wwPDB EM Validation Summary Report

Nov 2, 2024 – 02:33 PM EDT

PDB ID	:	5TB4
EMDB ID	:	EMD-8395
Title	:	Structure of rabbit RyR1 (EGTA-only dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-11
Resolution	:	4.50 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 ⓘ symbol.

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

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

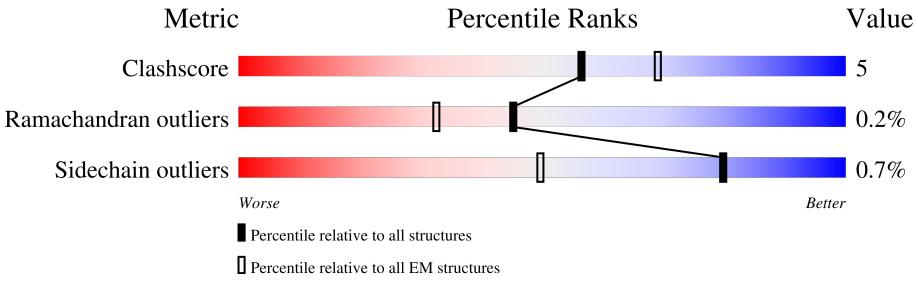
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	27% 84% 15%
1	F	108	28% 81% 19%
1	H	108	26% 85% 14%
1	J	108	28% 83% 16%
2	B	4416	39% 84% 10% 5%
2	E	4416	39% 84% 10% 5%
2	G	4416	39% 84% 10% 5%
2	I	4416	39% 84% 10% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 121272 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

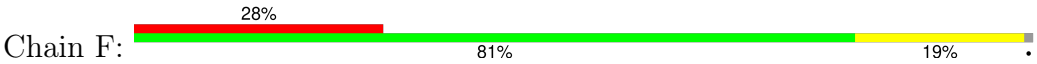
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

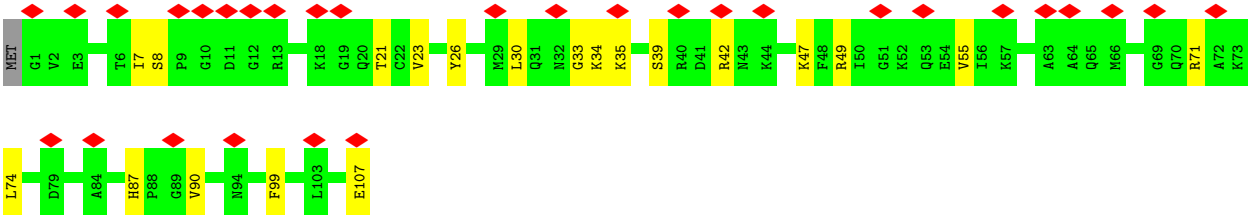
3 Residue-property plots (i)

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: Peptidyl-prolyl cis-trans isomerase FKBP1B

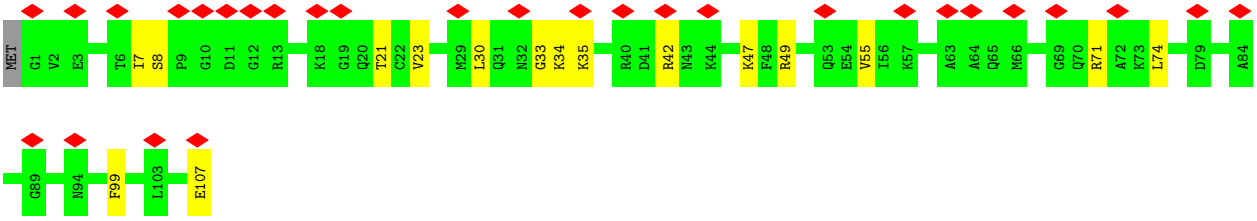
Chain F:





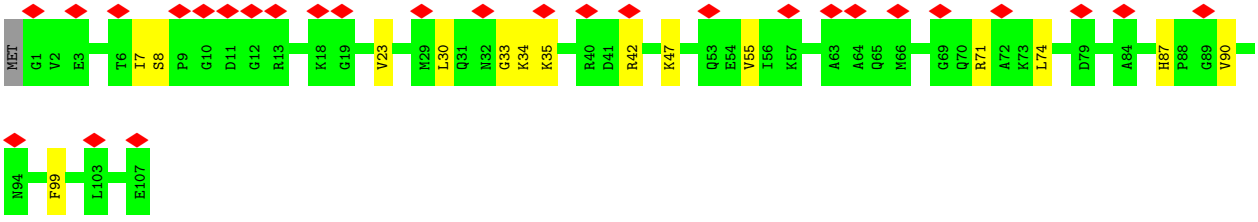
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



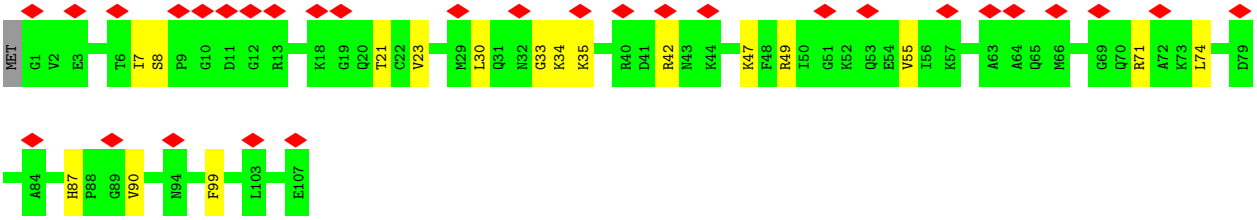
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



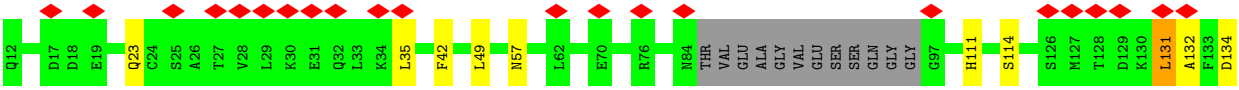
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

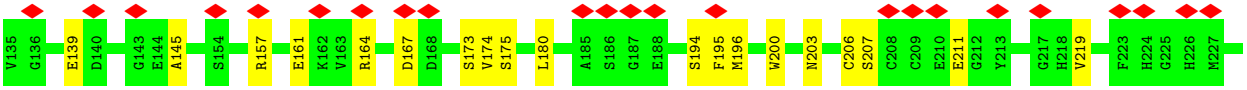
Chain J:

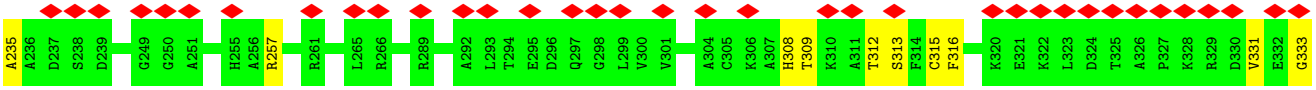


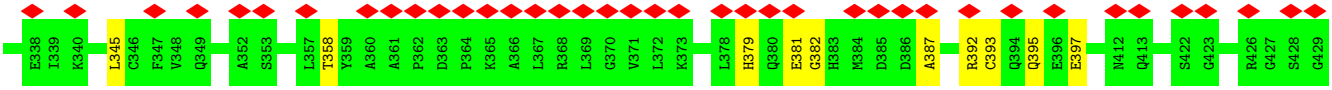
• Molecule 2: Ryanodine receptor 1

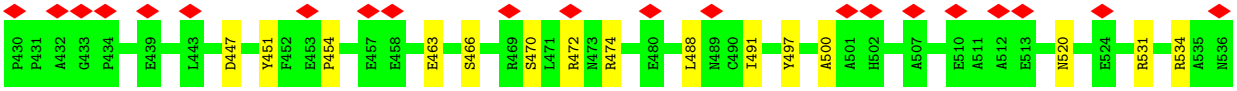
Chain B:

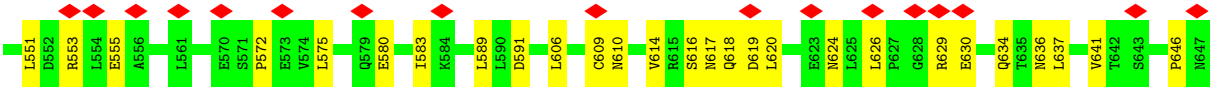


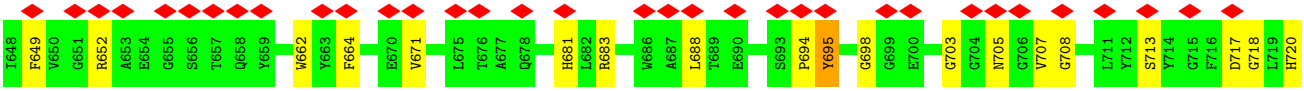


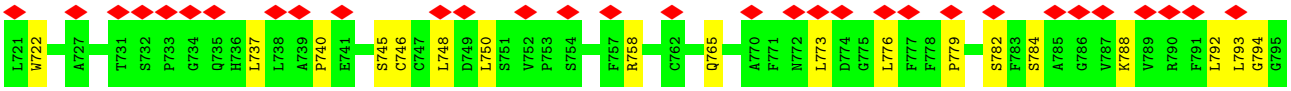


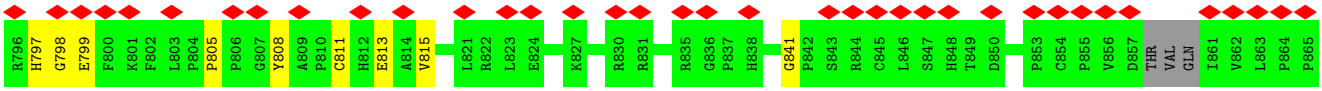


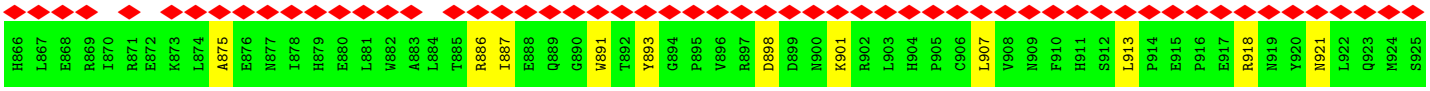


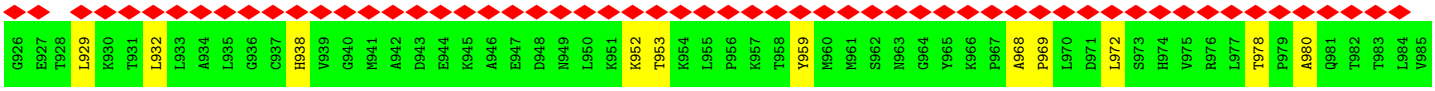


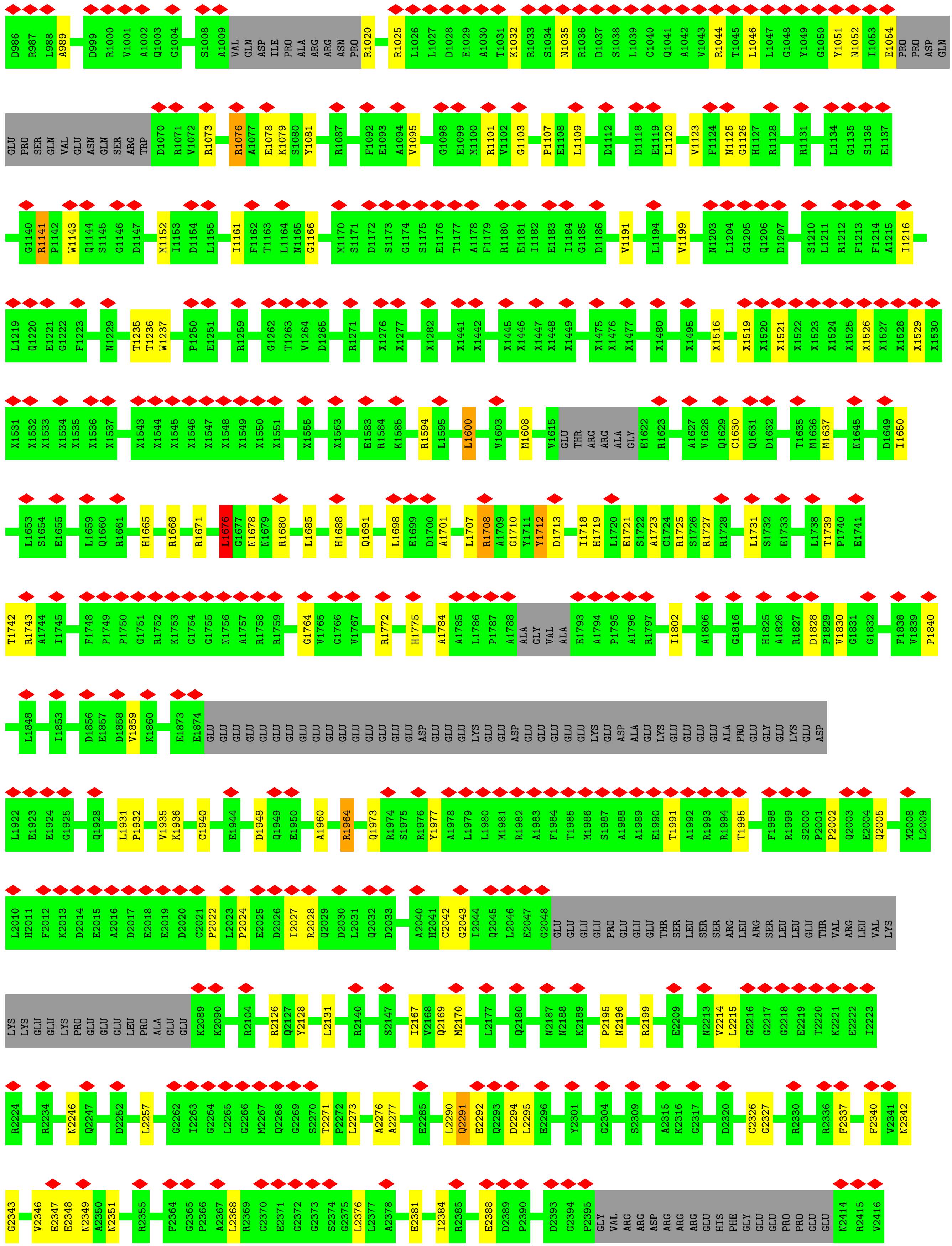








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GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 R1076 A1077 E1078 K1079 S1080 Y1081 R1087 F1092 E1093 A1094 V1095 G1098 E1099 M1100 R1101 V1102 G1103 P1107 E1108 L1109 D1112 D1118 E1119 L1120 V1123 F1124 N1125 G1126 H1127 R1128 R1131 L1134 G1135 S1136 E1137
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T1742 R1743 A1744 I1745 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 G1764 V1765 G1766 V1767 R1772 H1775 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 I1802 A1806 G1816 H1825 A1826 R1827 D1828 P1829 V1830 G1831 G1832 F1838 V1839 P1840
L1848 I1853 D1856 E1857 D1858 V1859 K1860 E1873 E1874 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
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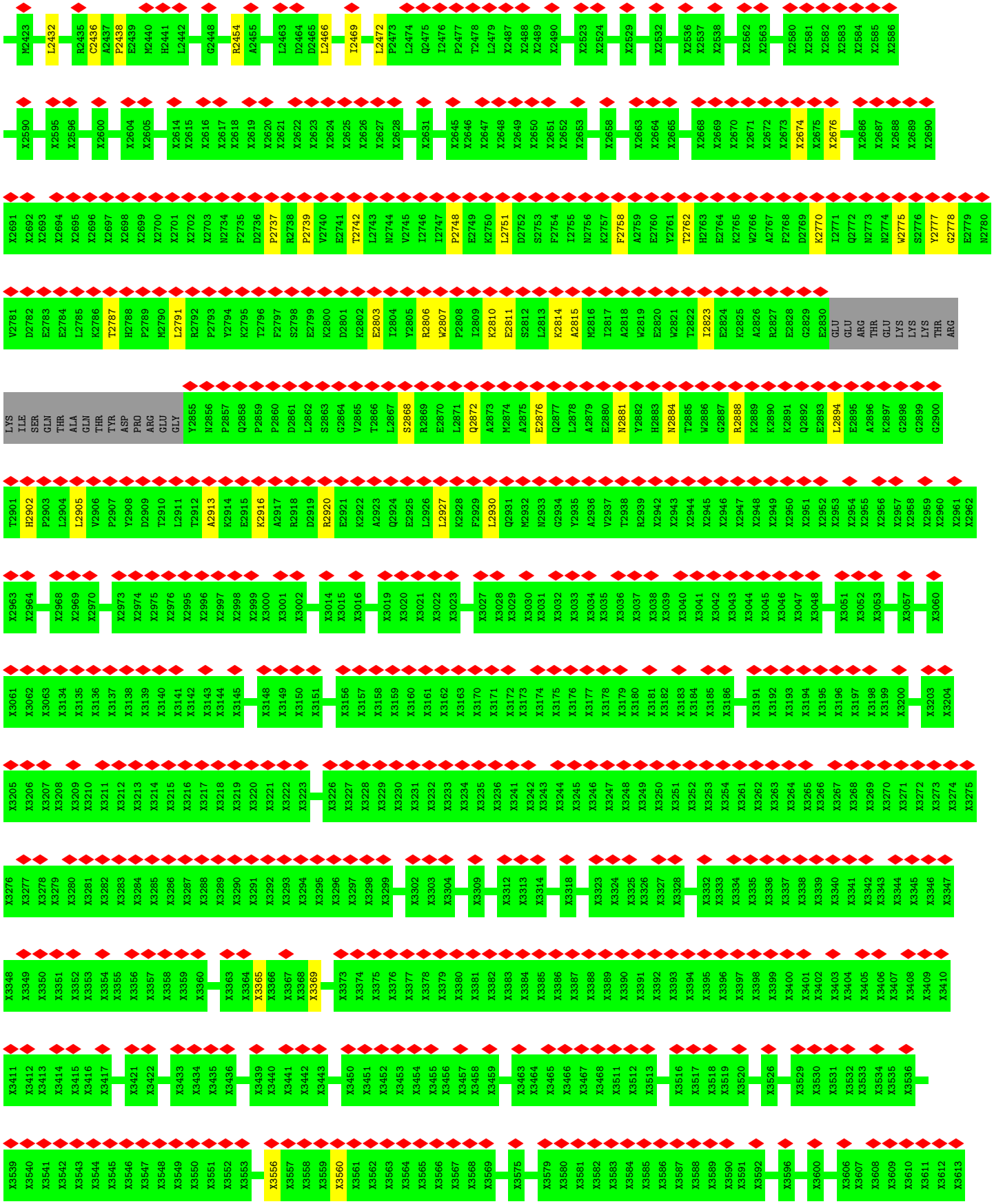
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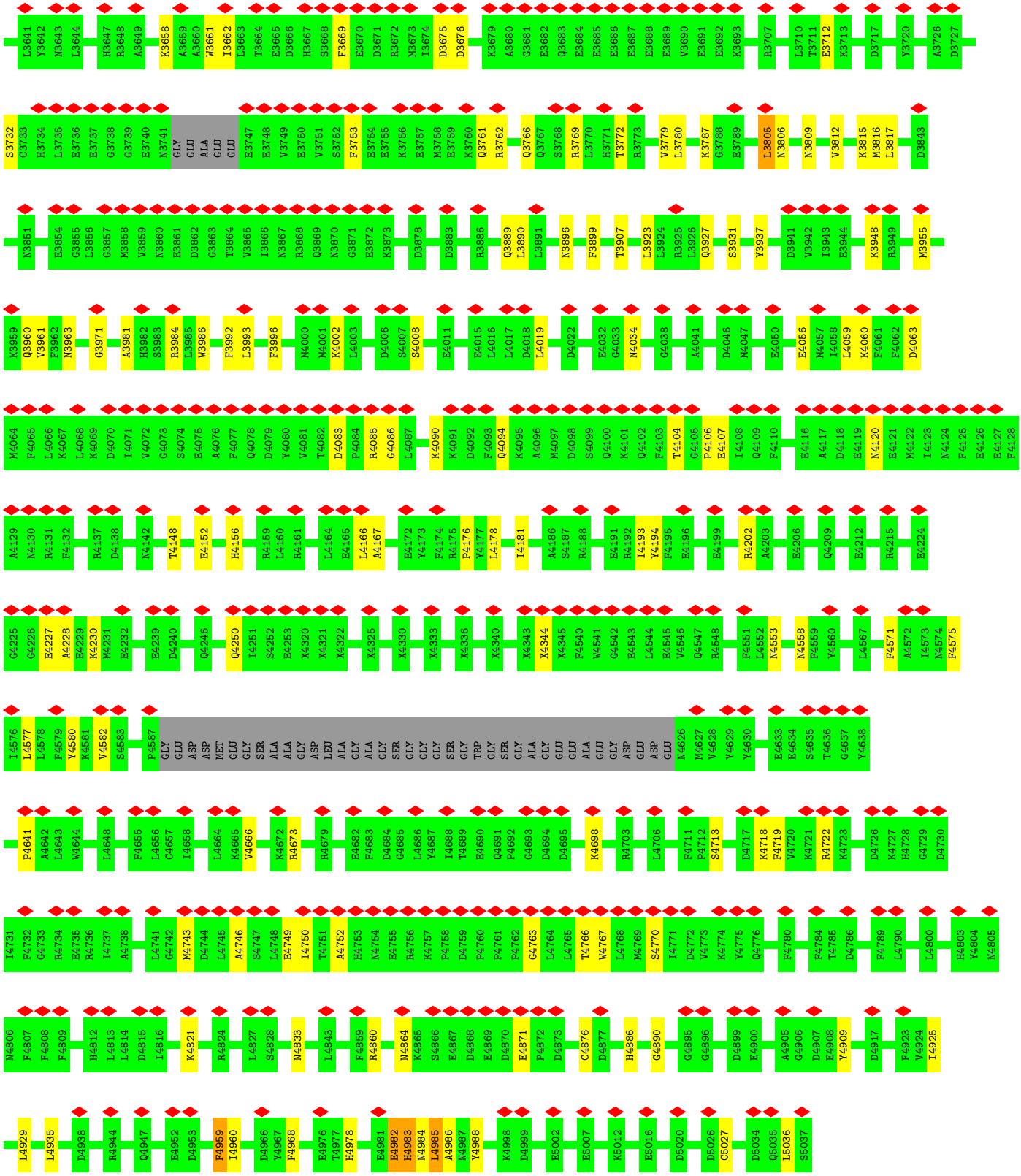

• Molecule 2: Ryanodine receptor 1

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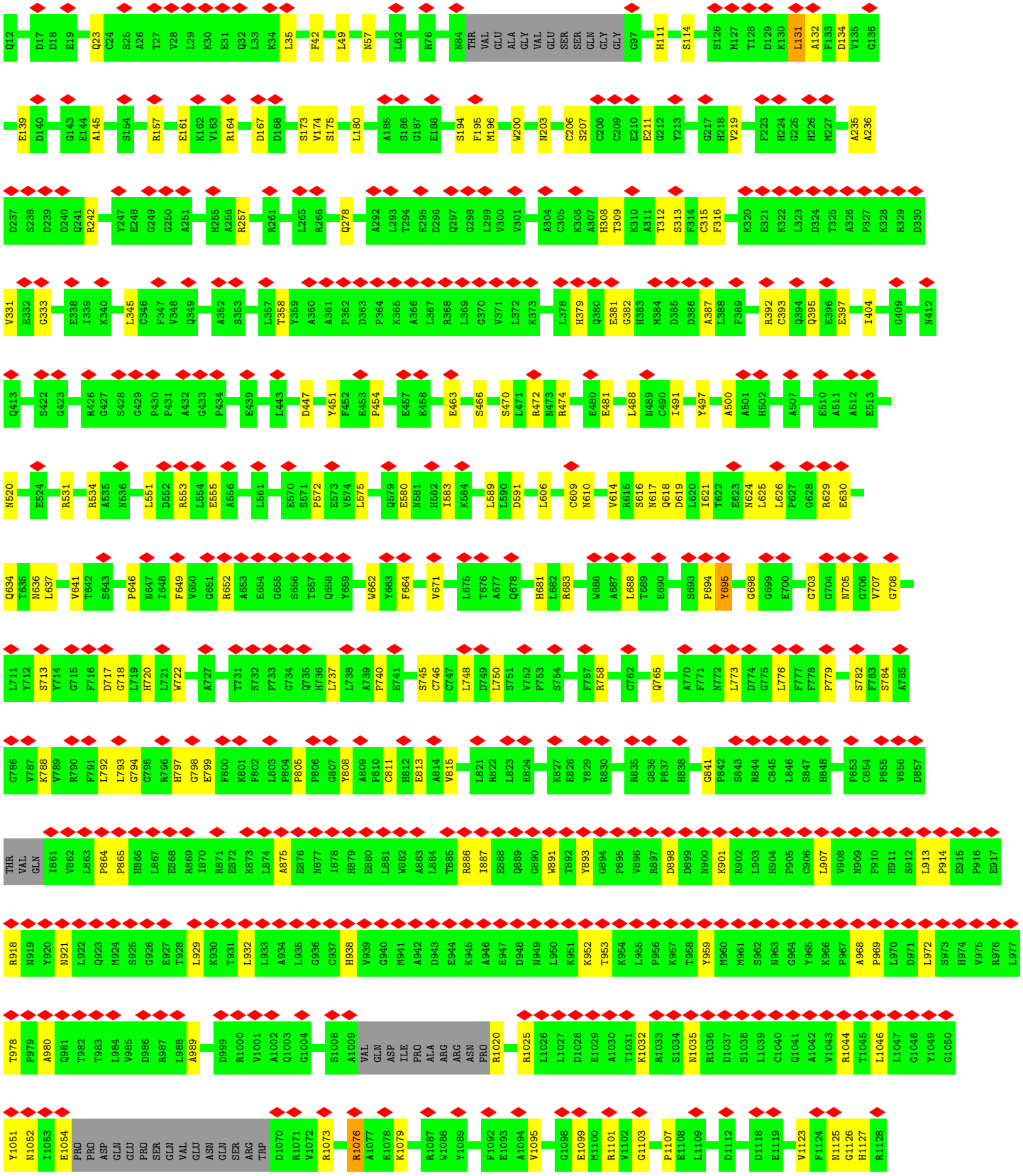
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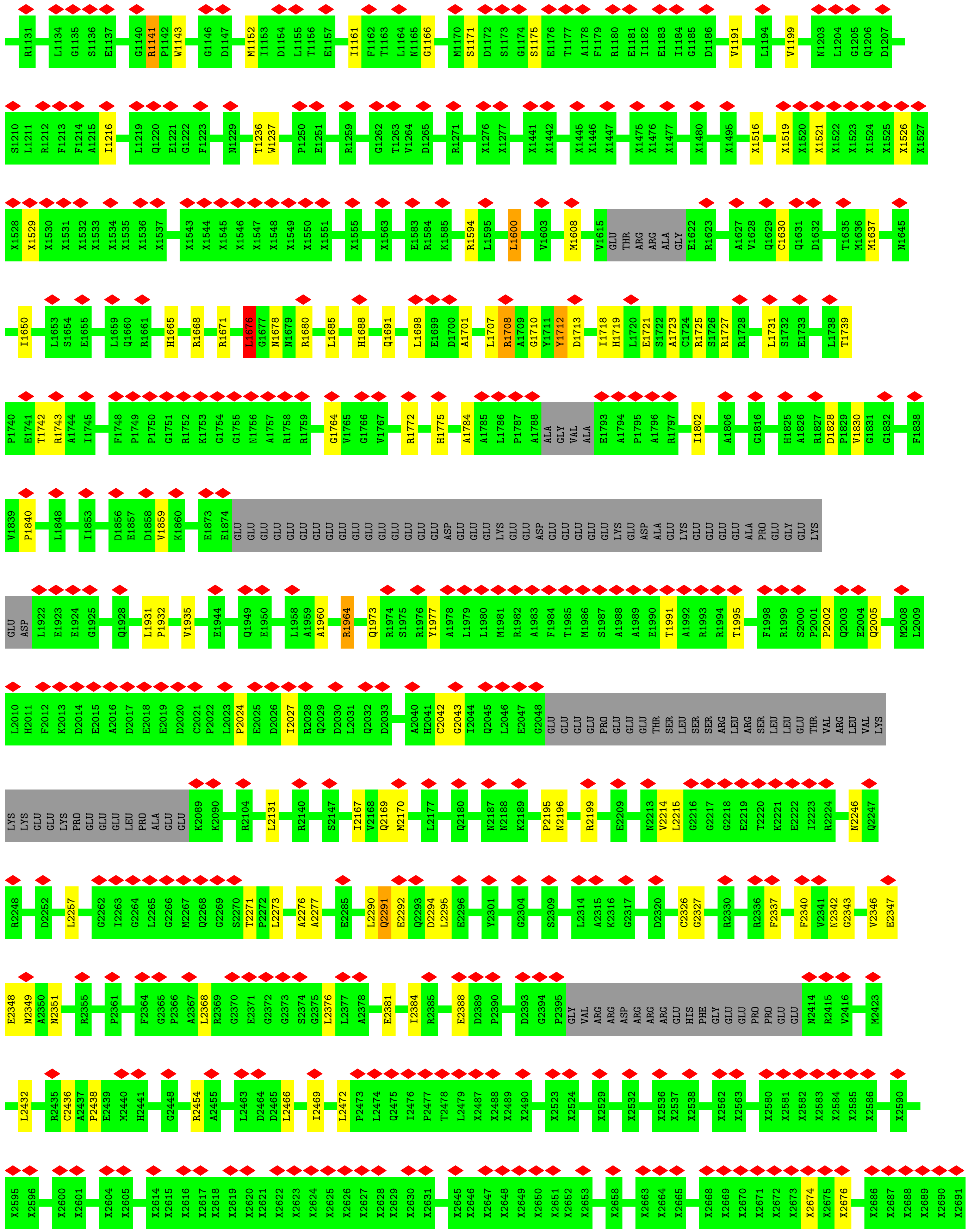
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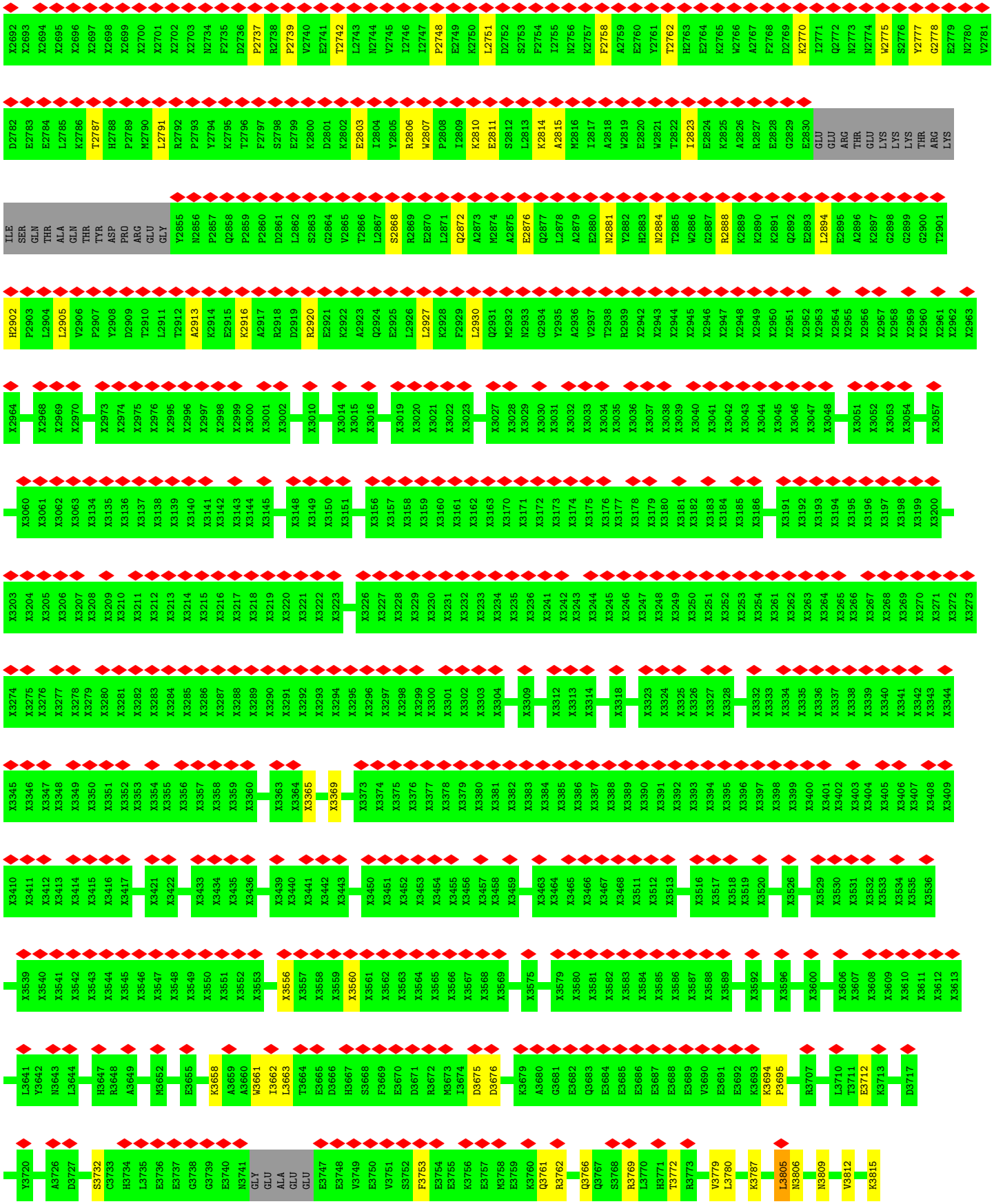
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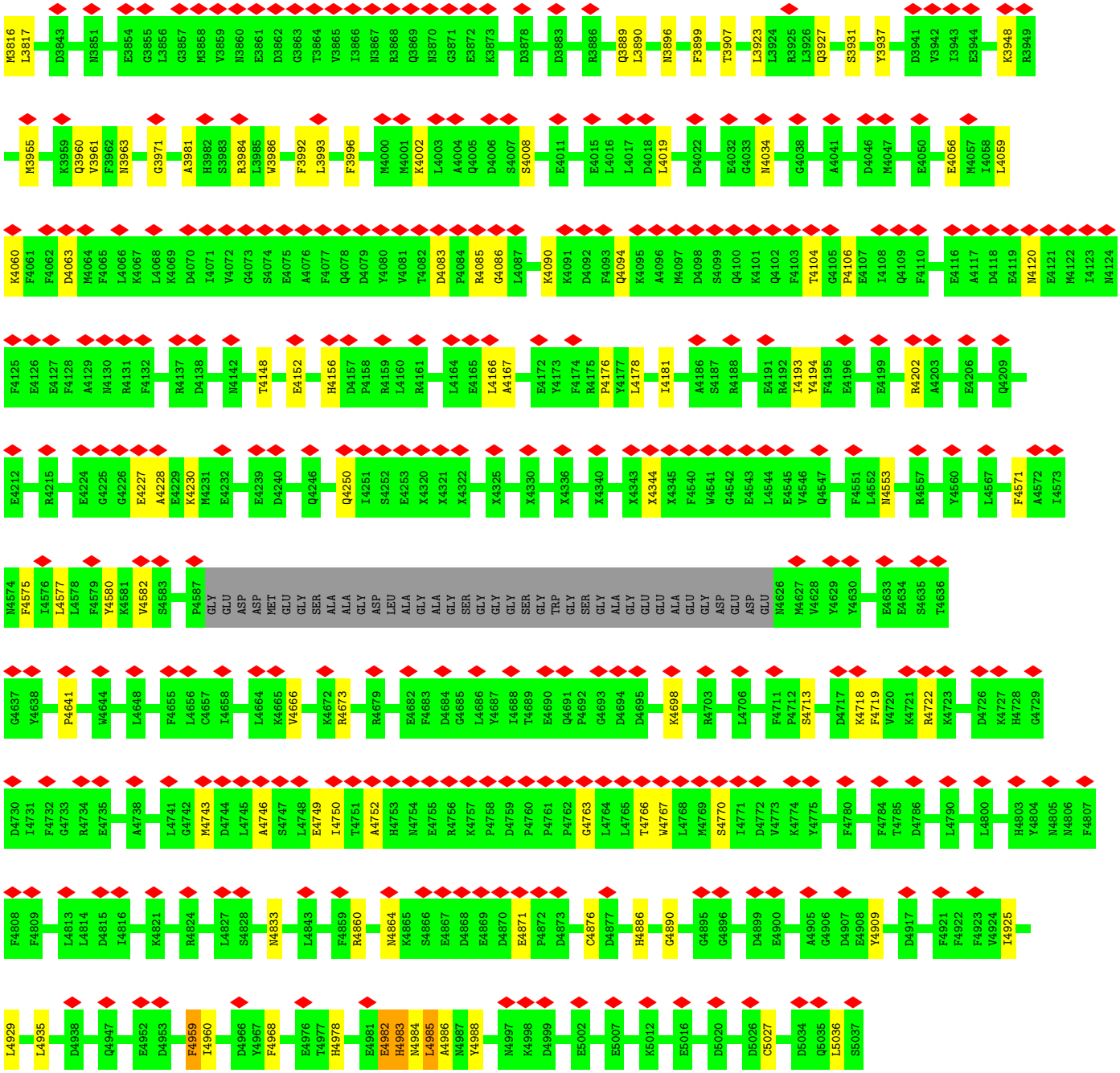
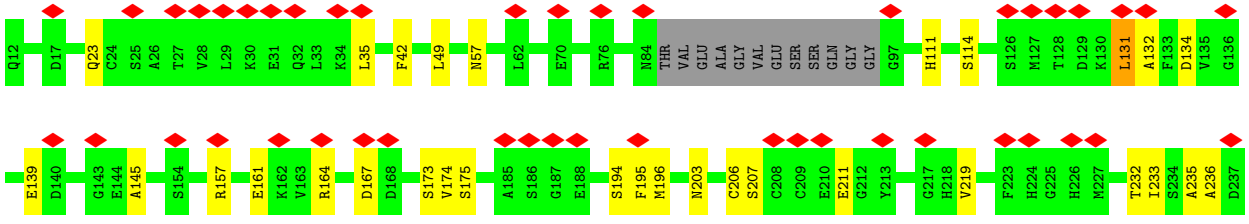
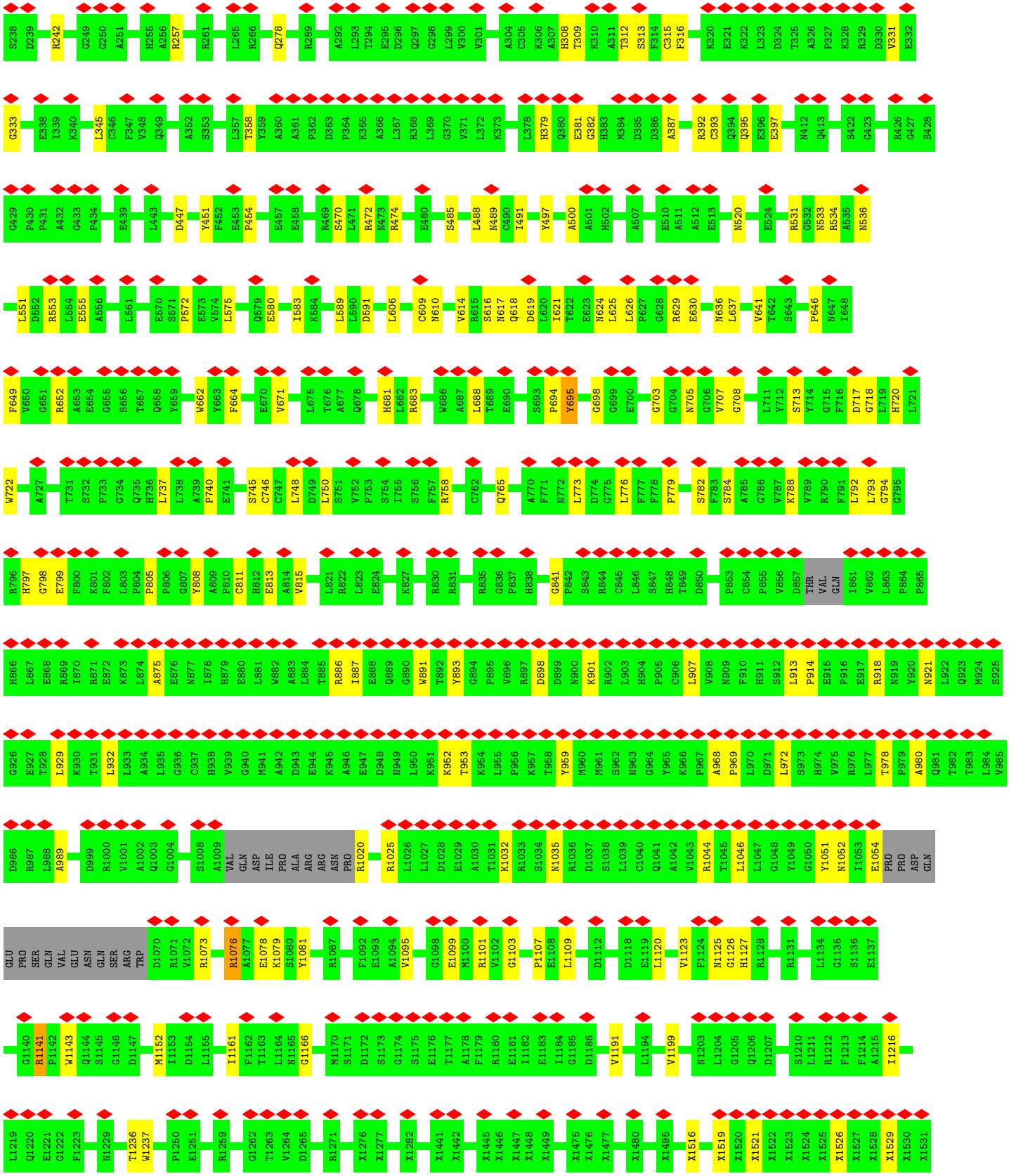


• Molecule 2: Ryanodine receptor 1

Chain I:

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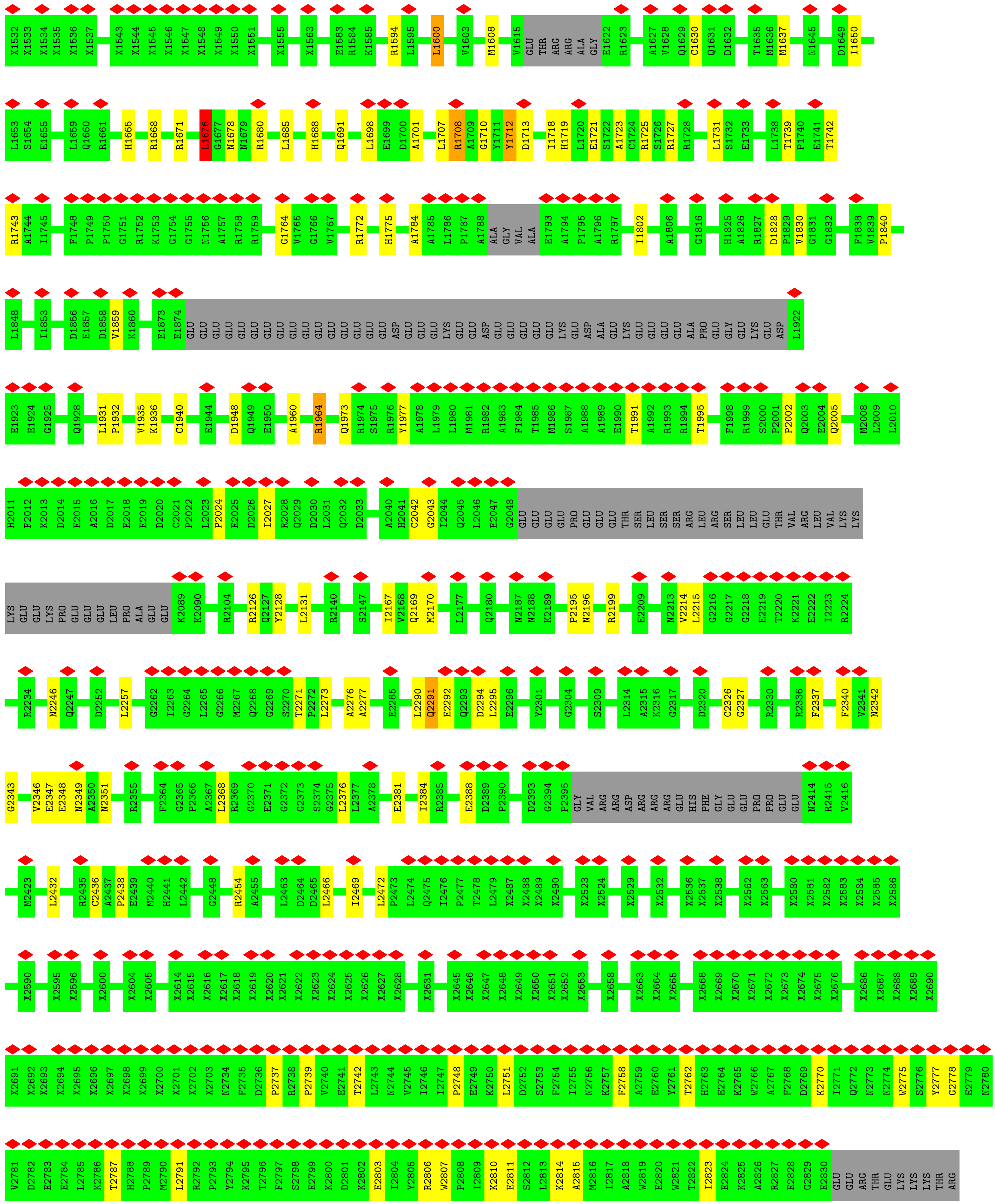
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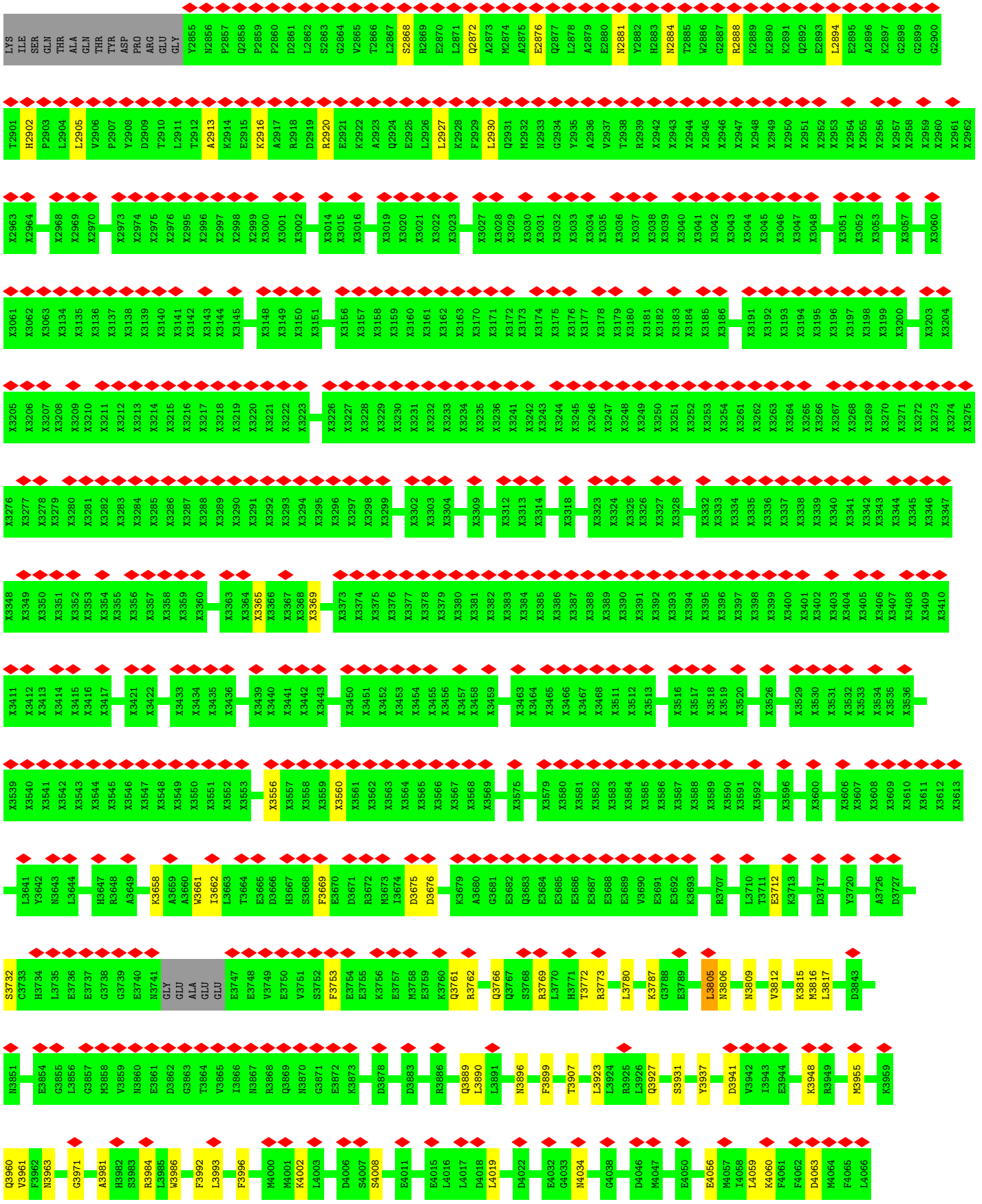
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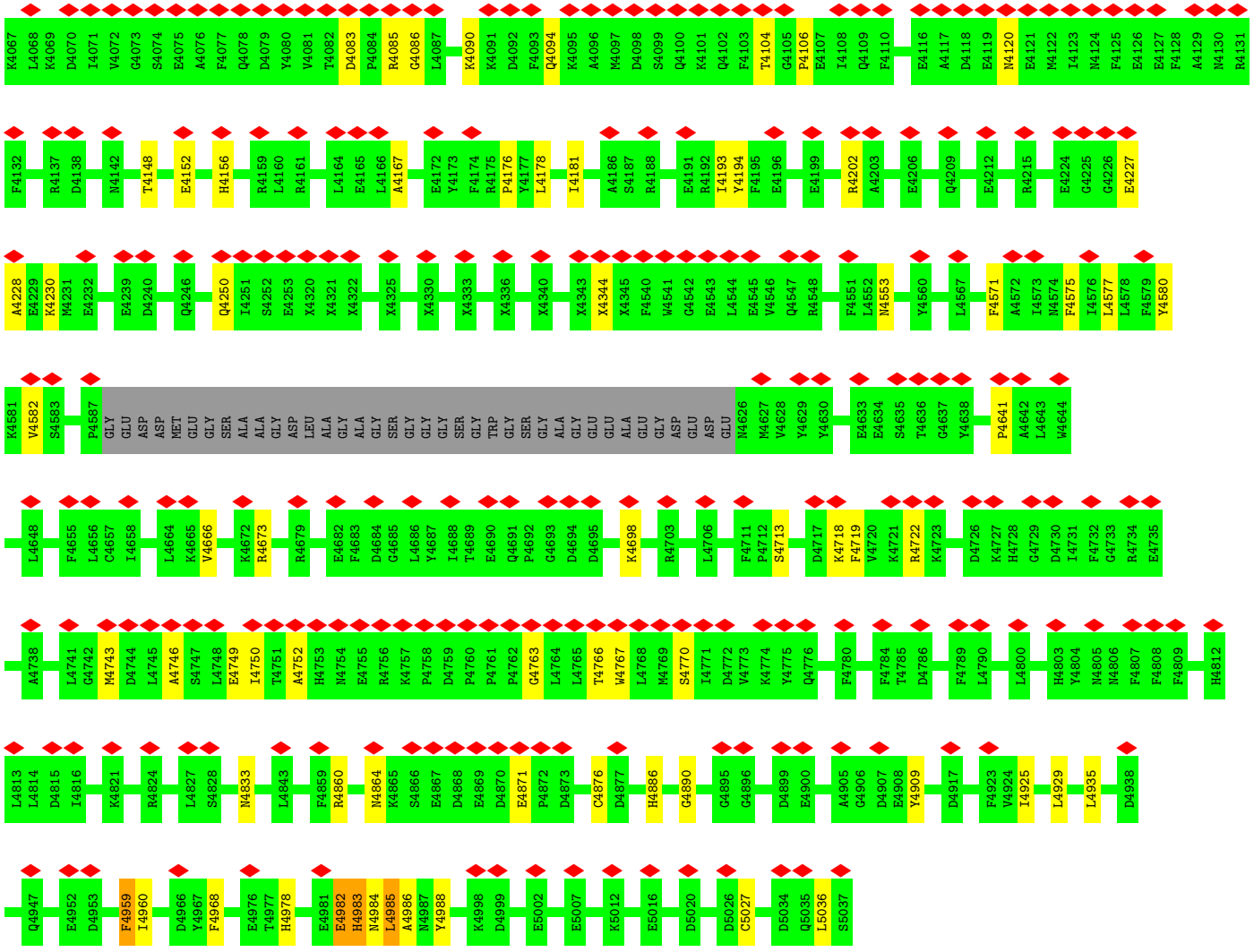
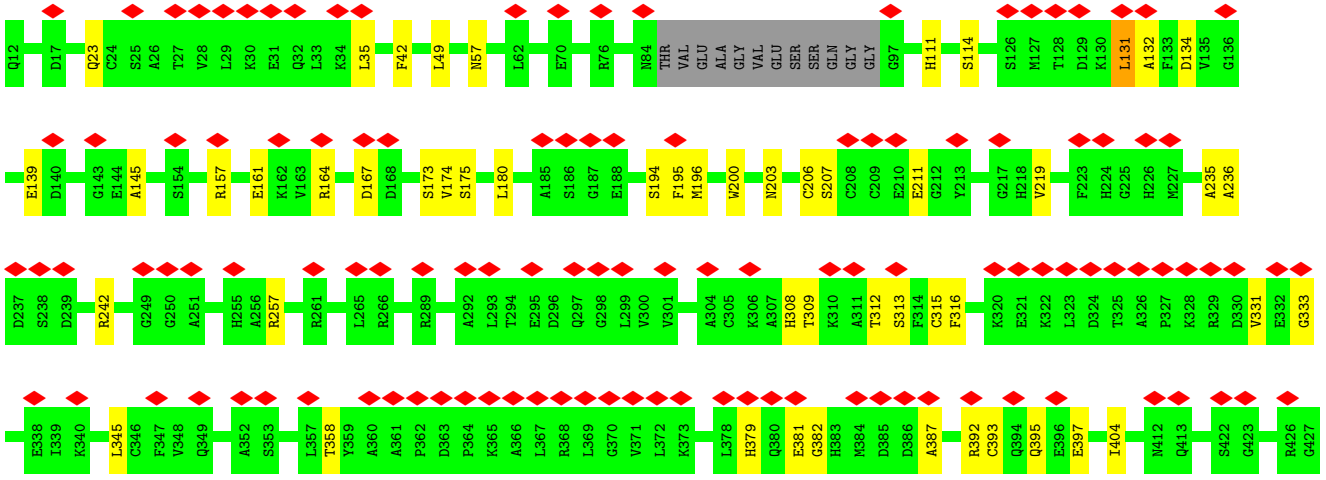
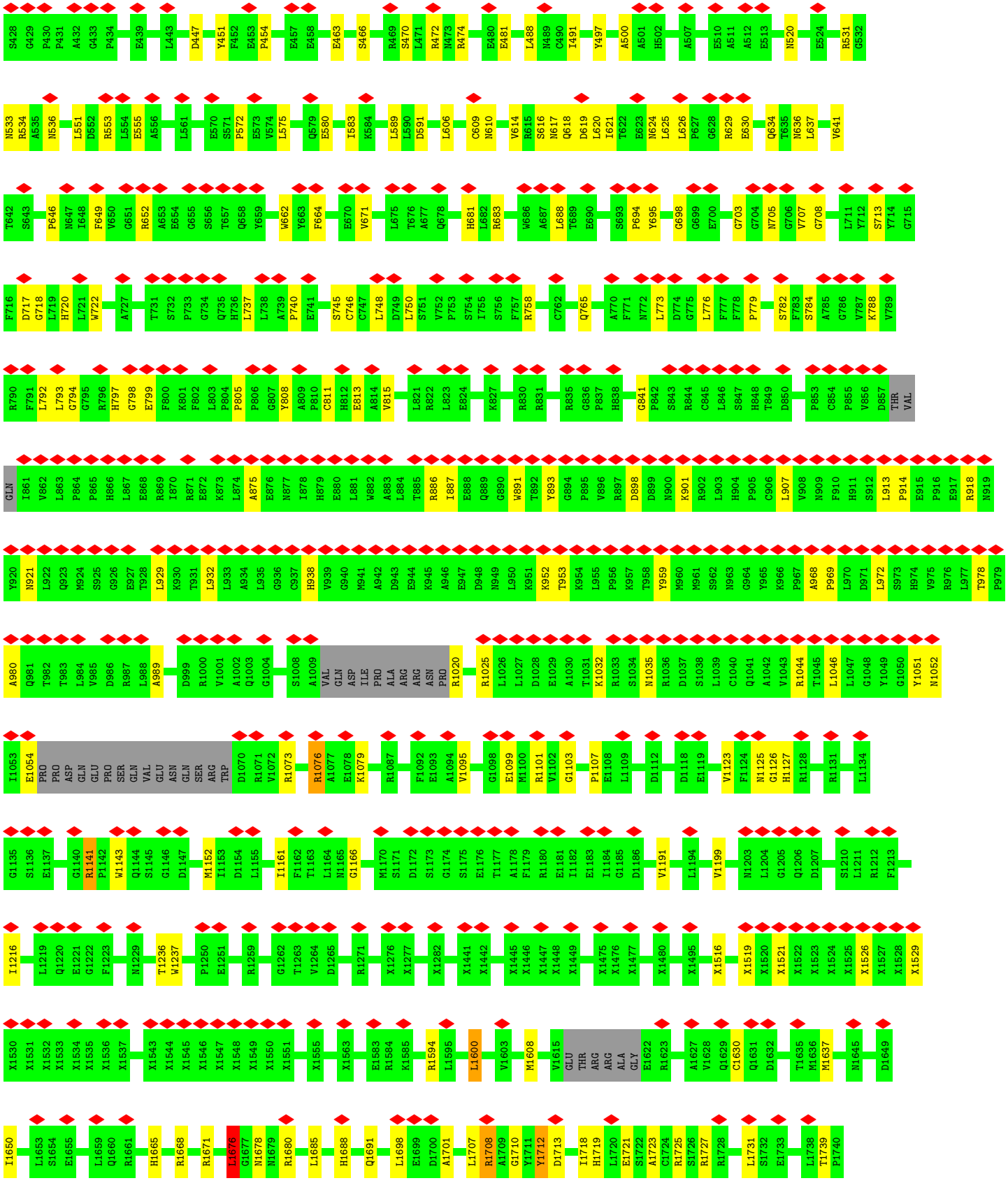


• Molecule 2: Ryanodine receptor 1

Chain G:

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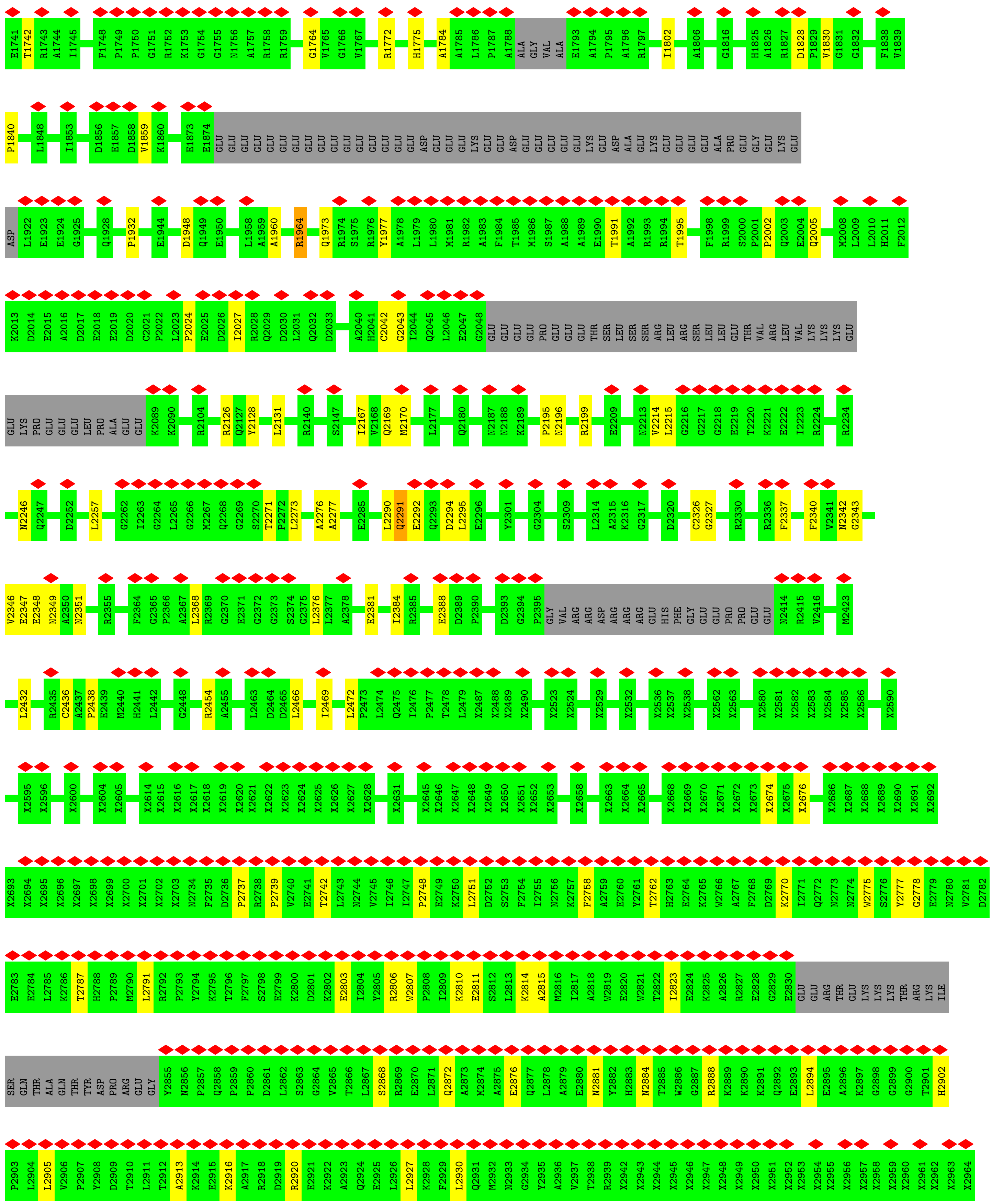
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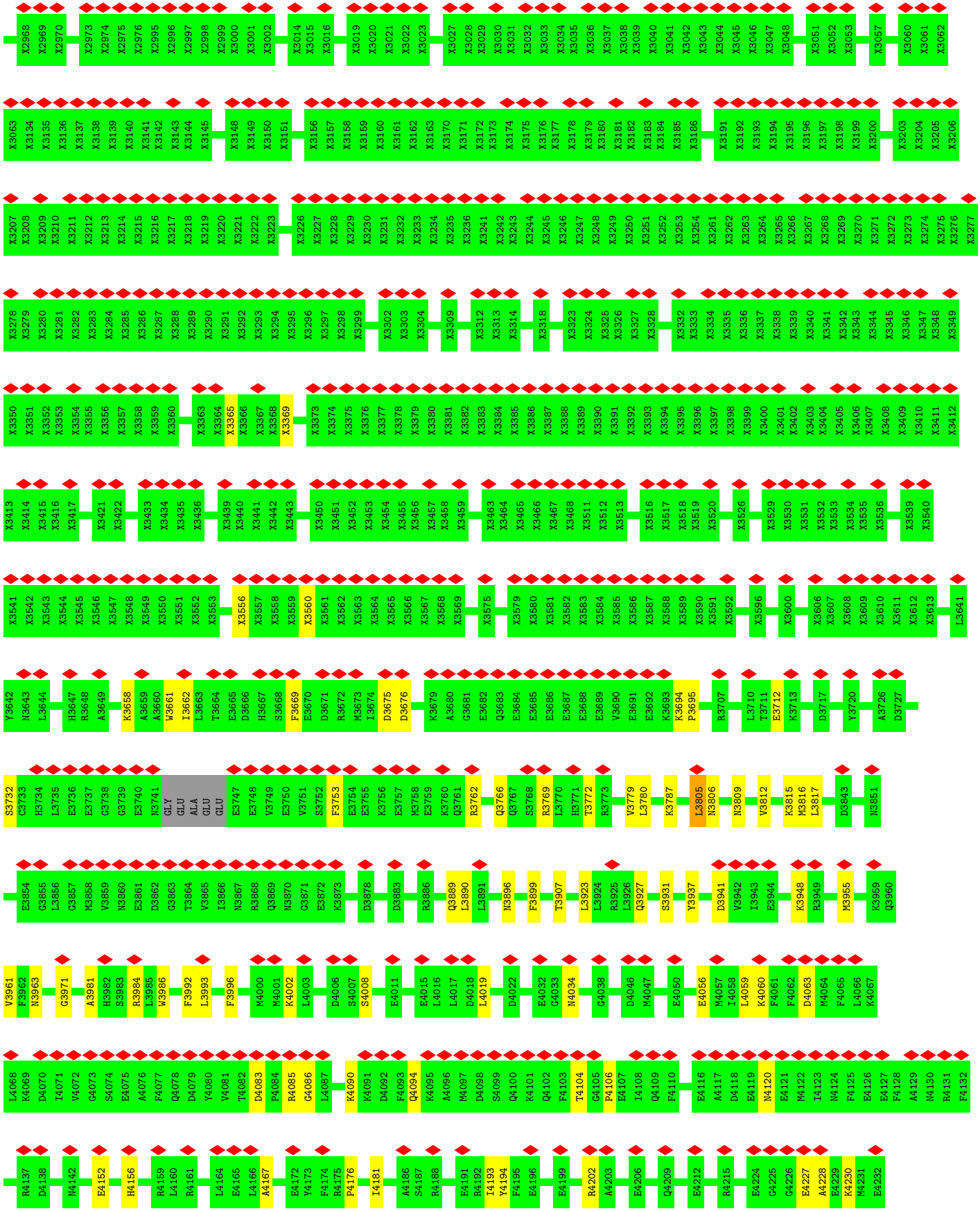
E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 Y2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE
SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902
P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2956 X2957 X2958 X2959 X2960 X2961 X2962 X2963 X2964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X3063 X3134 X3135 X3136 X3137 X3138 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3148 X3149 X3150 X3151 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3183 X3184 X3185 X3186 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3198 X3199 X3200 X3203 X3204 X3205 X3206
X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3226 X3227 X3228 X3229 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277
X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3302 X3303 X3304 X3309 X3312 X3313 X3314 X3318 X3323 X3324 X3325 X3326 X3327 X3328 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349
X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3373 X3374 X3375 X3376 X3377 X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412
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Y3642 N3643 L3644 H3647 R3648 A3649 K3658 A3659 A3660 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 E3670 D3671 R3672 M3673 I3674 D3675 D3676 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 R3707 L3710 T3711 E3712 K3713 D3717 Y3720 A3726 D3727
S3732 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 Q3766 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 V3779 L3780 K3787 L3805 N3806 N3809 V3812 K3815 M3816 L3817 D3843 N3851
E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 D3878 D3883 R3886 Q3889 L3890 L3891 N3896 F3899 T3907 L3923 L3924 R3925 L3926 Q3927 S3931 Y3937 D3941 V3942 I3943 E3944 K3948 R3949 M3955 K3959 Q3960
V3961 F3962 N3963 G3971 A3981 H3982 S3983 R3984 L3985 W3986 F3992 L3993 F3996 M4000 M4001 K4002 L4003 D4006 S4007 S4008 E4011 E4015 L4016 L4017 D4018 L4019 D4022 E4032 G4033 N4034 G4038 D4046 M4047 E4050 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 F4065 L4066 K4067
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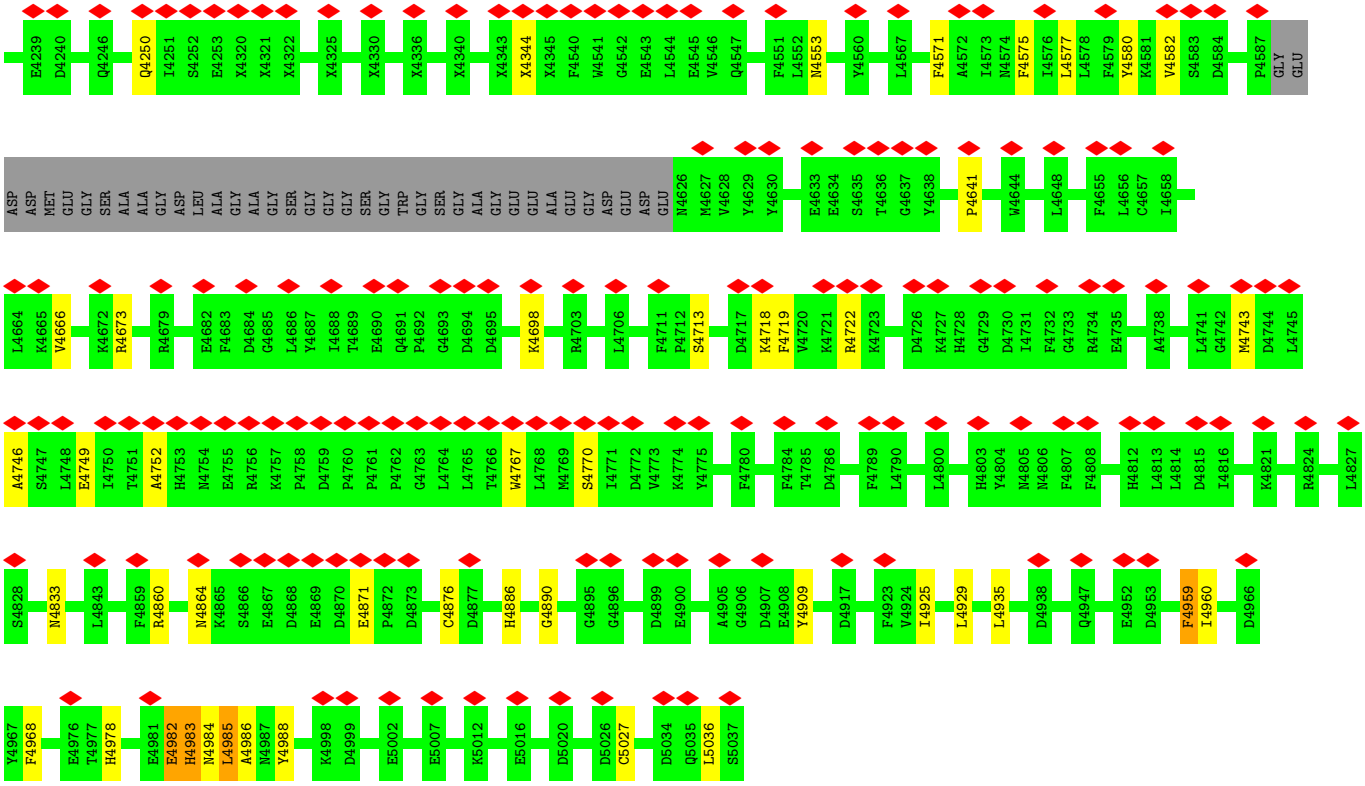
R4137 D4138 N4142 E4152 H4156 R4159 L4160 R4161 L4164 E4165 L4166 A4167 E4172 Y4173 F4174 R4175 P4176 I4181 A4186 S4187 R4188 E4191 R4192 I4193 Y4194 F4195 E4196 E4199 R4202 A4203 E4206 Q4209 E4212 R4215 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232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ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU GLU N4626 M4627 V4628 Y4629 Y4630 E4633 E4634 S4635 T4636 G4637 Y4638 P4641 W4644 L4648 F4655 L4656 C4657 I4658
L4664 K4665 V4666 K4672 R4673 R4679 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 K4698 R4703 L4706 F4711 P4712 S4713 D4717 K4718 F4719 V4720 K4721 R4722 K4723 D4726 K4727 H4728 G4729 D4730 I4731 F4732 G4733 R4734 E4735 A4738 L4741 G4742 M4743 D4744 L4745
A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 D4772 V4773 K4774 Y4775 F4780 F4784 T4785 D4786 F4789 L4790 L4800 H4803 Y4804 N4805 N4806 F4807 F4808 H4812 L4813 L4814 D4815 I4816 K4821 R4824 L4827
S4828 N4833 L4843 F4859 R4860 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 C4876 D4877 H4886 G4890 G4895 G4896 D4899 E4900 A4905 G4906 D4907 E4908 Y4909 D4917 F4923 V4924 I4925 L4929 L4935 D4938 Q4947 E4952 D4953 F4959 I4960 D4966
Y4967 F4968 E4976 T4977 H4978 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 K4998 D4999 E5002 E5007 K5012 E5016 D5020 D5026 C5027 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	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 ($e^-/Å^2$)	50	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	0.076	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.31	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.55	24/142628 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	TYR	C-N	5.28	1.44	1.34
2	I	695	TYR	C-N	5.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	5.28	1.44	1.34
2	E	695	TYR	C-N	5.26	1.44	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	E	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	G	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	I	1600	LEU	CA-CB-CG	6.73	130.78	115.30

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	12	0
1	H	818	0	824	9	0
1	J	818	0	824	11	0
2	B	29499	0	24757	259	0
2	E	29499	0	24757	259	0
2	G	29499	0	24757	251	0
2	I	29499	0	24757	256	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1	0	0	0	0
All	All	121272	0	102324	1040	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 5.

The worst 5 of 1040 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)
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.51	0.76
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.51	0.76
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.51	0.75
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.51	0.74
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.57	0.70

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	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	44	78
2	E	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	44	78
2	G	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	44	78
2	I	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	44	78
All	All	13360/18096 (74%)	11956 (90%)	1376 (10%)	28 (0%)	45	78

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	81	87
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	80	87

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1676	LEU
2	G	3762	ARG
2	G	4120	ASN
2	E	1964	ARG
2	E	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	379	HIS
2	I	3896	ASN
2	G	4034	ASN
2	I	520	ASN
2	I	1775	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.04
1	E	4345:UNK	C	4540:PHE	N	74.04
1	I	4345:UNK	C	4540:PHE	N	74.04
1	G	4345:UNK	C	4540:PHE	N	74.04
1	B	3613:UNK	C	3639:THR	N	46.14

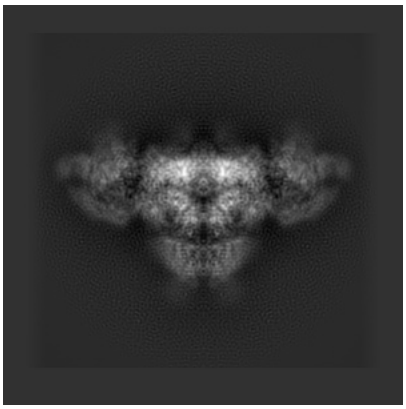
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8395. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map



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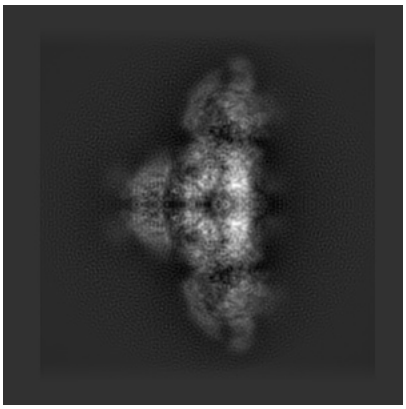

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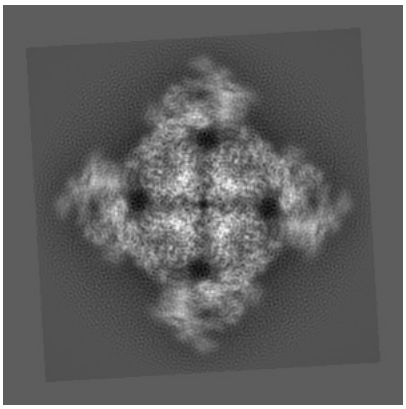

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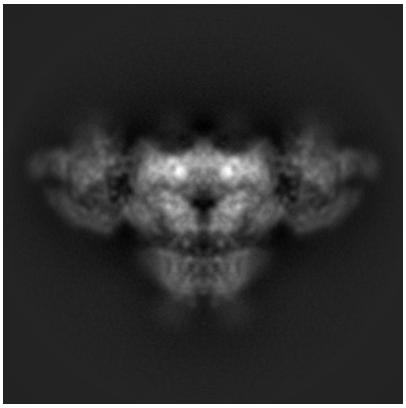
6.1.2 Raw map



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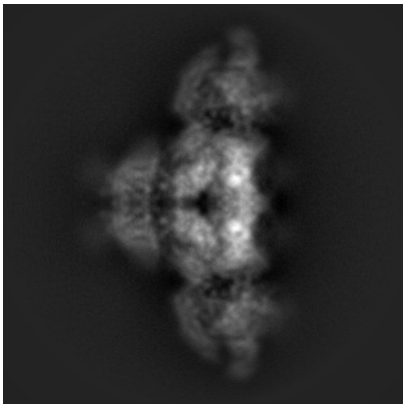
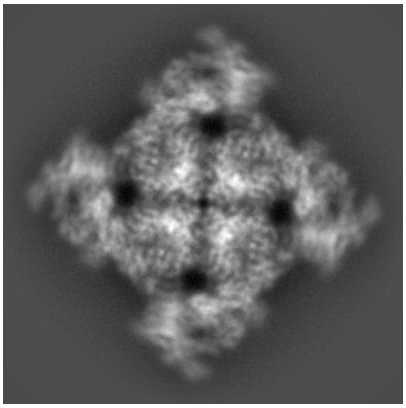


Y



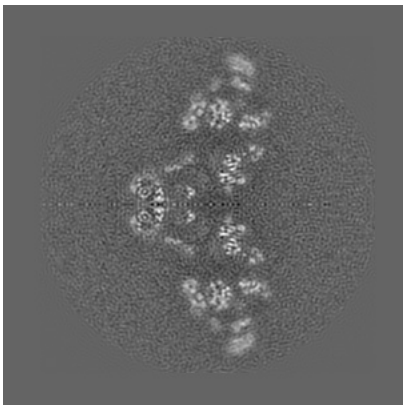
Z

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

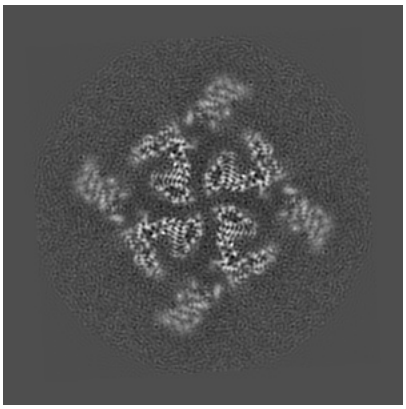
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

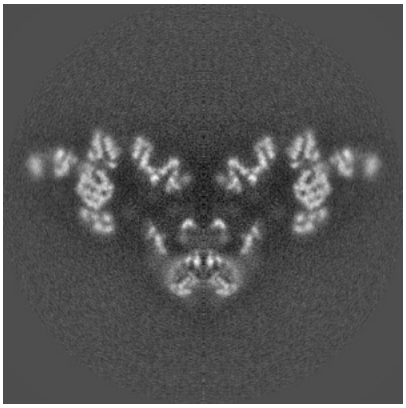


Y Index: 200

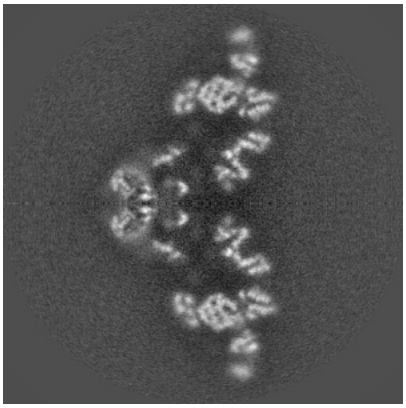


Z Index: 200

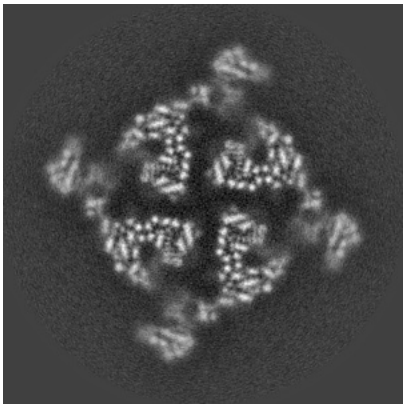
6.2.2 Raw map



X Index: 168



Y Index: 168

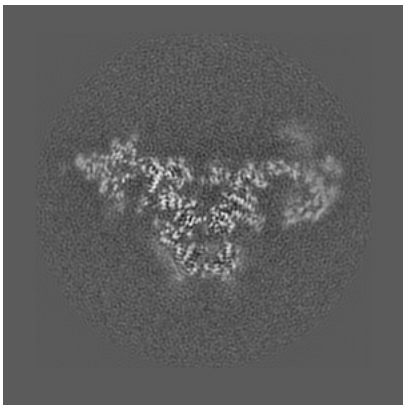


Z Index: 168

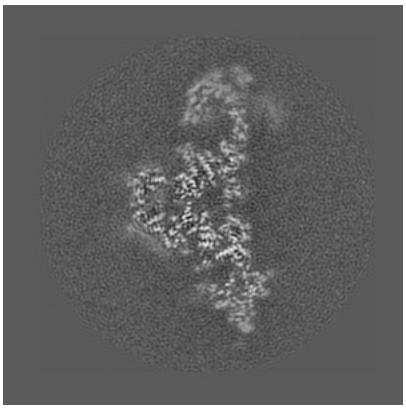
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

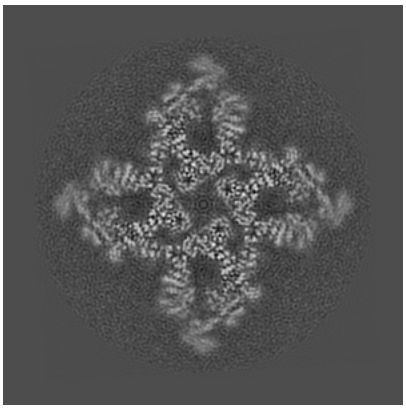
6.3.1 Primary map



X Index: 217

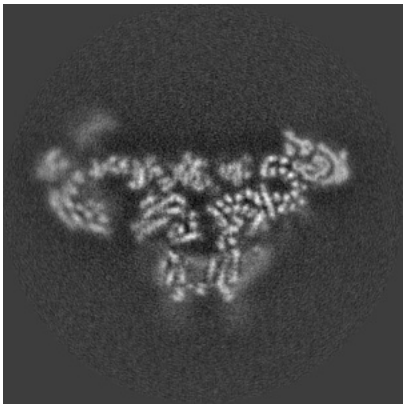


Y Index: 183

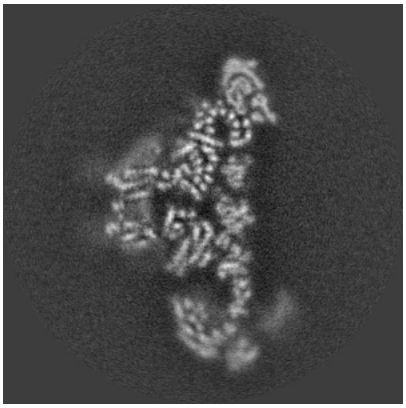


Z Index: 232

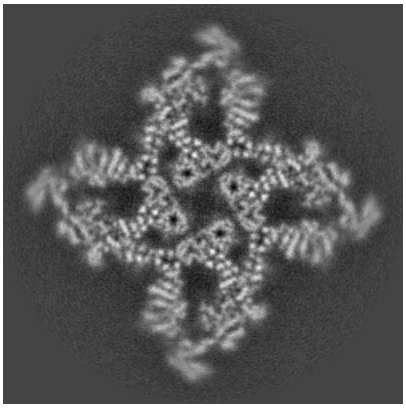
6.3.2 Raw map



X Index: 147



Y Index: 189

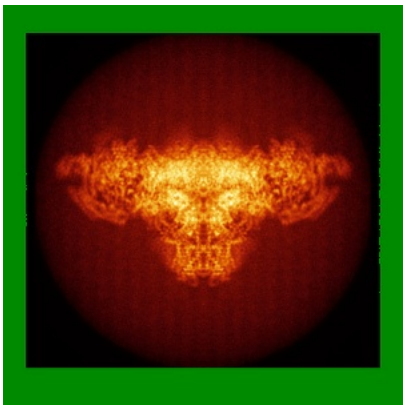


Z Index: 195

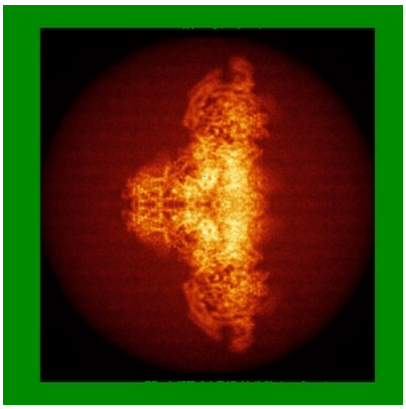
The images above show the largest variance slices of the map in three orthogonal directions.

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

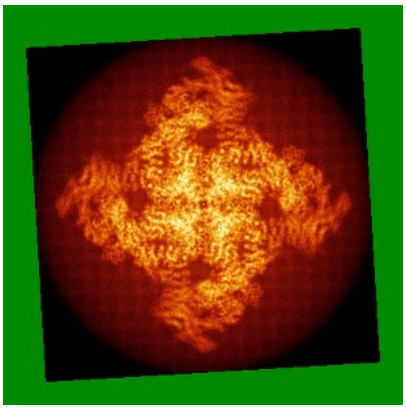
6.4.1 Primary map



X

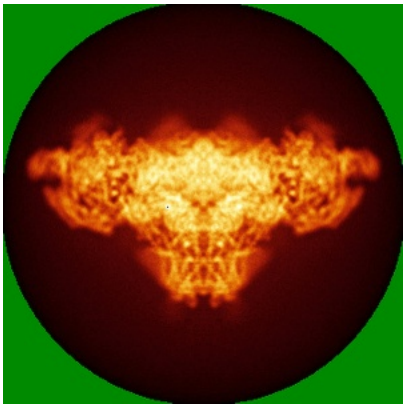


Y

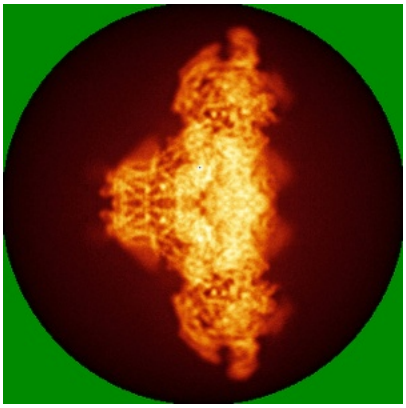


Z

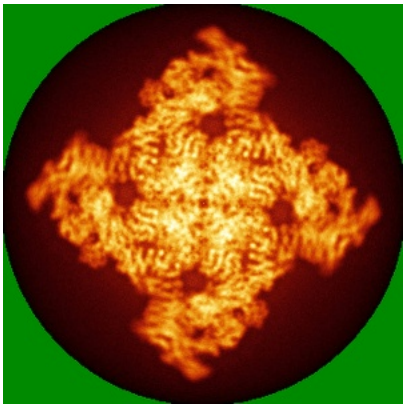
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

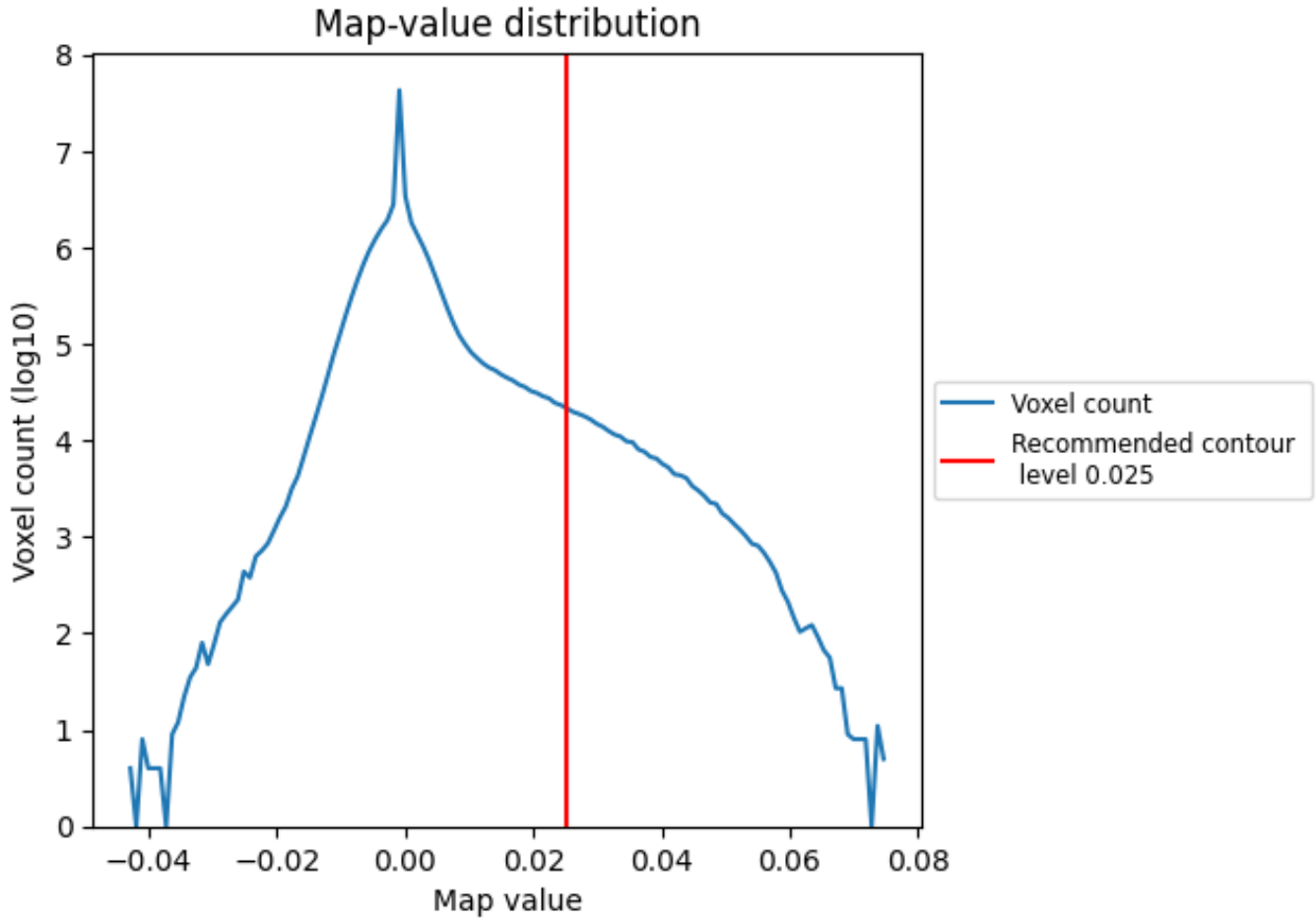
6.6 Mask visualisation (i)

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

7 Map analysis

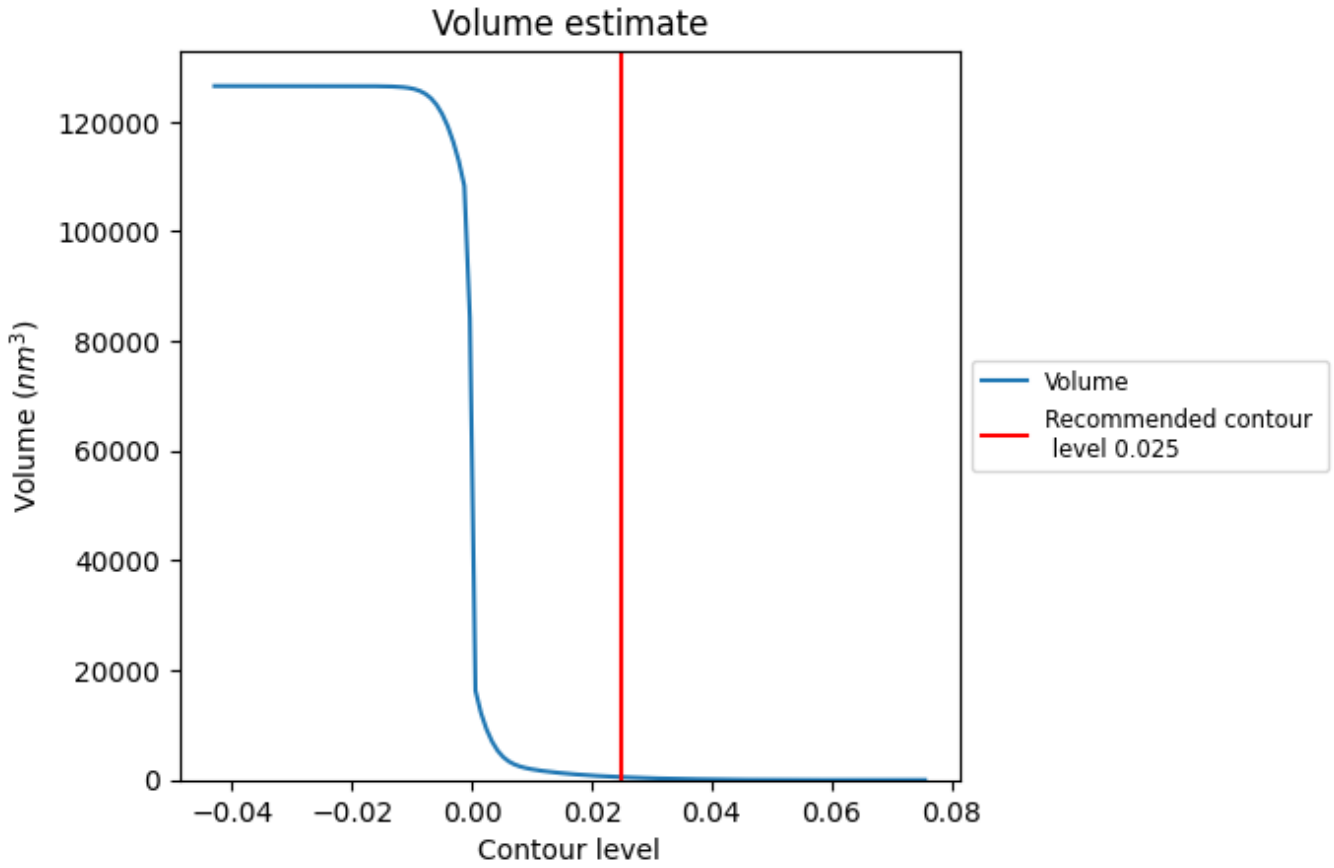
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

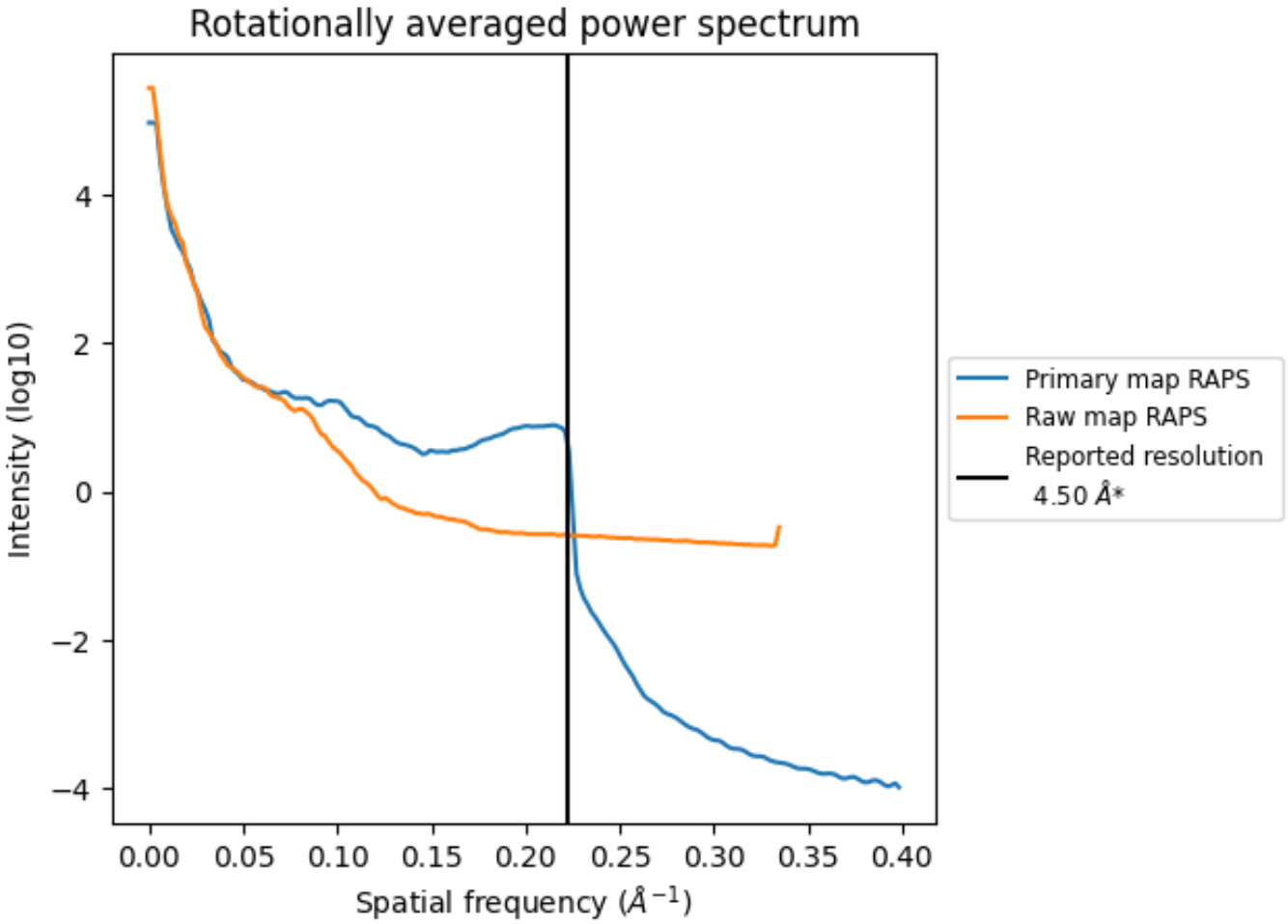
7.2 Volume estimate (i)



The volume at the recommended contour level is 516 nm^3; this corresponds to an approximate mass of 466 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)

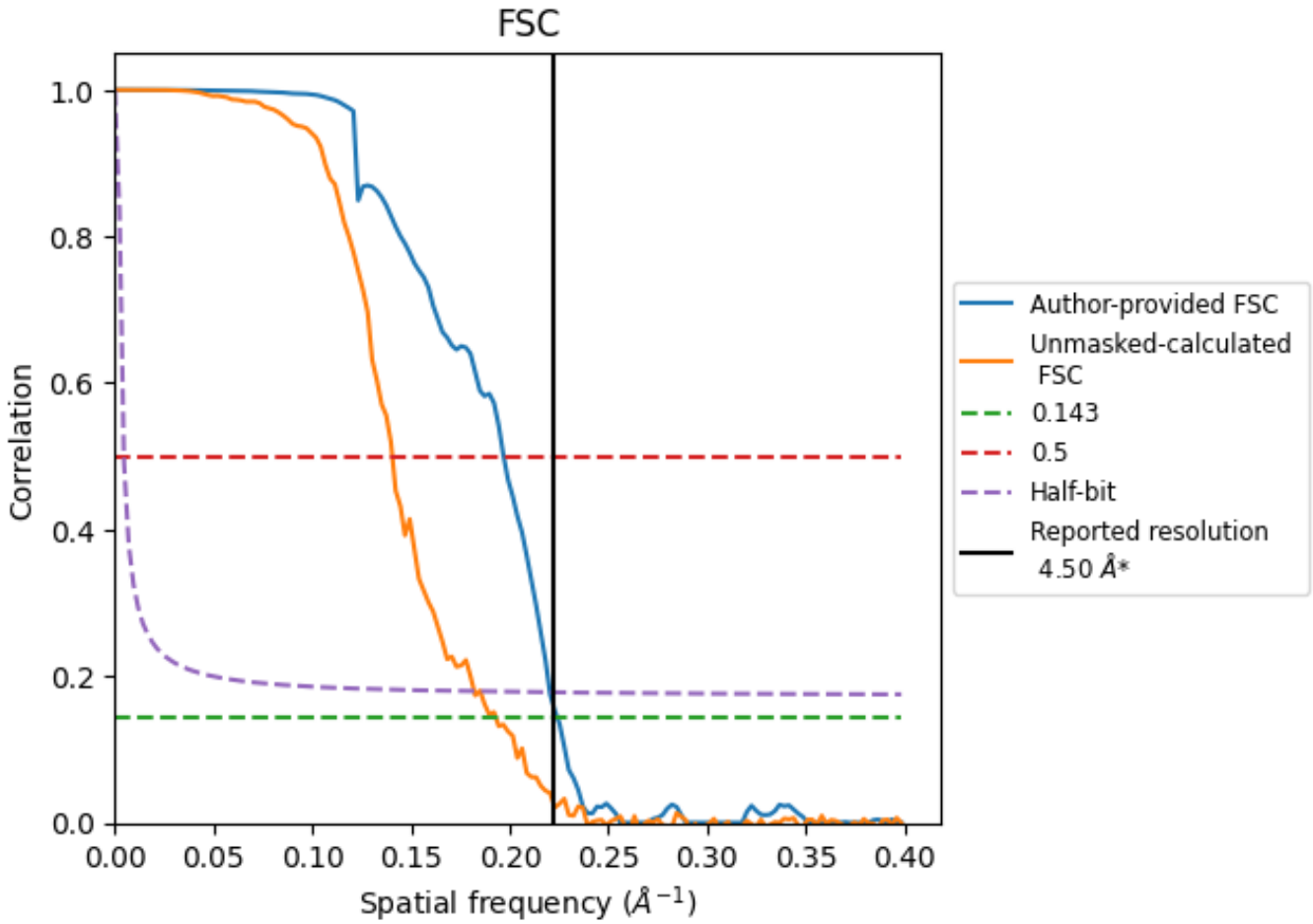


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

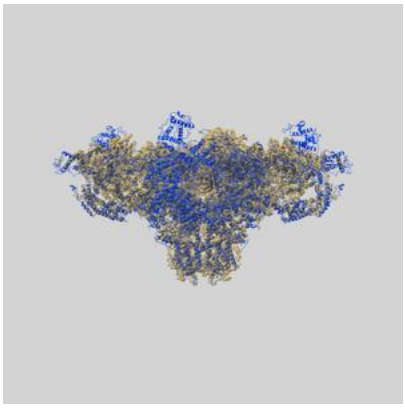
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	5.08	4.54
Unmasked-calculated*	5.18	7.11	5.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.18 differs from the reported value 4.5 by more than 10 %

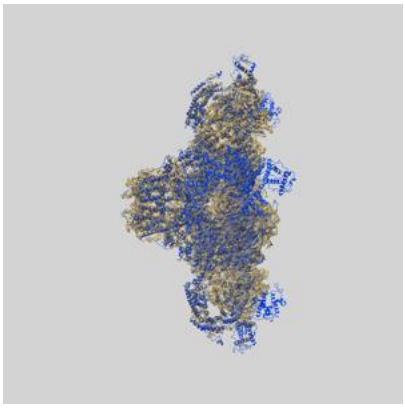
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8395 and PDB model 5TB4. Per-residue inclusion information can be found in section 3 on page 4.

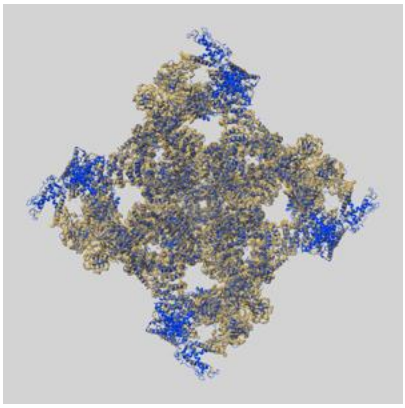
9.1 Map-model overlay



X



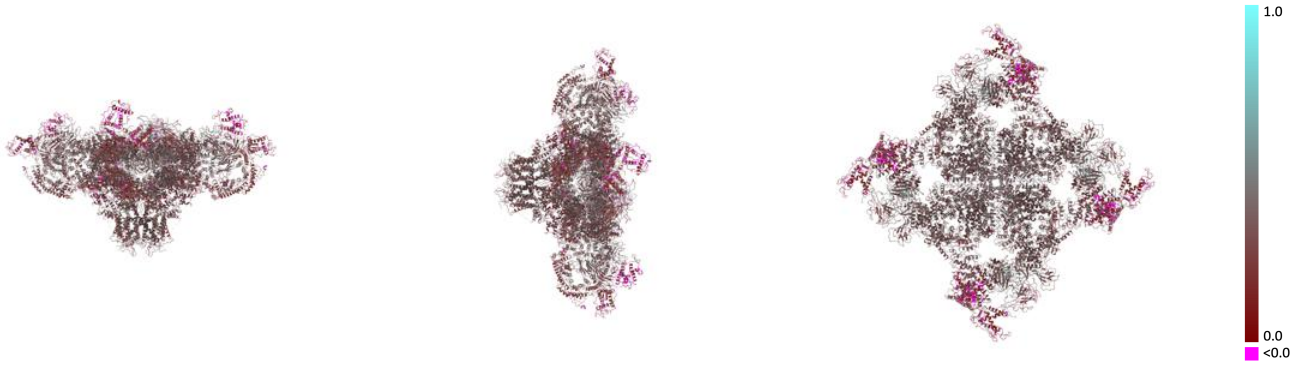
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

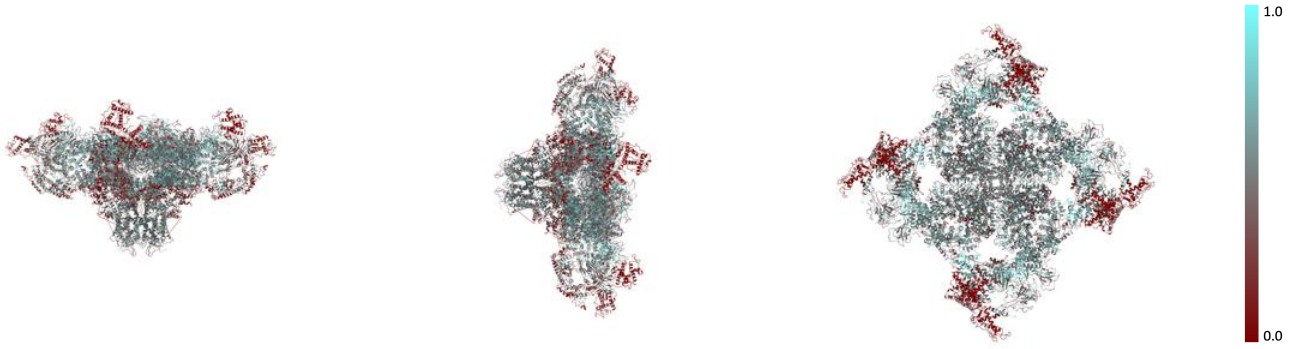
9.2 Q-score mapped to coordinate model



X Y Z

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

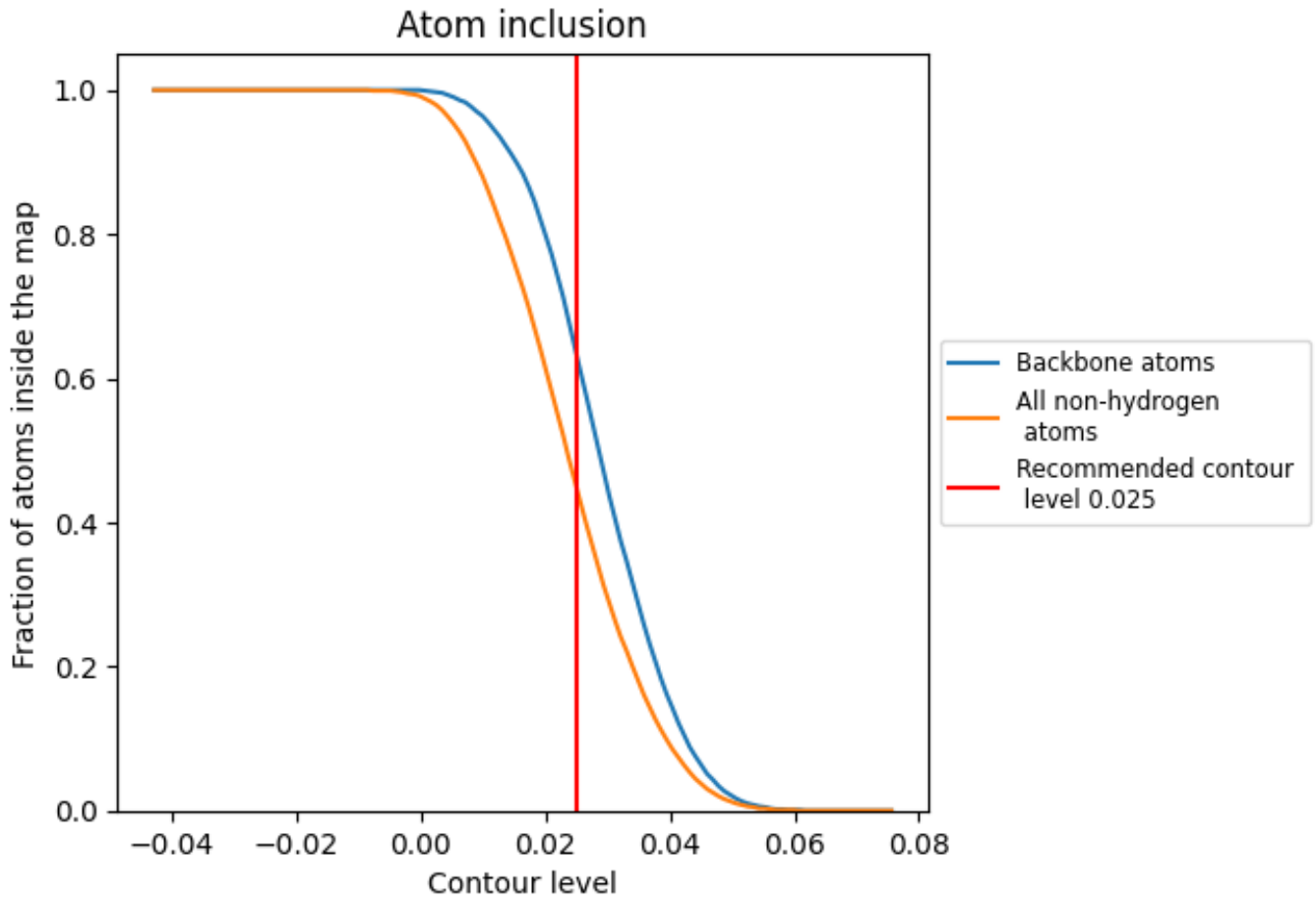
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 45% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4480	0.3170
A	0.4810	0.3380
B	0.4470	0.3160
E	0.4470	0.3160
F	0.4740	0.3420
G	0.4470	0.3160
H	0.4790	0.3410
I	0.4470	0.3160
J	0.4800	0.3400