wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 06:06 PM JST

PDB ID	:	6JI8
EMDB ID	:	EMD-9833
Title	:	Structure of RyR2 (F/apoCaM dataset)
Authors	:	Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on	:	2019-02-20
Resolution	:	3.60 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:

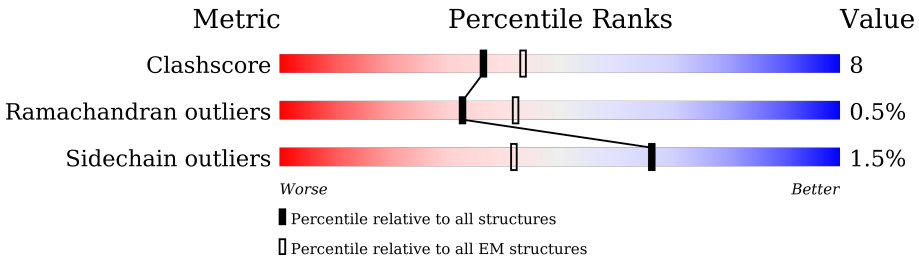
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	4968	11% 58% 12% • 29%
1	D	4968	11% 58% 12% • 29%
1	G	4968	11% 58% 12% • 29%
1	J	4968	11% 57% 13% • 29%
2	B	108	80% 19% ••
2	E	108	80% 19% ••
2	H	108	82% 16% ••
2	K	108	80% 19% ••

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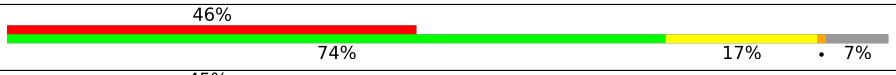
Mol	Chain	Length	Quality of chain
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 115060 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		
1	D	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		
1	G	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		
1	J	3511	Total	C	N	O	S	0	0
			26851	17104	4605	4982	160		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		
3	F	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		
3	I	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		
3	L	138	Total	C	N	O	S	0	0
			1094	676	176	233	9		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

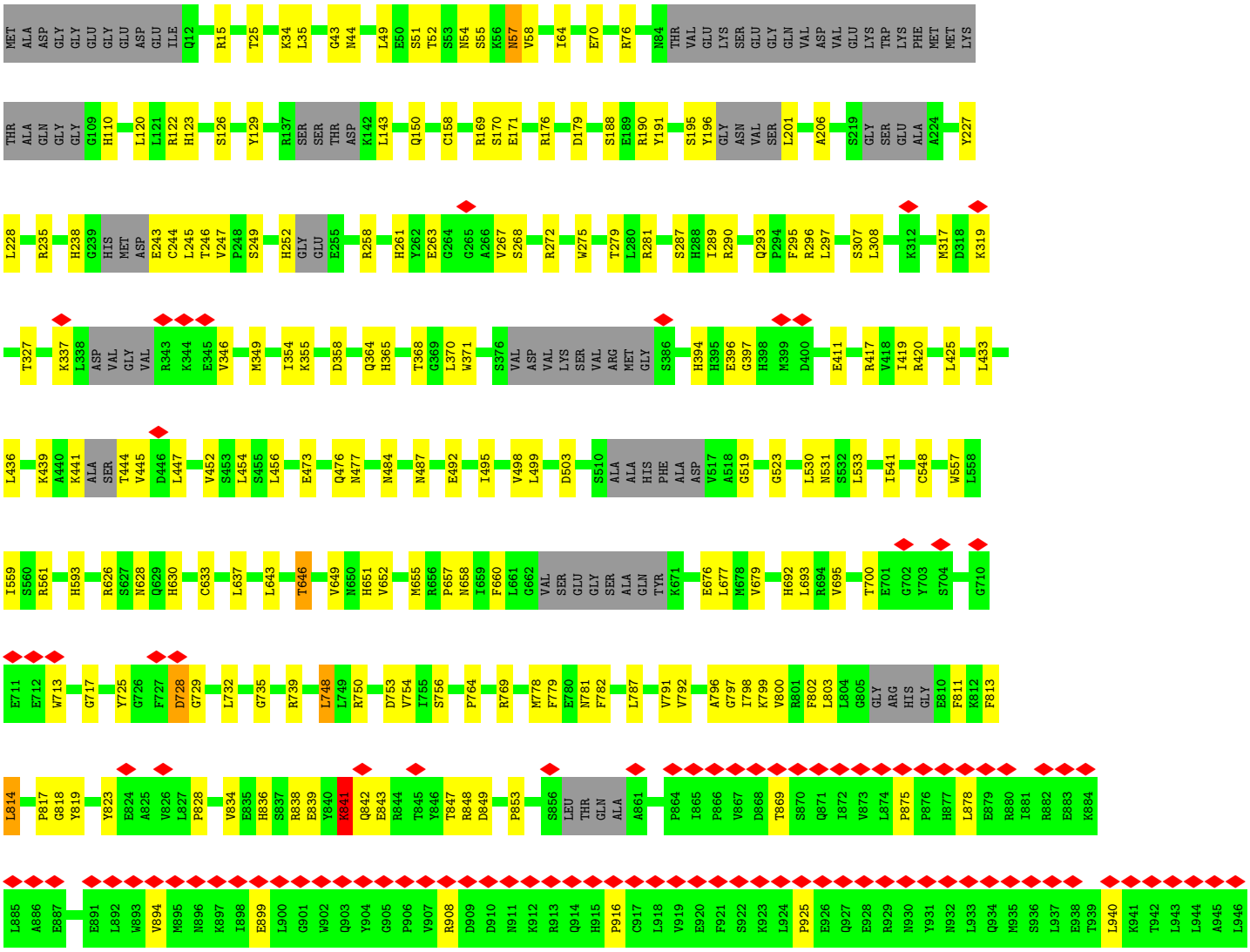
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Zn 1 1	0
4	D	1	Total Zn 1 1	0
4	G	1	Total Zn 1 1	0
4	J	1	Total Zn 1 1	0

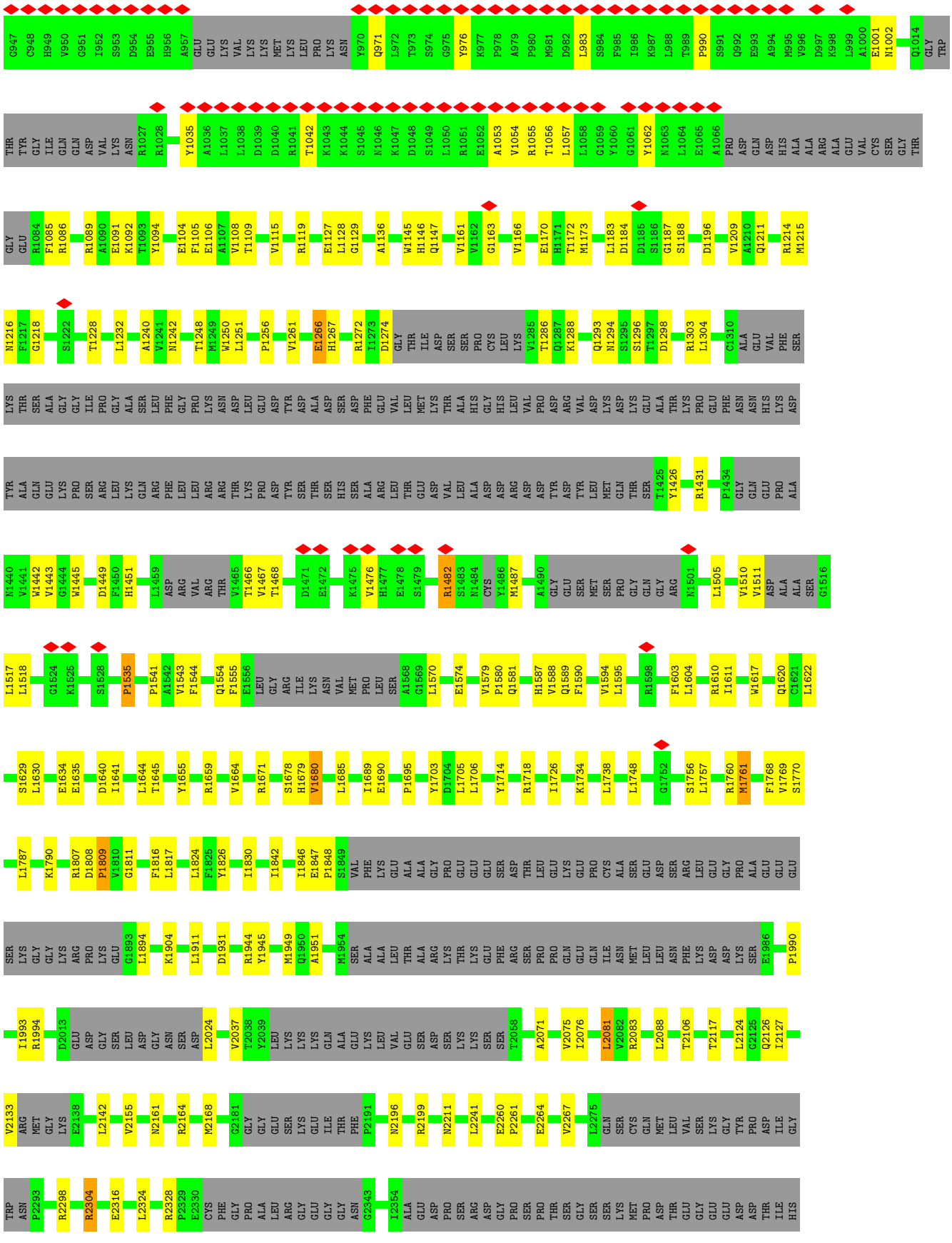
3 Residue-property plots (i)

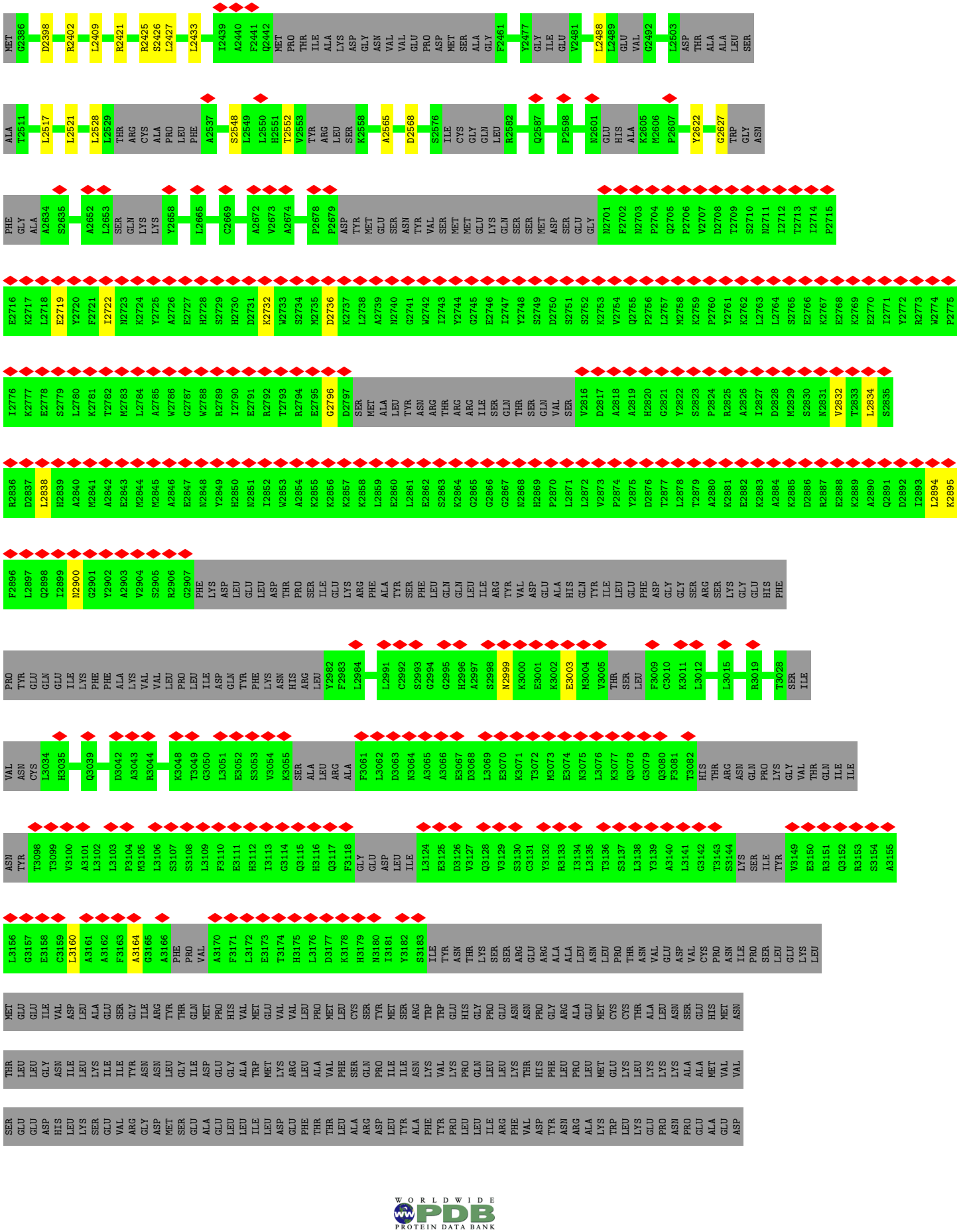
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RyR2

Chain A:



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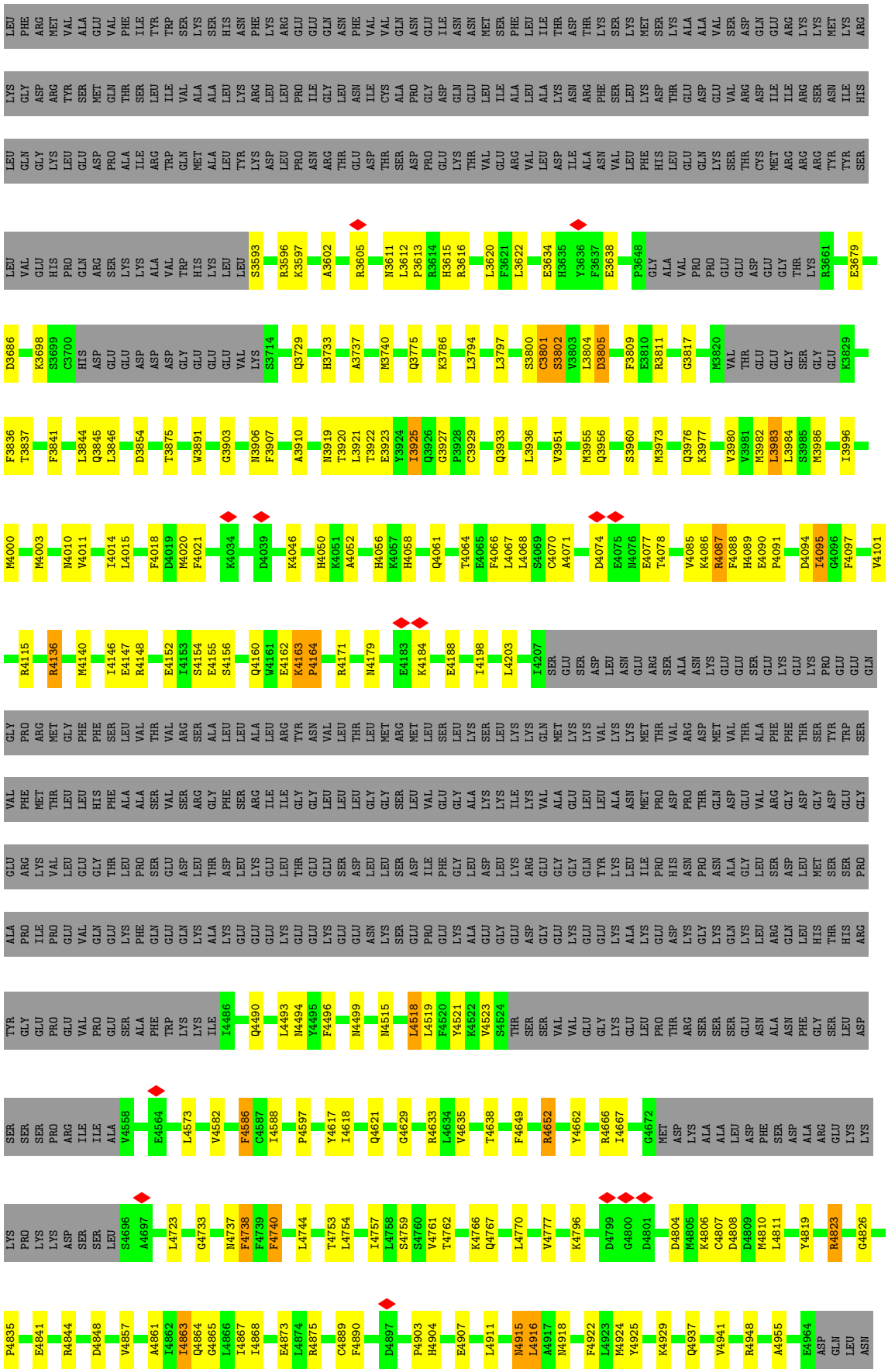
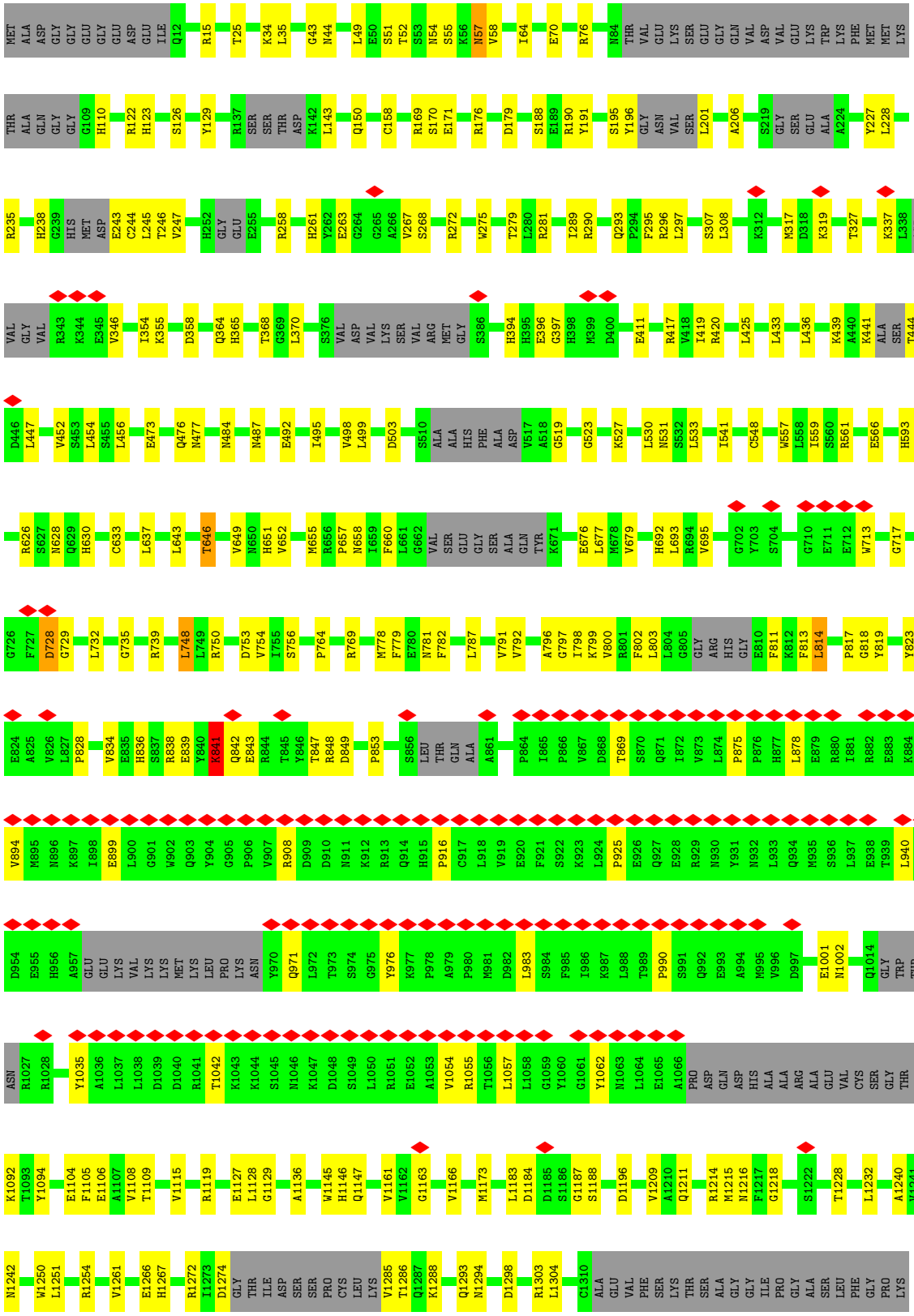
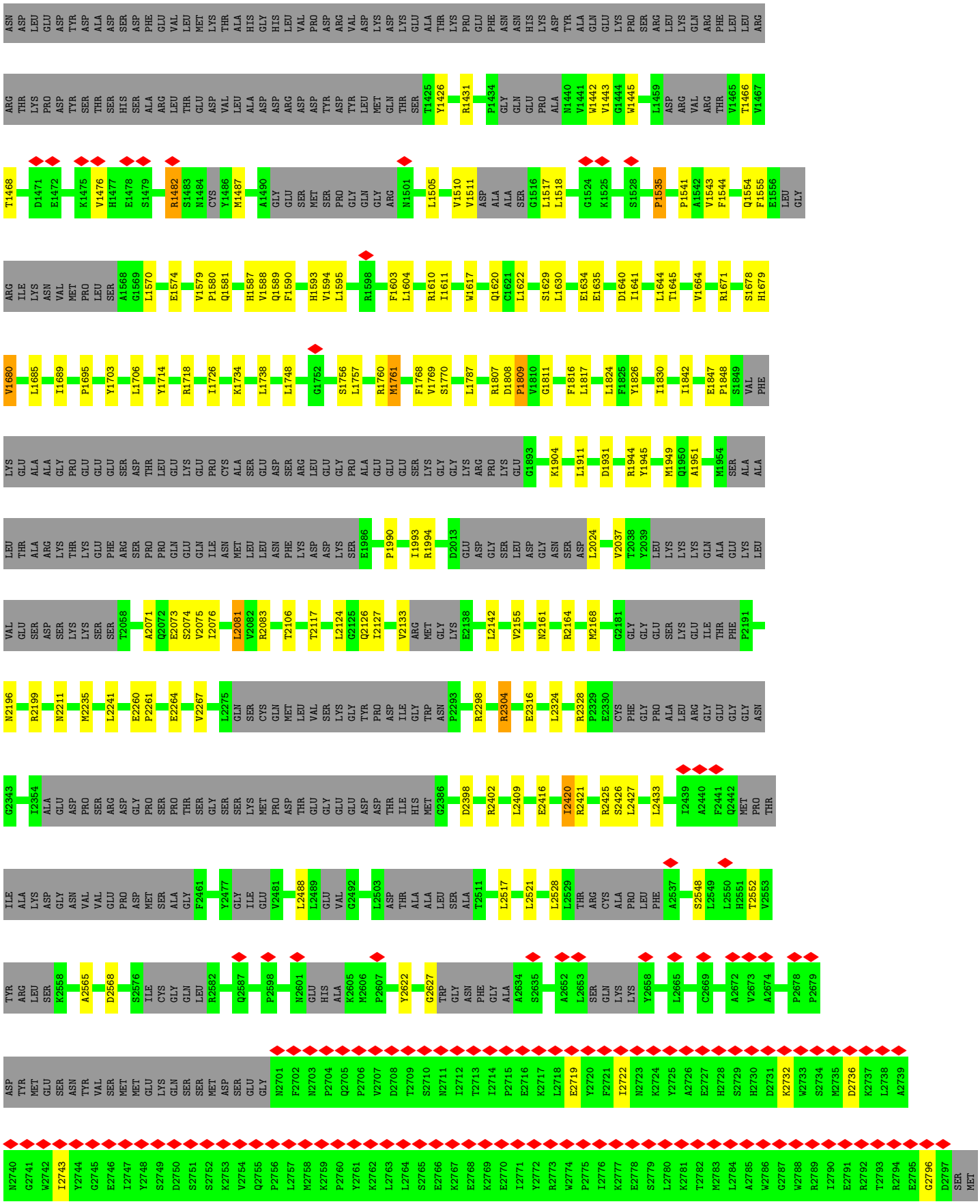
ALA T2511 L2517 L2521 L2528 L2529 THR ARG CYS ALA PRO LEU PHE A2537 S2548 L2549 L2550 H2551 T2552 V2553 TYR ARG LEU SER K2558 A2565 D2568 S2576 ILE CYS GLY GLN LEU R2582 Q2587 P2598 N2601 GLU HIS ALA K2605 M2606 P2607 Y2622 G2627 TRP GLY ASN
PHE GLY ALA A2634 S2635 A2652 L2653 SER GLN LYS LYS Y2658 L2665 C2669 A2672 V2673 A2674 P2678 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715
E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728 S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775
I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788 R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER V2816 D2817 A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835
R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895
F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE
PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 F2983 L2984 L2991 C2992 S2993 G2994 G2996 H2996 A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 L3015 R3019 T3028 SER ILE
VAL ASN CYS L3034 H3035 Q3039 D3042 A3043 R3044 K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070 K3071 T3072 M3073 E3074 N3075 L3076 K3077 Q3078 G3079 Q3080 F3081 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE
ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 F3110 E3111 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135 T3136 S3137 L3138 Y3139 A3140 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 E3150 R3151 Q3152 R3153 S3154 A3155
L3156 G3157 E3158 C3159 L3160 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU
MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN
THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL
SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU ALA ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU GLU ASP

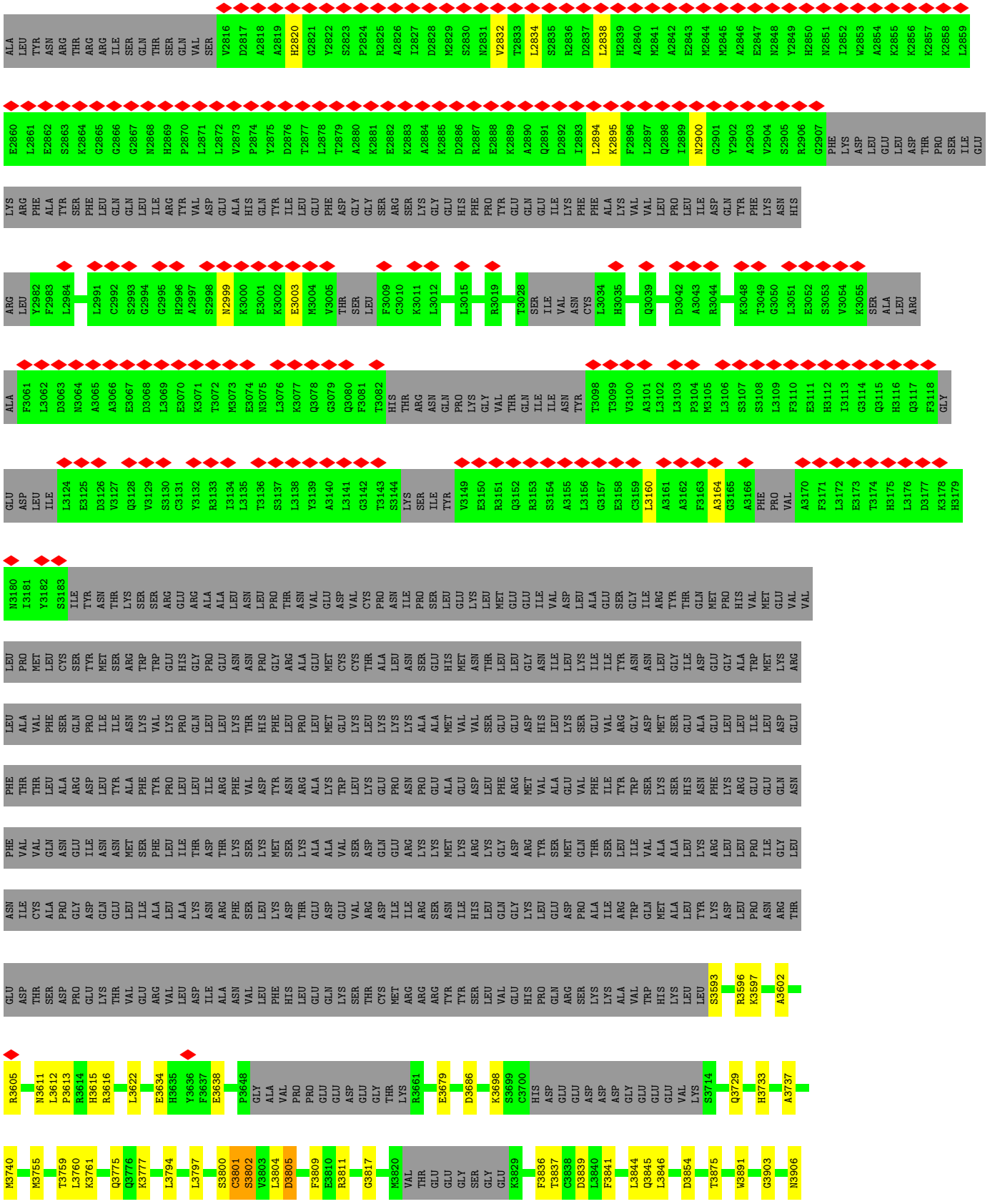


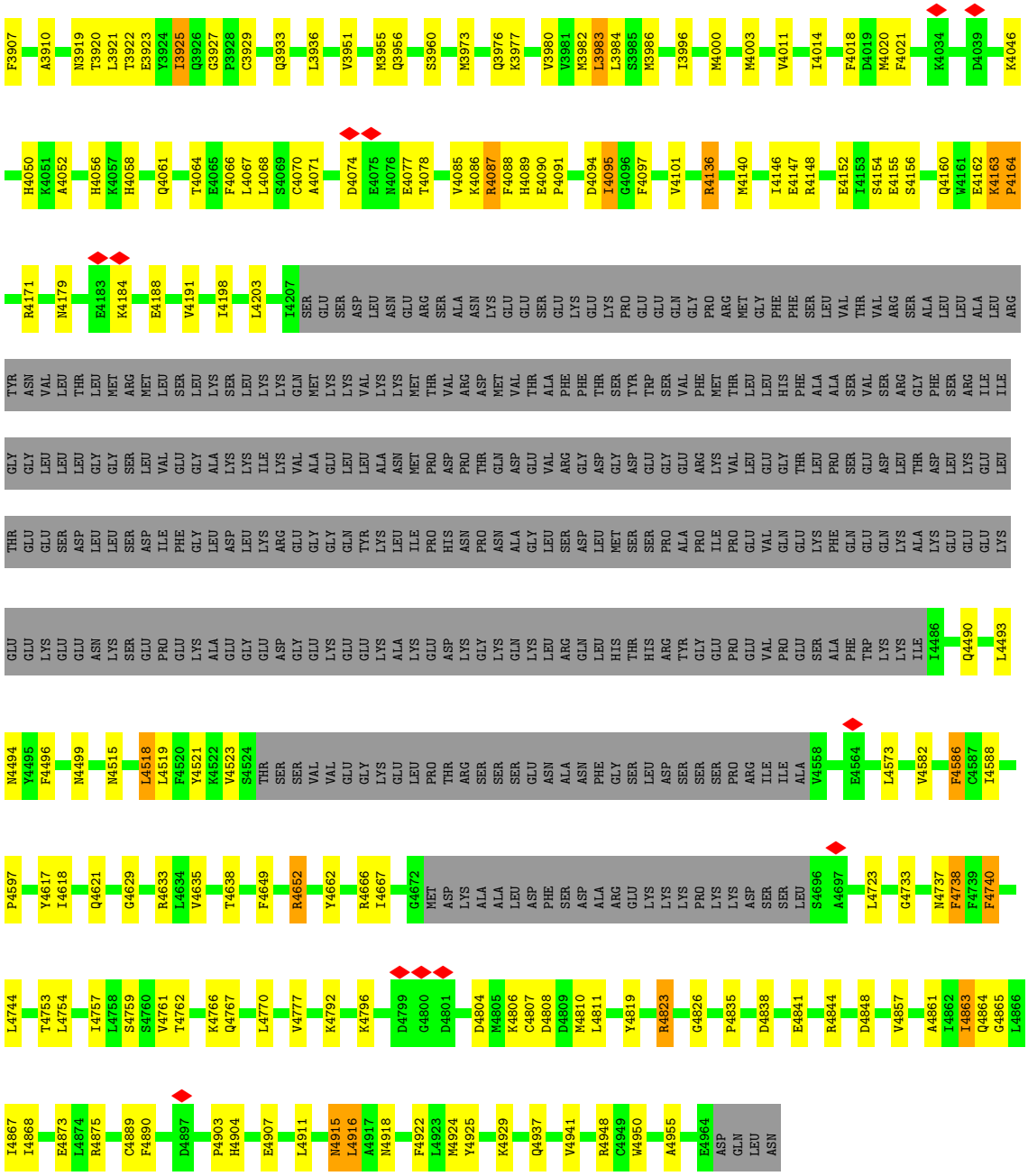
• Molecule 1: RyR2

Chain D:



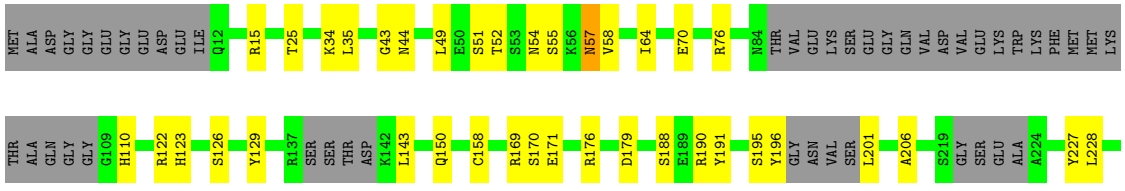


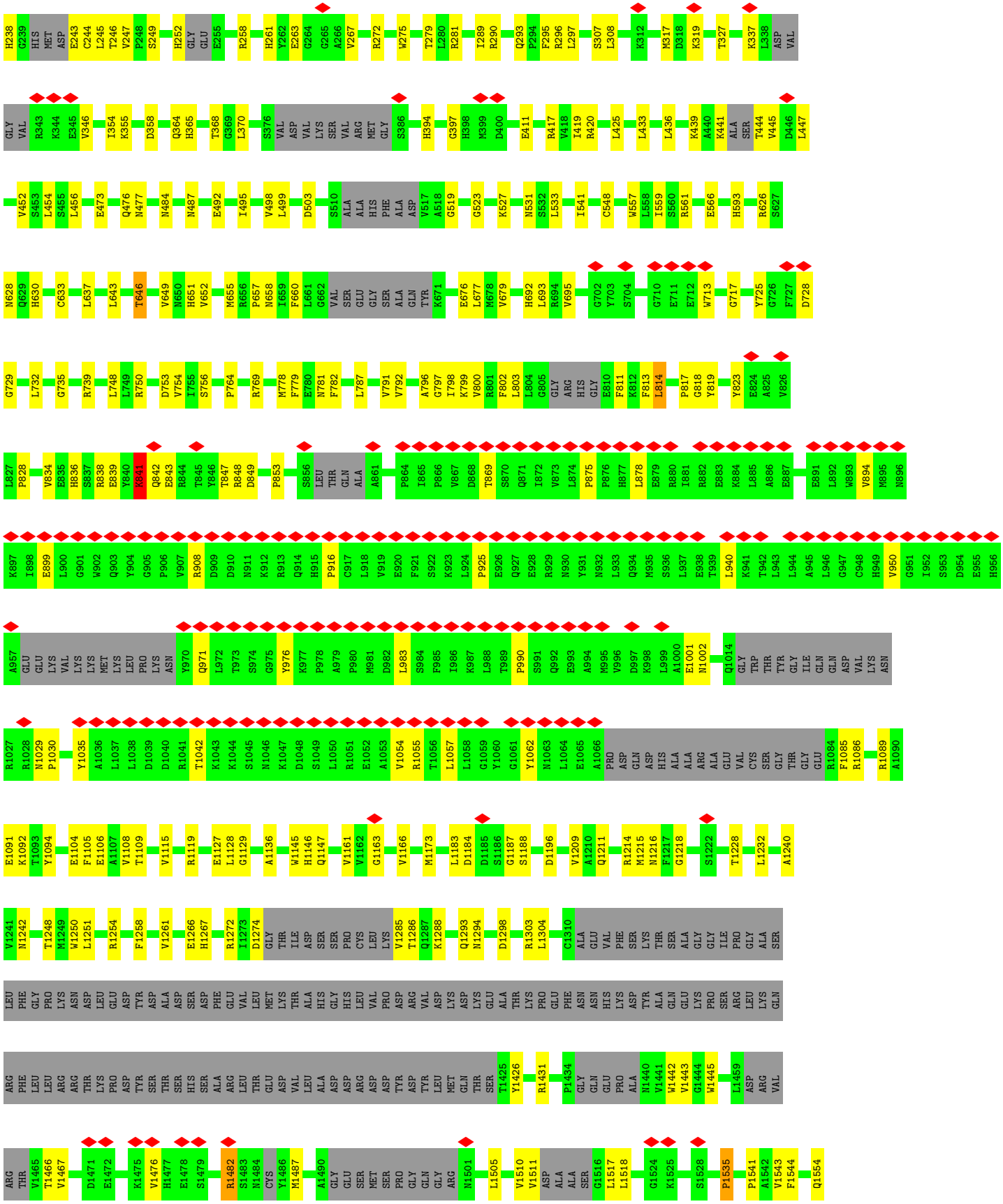

ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER V2816 D2817 A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859
E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU
LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO TYR PHE LYS ASN HIS
ARG LEU Y2982 F2983 L2984 L2991 C2992 S2993 G2994 G2995 H2996 A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 L3015 R3019 T3028 SER ILE VAL ASN CYS L3034 H3035 Q3039 D3042 A3043 R3044 K3048 T3049 G3050 L3051 E3052 S3053 V3054 K3055 SER ALA LEU ARG
ALA F3061 L3062 D3063 N3064 A3065 A3066 E3067 D3068 L3069 E3070 K3071 T3072 M3073 E3074 N3075 L3076 K3077 Q3078 G3079 Q3080 F3081 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 F3110 E3111 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY
GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135 T3136 S3137 L3138 Y3139 A3140 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 E3150 R3151 Q3152 R3153 S3154 A3155 L3156 G3157 E3158 C3159 L3160 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179
N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL
LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG
LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO PRO LEU MET GLU LYS LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU
PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN
PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS SER MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU
ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR
GLU ASP THR SER ASP PRO GLU VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU LEU S3593 R3596 K3597 A3602
R3605 N3611 L3612 P3613 R3614 H3615 R3616 L3622 E3634 H3635 Y3636 F3637 E3638 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 E3679 D3686 K3698 S3699 C3700 HIS ASP GLU GLU ASP ASP GLY GLU GLU GLU VAL LYS S3714 Q3729 H3733 A3737
M3740 M3755 T3759 L3760 K3761 Q3775 Q3776 K3777 L3794 L3797 S3800 C3801 S3802 V3803 L3804 D3805 F3809 E3810 R3811 G3817 M3820 VAL THR GLU GLU GLY SER GLY GLU K3829 F3836 T3837 C3838 D3839 L3840 F3841 L3844 Q3845 L3846 D3854 T3875 W3891 G3903 N3906



• Molecule 1: RyR2

Chain G:

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GLY VAL R343 K344 E345 V346 I354 K355 D358 Q364 H365 T368 G369 L370 S376 VAL ASP VAL LYS SER VAL ARG MET GLY S386 H394 G397 H398 M399 D400 E411 R417 V418 I419 R420 L425 L433 L436 K439 A440 K441 ALA SER T444 V445 D446 L447
V452 S453 L454 S455 L456 E473 Q476 N477 N484 N487 E492 I495 V498 L499 D503 S510 ALA ALA HIS PHE ALA ASP V517 A518 G519 G523 K527 N531 S532 L533 I541 C548 W557 L558 I559 S560 R561 E566 H593 R626 S627
N628 Q629 H630 C633 L637 L643 T646 V649 N650 H651 V652 M655 H656 P657 N658 I659 F660 L661 G662 VAL SER GLU GLY SER ALA GLN TYR K671 E676 L677 M678 V679 H692 L693 R694 V695 G702 Y703 S704 G710 E711 E712 W713 G717 Y725 G726 F727 D728
G729 L732 G735 R739 L748 L749 R750 D753 V754 I755 S756 P764 R769 M778 F779 E780 N781 F782 L787 V791 V792 A796 G797 I798 K799 V800 R801 F802 L803 L804 G805 GLY ARG HIS GLY E810 F811 K812 F813 L814 P817 G818 Y819 Y823 E824 A825 V826
L827 P828 V834 E835 H836 S837 R838 E839 Y840 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 P853 S856 LEU THR GLN ALA A861 P864 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 E887 E891 L892 W893 V894 M895 N896
K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956
A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN
R1027 R1028 N1029 P1030 Y1035 A1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 R1089 A1090
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V1241 N1242 T1248 M1249 W1250 L1251 R1254 F1258 V1261 E1266 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 Q1293 N1294 D1298 R1303 L1304 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY GLY ILE PRO GLY ALA SER
LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN
ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 Y1426 R1431 P1434 GLY GLN GLU PRO ALA N1440 V1441 W1442 V1443 G1444 W1445 L1459 ASP ARG VAL
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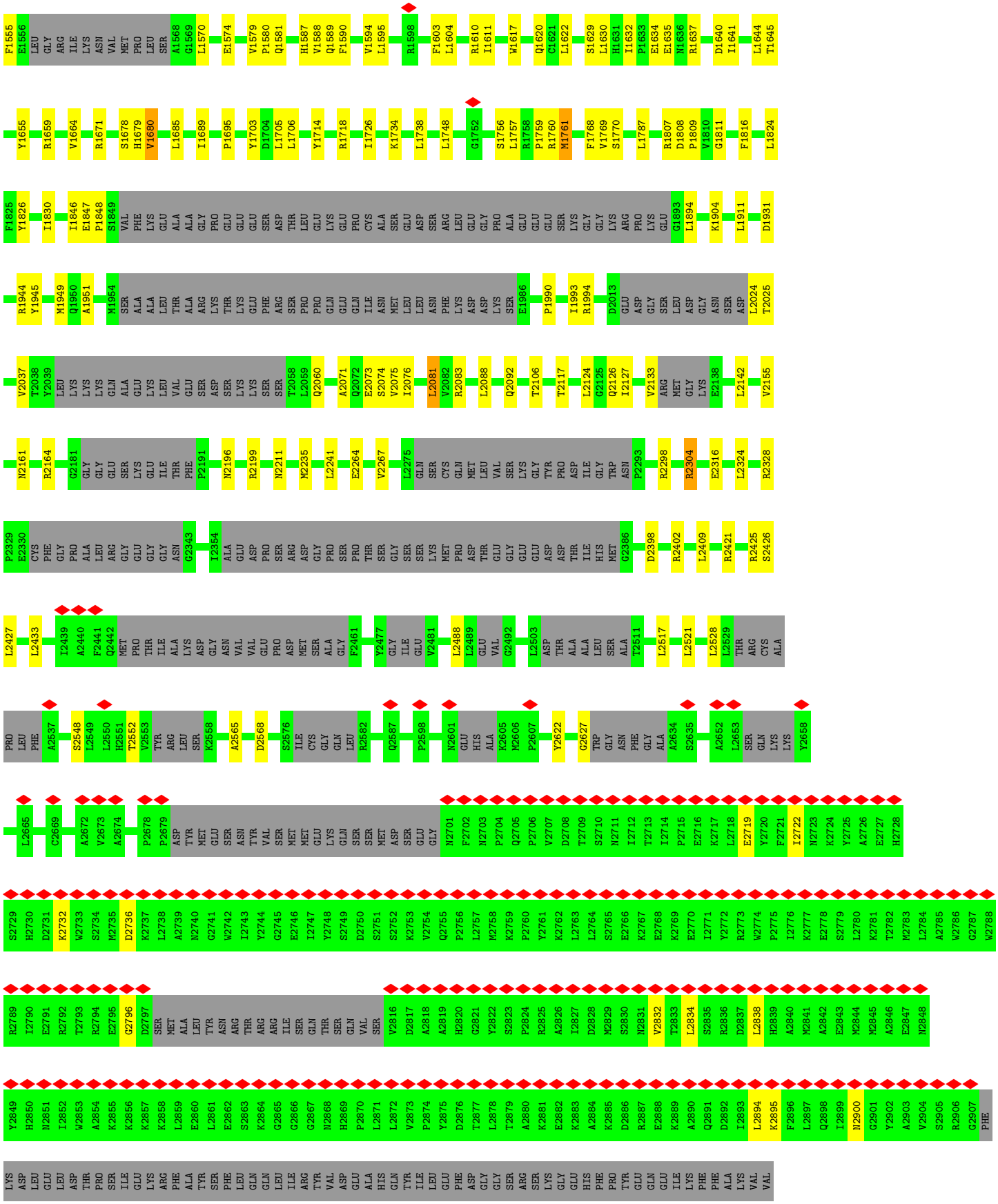
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F1825 Y1826 I1830 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS GLU G1893 L1894 K1904 L1911 D1931
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L2665 C2669 A2672 V2673 A2674 P2678 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728
S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788
R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER V2816 D2817 A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848
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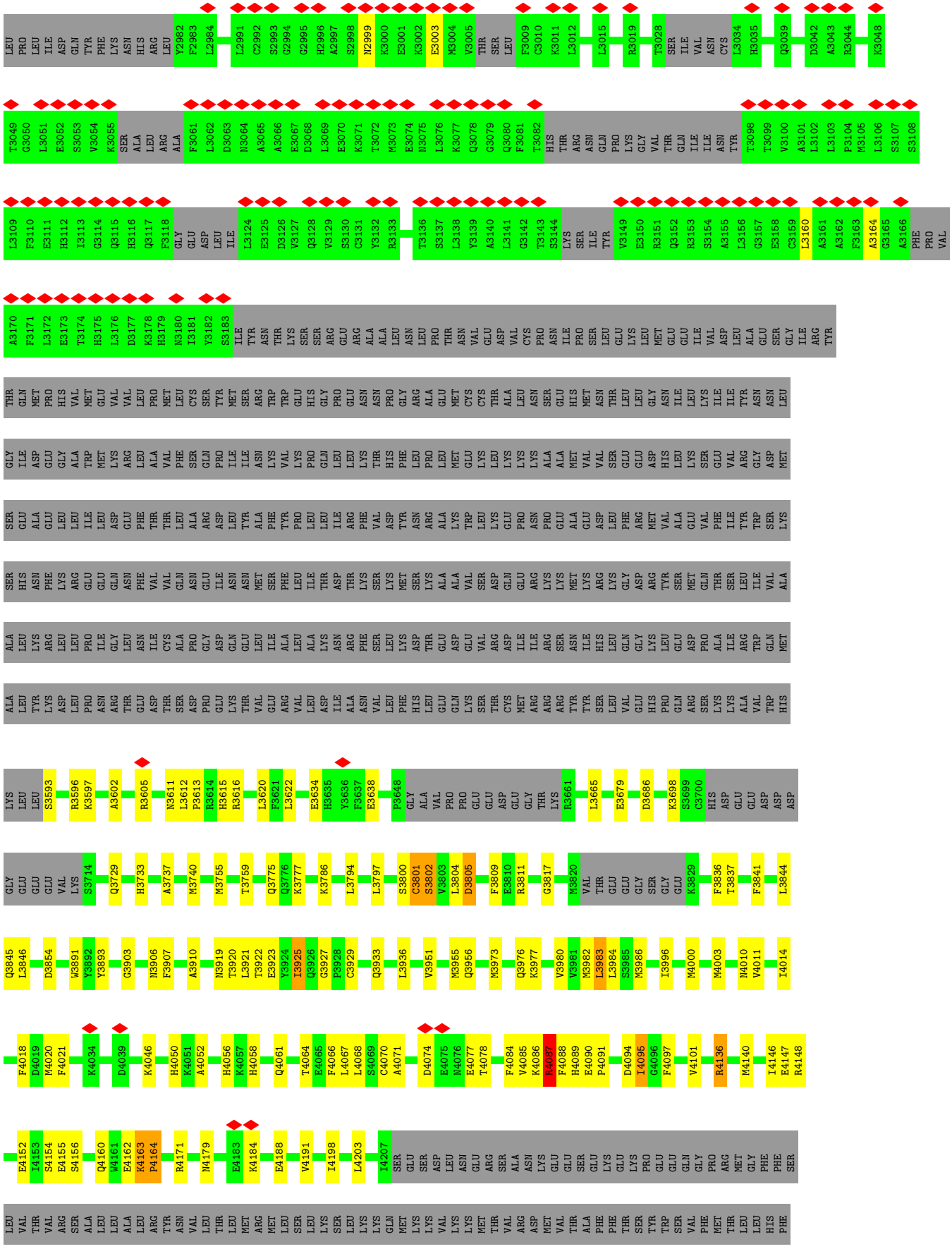
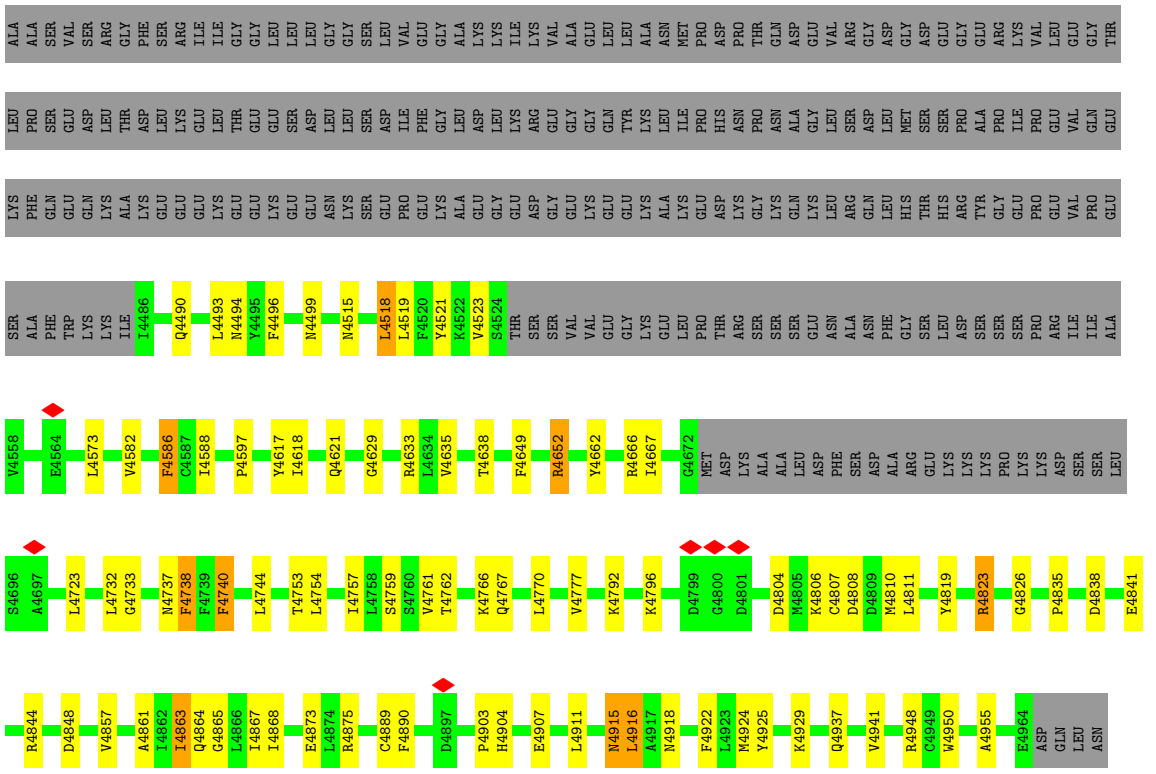
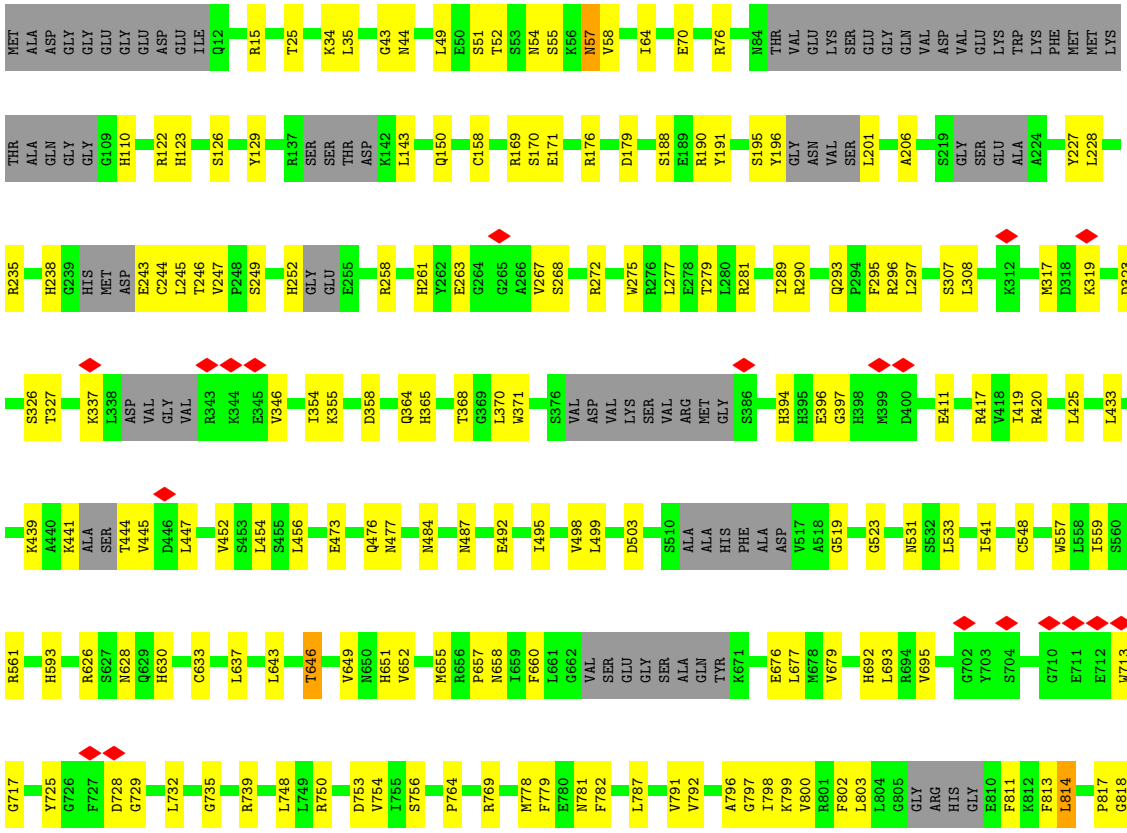
LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL

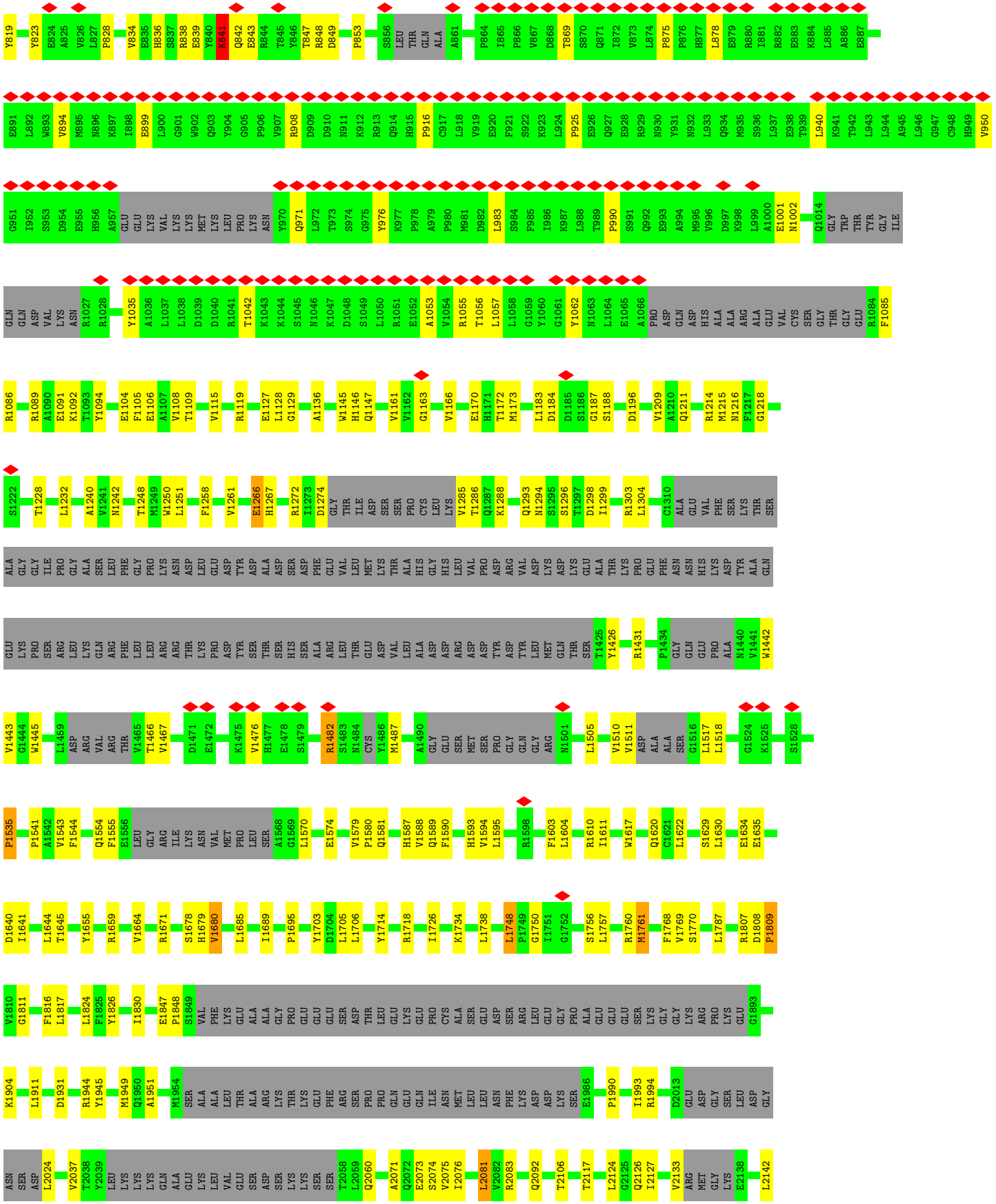




- Molecule 1: RyR2

Chain J:

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E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 Y907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950
G951 I952 S953 D954 E955 H956 A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 Q1014 GLY TRP THR TYR GLY ILE
GLN GLN ASP VAL LYS ASN R1027 R1028 Y1035 A1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085
R1086 R1089 A1090 E1091 K1092 T1093 Y1094 E1104 F1105 E1106 A1107 V1108 T1109 V1115 R1119 E1127 L1128 G1129 A1136 W1145 H1146 Q1147 V1161 V1162 G1163 V1166 E1170 H1171 T1172 M1173 L1183 D1184 D1185 S1186 G1187 S1188 D1196 V1209 A1210 Q1211 R1214 M1215 N1216 F1217 G1218
S1222 T1228 L1232 A1240 Y1241 N1242 T1248 M1249 W1250 L1251 F1258 V1261 E1266 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 Q1293 N1294 S1295 S1296 T1297 D1298 I1299 R1303 L1304 C1310 ALA GLU VAL PHE SER LYS THR SER
ALA GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLN PHE ASN ASN HIS LYS ASP TYR ALA GLN
GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 Y1426 R1431 P1434 GLY GLN GLU PRO ALA N1440 V1441 W1442
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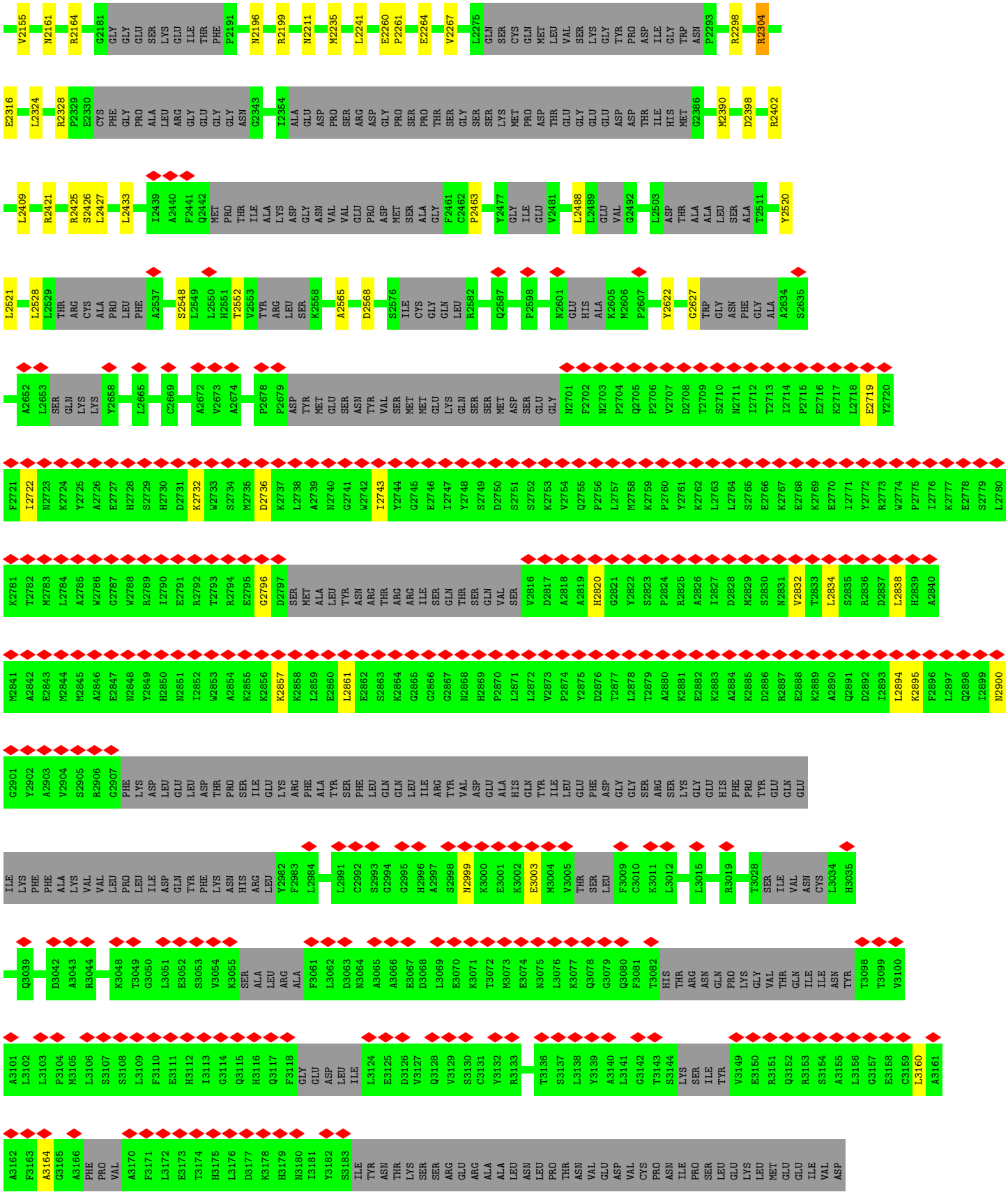
ASN SER ASP L2024 V2037 T2038 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 L2059 Q2060 A2071 Q2072 E2073 S2074 V2075 I2076 L2081 V2082 R2083 Q2092 T2106 T2117 L2124 G2125 Q2126 I2127 V2133 ARG MET GLY LYS E2138 L2142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G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU
ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 F2983 L2984 L2991 C2992 S2993 G2994 G2995 H2996 A2997 S2998 N2999 K3000 E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 C3010 K3011 L3012 L3015 R3019 T3028 SER ILE VAL ASN CYS L3034 H3035
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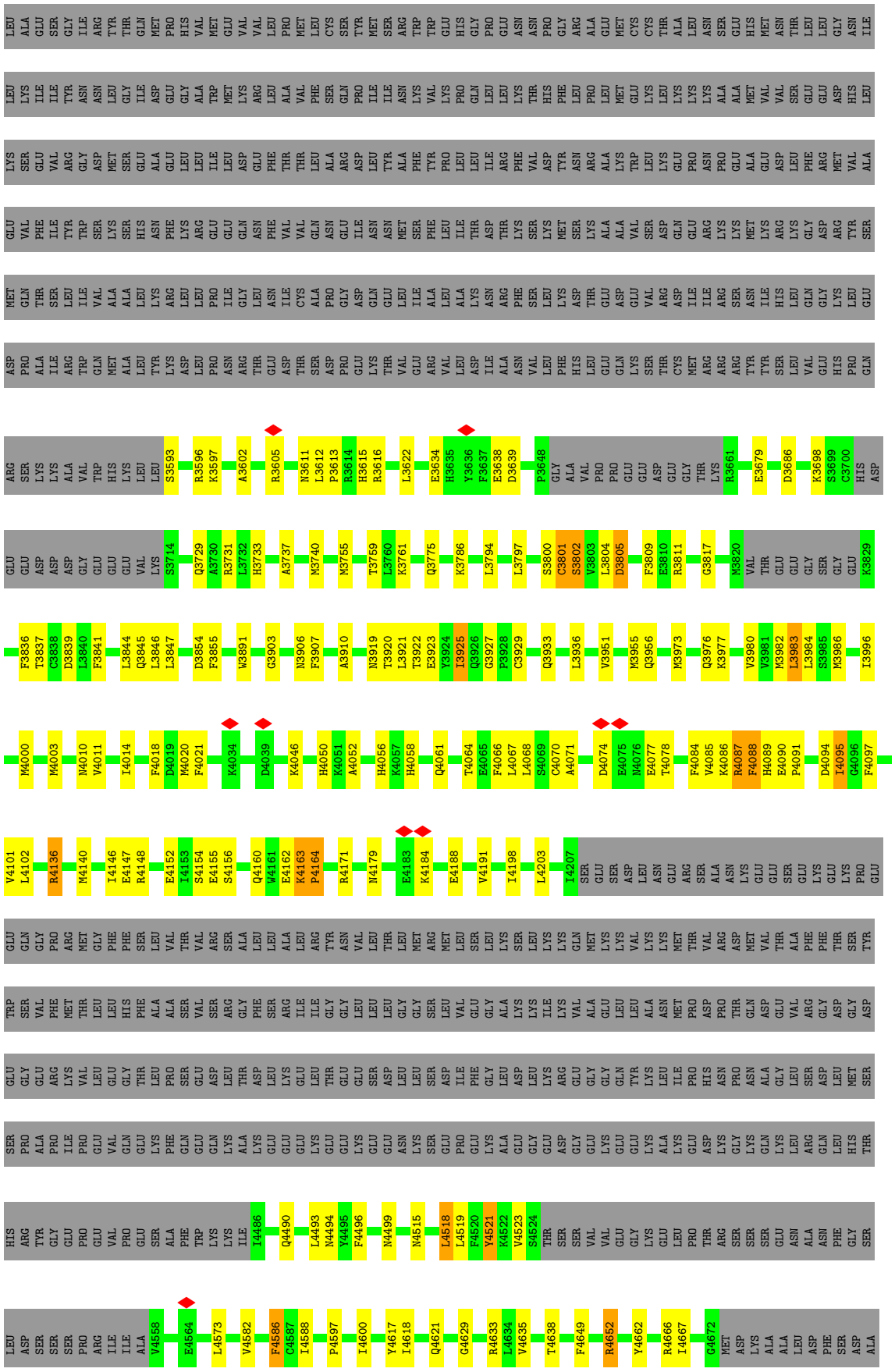
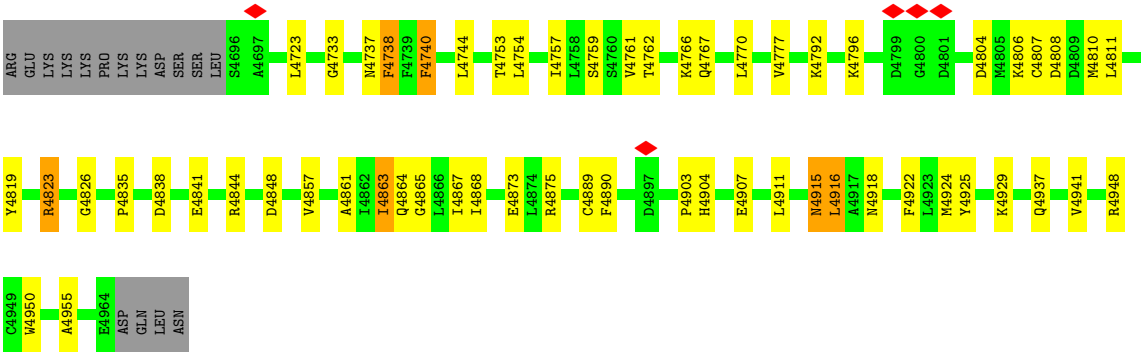
A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP





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

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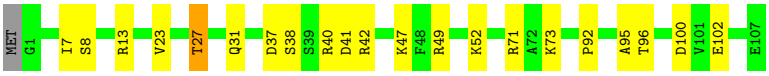

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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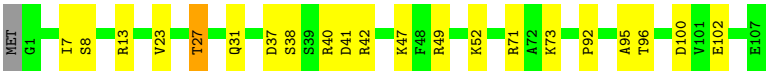

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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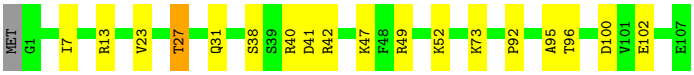
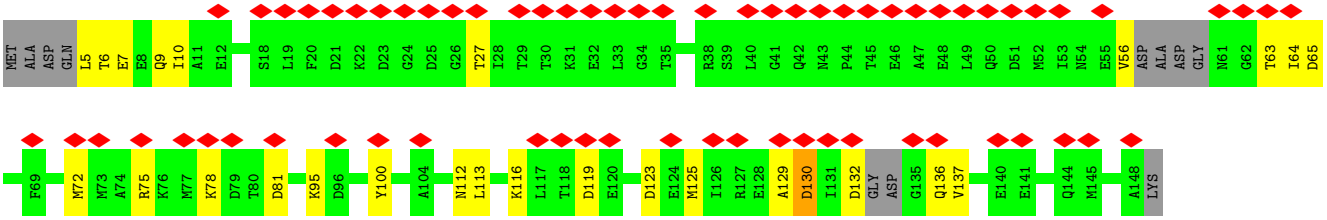


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:

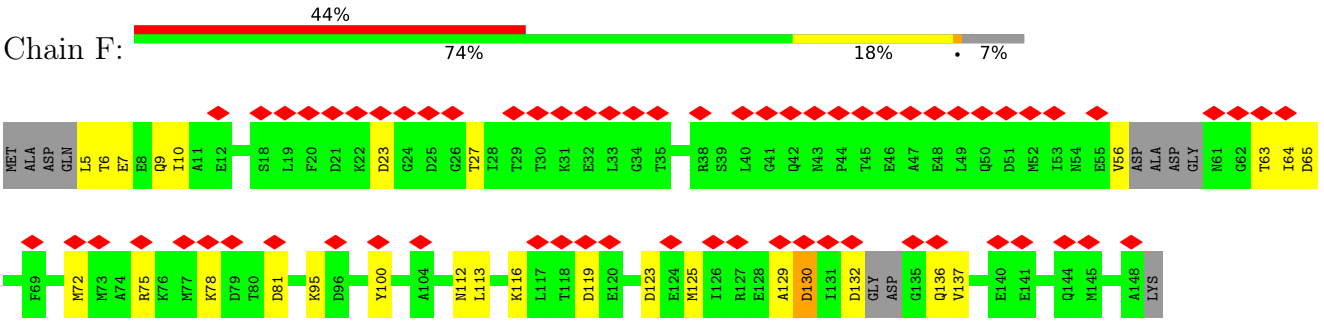
• Molecule 3: Calmodulin-1

Chain C:



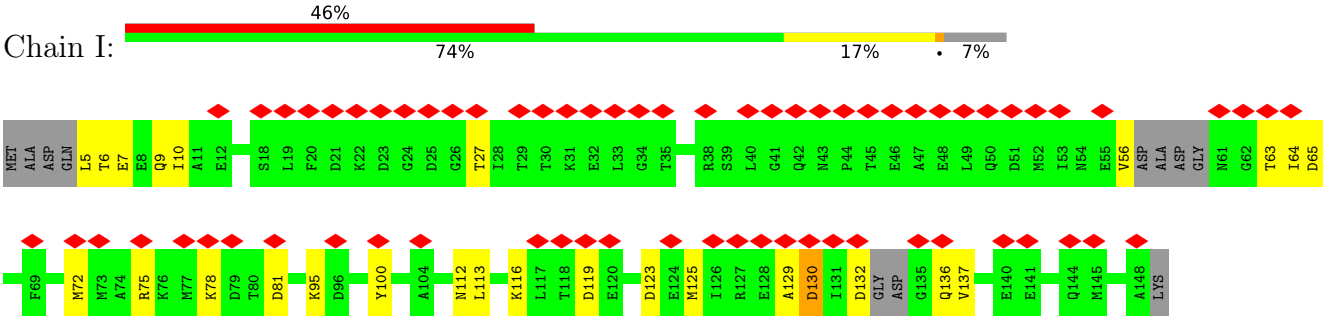
• Molecule 3: Calmodulin-1

Chain F:



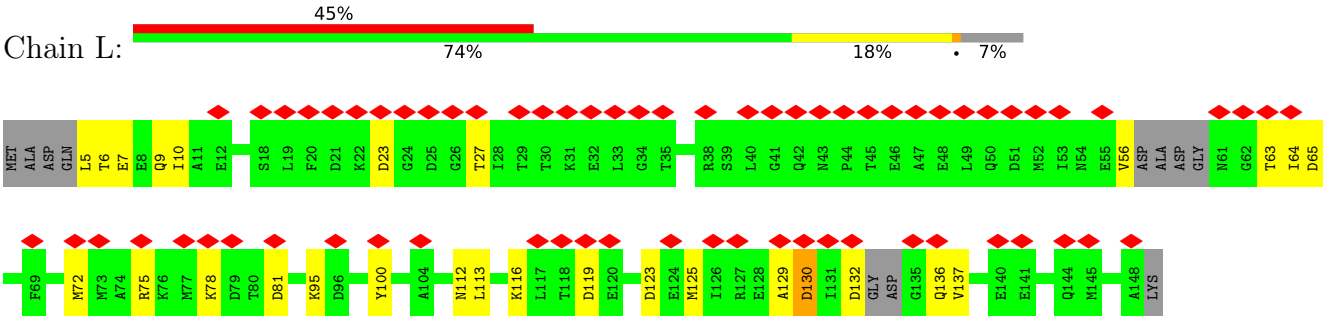
• Molecule 3: Calmodulin-1

Chain I:



• Molecule 3: Calmodulin-1

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	208715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	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	0.48	0/27354	0.68	11/36987 (0.0%)
1	D	0.48	0/27354	0.68	11/36987 (0.0%)
1	G	0.48	0/27354	0.68	11/36987 (0.0%)
1	J	0.48	0/27354	0.68	10/36987 (0.0%)
2	B	0.41	0/835	0.60	0/1123
2	E	0.41	0/835	0.60	0/1123
2	H	0.41	0/835	0.60	0/1123
2	K	0.41	0/835	0.60	0/1123
3	C	0.33	0/1104	0.59	0/1479
3	F	0.33	0/1104	0.59	0/1479
3	I	0.33	0/1104	0.59	0/1479
3	L	0.33	0/1104	0.59	0/1479
All	All	0.48	0/117172	0.67	43/158356 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	32
1	D	0	32
1	G	0	32
1	J	0	32
All	All	0	128

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1911	LEU	CA-CB-CG	7.19	131.83	115.30
1	D	1911	LEU	CA-CB-CG	7.19	131.83	115.30
1	G	1911	LEU	CA-CB-CG	7.19	131.83	115.30
1	J	1911	LEU	CA-CB-CG	7.19	131.83	115.30
1	G	4518	LEU	CB-CG-CD1	-6.50	99.96	111.00

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	HIS	Peptide
1	A	729	GLY	Peptide
1	A	748	LEU	Peptide
1	A	791	VAL	Peptide
1	A	817	PRO	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	26851	0	25388	500	0
1	D	26851	0	25388	500	0
1	G	26851	0	25388	497	0
1	J	26851	0	25388	508	0
2	B	819	0	824	10	0
2	E	819	0	824	10	0
2	H	819	0	824	8	0
2	K	819	0	824	10	0
3	C	1094	0	1036	16	0
3	F	1094	0	1036	17	0
3	I	1094	0	1036	16	0
3	L	1094	0	1036	17	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
All	All	115060	0	108992	1872	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 1872 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:G:4518:LEU:HD21	1:G:4738:PHE:CE1	1.58	1.39
1:D:4518:LEU:HD21	1:D:4738:PHE:CE1	1.58	1.38
1:A:4518:LEU:HD21	1:A:4738:PHE:CE1	1.58	1.37
1:J:4518:LEU:HD21	1:J:4738:PHE:CE1	1.58	1.36
1:D:4733:GLY:HA3	1:D:4740:PHE:CE1	1.68	1.28

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	3389/4968 (68%)	3012 (89%)	360 (11%)	17 (0%)	29	68
1	D	3389/4968 (68%)	3013 (89%)	359 (11%)	17 (0%)	29	68
1	G	3389/4968 (68%)	3015 (89%)	356 (10%)	18 (0%)	29	68
1	J	3389/4968 (68%)	3012 (89%)	360 (11%)	17 (0%)	29	68
2	B	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	E	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	K	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
3	C	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	59
3	F	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	59
3	I	132/149 (89%)	118 (89%)	13 (10%)	1 (1%)	19	59
3	L	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	19	59
All	All	14504/20900 (69%)	12911 (89%)	1520 (10%)	73 (0%)	32	68

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4916	LEU
1	D	4916	LEU
1	G	4916	LEU
1	J	4916	LEU
1	A	1580	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	2704/4355 (62%)	2667 (99%)	37 (1%)	67	85
1	D	2704/4355 (62%)	2666 (99%)	38 (1%)	67	85
1	G	2704/4355 (62%)	2666 (99%)	38 (1%)	67	85
1	J	2704/4355 (62%)	2666 (99%)	38 (1%)	67	85
2	B	88/89 (99%)	84 (96%)	4 (4%)	27	62
2	E	88/89 (99%)	84 (96%)	4 (4%)	27	62
2	H	88/89 (99%)	84 (96%)	4 (4%)	27	62
2	K	88/89 (99%)	84 (96%)	4 (4%)	27	62
3	C	119/127 (94%)	118 (99%)	1 (1%)	81	91
3	F	119/127 (94%)	118 (99%)	1 (1%)	81	91
3	I	119/127 (94%)	118 (99%)	1 (1%)	81	91
3	L	119/127 (94%)	118 (99%)	1 (1%)	81	91
All	All	11644/18284 (64%)	11473 (98%)	171 (2%)	66	84

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	4499	ASN
1	J	1760	ARG
1	G	4738	PHE
1	J	439	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	3906	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1679	HIS
1	J	193	HIS
1	G	2211	ASN
1	G	4499	ASN
1	J	544	ASN

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.

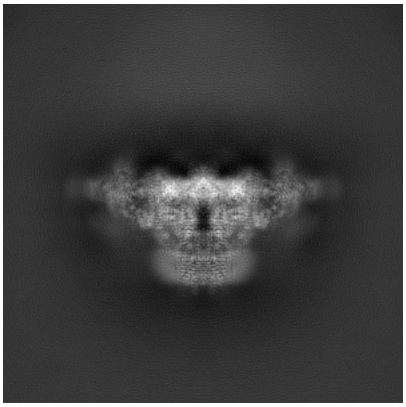
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9833. These allow visual inspection of the internal detail of the map and identification of artifacts.

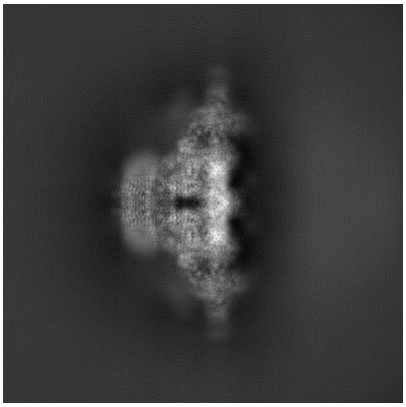
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

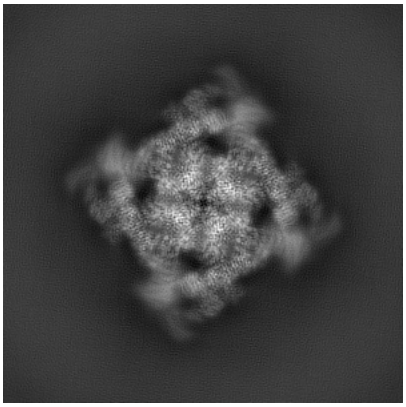
6.1.1 Primary map



X



Y

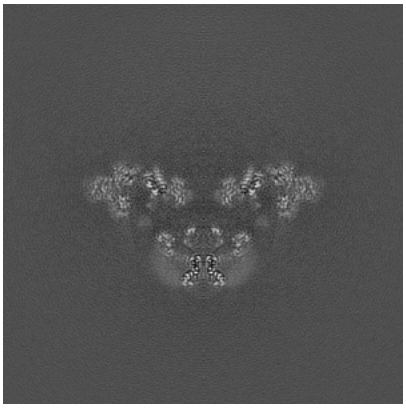


Z

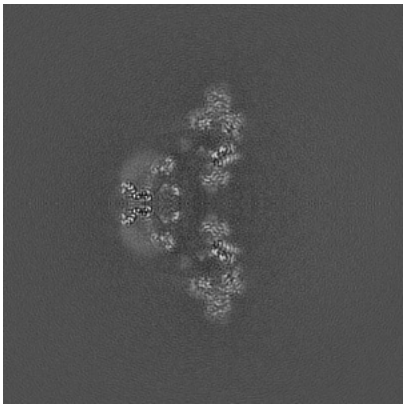
The images above show the map projected in three orthogonal directions.

6.2 Central slices

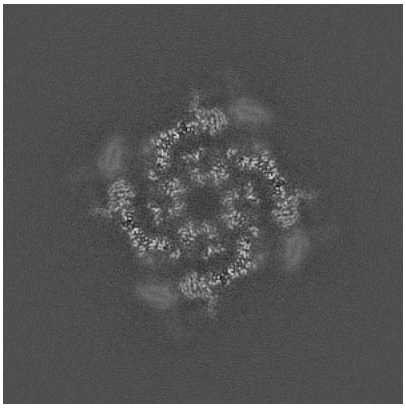
6.2.1 Primary map



X Index: 200



Y Index: 200

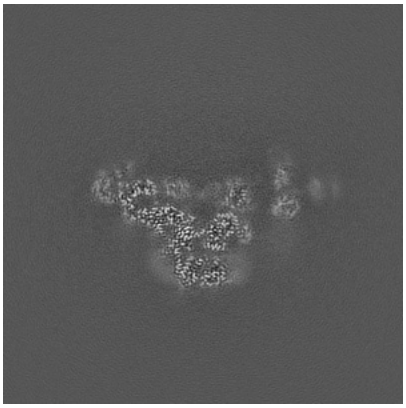


Z Index: 200

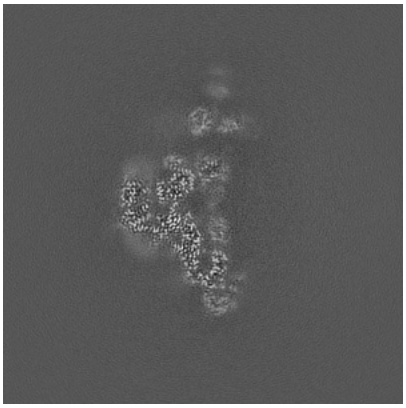
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

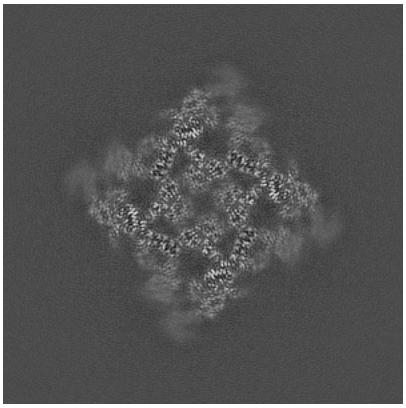
6.3.1 Primary map



X Index: 214



Y Index: 186

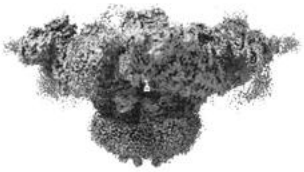


Z Index: 209

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

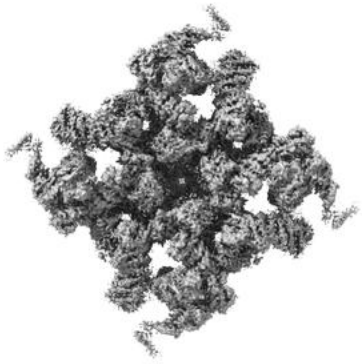
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

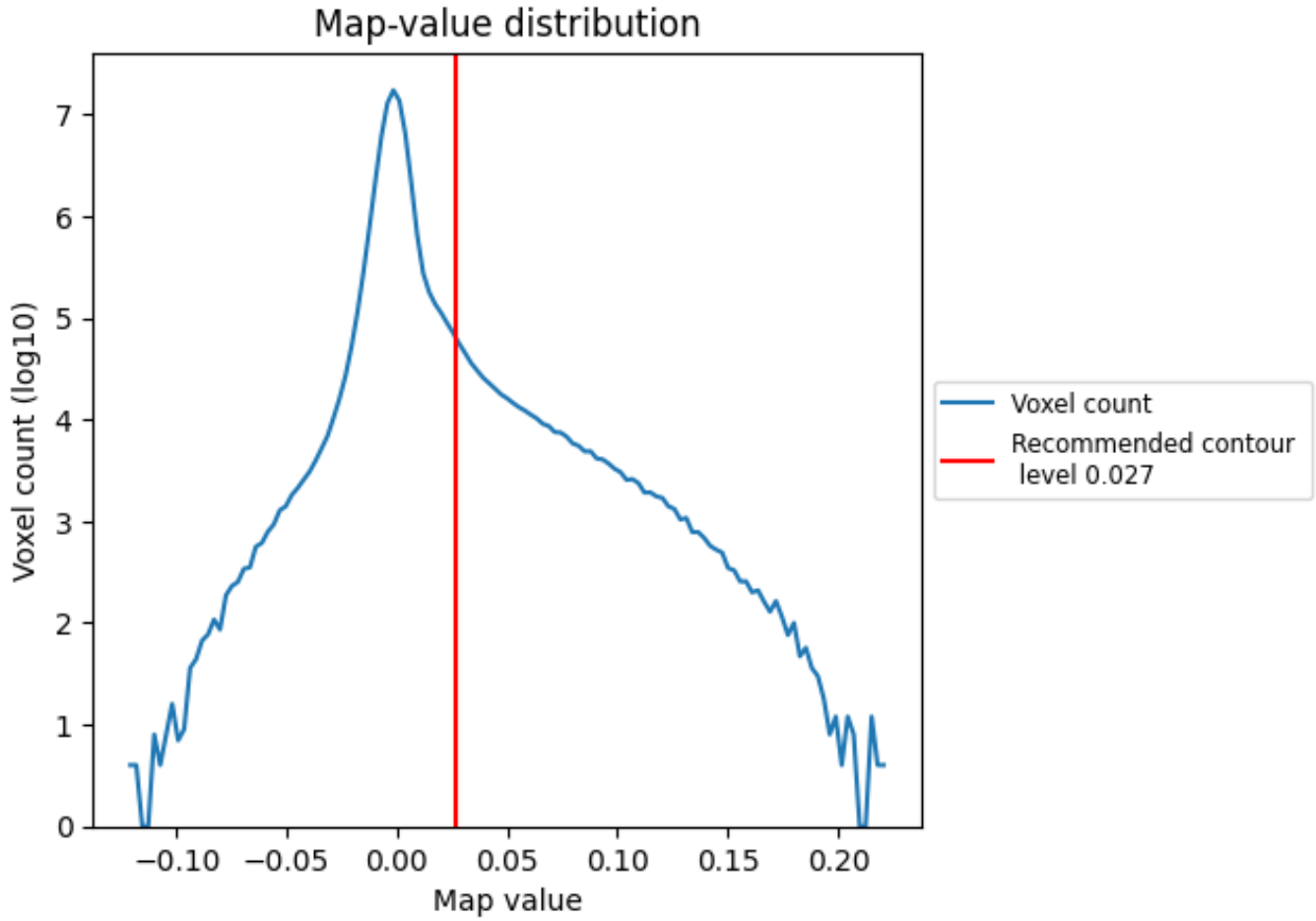
6.5 Mask visualisation (i)

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

7 Map analysis

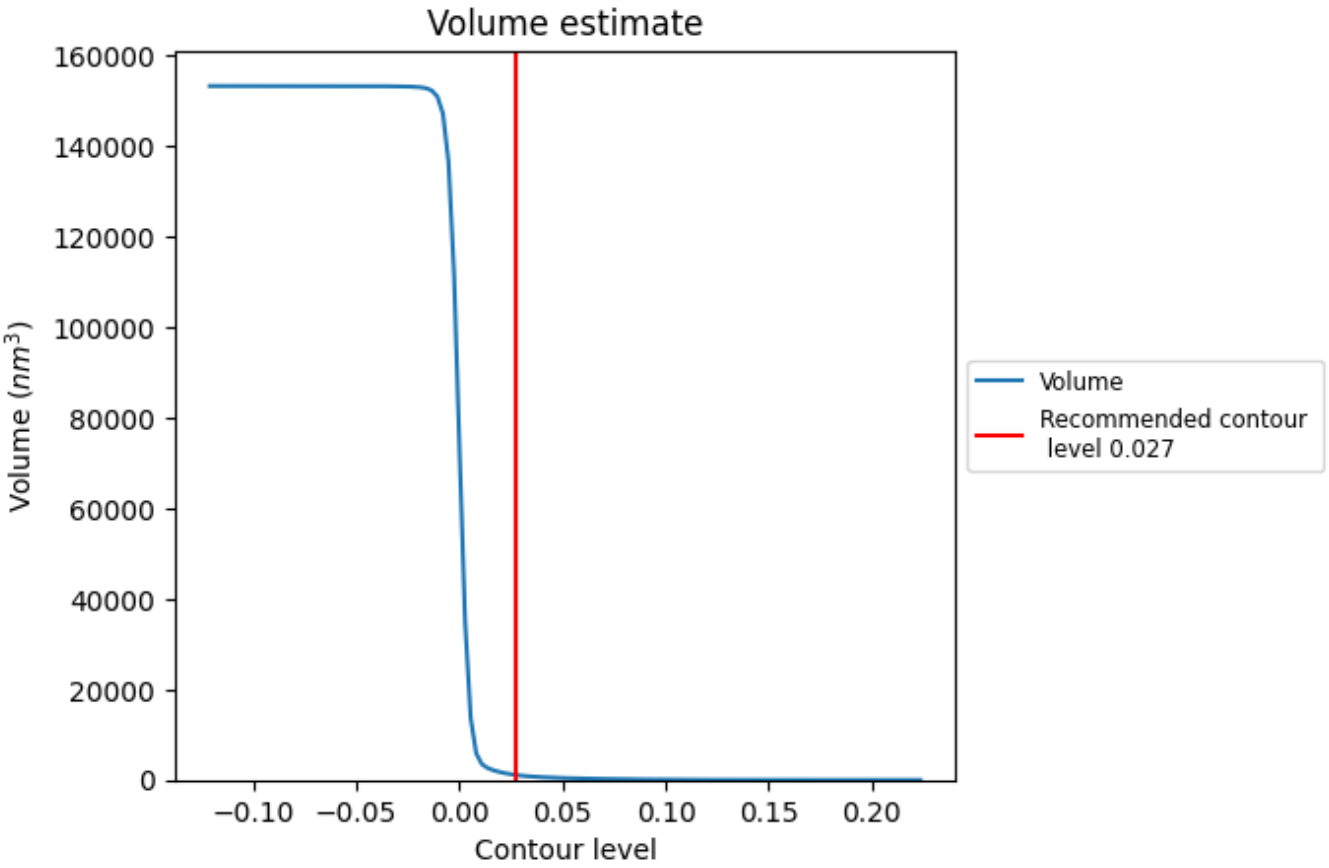
This section contains the results of statistical analysis of the map.

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.

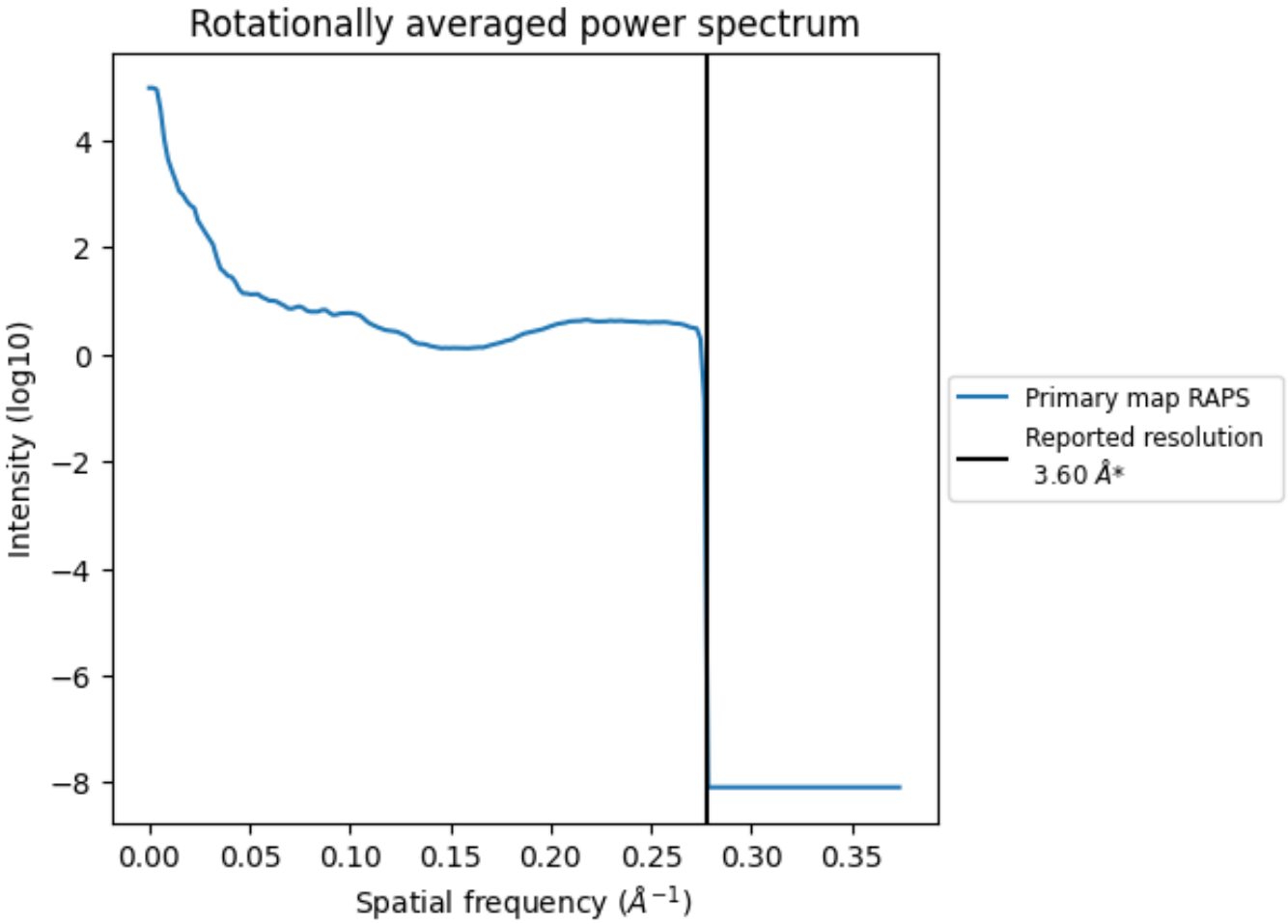
7.2 Volume estimate (i)



The volume at the recommended contour level is 1114 nm^3; this corresponds to an approximate mass of 1007 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)

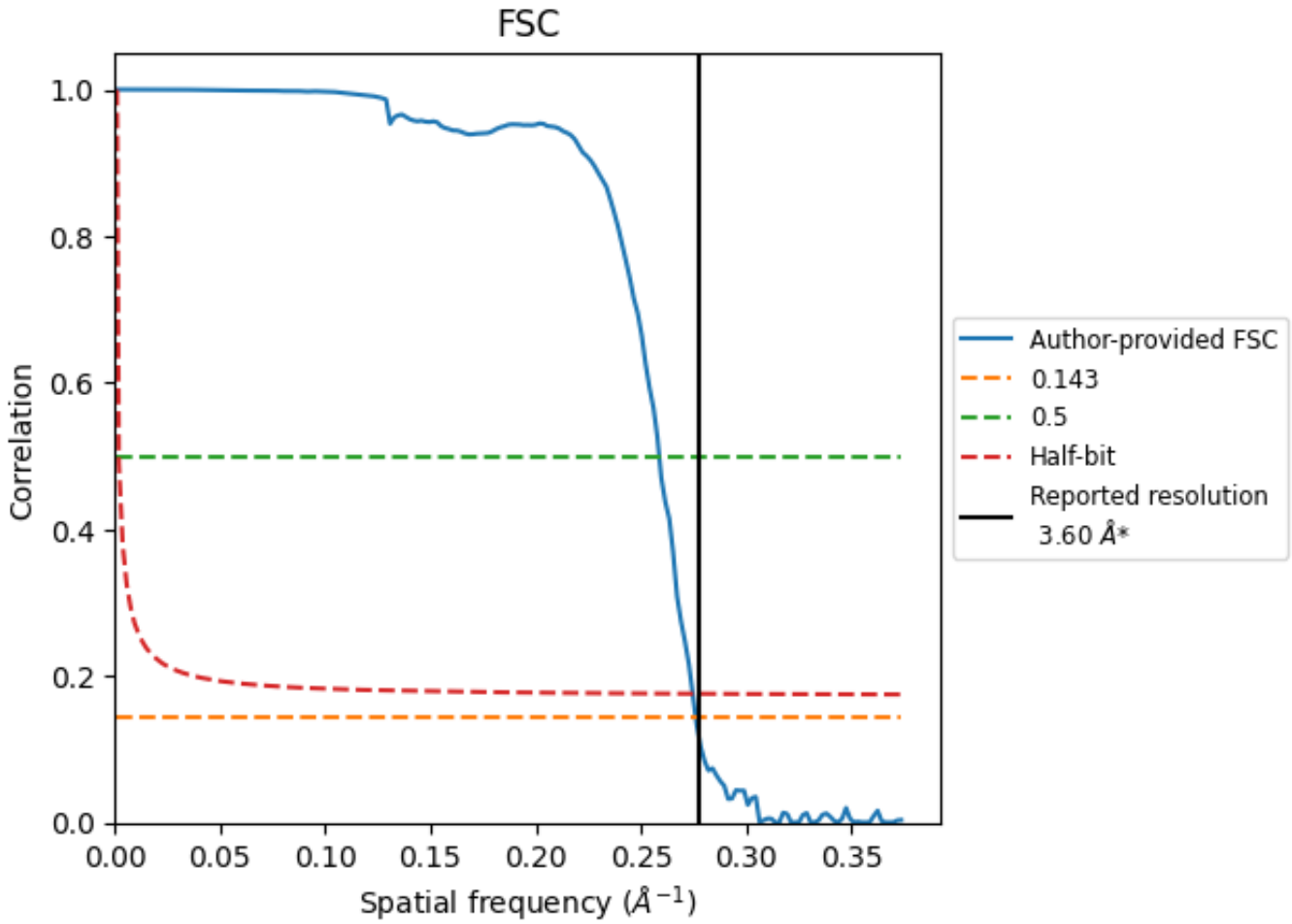


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

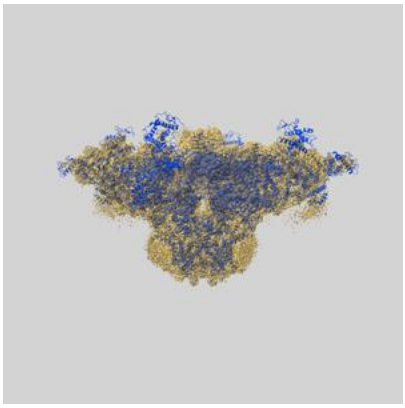
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	3.87	3.64
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

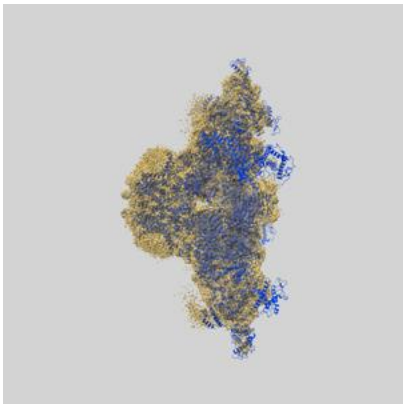
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9833 and PDB model 6JI8. Per-residue inclusion information can be found in section 3 on page 6.

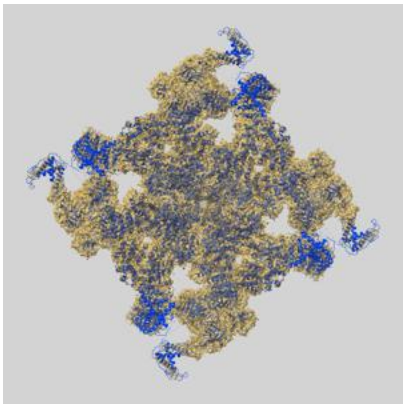
9.1 Map-model overlay



X



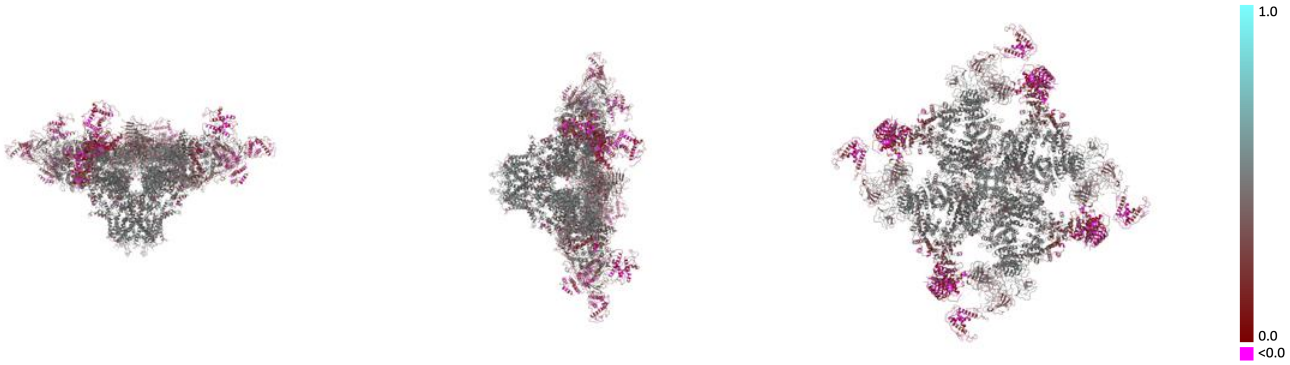
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

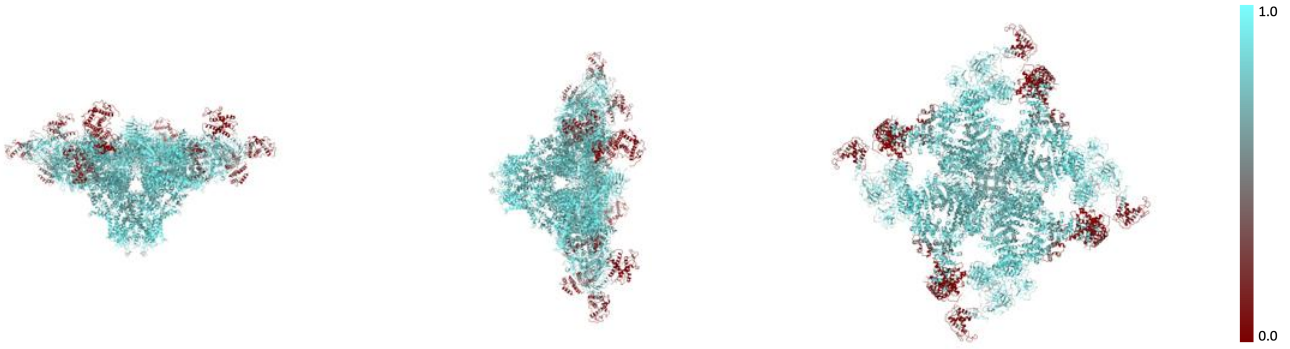
9.2 Q-score mapped to coordinate model (i)



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.

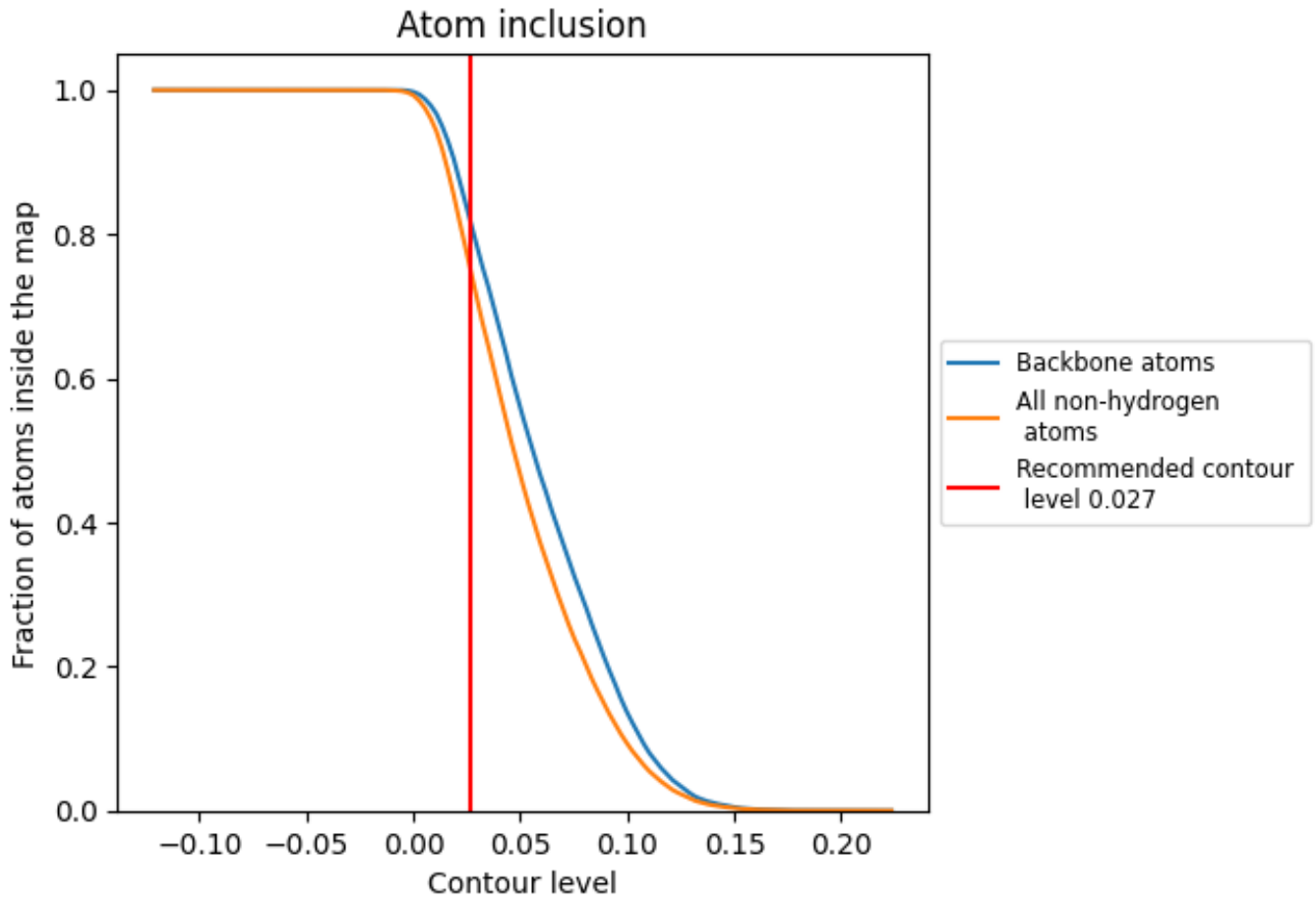
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7479	0.3840
A	0.7586	0.3880
B	0.8327	0.4310
C	0.4250	0.2340
D	0.7584	0.3880
E	0.8327	0.4310
F	0.4250	0.2340
G	0.7587	0.3880
H	0.8340	0.4320
I	0.4231	0.2350
J	0.7586	0.3880
K	0.8340	0.4310
L	0.4241	0.2360