wwPDB EM Validation Summary Report

Feb 13, 2024 – 08:52 PM EST

PDB ID	:	3J8H
EMDB ID	:	EMD-2807
Title	:	Structure of the rabbit ryanodine receptor RyR1 in complex with FKBP12 at 3.8 Angstrom resolution
Authors	:	Yan, Z.; Bai, X.; Yan, C.; Wu, J.; Scheres, S.H.W.; Shi, Y.; Yan, N.
Deposited on	:	2014-10-26
Resolution	:	3.80 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:

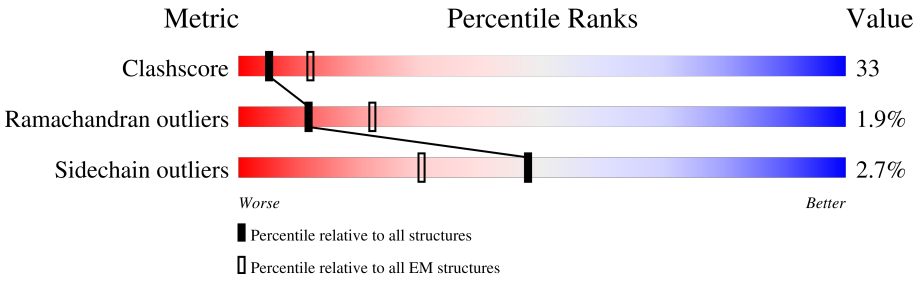
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 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	4599	48% 30% 20%
1	C	4599	48% 30% 20%
1	E	4599	48% 29% 20%
1	G	4599	48% 30% 20%
2	B	107	60% 39%
2	D	107	62% 37%
2	F	107	60% 39%
2	H	107	59% 40%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	6000	-	-	X	-
3	ZN	C	6000	-	-	X	-
3	ZN	E	6000	-	-	X	-
3	ZN	G	6000	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 111160 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 26957	C 17143	N 4683	O 4974	S 157	1	0
1	C	3660	Total 26957	C 17143	N 4683	O 4974	S 157	1	0
1	E	3660	Total 26957	C 17143	N 4683	O 4974	S 157	1	0
1	G	3660	Total 26957	C 17143	N 4683	O 4974	S 157	1	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).

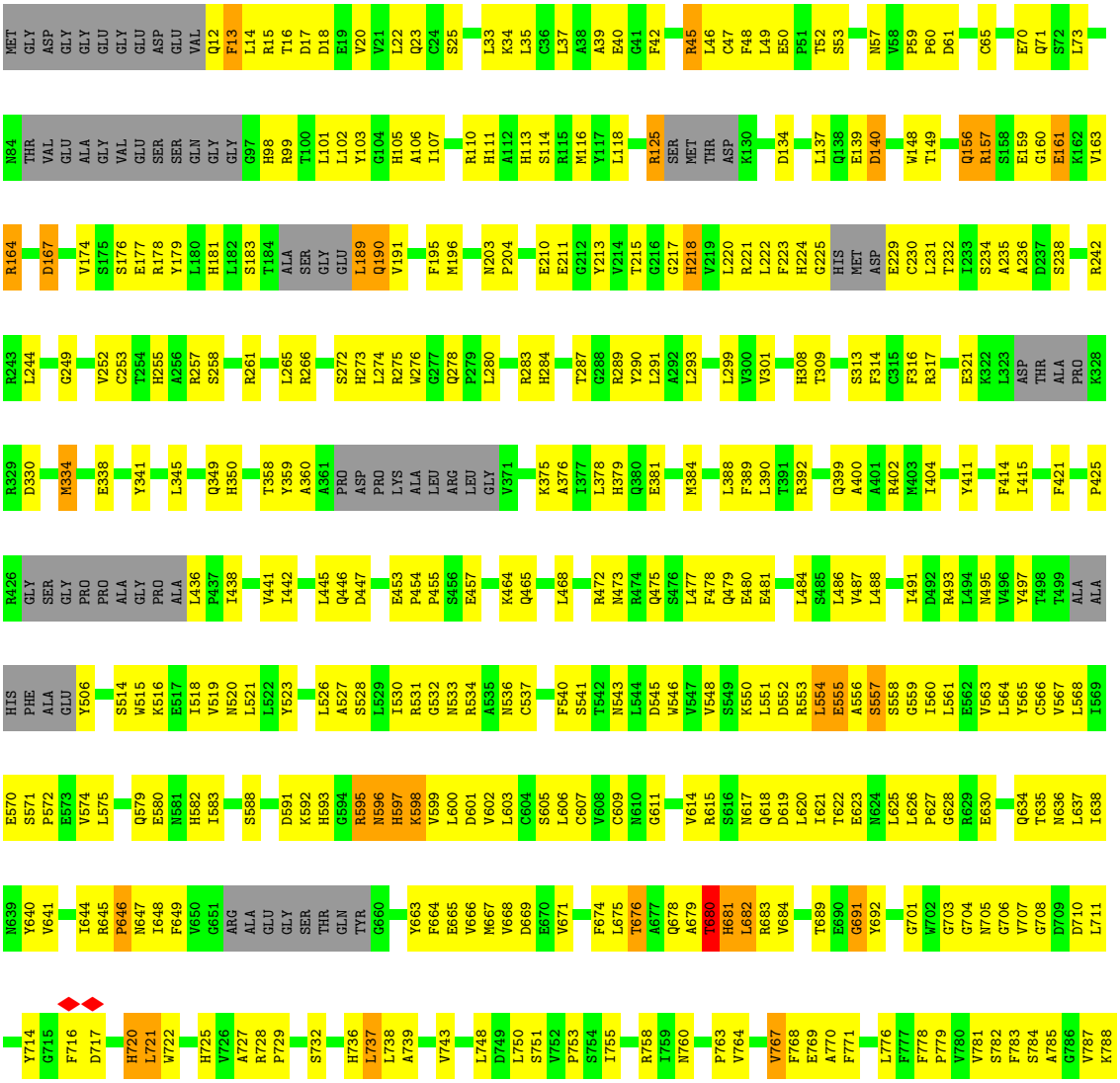
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	E	1	Total 1	Zn 1	0
3	G	1	Total 1	Zn 1	0

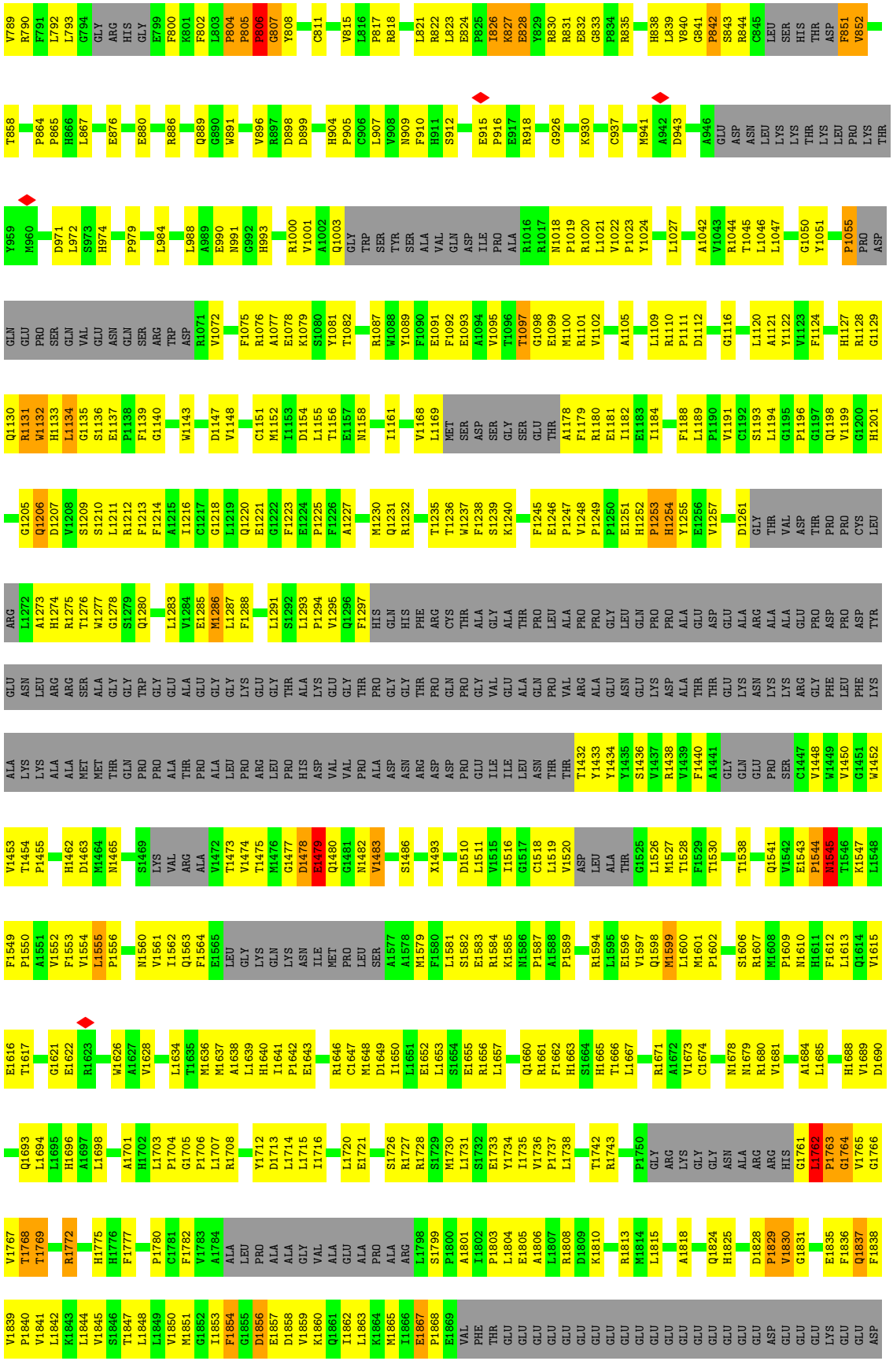
3 Residue-property plots (i)

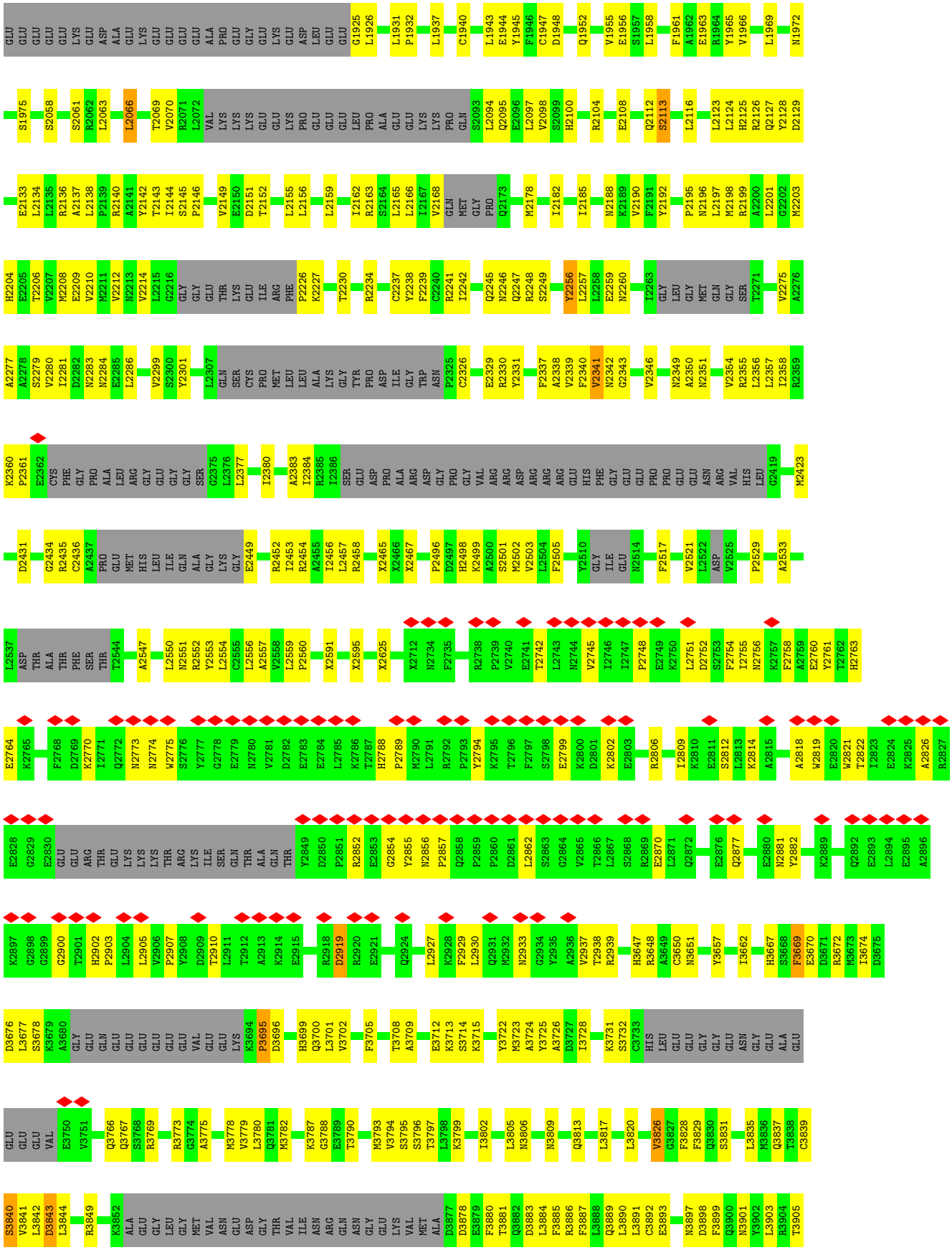
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

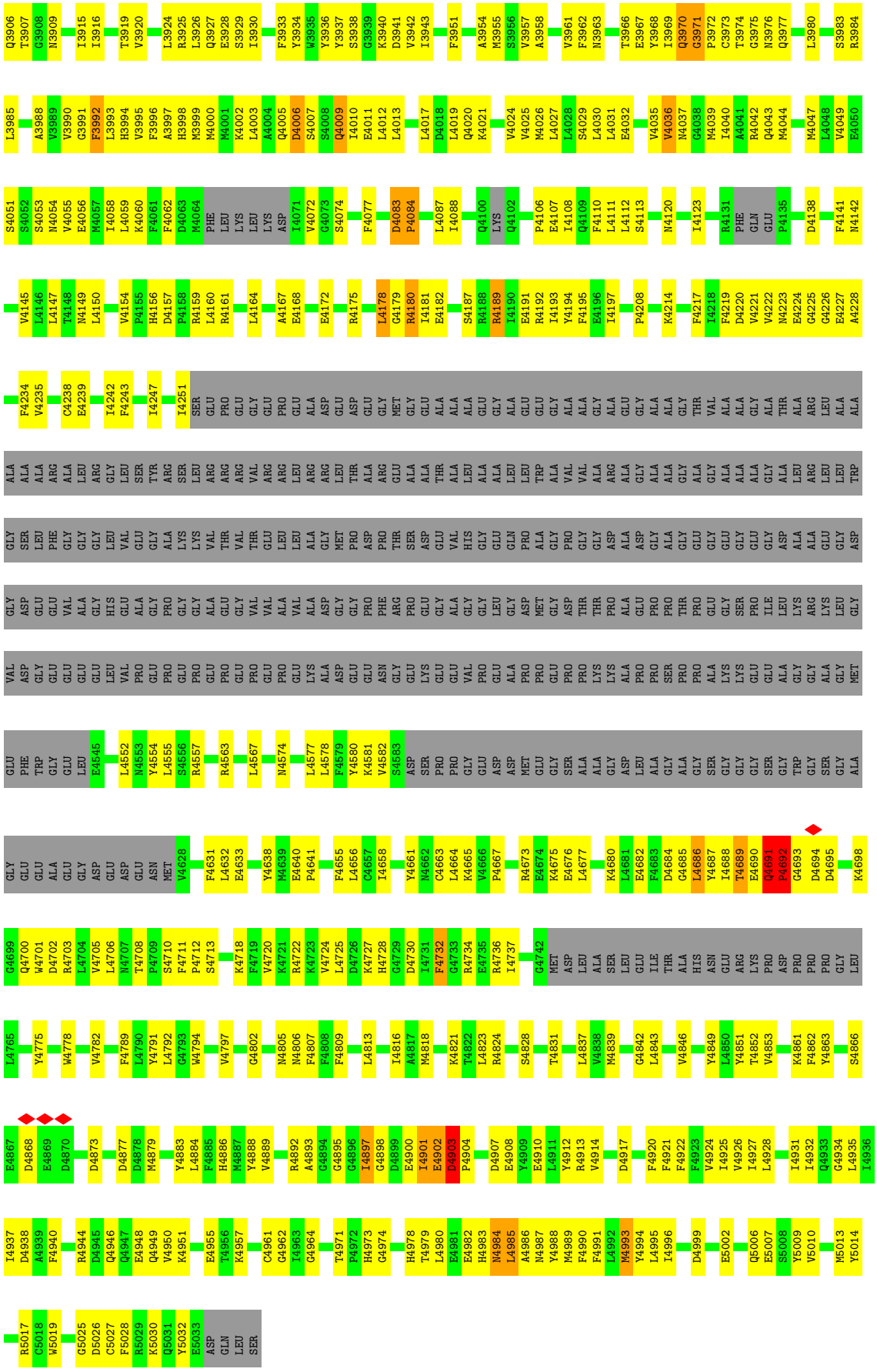
- Molecule 1: Ryanodine receptor 1

Chain A:



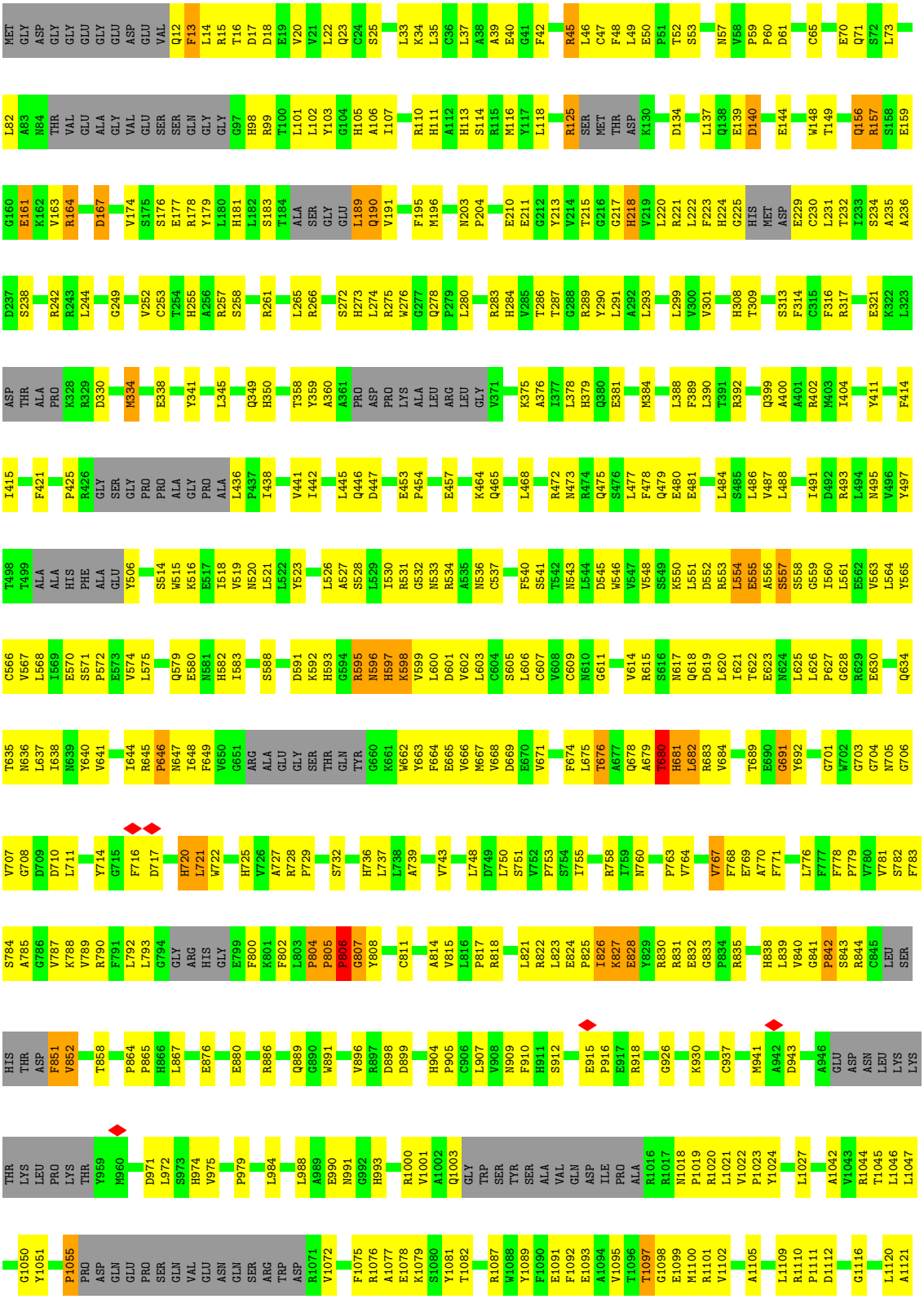


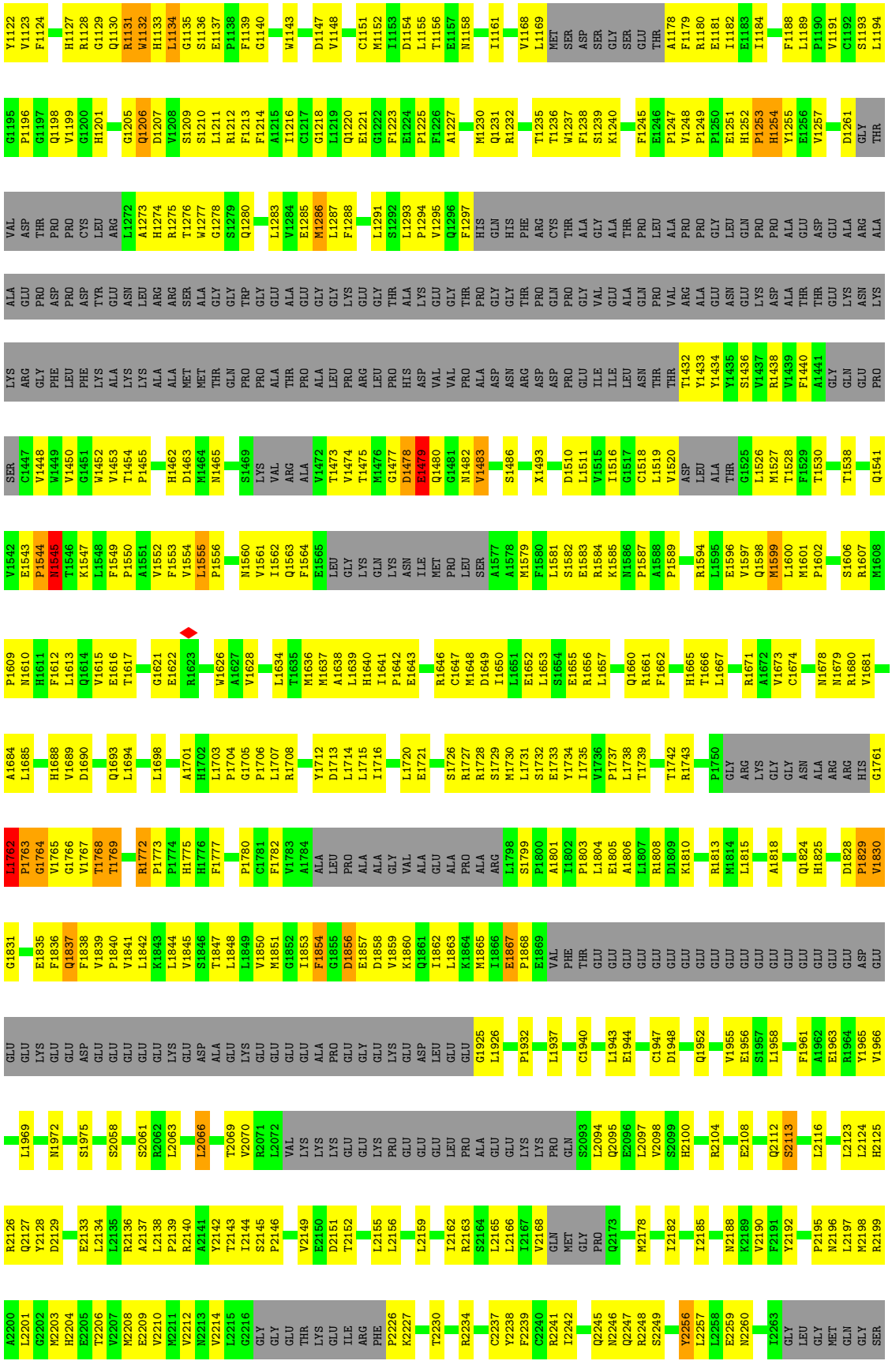


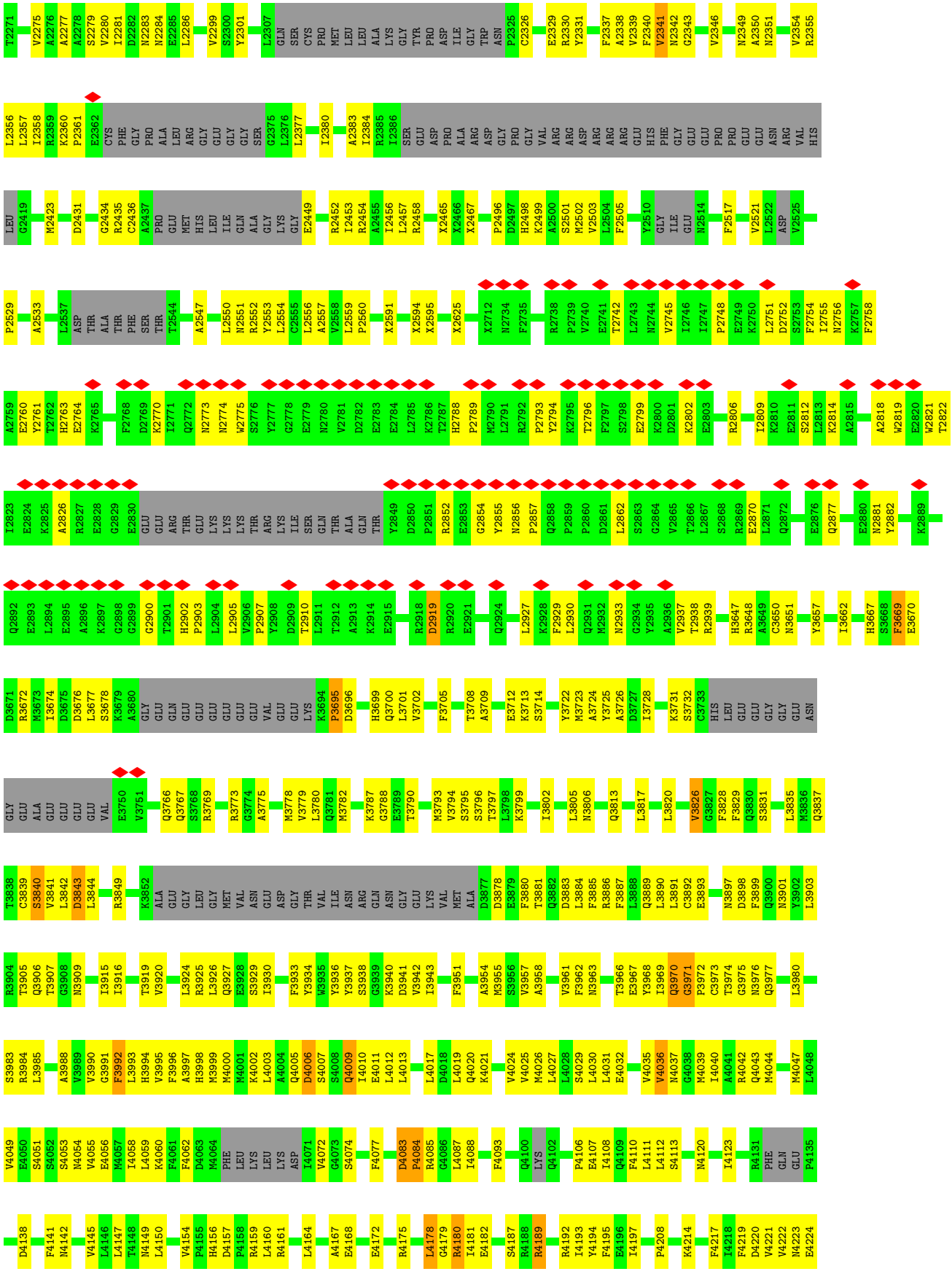


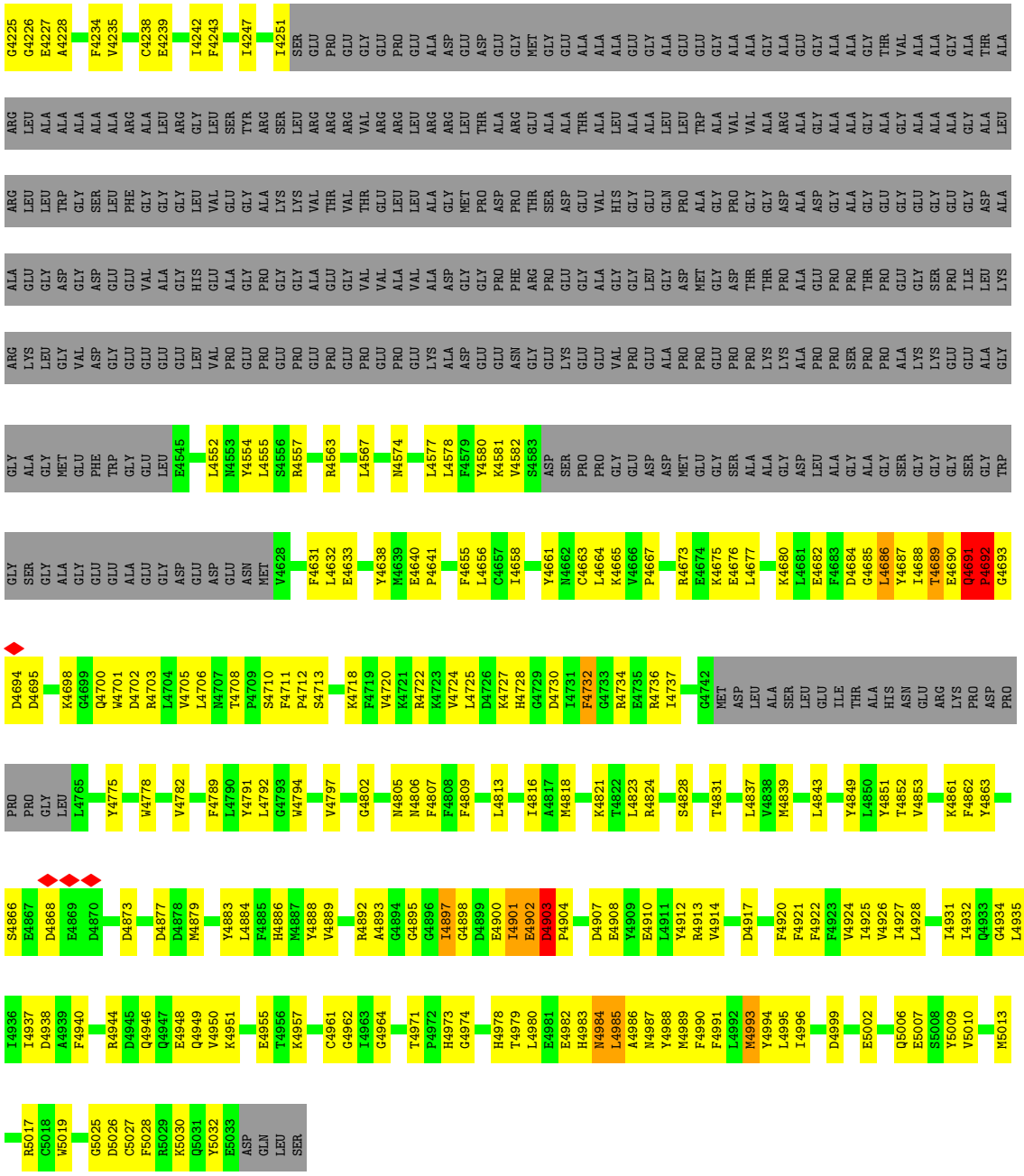
• Molecule 1: Ryanodine receptor 1

Chain C:



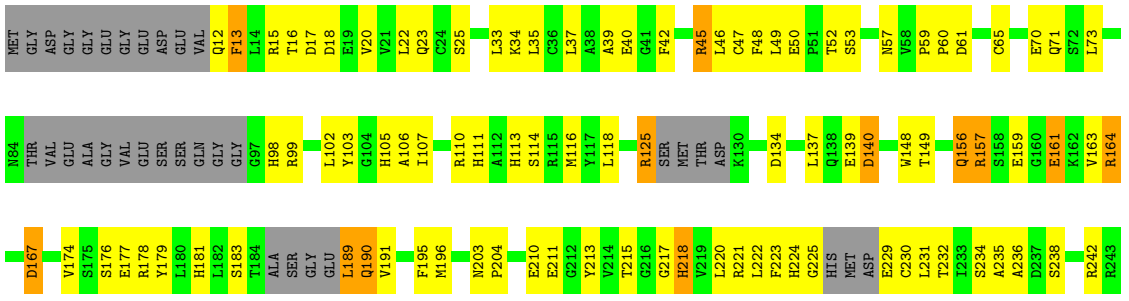


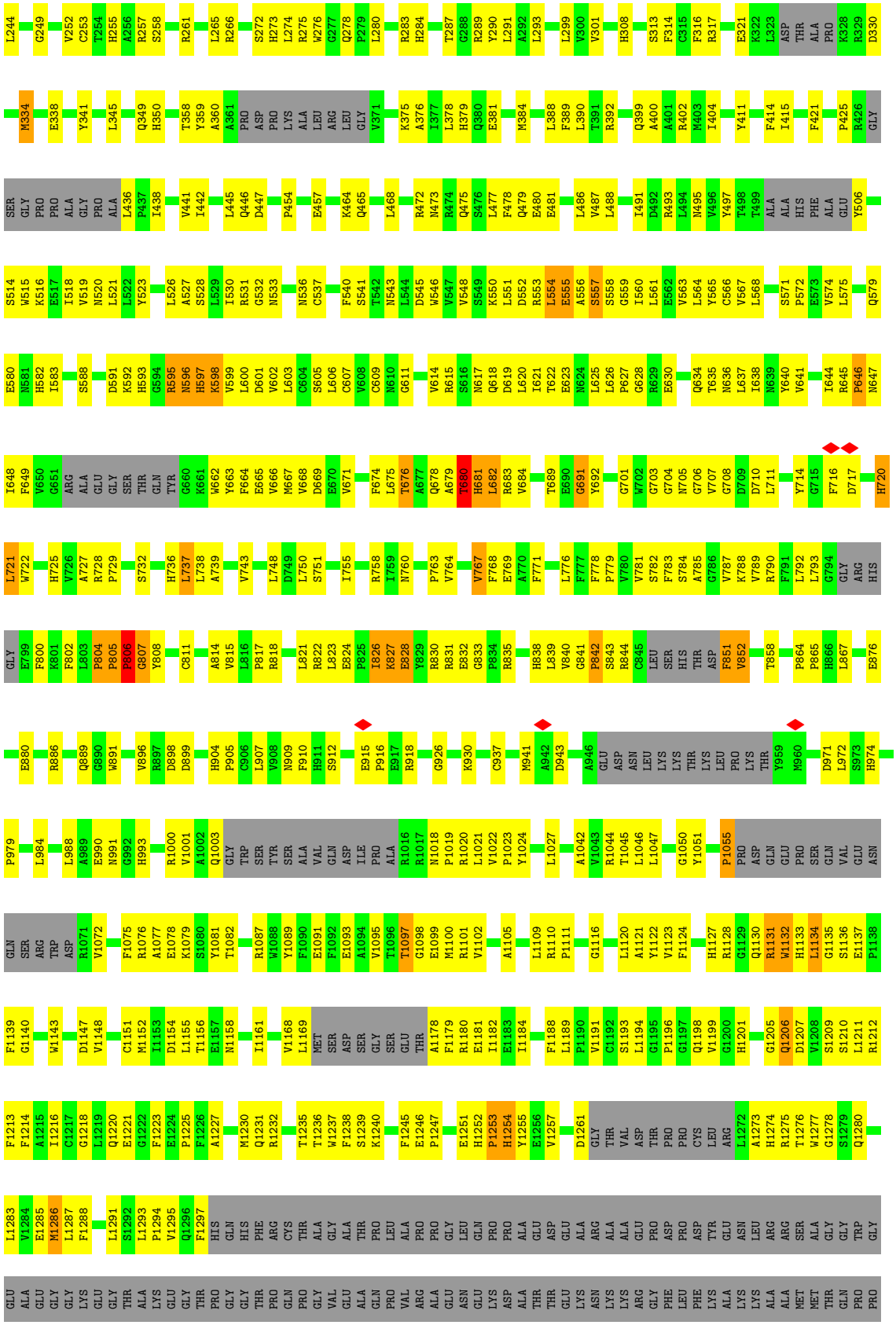


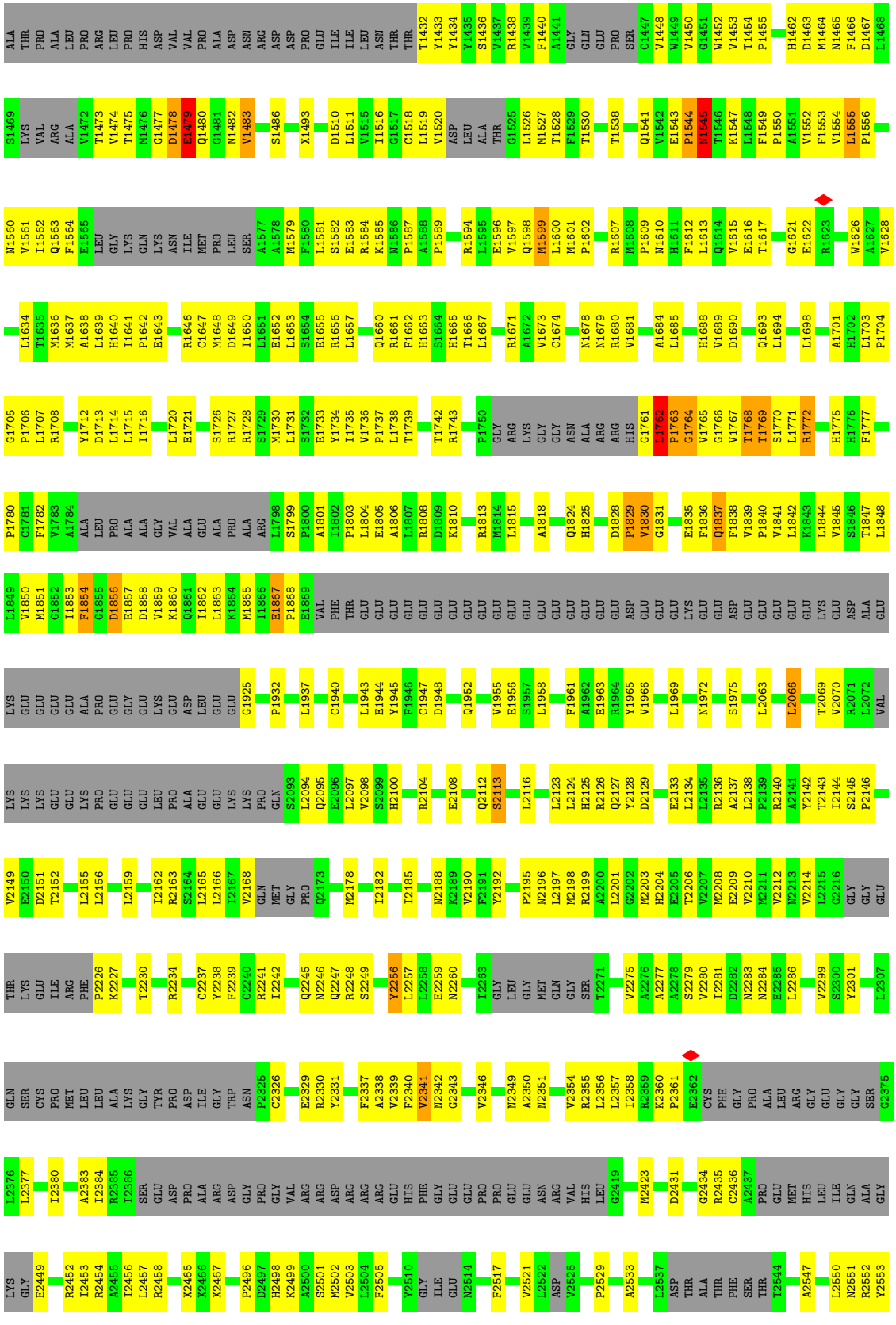


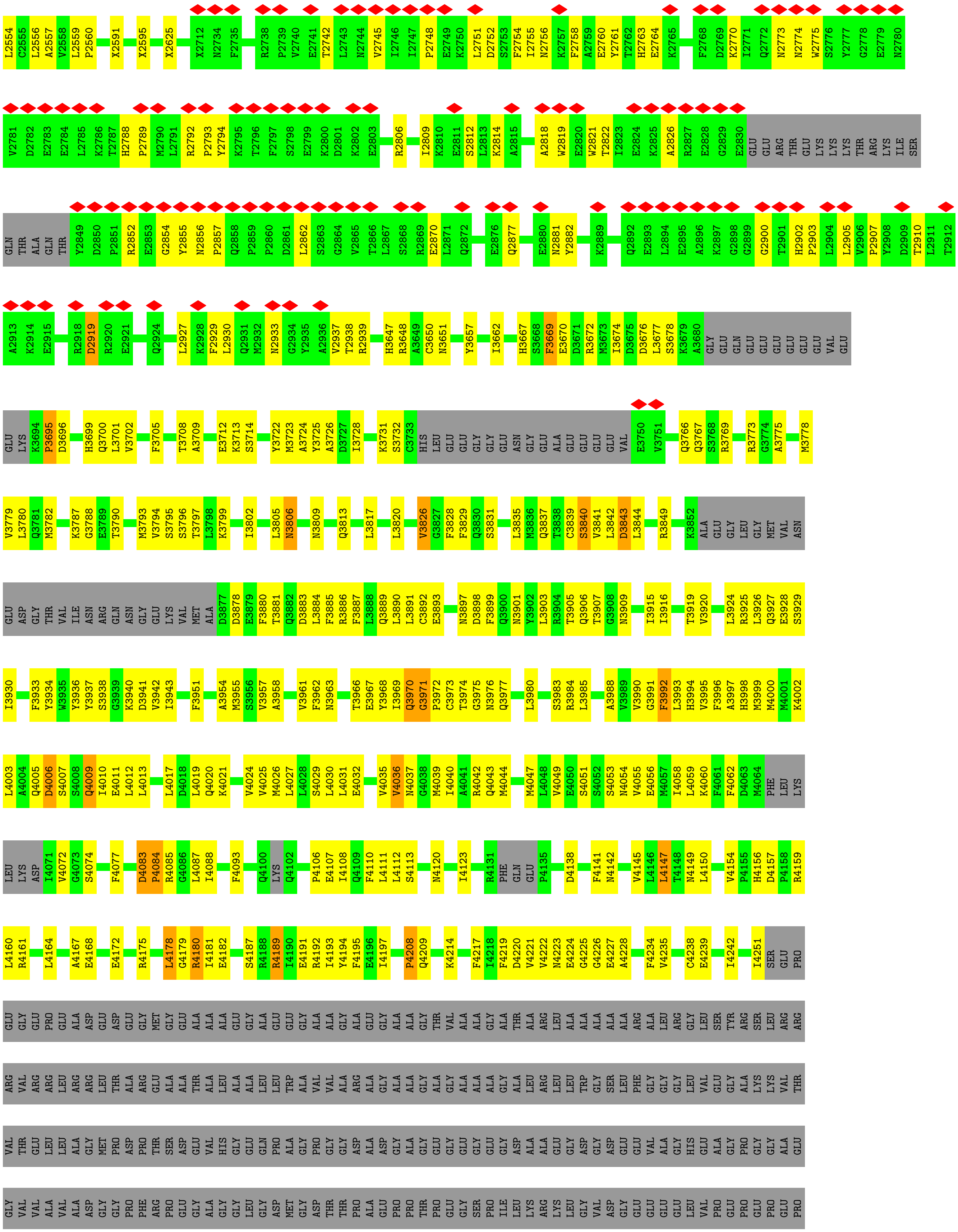
• Molecule 1: Ryanodine receptor 1

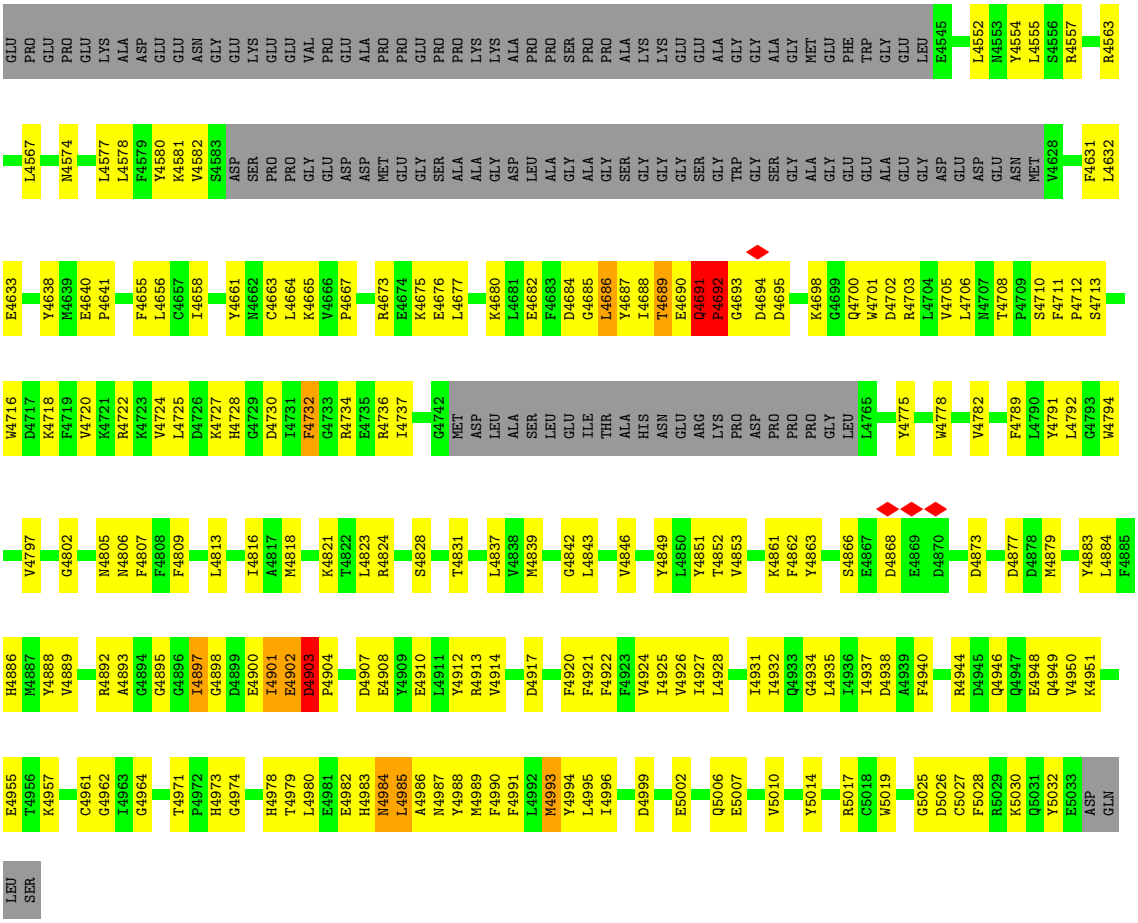
Chain E:





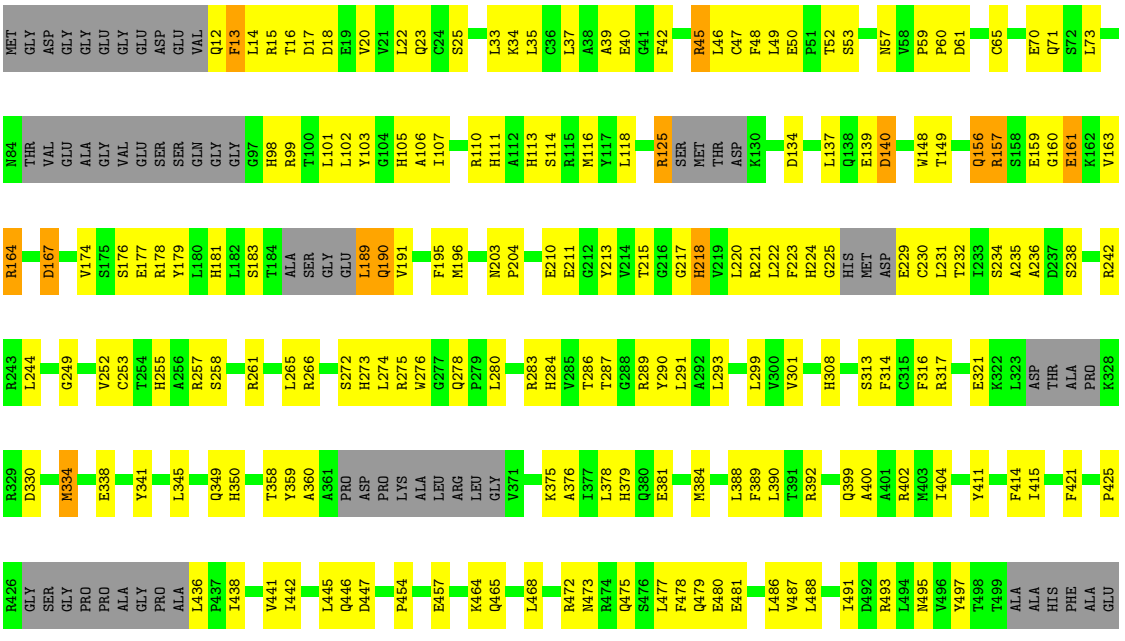


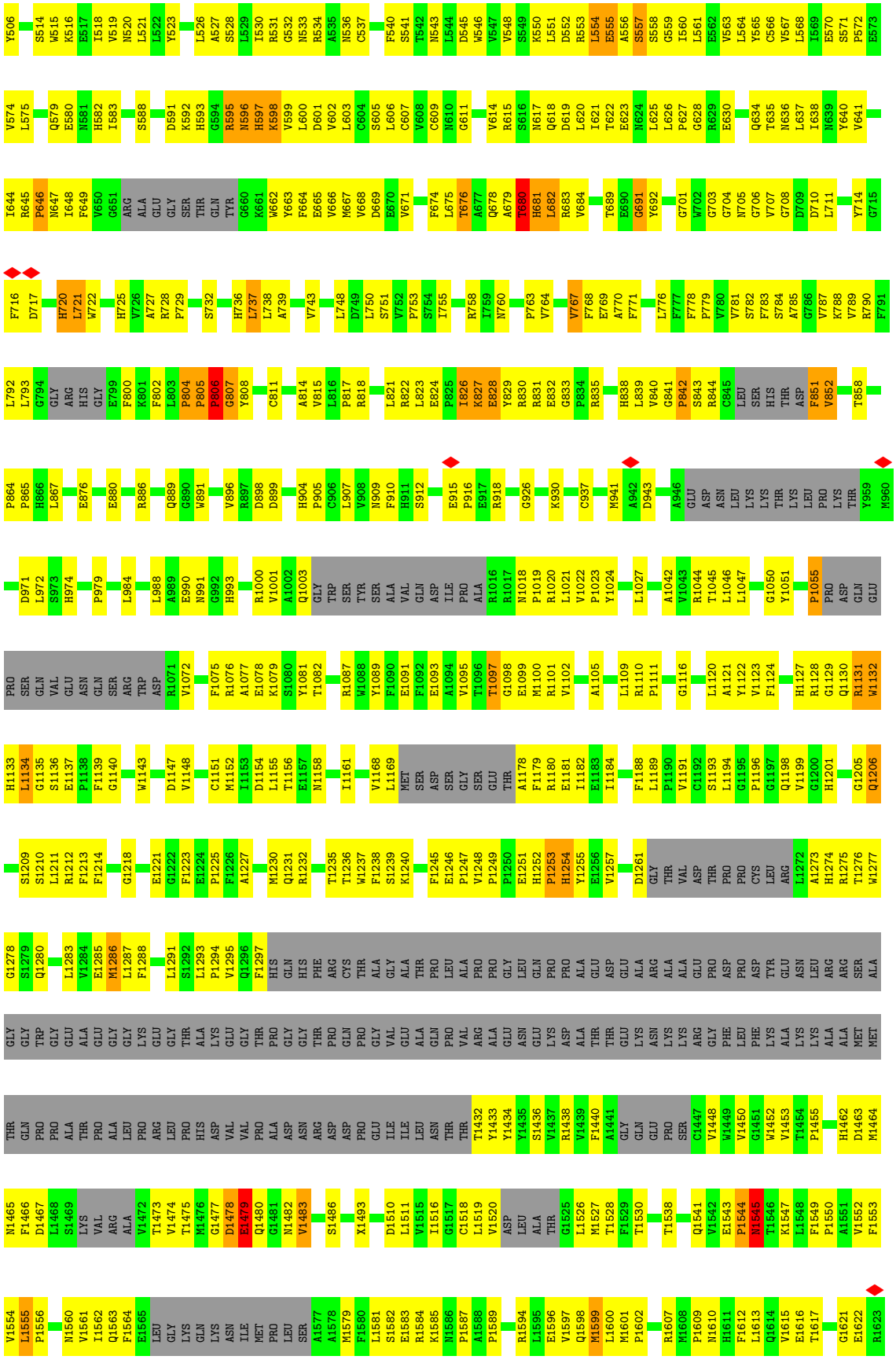

L2554 C2555 L2556 A2557 V2558 L2559 P2560 K2591 K2595 K2625 K2712 N2734 F2735 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 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 R2806 I2809 K2810 E2811 S2812 L2813 K2814 A2815 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 E2876 Q2877 E2880 N2881 Y2882 K2889 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912
A2913 K2914 E2915 R2918 D2919 R2920 E2921 Q2924 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 H3647 R3648 A3649 C3650 N3651 Y3657 I3662 H3667 S3668 F3669 E3670 D3671 R3672 M3673 I3674 D3675 D3676 L3677 S3678 K3679 A3680 GLY GLU GLN GLU GLU GLU GLU GLU GLU VAL GLU
GLU LYS K3694 P3695 D3696 H3699 Q3700 L3701 V3702 F3705 T3708 A3709 E3712 K3713 S3714 Y3722 M3723 A3724 Y3725 A3726 D3727 I3728 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 Q3766 Q3767 S3768 R3769 R3773 G3774 A3775 M3778
V3779 L3780 Q3781 M3782 K3787 G3788 E3789 T3790 M3793 V3794 S3795 S3796 T3797 L3798 K3799 I3802 L3805 N3806 N3809 Q3813 L3817 L3820 V3826 G3827 F3828 F3829 Q3830 S3831 L3835 M3836 Q3837 T3838 C3839 S3840 V3841 L3842 D3843 L3844 R3849 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 N3897 D3898 F3899 Q3900 N3901 Y3902 L3903 R3904 T3905 Q3906 T3907 G3908 N3909 I3915 I3916 T3919 V3920 L3924 R3925 L3926 Q3927 E3928 S3929
I3930 F3933 Y3934 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 F3951 A3954 M3955 S3956 V3957 A3958 V3961 F3962 N3963 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 T3974 G3975 N3976 Q3977 L3980 S3983 R3984 L3985 A3988 V3989 V3990 G3991 F3992 L3993 H3994 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002
L4003 A4004 Q4005 D4006 S4007 S4008 Q4009 I4010 E4011 L4012 L4013 L4017 D4018 L4019 Q4020 K4021 V4024 V4025 M4026 L4027 L4028 S4029 L4030 L4031 E4032 V4035 V4036 N4037 G4038 M4039 I4040 A4041 R4042 Q4043 M4044 M4047 L4048 V4049 E4050 S4051 S4052 S4053 N4054 V4055 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 PHE LEU LYS
LEU LYS ASP I4071 V4072 G4073 S4074 F4077 D4083 P4084 R4085 G4086 L4087 I4088 F4093 Q4100 LYS Q4102 P4106 E4107 I4108 Q4109 F4110 L4111 L4112 S4113 N4120 I4123 R4131 PHE GLN GLU P4135 D4138 F4141 N4142 V4145 L4146 L4147 T4148 N4149 L4150 V4154 P4155 H4156 D4157 P4158 R4159
L4160 R4161 L4164 A4167 E4168 E4172 R4175 L4178 G4179 R4180 I4181 E4182 S4187 R4188 R4189 I4190 E4191 R4192 I4193 Y4194 F4195 E4196 I4197 P4208 Q4209 K4214 F4217 I4218 F4219 D4220 V4221 V4222 N4223 E4224 G4225 G4226 E4227 A4228 F4234 V4235 C4238 E4239 I4242 I4251 SER GLU PRO
GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG
ARG VAL ARG ARG LEU ARG ARG LEU THR THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR
VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU
GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO ASP GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO

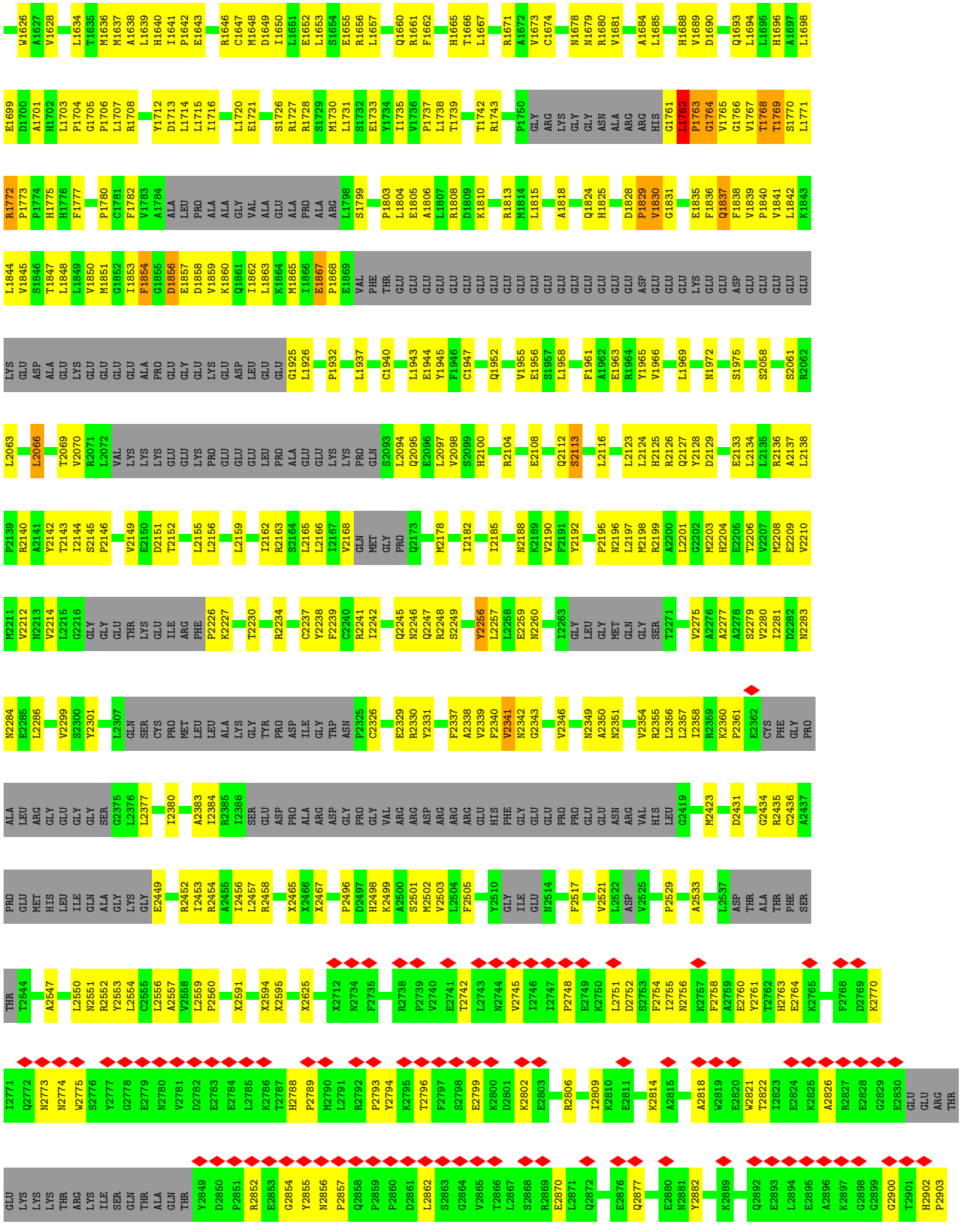


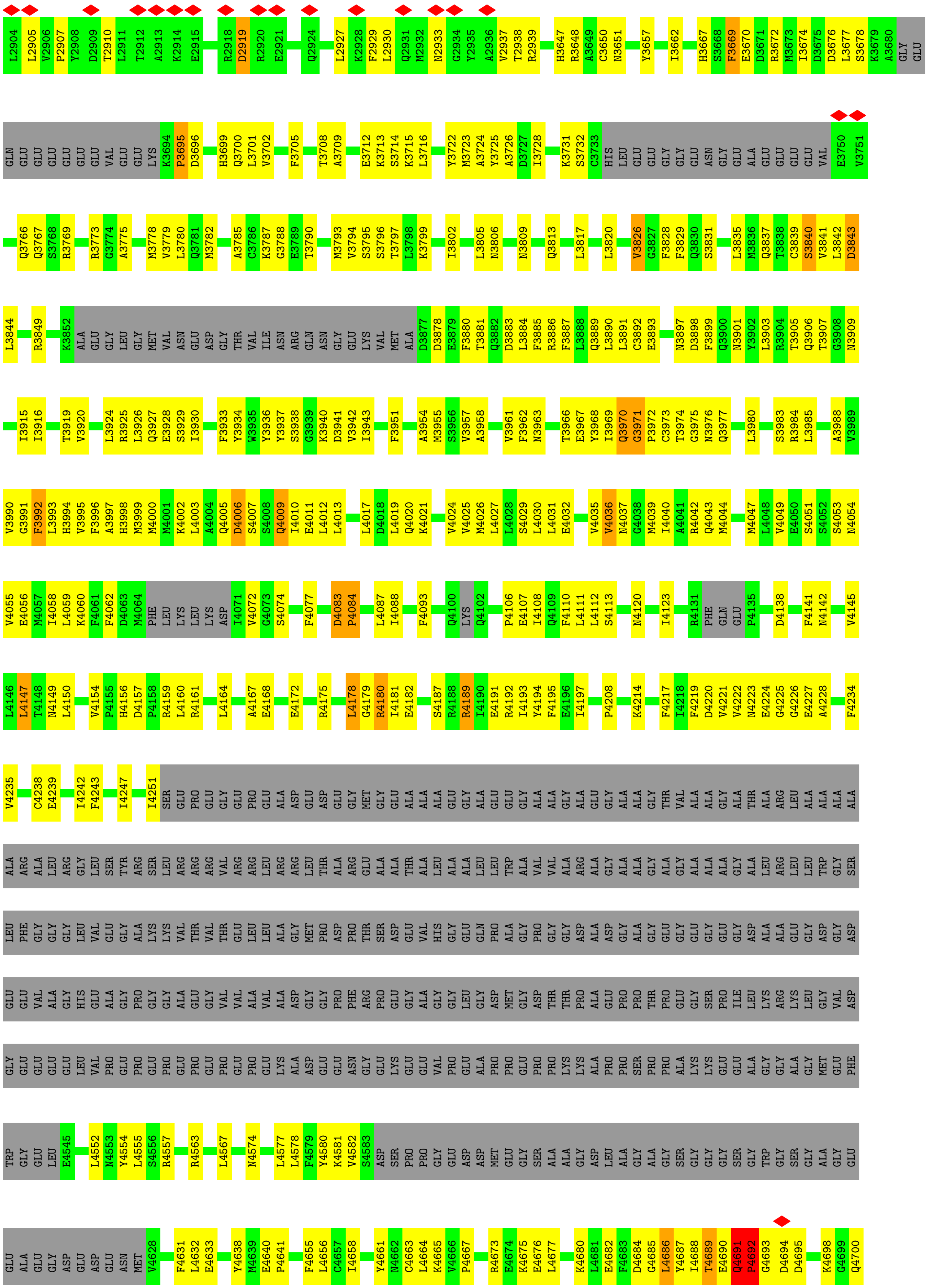
• Molecule 1: Ryanodine receptor 1

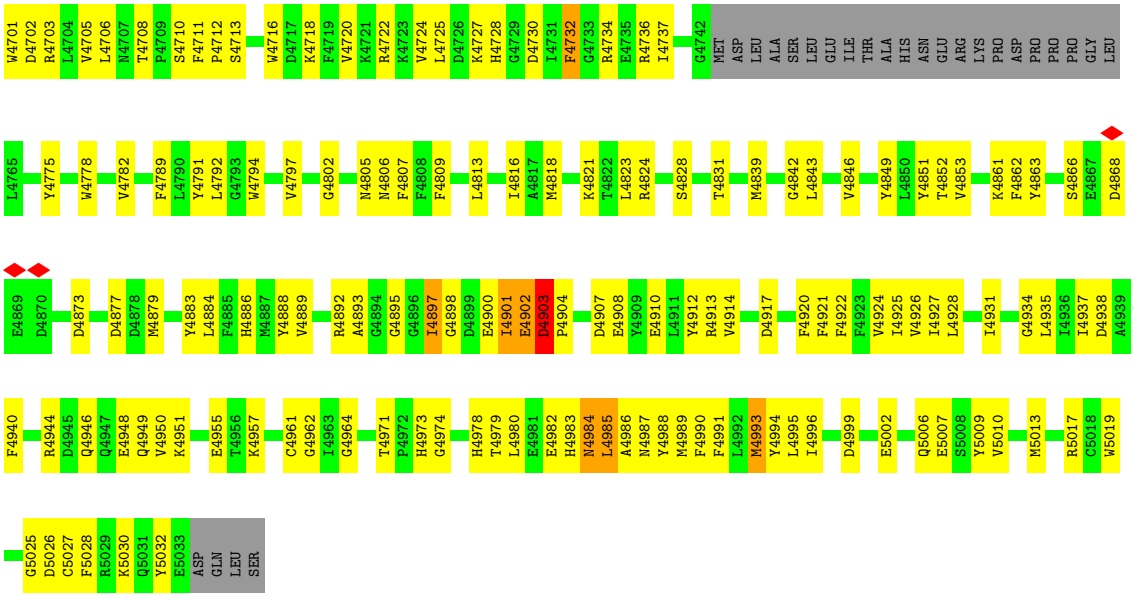
Chain G:








L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 R2918 D2919 R2920 E2921 Q2924 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 H3647 R3648 A3649 C3650 N3651 Y3657 I3662 H3667 S3668 F3669 E3670 D3671 R3672 M3673 I3674 D3675 D3676 L3677 S3678 K3679 A3680 GLY GLU
GLN GLU GLU GLU GLU GLU GLU VAL GLU GLU LYS K3694 P3695 D3696 H3699 Q3700 L3701 V3702 F3705 T3708 A3709 E3712 K3713 S3714 K3715 L3716 Y3722 M3723 A3724 Y3725 A3726 D3727 I3728 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751
Q3766 Q3767 S3768 R3769 R3773 G3774 A3775 M3778 V3779 L3780 Q3781 M3782 A3785 C3786 K3787 G3788 E3789 T3790 M3793 V3794 S3795 S3796 T3797 L3798 K3799 I3802 L3805 N3806 N3809 Q3813 L3817 L3820 V3826 G3827 F3828 F3829 Q3830 S3831 L3835 M3836 Q3837 T3838 C3839 S3840 V3841 L3842 D3843
L3844 R3849 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 N3897 D3898 F3899 Q3900 N3901 Y3902 L3903 R3904 T3905 Q3906 T3907 G3908 N3909
I3915 I3916 T3919 V3920 L3924 R3925 L3926 Q3927 E3928 S3929 I3930 F3933 Y3934 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 F3951 A3954 M3955 S3956 V3957 A3958 V3961 F3962 N3963 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 T3974 G3975 N3976 Q3977 L3980 S3983 R3984 L3985 A3988 V3989
V3990 G3991 F3992 L3993 H3994 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002 L4003 A4004 Q4005 D4006 S4007 S4008 Q4009 I4010 E4011 L4012 L4013 L4017 D4018 L4019 Q4020 K4021 V4024 V4025 M4026 L4027 L4028 S4029 L4030 L4031 E4032 V4035 V4036 N4037 G4038 M4039 I4040 A4041 R4042 Q4043 M4044 M4047 L4048 V4049 E4050 S4051 S4052 S4053 N4054
V4055 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 PHE LEU LYS LEU LYS ASP I4071 V4072 G4073 S4074 F4077 D4083 P4084 L4087 I4088 F4093 Q4100 LYS Q4102 P4106 E4107 I4108 Q4109 F4110 L4111 L4112 S4113 N4120 I4123 R4131 PHE GLN GLU P4135 D4138 F4141 N4142 V4145
L4146 L4147 T4148 N4149 L4150 V4154 P4155 H4156 D4157 P4158 R4159 L4160 R4161 L4164 A4167 E4168 E4172 R4175 L4178 G4179 R4180 I4181 E4182 S4187 R4188 R4189 I4190 E4191 R4192 I4193 Y4194 F4195 E4196 I4197 P4208 K4214 F4217 I4218 F4219 D4220 V4221 V4222 N4223 E4224 G4225 G4226 E4227 A4228 F4234
V4235 C4238 E4239 I4242 F4243 I4247 I4251 SER GLU PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA
ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER
LEU PHE GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP
GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP
GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU PHE
TRP GLY GLU LEU E4545 L4552 N4553 Y4554 L4555 S4556 R4557 R4563 L4567 N4574 L4577 L4578 F4579 Y4580 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 LYS GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU
GLU ALA GLU GLY ASP GLU ASP GLU ASN MET V4628 F4631 L4632 E4633 Y4638 M4639 E4640 P4641 F4655 L4656 C4657 I4658 Y4661 N4662 C4663 L4664 K4665 V4666 P4667 R4673 E4674 K4675 E4676 L4677 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 K4698 G4699 Q4700

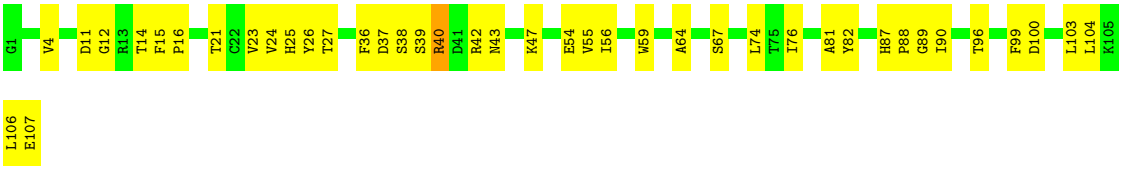


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain B:

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

Chain D:

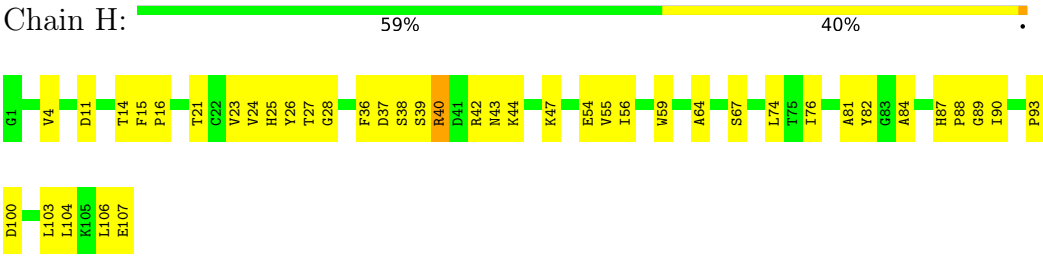


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:

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

Chain H:


59%
40%
G1
V4
D11
T14
F15
P16
T21
C22
V23
V24
H25
Y26
T27
G28
F36
D37
S38
S39
R40
D41
R42
N43
K44
K47
E54
V55
I56
W59
A64
S67
L74
T75
I76
A81
Y82
G83
A84
H87
P88
G89
I90
P93
T96
F99
D100
L103
L104
K105
L106
E107

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	65872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Contrast transfer function parameters were estimated using CTFFIND3	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	5600	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.04	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	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	C	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	E	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
1	G	0.33	2/24616 (0.0%)	0.59	19/33295 (0.1%)
2	B	0.26	0/851	0.45	0/1146
2	D	0.26	0/851	0.45	0/1146
2	F	0.26	0/851	0.45	0/1146
2	H	0.26	0/851	0.45	0/1146
All	All	0.33	8/101868 (0.0%)	0.59	76/137764 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
1	E	0	3
1	G	0	3
All	All	0	12

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1544	PRO	N-CD	5.20	1.55	1.47
1	C	1544	PRO	N-CD	5.20	1.55	1.47
1	E	1544	PRO	N-CD	5.20	1.55	1.47
1	G	1544	PRO	N-CD	5.20	1.55	1.47
1	A	1763	PRO	N-CD	5.05	1.54	1.47

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1764	GLY	N-CA-C	14.38	149.05	113.10
1	C	1764	GLY	N-CA-C	14.38	149.05	113.10
1	E	1764	GLY	N-CA-C	14.38	149.05	113.10
1	G	1764	GLY	N-CA-C	14.38	149.05	113.10
1	A	1765	VAL	N-CA-CB	-9.67	90.23	111.50

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1253	PRO	Peptide
1	A	1867	GLU	Peptide
1	A	646	PRO	Peptide
1	C	1253	PRO	Peptide
1	C	646	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	26957	0	23849	1705	0
1	C	26957	0	23849	1709	0
1	E	26957	0	23849	1698	0
1	G	26957	0	23849	1714	0
2	B	832	0	831	41	0
2	D	832	0	831	42	0
2	F	832	0	831	42	0
2	H	832	0	831	43	0
3	A	1	0	0	2	0
3	C	1	0	0	2	0
3	E	1	0	0	2	0
3	G	1	0	0	2	0
All	All	111160	0	98720	6845	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 33.

The worst 5 of 6845 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:554:LEU:HD11	1:E:593:HIS:CE1	1.12	1.64
1:G:554:LEU:HD11	1:G:593:HIS:CE1	1.12	1.63
1:A:554:LEU:HD11	1:A:593:HIS:CE1	1.12	1.62
1:C:554:LEU:HD11	1:C:593:HIS:CE1	1.12	1.61
1:G:1961:PHE:CZ	1:G:2063:LEU:HD23	1.36	1.60

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	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7 41
1	C	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7 41
1	E	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7 41
1	G	2991/4599 (65%)	2776 (93%)	155 (5%)	60 (2%)	7 41
2	B	105/107 (98%)	97 (92%)	8 (8%)	0	100 100
2	D	105/107 (98%)	97 (92%)	8 (8%)	0	100 100
2	F	105/107 (98%)	97 (92%)	8 (8%)	0	100 100
2	H	105/107 (98%)	97 (92%)	8 (8%)	0	100 100
All	All	12384/18824 (66%)	11492 (93%)	652 (5%)	240 (2%)	11 42

5 of 240 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	LEU
1	A	807	GLY
1	A	827	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	852	VAL
1	A	1254	HIS

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	2507/3406 (74%)	2439 (97%)	68 (3%)	44	69
1	C	2507/3406 (74%)	2439 (97%)	68 (3%)	44	69
1	E	2507/3406 (74%)	2439 (97%)	68 (3%)	44	69
1	G	2507/3406 (74%)	2439 (97%)	68 (3%)	44	69
2	B	89/89 (100%)	88 (99%)	1 (1%)	73	85
2	D	89/89 (100%)	88 (99%)	1 (1%)	73	85
2	F	89/89 (100%)	88 (99%)	1 (1%)	73	85
2	H	89/89 (100%)	88 (99%)	1 (1%)	73	85
All	All	10384/13980 (74%)	10108 (97%)	276 (3%)	48	69

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	851	PHE
1	G	1055	PRO
1	G	4006	ASP
1	C	979	PRO
1	C	865	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	156	GLN
1	E	2100	HIS
2	H	25	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	2196	ASN
1	E	278	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	36

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	C	36
1	E	36
1	G	36

The worst 5 of 144 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3572:UNK	C	3645:PRO	N	56.50
1	C	3572:UNK	C	3645:PRO	N	56.50
1	E	3572:UNK	C	3645:PRO	N	56.50
1	G	3572:UNK	C	3645:PRO	N	56.50
1	A	2712:UNK	C	2734:ASN	N	35.36

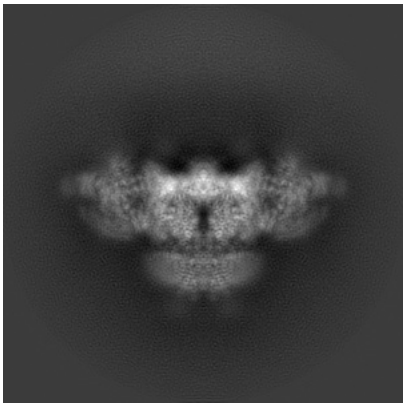
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2807. These allow visual inspection of the internal detail of the map and identification of artifacts.

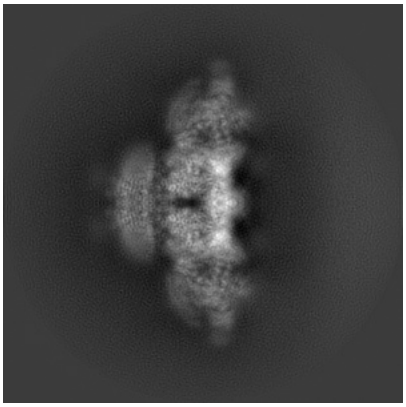
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

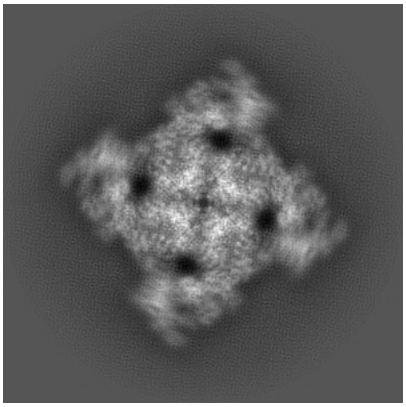
6.1.1 Primary map



X



Y

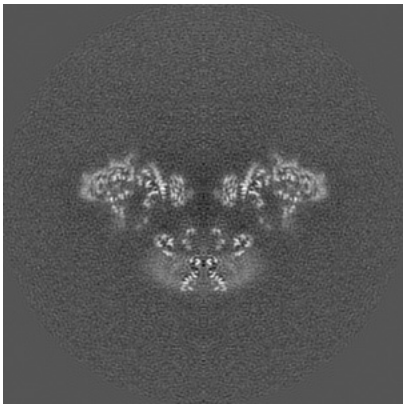


Z

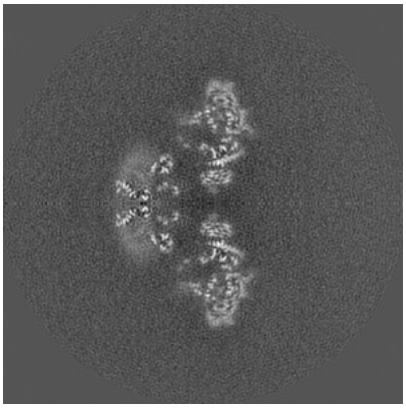
The images above show the map projected in three orthogonal directions.

6.2 Central slices

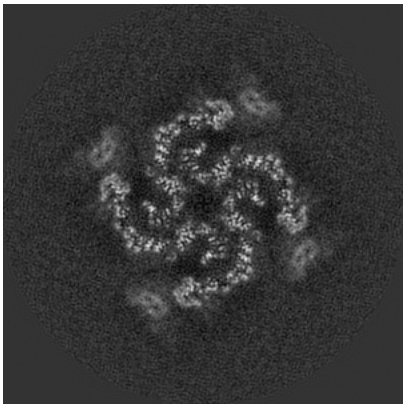
6.2.1 Primary map



X Index: 180



Y Index: 180

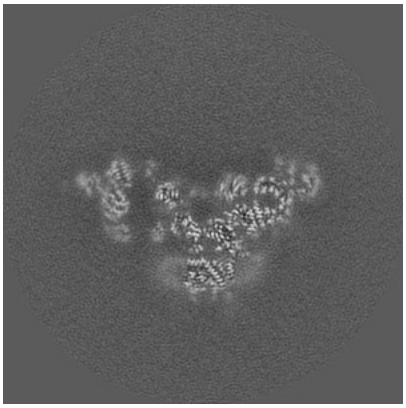


Z Index: 180

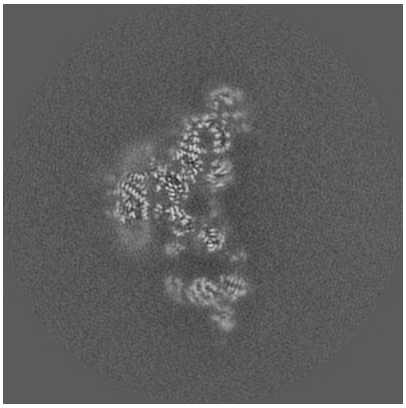
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

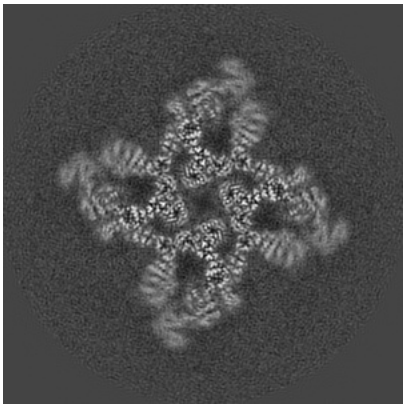
6.3.1 Primary map



X Index: 169



Y Index: 191

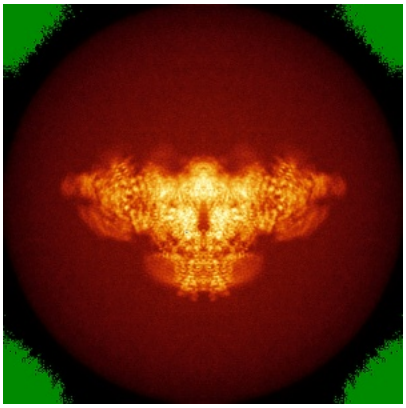


Z Index: 193

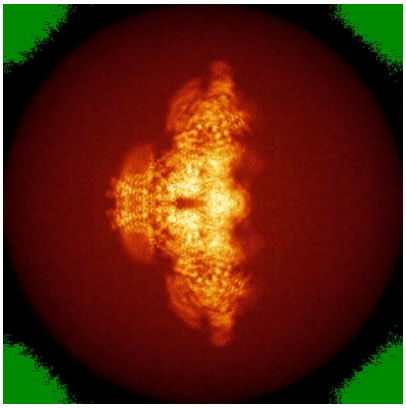
The images above show the largest variance slices of the map in three orthogonal directions.

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

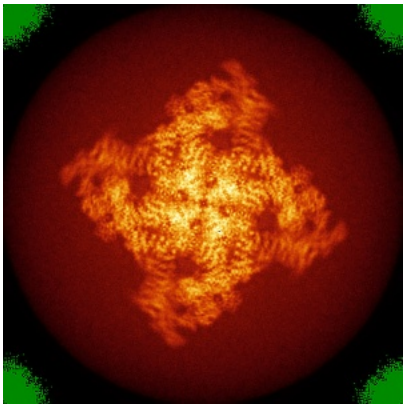
6.4.1 Primary map



X



Y

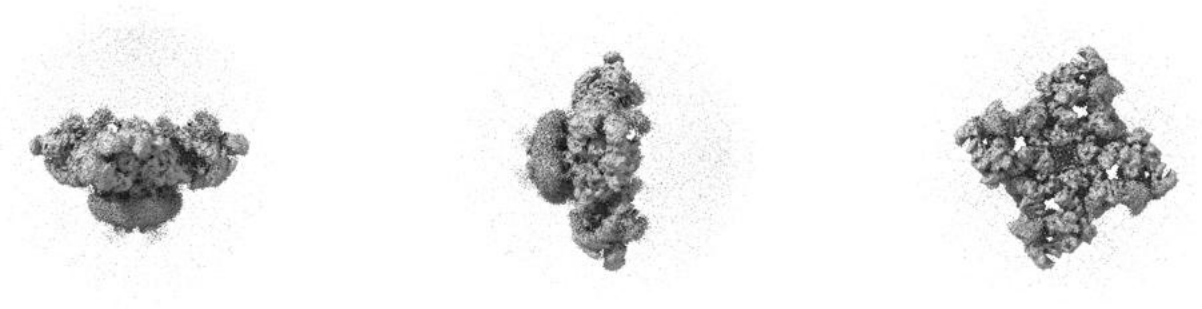


Z

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

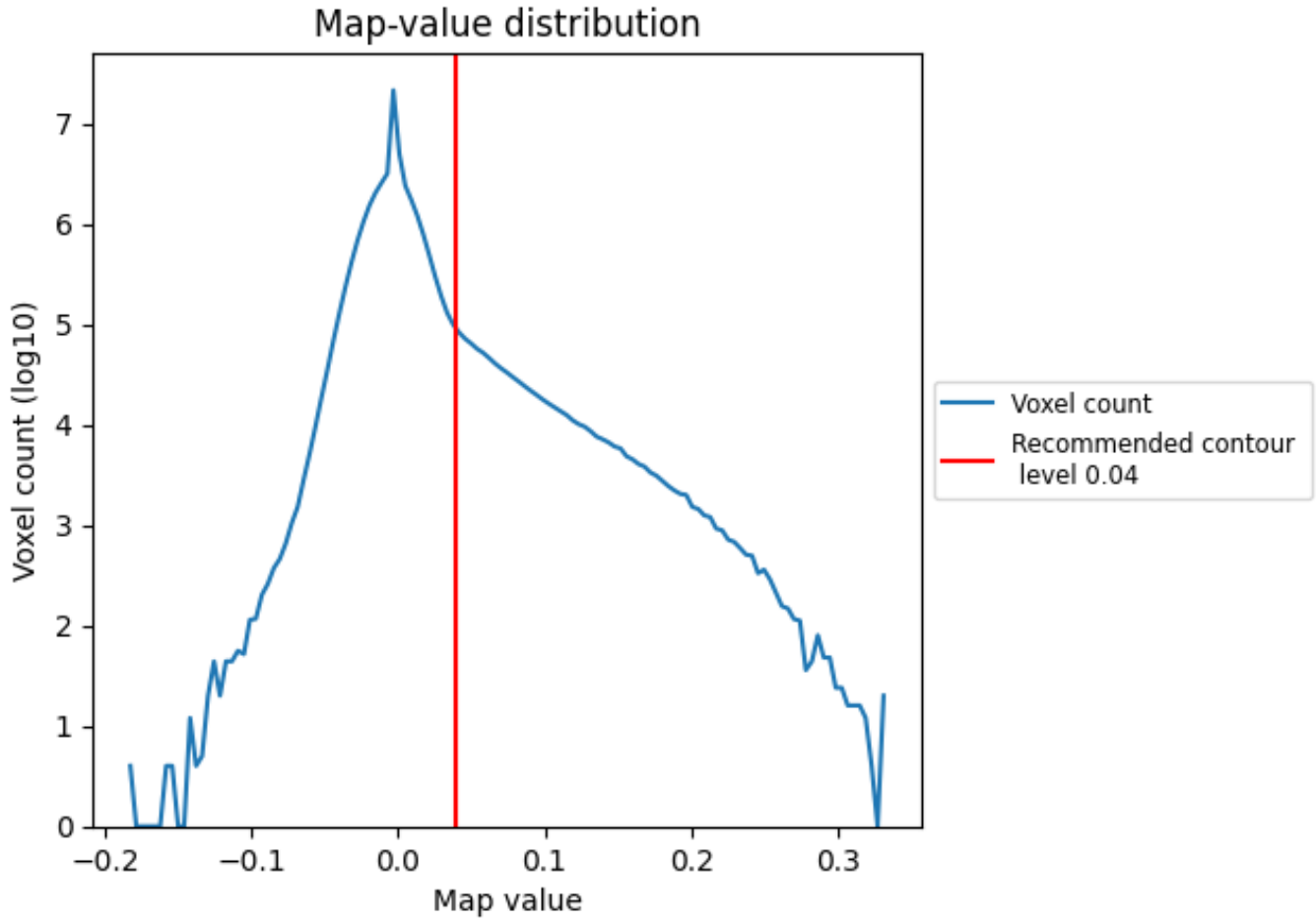
6.6 Mask visualisation (i)

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

7 Map analysis

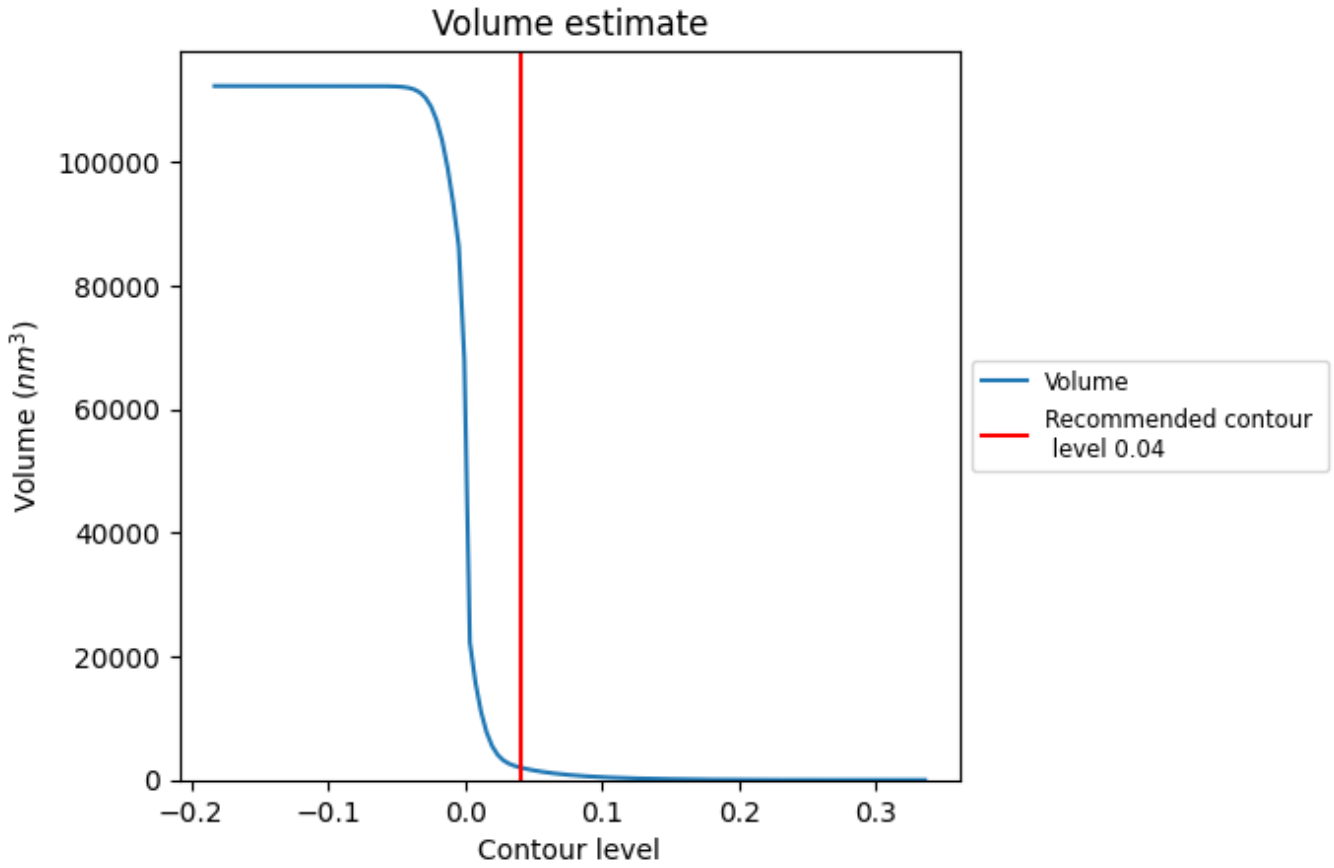
This section contains the results of statistical analysis of the map.

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.

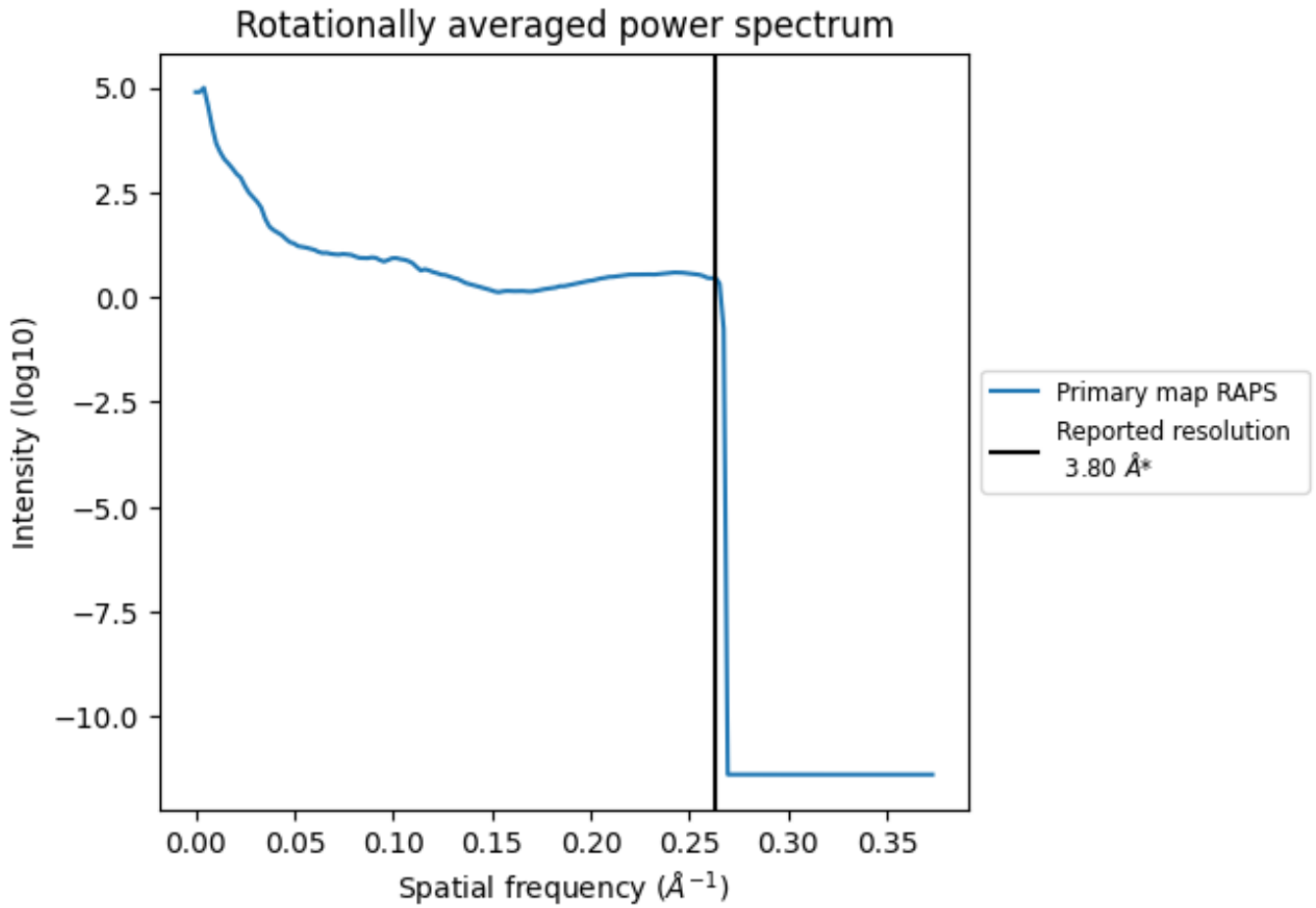
7.2 Volume estimate (i)



The volume at the recommended contour level is 2026 nm^3; this corresponds to an approximate mass of 1830 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 0.263 Å^{-1}

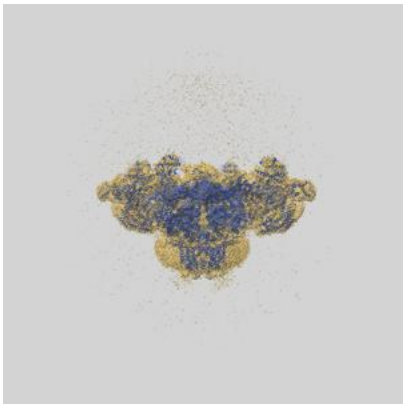
8 Fourier-Shell correlation

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

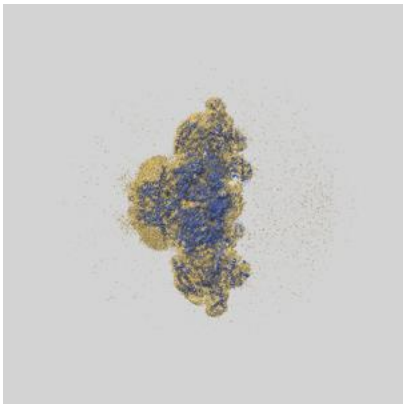
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2807 and PDB model 3J8H. Per-residue inclusion information can be found in section 3 on page 5.

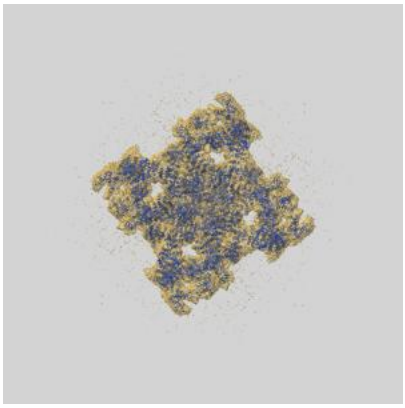
9.1 Map-model overlay



X



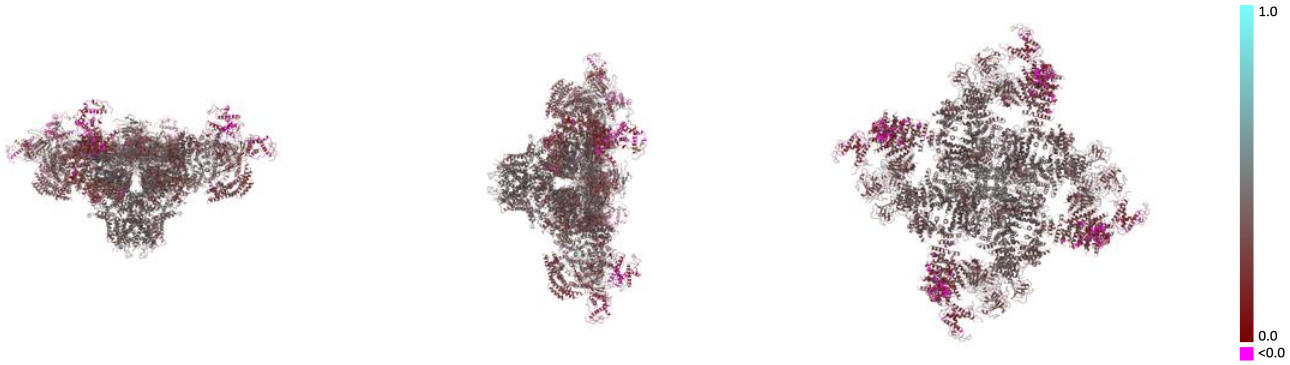
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

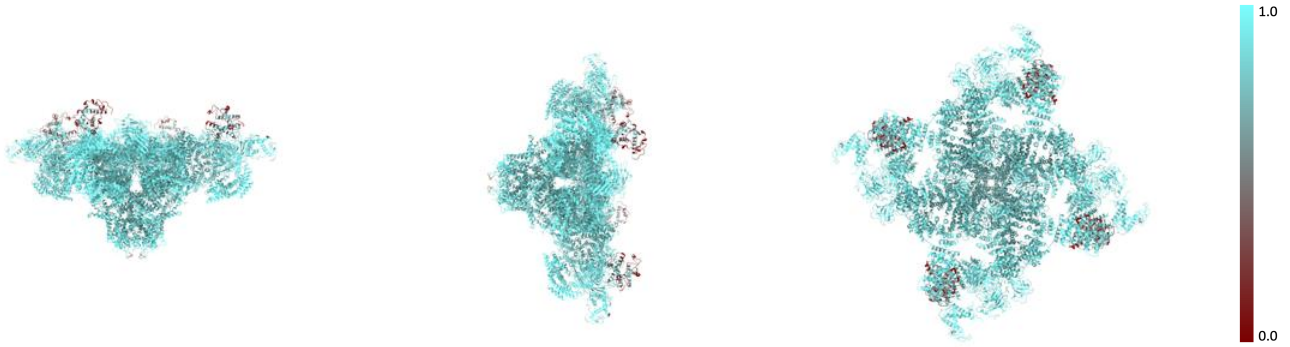
9.2 Q-score mapped to coordinate model (i)



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.

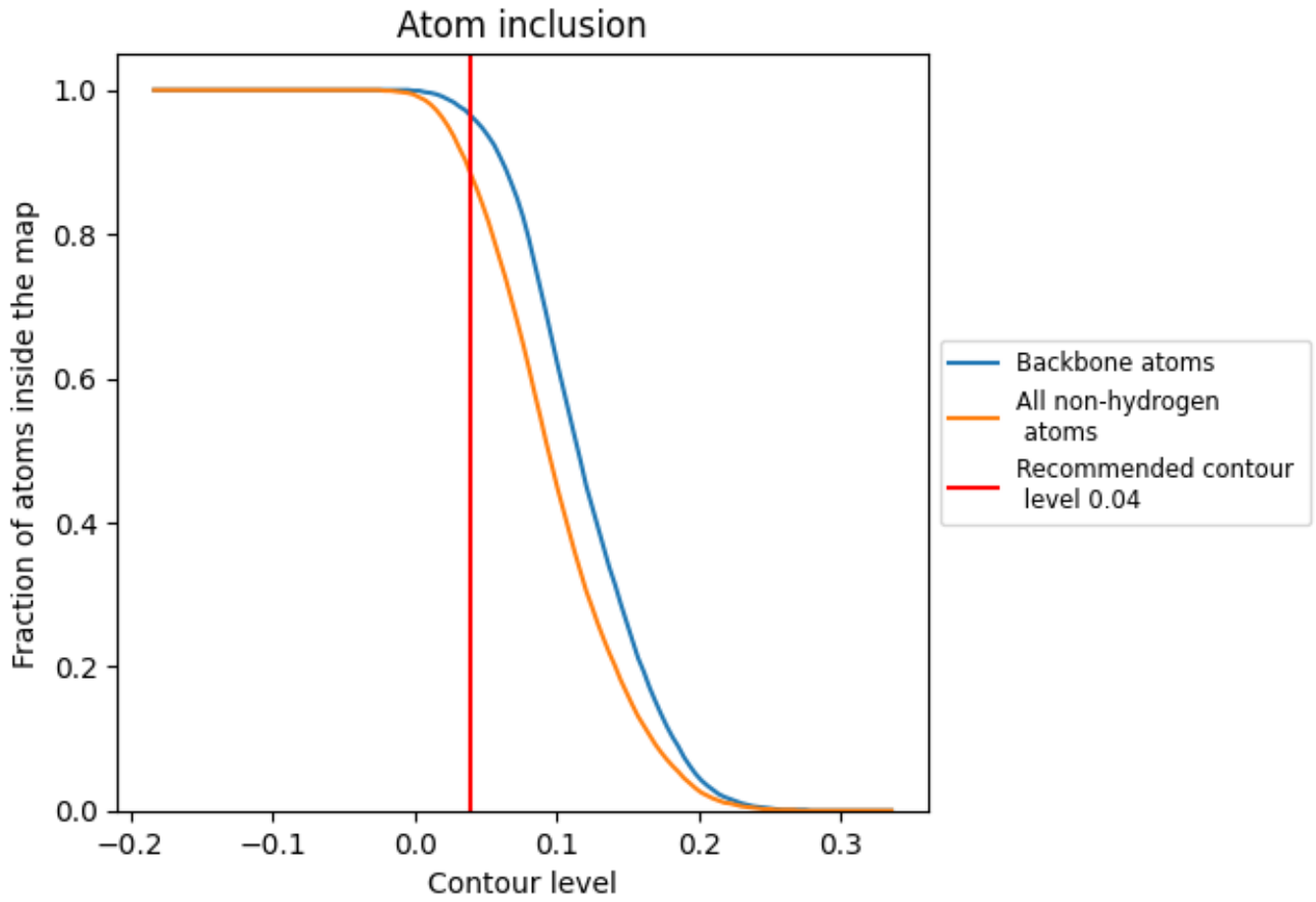
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.3380
A	0.8810	0.3380
B	0.9190	0.3580
C	0.8810	0.3380
D	0.9190	0.3570
E	0.8810	0.3380
F	0.9190	0.3540
G	0.8810	0.3380
H	0.9190	0.3590