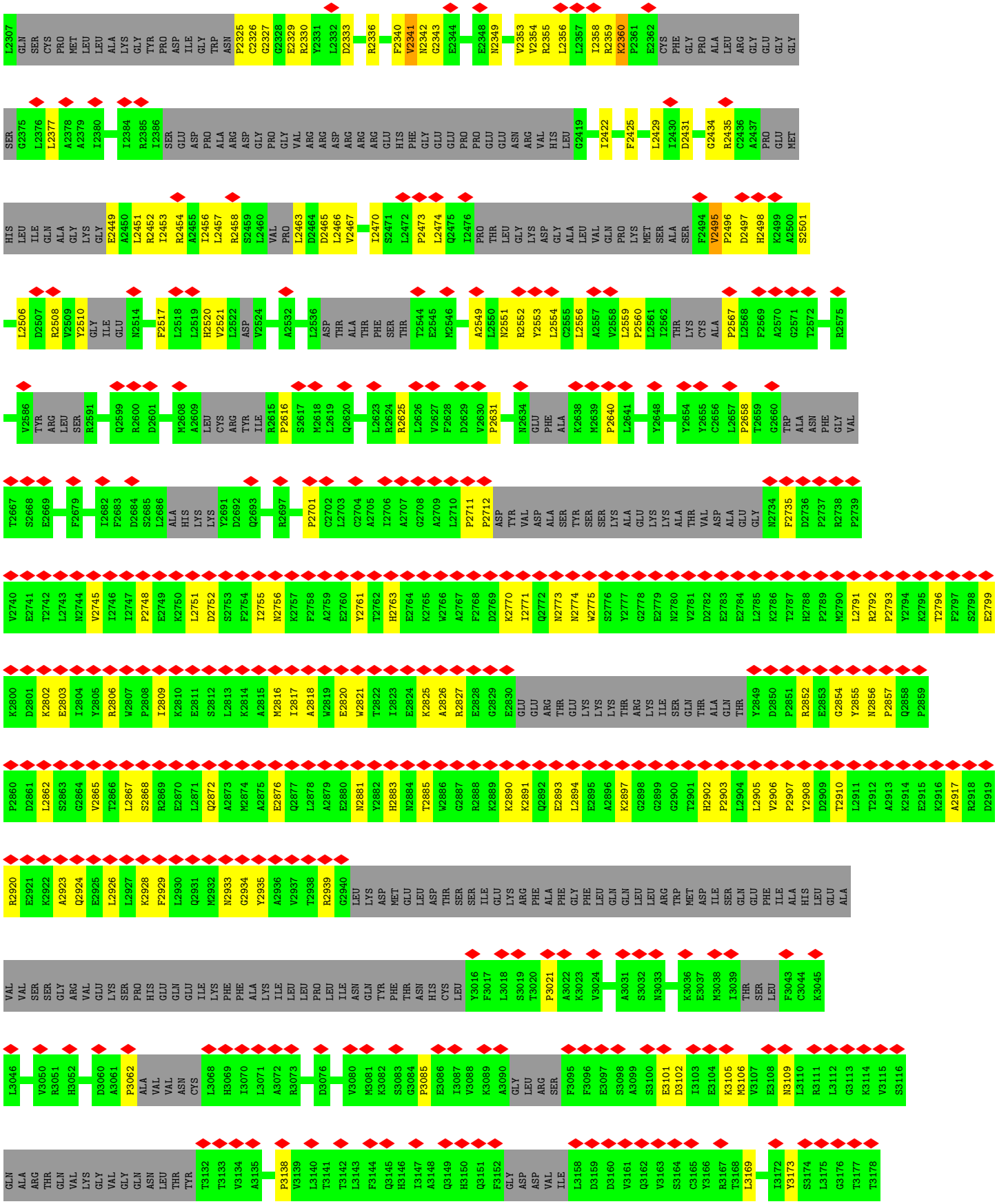
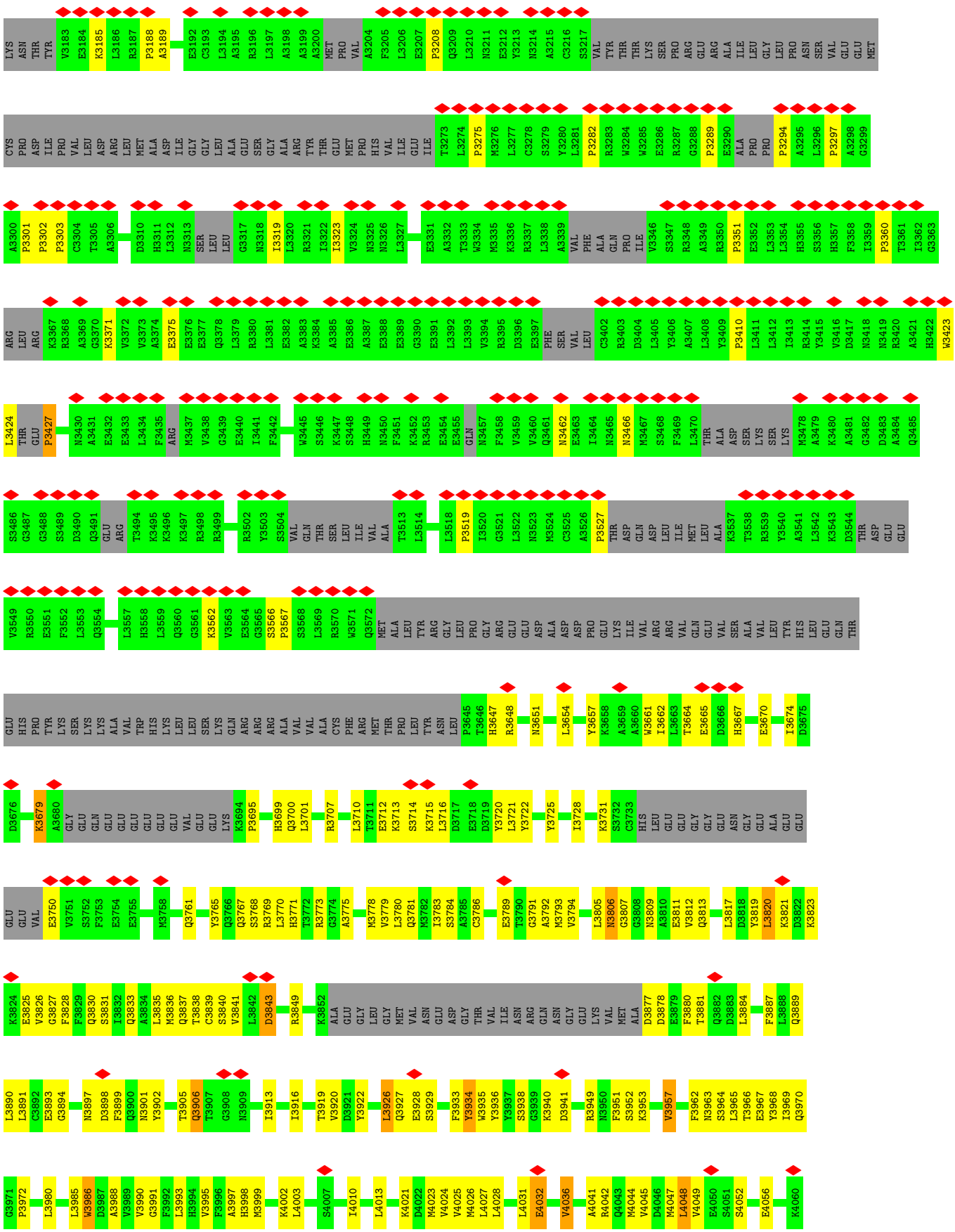
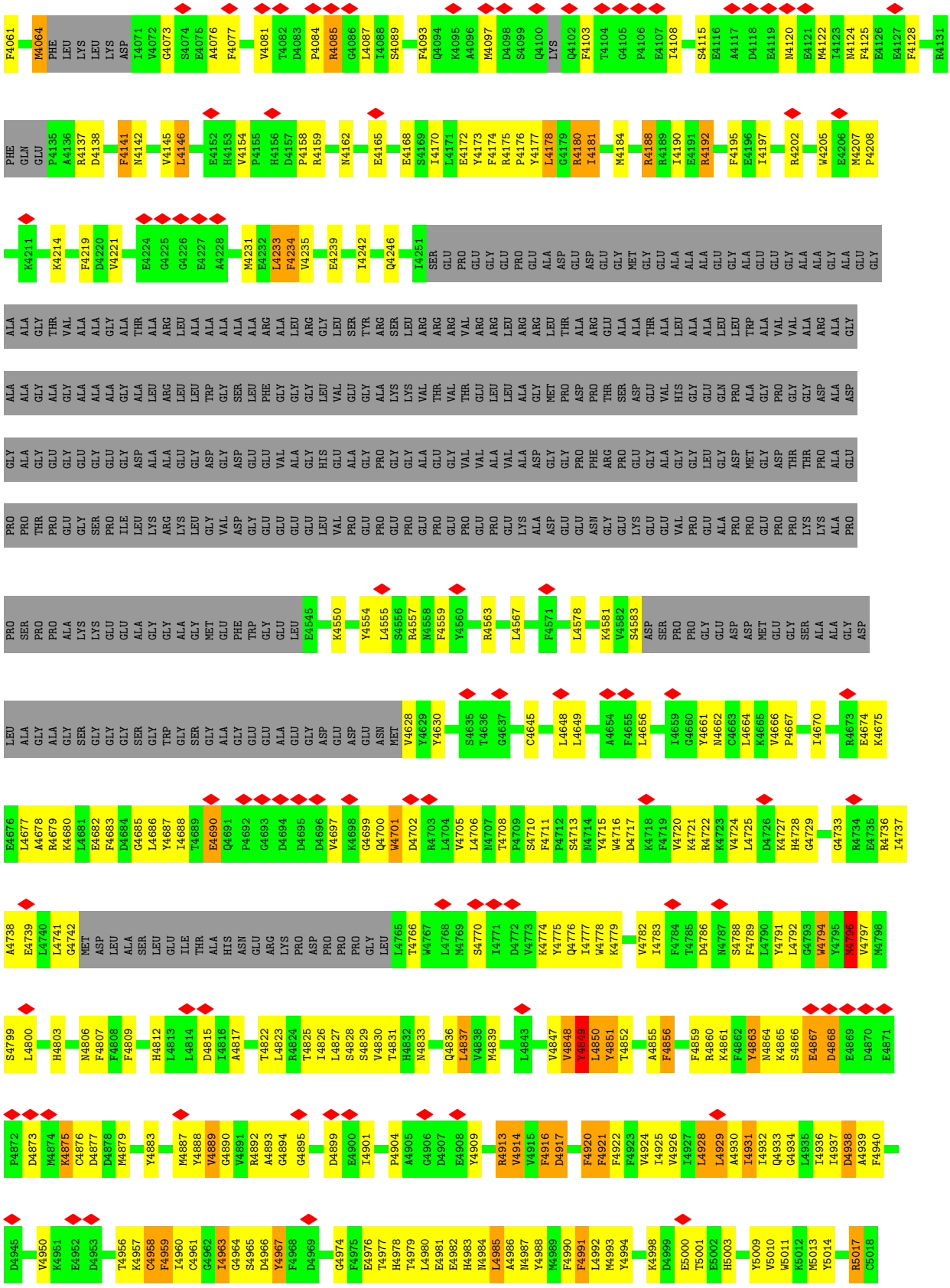
THR PRO PRO CYS LEU ARG L1272 A1273 H1274 R1275 T1276 W1277 G1278 S1279 Q1280 N1281 S1282 L1283 V1284 E1285 M1286 L1287 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY GLN ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS
ALA GLU 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 GLY THR PRO GLY GLY GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS





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PHE GLN GLU P4135 A4136 R4137 D4138 F4141 N4142 V4145 L4146 E4152 H4153 V4154 P4155 H4156 D4157 P4158 R4159 N4162 E4165 E4168 S4169 I4170 L4171 E4172 Y4173 F4174 R4175 P4176 Y4177 L4178 G4179 R4180 I4181 N4184 R4188 R4189 I4190 E4191 R4192 F4195 E4196 I4197 R4202 W4205 E4206 M4207 P4208
K4211 K4214 F4219 D4220 V4221 E4224 G4225 G4226 E4227 A4228 M4231 E4232 L4233 F4234 V4235 E4239 I4242 Q4246 I4251 SER GLU PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLU GLY ALA ALA GLY GLU GLY
ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU ARG ALA ALA ARG GLU ALA ALA THR ALA ALA LEU ALA ALA ALA ALA LEU 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 ALA ASP
GLY ALA 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 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 GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU 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 GLY GLY MET GLU PHE TRP GLY GLU LEU E4545 K4550 Y4554 L4555 S4556 R4557 N4558 F4559 Y4560 R4563 L4567 F4571 L4578 K4581 V4582 S4583 ASP SER PRO PRO GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP
LEU ALA GLY ALA GLY SER GLY GLY GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASN MET V4628 Y4629 Y4630 S4635 T4636 G4637 C4645 L4648 L4649 A4654 F4655 L4656 I4659 G4660 Y4661 N4662 C4663 L4664 K4665 V4666 P4667 I4670 R4673 E4674 K4675
E4676 L4677 A4678 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 V4705 L4706 N4707 T4708 P4709 S4710 F4711 P4712 S4713 N4714 Y4715 W4716 D4717 K4718 F4719 V4720 K4721 R4722 K4723 V4724 L4725 D4726 K4727 H4728 G4729 G4733 R4734 E4735 R4736 I4737
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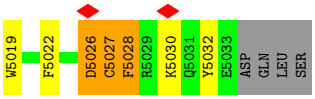
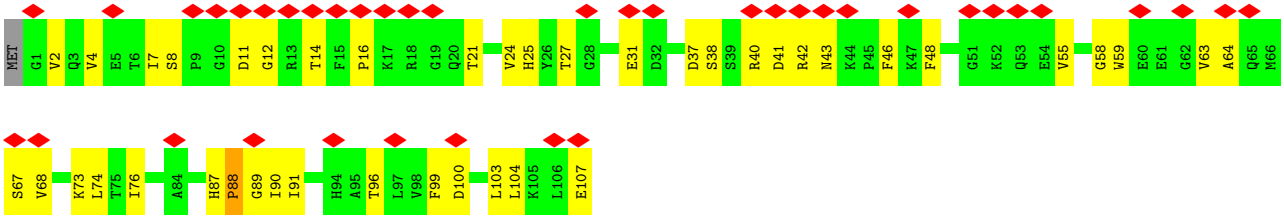
D4945 V4950 K4951 E4962 D4953 T4956 K4957 C4958 F4959 I4960 C4961 G4962 I4963 G4964 S4965 D4966 Y4967 F4968 D4969 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 M4989 F4990 F4991 L4992 M4993 Y4994 K4998 D4999 E5000 T5001 E5002 H5003 Y5009 V5010 W5011 K5012 M5013 Y5014 R5017 C5018



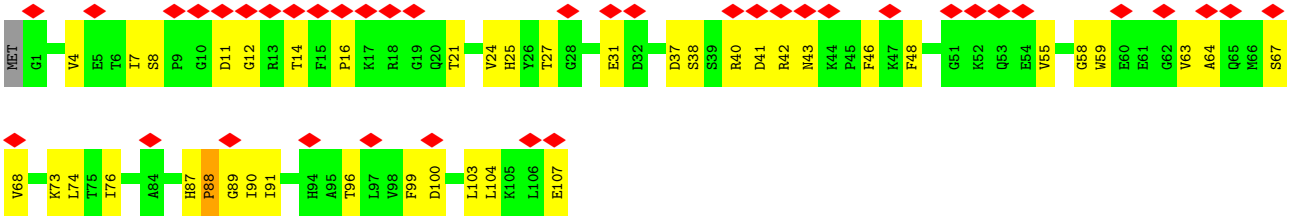
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain B:



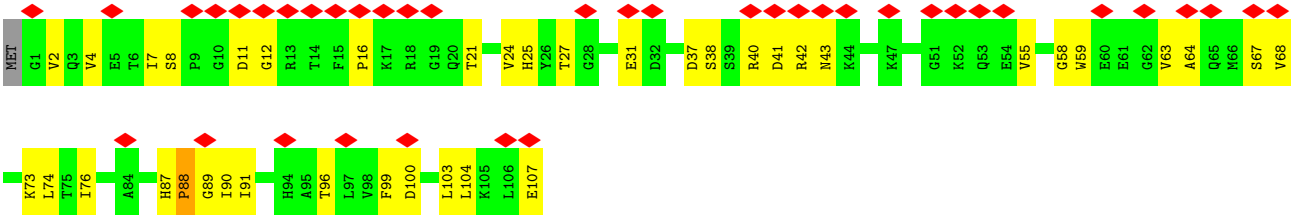
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain D:



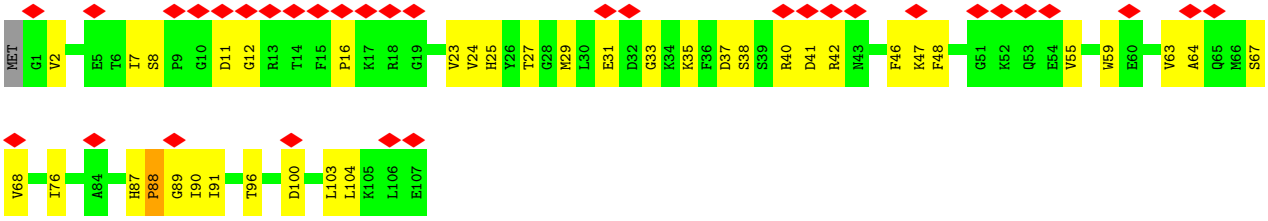
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.93	55/27385 (0.2%)	0.86	90/37104 (0.2%)
1	C	0.93	56/27385 (0.2%)	0.87	92/37104 (0.2%)
1	E	0.93	53/27385 (0.2%)	0.86	91/37104 (0.2%)
1	G	0.93	55/27385 (0.2%)	0.85	90/37104 (0.2%)
2	B	0.58	0/851	0.67	0/1146
2	D	0.58	0/851	0.67	0/1146
2	F	0.58	0/851	0.67	0/1146
2	H	0.60	0/851	0.67	0/1146
All	All	0.92	219/112944 (0.2%)	0.86	363/153000 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	C	0	19
1	E	0	19
1	G	0	19
All	All	0	76

The worst 5 of 219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-12.12	1.23	1.39
1	A	5014	TYR	CG-CD1	-11.55	1.24	1.39
1	E	5014	TYR	CG-CD1	-11.43	1.24	1.39
1	C	3922	TYR	CE1-CZ	-11.19	1.24	1.38
1	E	3922	TYR	CE1-CZ	-11.12	1.24	1.38

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	4128	PHE	CB-CG-CD2	-10.00	113.80	120.80
1	E	4128	PHE	CB-CG-CD2	-9.73	113.99	120.80
1	C	4128	PHE	CB-CG-CD2	-9.69	114.02	120.80
1	A	4128	PHE	CB-CG-CD2	-9.62	114.07	120.80
1	E	4064	MET	CG-SD-CE	8.87	114.39	100.20

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1252	HIS	Peptide
1	A	1253	PRO	Peptide
1	A	1464	PHE	Mainchain
1	A	332	GLU	Mainchain,Peptide
1	A	841	GLY	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	26917	0	24461	1094	0
1	C	26917	0	24461	1105	0
1	E	26917	0	24461	1108	0
1	G	26917	0	24461	1100	0
2	B	832	0	831	38	0
2	D	832	0	831	37	0
2	F	832	0	831	36	0
2	H	832	0	831	34	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111000	0	101168	4395	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 21.

The worst 5 of 4395 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:E:4826:ILE:CG2	1:G:4931:ILE:HD11	1.79	1.10
1:A:4879:MET:SD	1:G:4578:LEU:HA	1.92	1.10
1:A:4826:ILE:CG2	1:C:4931:ILE:HD11	1.86	1.05
1:E:4578:LEU:HA	1:G:4879:MET:SD	1.99	1.03
1:C:4826:ILE:CG2	1:E:4931:ILE:HD11	1.91	1.00

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	3496/5037 (69%)	3173 (91%)	220 (6%)	103 (3%)	4	32
1	C	3496/5037 (69%)	3169 (91%)	223 (6%)	104 (3%)	4	32
1	E	3496/5037 (69%)	3169 (91%)	223 (6%)	104 (3%)	4	32
1	G	3496/5037 (69%)	3169 (91%)	226 (6%)	101 (3%)	4	32
2	B	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	15	54
2	D	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	15	54
2	F	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	15	54
2	H	105/108 (97%)	89 (85%)	15 (14%)	1 (1%)	15	54
All	All	14404/20580 (70%)	13045 (91%)	943 (6%)	416 (3%)	7	32

5 of 416 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	THR
1	A	720	HIS
1	A	806	PRO

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Mol	Chain	Res	Type
1	A	916	PRO
1	A	1253	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2500/4276 (58%)	2486 (99%)	14 (1%)	86 92
1	C	2501/4276 (58%)	2487 (99%)	14 (1%)	86 92
1	E	2502/4276 (58%)	2486 (99%)	16 (1%)	86 92
1	G	2501/4276 (58%)	2482 (99%)	19 (1%)	81 89
2	B	89/90 (99%)	89 (100%)	0	100 100
2	D	89/90 (99%)	89 (100%)	0	100 100
2	F	89/90 (99%)	89 (100%)	0	100 100
2	H	89/90 (99%)	89 (100%)	0	100 100
All	All	10360/17464 (59%)	10297 (99%)	63 (1%)	86 92

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	806	PRO
1	G	1513	ASP
1	E	979	PRO
1	G	1055	PRO
1	G	3926	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	203	ASN
1	G	3699	HIS
1	G	465	GLN

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Mol	Chain	Res	Type
1	G	1631	GLN
1	G	5031	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

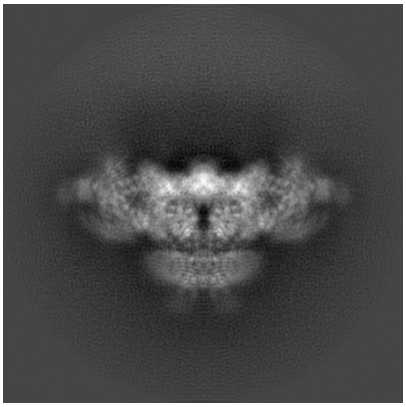
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9520. These allow visual inspection of the internal detail of the map and identification of artifacts.

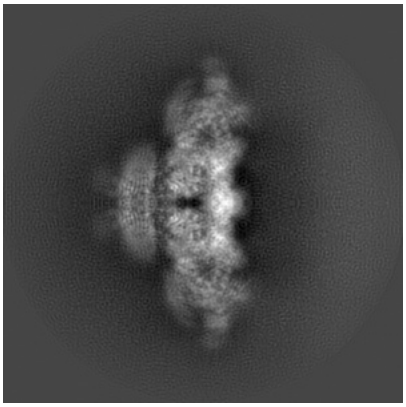
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

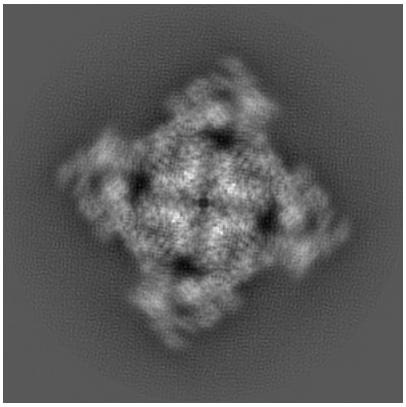
6.1.1 Primary map



X



Y

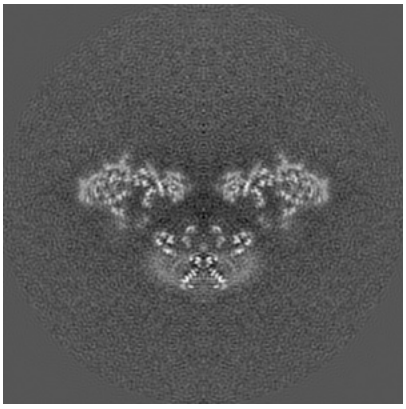


Z

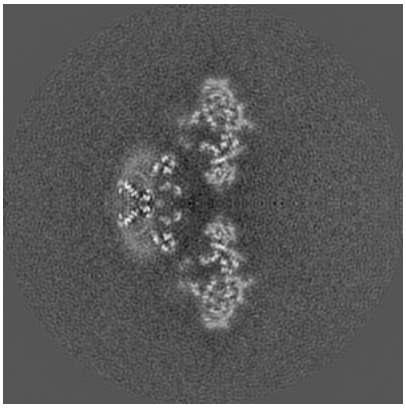
The images above show the map projected in three orthogonal directions.

6.2 Central slices

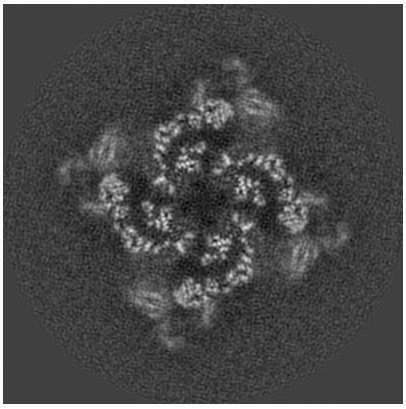
6.2.1 Primary map



X Index: 180



Y Index: 180

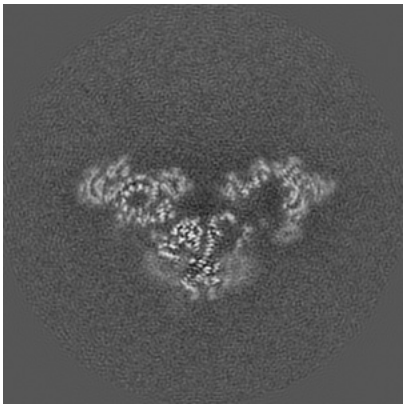


Z Index: 180

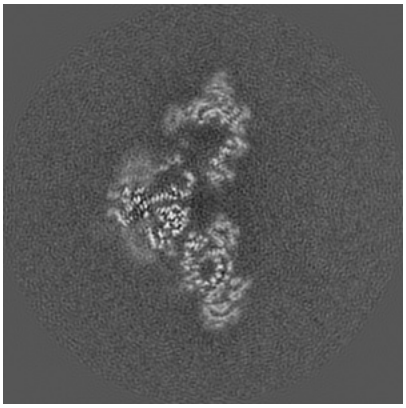
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

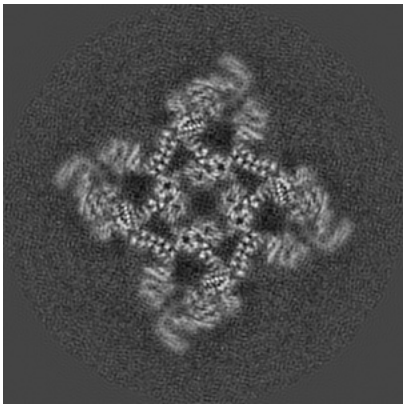
6.3.1 Primary map



X Index: 187



Y Index: 173

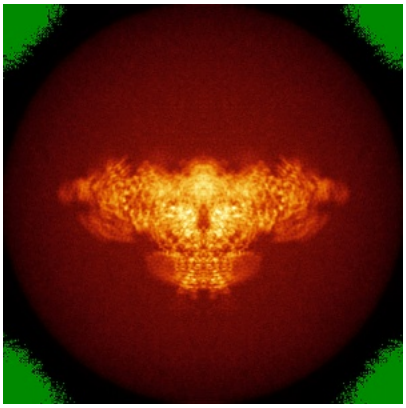


Z Index: 191

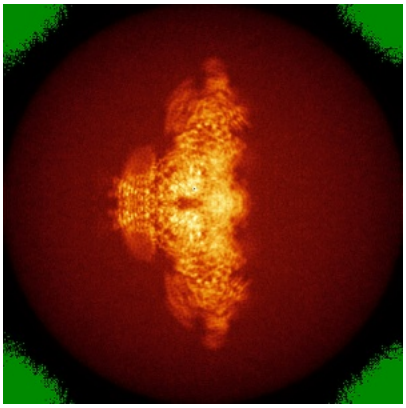
The images above show the largest variance slices of the map in three orthogonal directions.

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

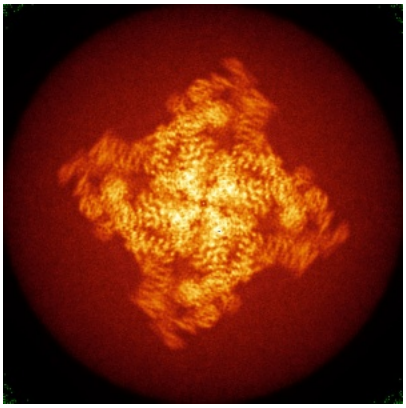
6.4.1 Primary map



X



Y

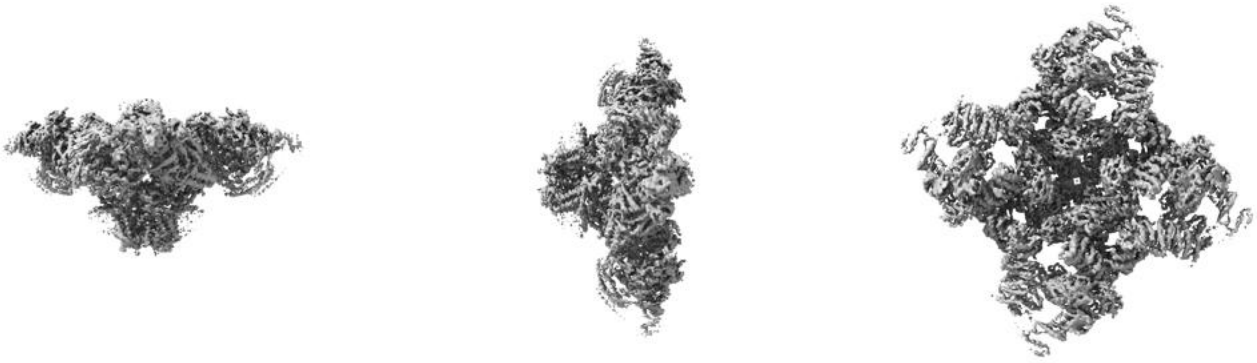


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

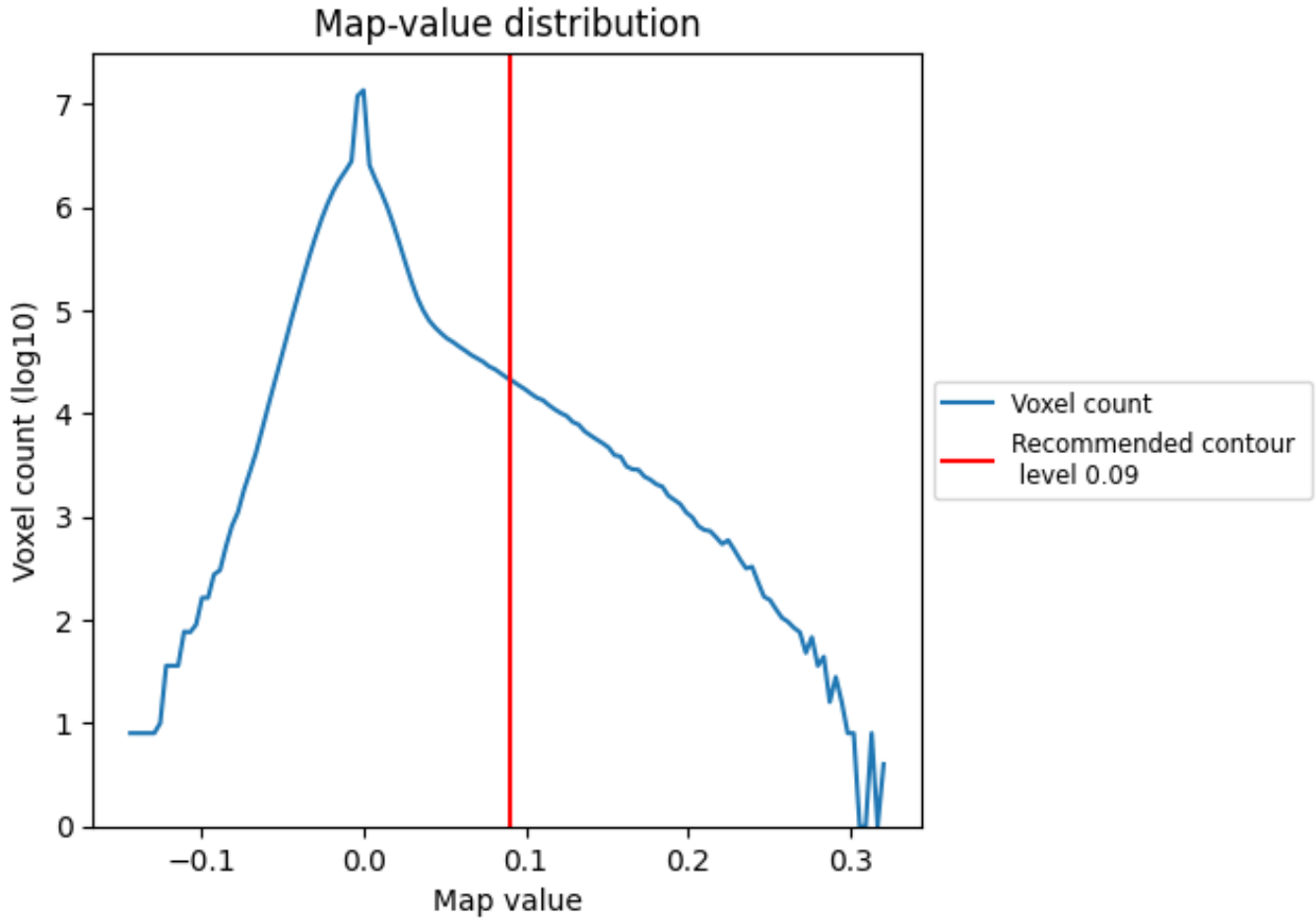
6.6 Mask visualisation (i)

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

7 Map analysis

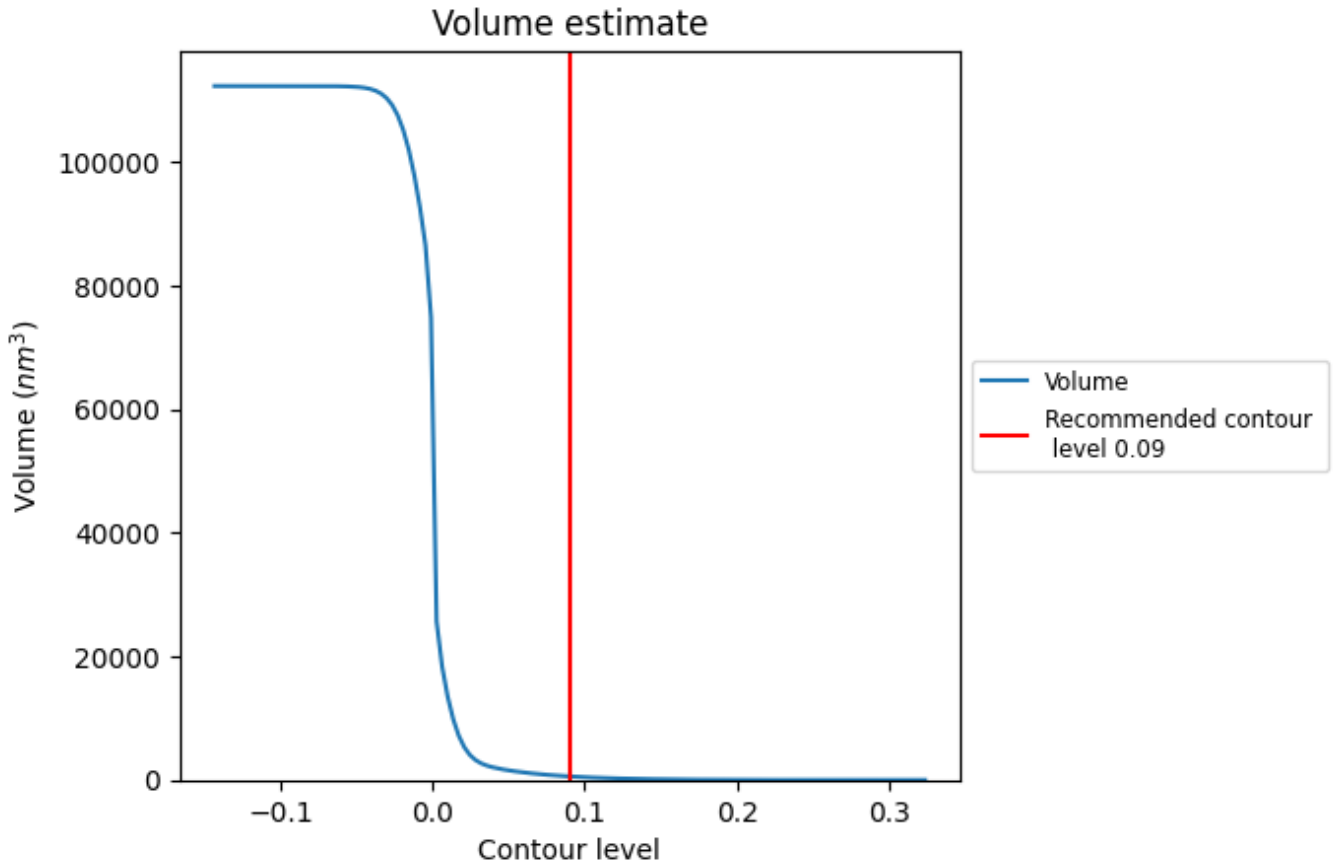
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

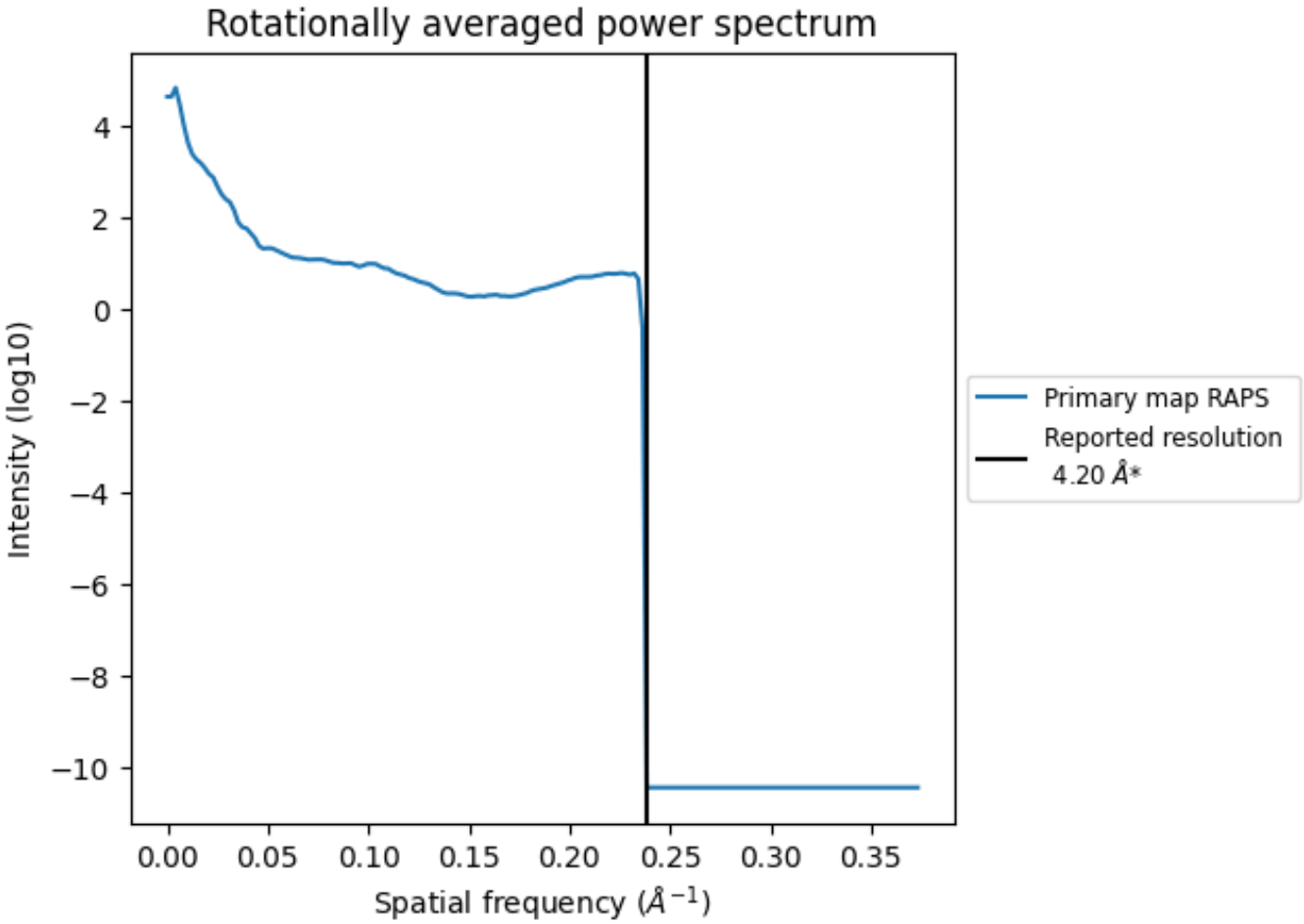
7.2 Volume estimate (i)



The volume at the recommended contour level is 572 nm^3; this corresponds to an approximate mass of 517 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 0.238 Å^{-1}

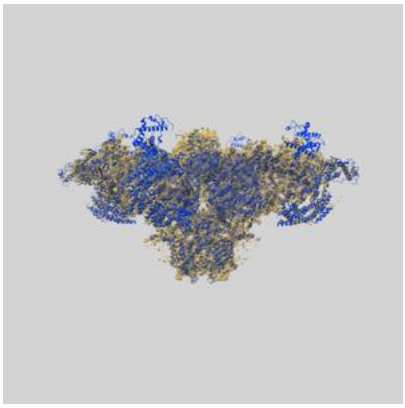
8 Fourier-Shell correlation (i)

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

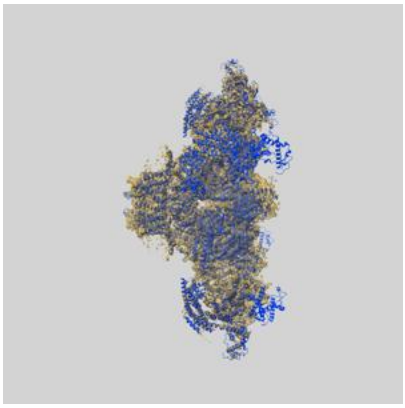
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9520 and PDB model 5GL0. Per-residue inclusion information can be found in section 3 on page 4.

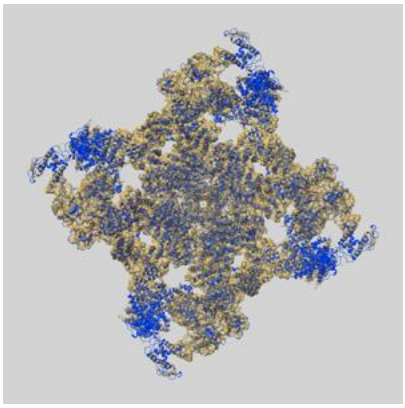
9.1 Map-model overlay



X



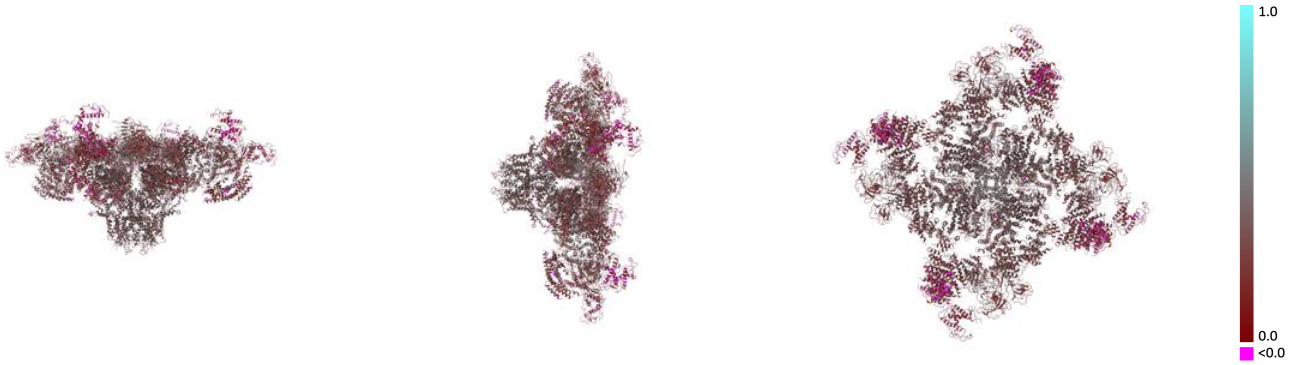
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

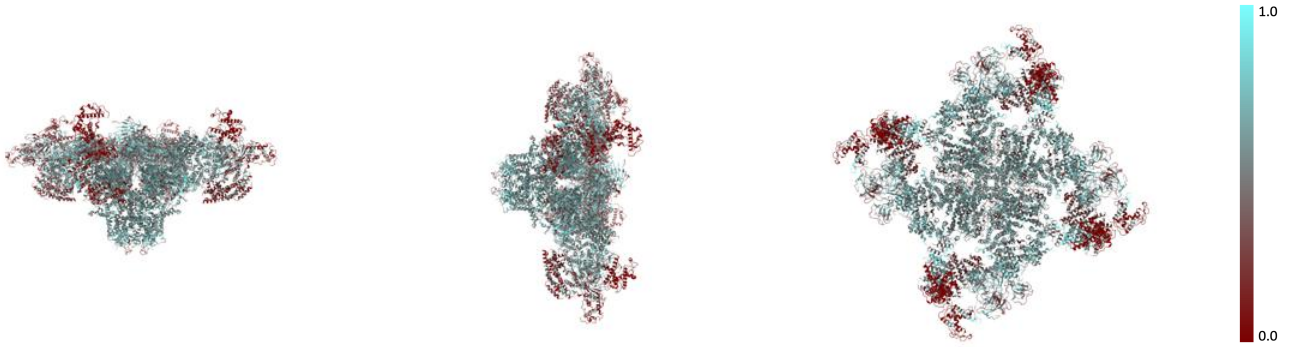
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

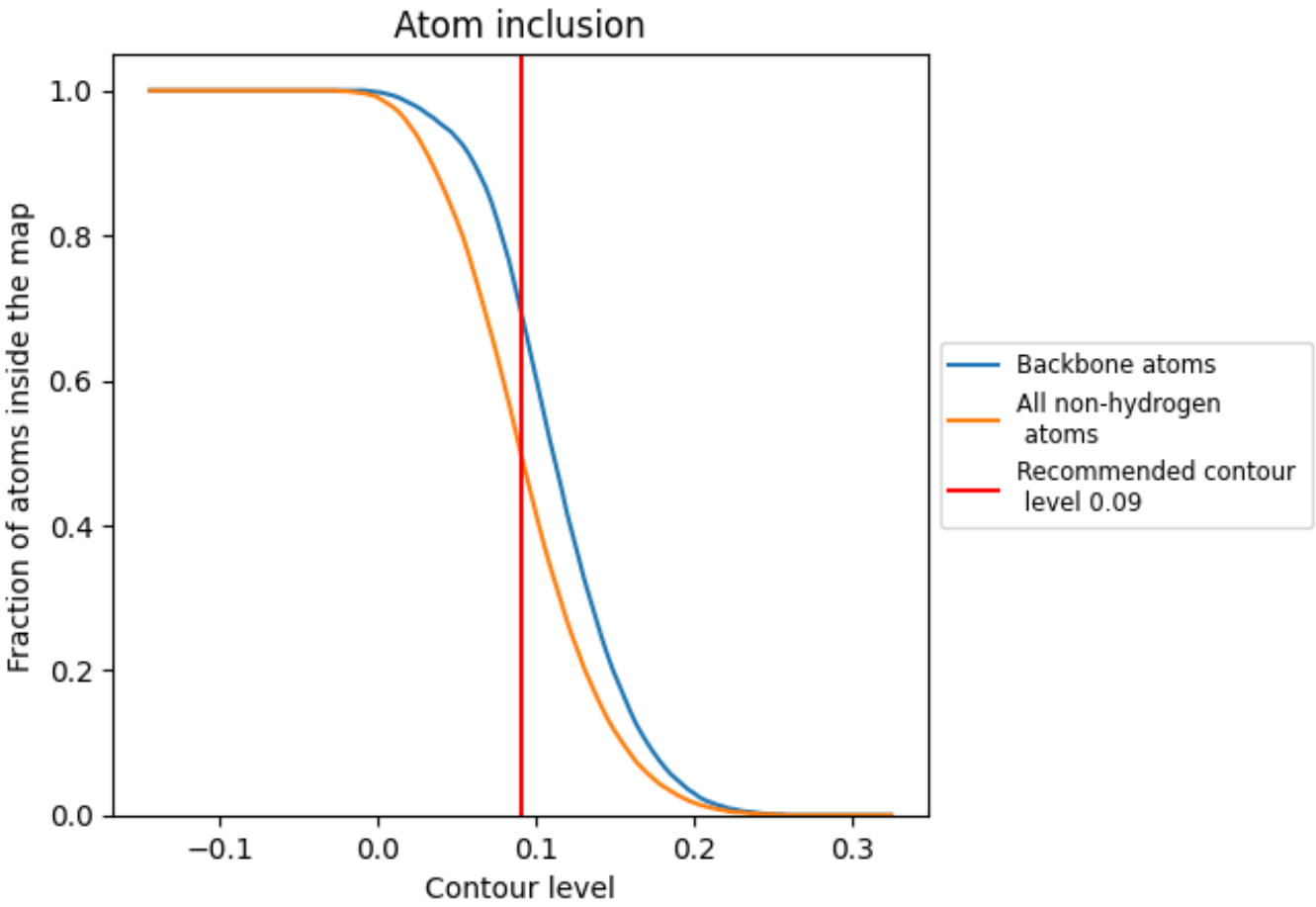
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 50% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5020	0.3090
A	0.5030	0.3090
B	0.4670	0.3060
C	0.5020	0.3090
D	0.4670	0.3070
E	0.5030	0.3090
F	0.4660	0.3010
G	0.5040	0.3100
H	0.4710	0.3070