



# wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 09:33 AM EST

PDB ID : 6PV6  
EMDB ID : EMD-20486  
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots  
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.  
Deposited on : 2019-07-19  
Resolution : 4.50 Å(reported)  
Based on initial model : 5TB4

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

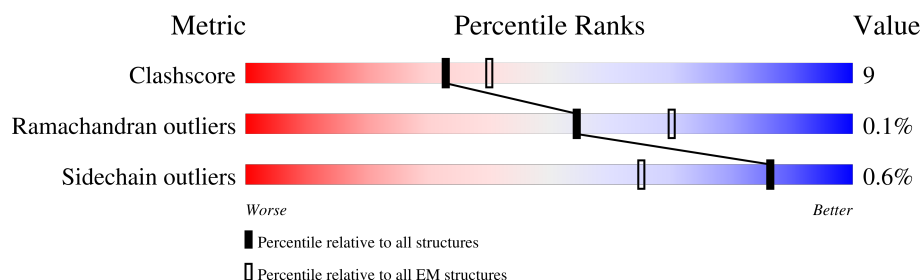
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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  $\leq 5\%$ . 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	B	4687	<div> <div>33%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>
1	E	4687	<div> <div>37%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>
1	G	4687	<div> <div>40%</div> <div>70%</div> <div>19%</div> <div>11%</div> </div>
1	I	4687	<div> <div>36%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>
2	A	108	<div> <div>37%</div> <div>69%</div> <div>31%</div> <div>.</div> </div>
2	F	108	<div> <div>47%</div> <div>70%</div> <div>29%</div> <div>.</div> </div>
2	H	108	<div> <div>54%</div> <div>69%</div> <div>31%</div> <div>.</div> </div>
2	J	108	<div> <div>43%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

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

- 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	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

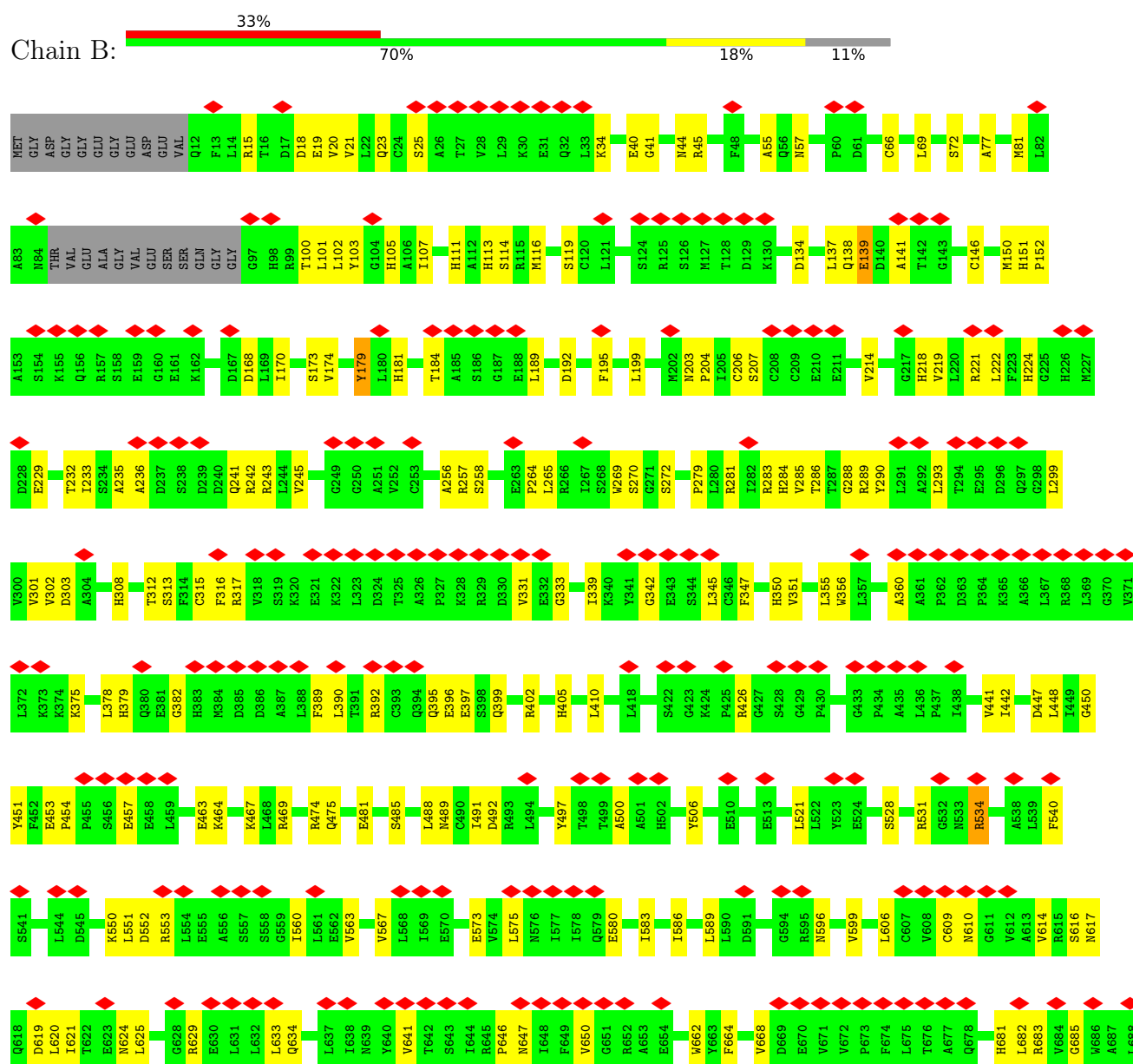
Interest" by depositor).

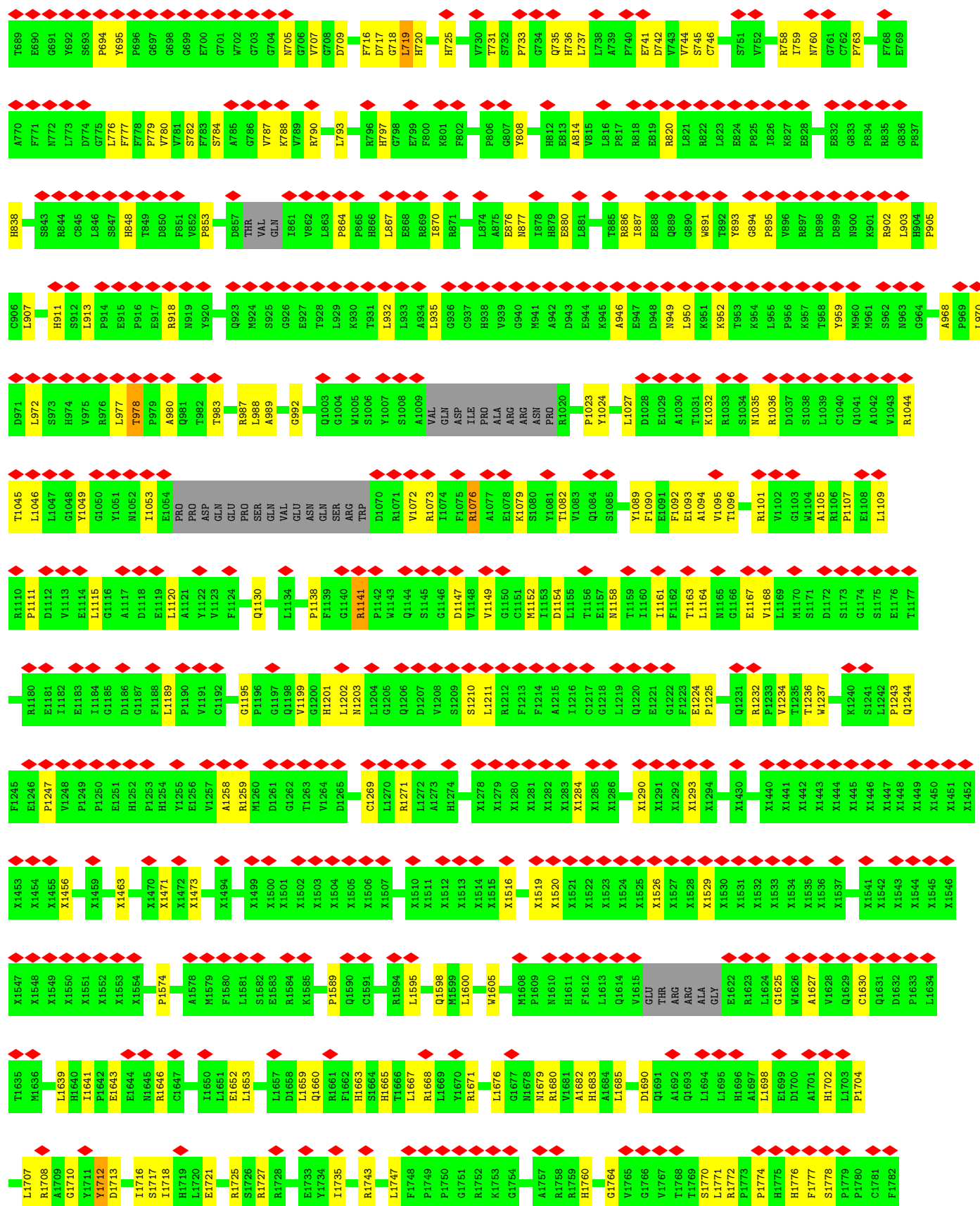
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

### 3 Residue-property plots

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

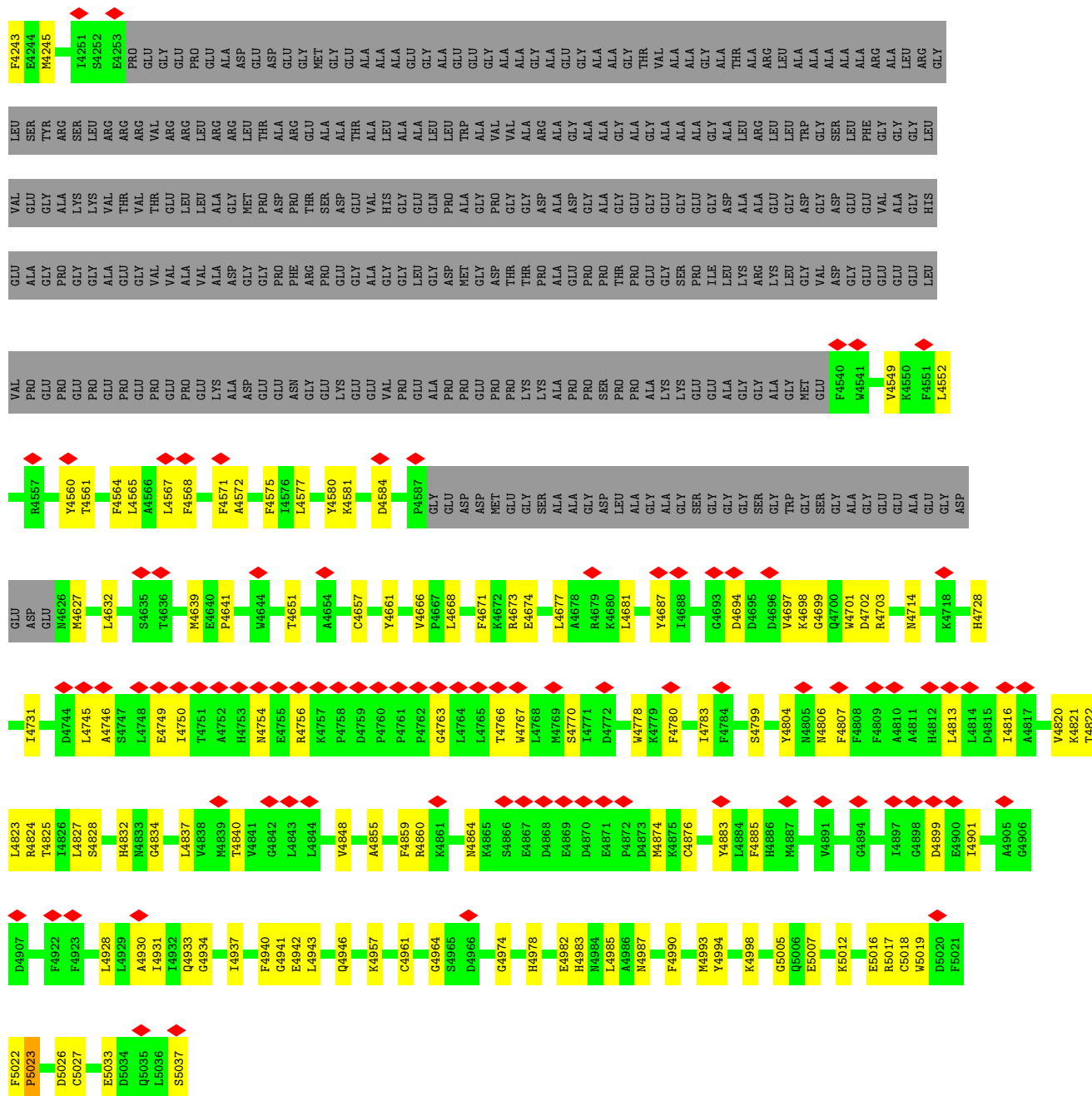




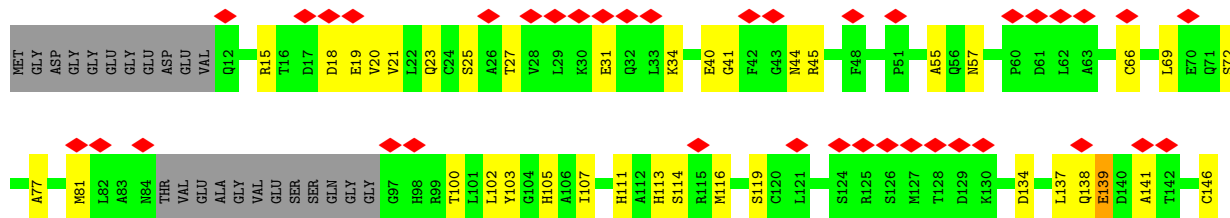
TLE	D2782	X2459	G2375	G2304	P2091	C2021	L1927	I1866	V1783
SER	E2783	X2591	L2376	C2305	Q2092	P2022	L1931	E1867	A1784
GLN	X2693	X2600	L2377	G2306	Q2095	L2023	L1831	V1870	A1785
THR	X2694	X2601	A2378	L2307	V2102	E2024	P1932	F1871	L1786
ALA	X2695	X2602	A2379	Q2308	V2103	E2025	V1935	T1872	P1787
GLN	X2696	X2603	T2380	S2309	R2104	L2026	F1946	E1873	A1788
THR	X2697	X2604	E2381	C2310	Q2107	R2028	E1950	ALA	ALA
TYR	X2698	X2605	T2384	P2311	E2222	L2039	L1951	GLY	GLY
ASP	X2699	X2606	E2388	M2312	E2223	C2042	Q1952	VAL	VAL
PRO	X2700	X2610	D2389	A2315	I2223	C2043	Q1953	ALA	ALA
GLU	X2701	X2614	D2390	K2316	L2116	L2044	R1954	E1793	E1793
GLY	X2702	X2617	A2391	G2317	M2120	Q2045	R1955	GLU	GLU
Y2855	X2703	X2618	P2395	Y2318	F2121	L2046	R1964	GLU	GLU
Y2856	X2704	X2619	GLY	P2320	L2124	E2047	Y1965	GLU	GLU
P2857	X2705	X2620	VAL	I2321	Q2127	Q2048	K1968	GLU	GLU
Q2858	X2706	X2621	ARG	D2326	Y2128	GLU	L1969	GLU	GLU
P2859	X2707	X2622	ARG	G2327	G2132	GLU	Q1970	GLU	GLU
P2860	X2708	X2623	ASP	R2330	R2136	PRO	Q1973	GLU	GLU
L2861	X2709	X2624	ARG	Y2331	R2140	GLU	R1976	ASP	P1803
K2795	X2710	X2625	HIS	L2332	A2141	THR	Y1977	GLU	L1804
K2796	X2711	X2626	GLY	L2335	S2147	LEU	A1978	GLU	E1805
K2797	X2712	X2627	GLU	A2338	L2155	SER	M1981	GLU	E1806
K2798	X2713	X2628	GLU	V2339	C2158	LEU	R1982	GLU	L1807
K2799	X2714	X2629	PRO	F2340	R2163	LEU	A1983	GLU	R1808
K2800	X2715	X2630	PRO	V2341	L2166	GLU	F1984	GLU	L1812
K2801	X2716	X2631	GLU	N2342	Q2169	THR	T1985	GLU	E1813
K2802	X2717	X2632	N2414	G2343	M2170	VAL	T1986	GLU	G1822
K2803	X2718	X2633	R2415	E2344	Q2173	LYS	S1987	GLU	G1823
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K2805	X2720	X2635	A2428	E2346	N2176	LYS	A1989	GLU	H1825
K2806	X2721	X2636	L2432	V2347	Q2180	VAL	E1990	ALA	D1828
K2807	X2722	X2637	C2436	N2349	Q2184	LYS	T1991	GLU	P1829
K2808	X2723	X2638	A2437	A2350	N2187	LYS	F1998	GLU	V1830
K2809	X2724	X2639	P2438	N2351	N2188	GLU	P2002	LYS	F1838
K2810	X2725	X2640	H2441	N2355	N2189	GLU	Q2003	LYS	V1839
K2811	X2726	X2641	A2445	L2356	N2191	GLU	Q2005	GLU	P1840
K2812	X2727	X2642	Q2446	K2359	F2192	GLU	I2006	GLU	V1841
K2813	X2728	X2643	K2447	P2360	Q2193	GLU	N2007	GLU	L1842
K2814	X2729	X2644	R2451	P2361	M2198	GLU	M2008	GLU	L1843
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K2816	X2731	X2646	I2456	C2363	Q2199	GLU	L2010	ALA	L1848
K2817	X2732	X2647	R2459	F2364	Q2199	GLU	L2011	GLY	G1852
K2818	X2733	X2648	X2459	A2367	Q2199	GLU	L2012	LYS	I1853
K2819	X2734	X2649	X2459	L2368	Q2199	GLU	A2016	GLU	D1856
K2820	X2735	X2650	X2459	K2369	Q2199	GLU	D2017	GLU	E1857
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K2822	X2737	X2652	X2459	E2371	Q2199	GLU	E2019	GLU	V1859
K2823	X2738	X2653	X2459	G2372	Q2199	GLU	D2020	GLU	Q1861
K2824	X2739	X2654	X2459	G2373	Q2199	GLU		GLU	I1862
K2825	X2740	X2655	X2459	S2374	Q2199	GLU		GLU	L1863
K2826	X2741	X2656	X2459		Q2199	GLU		GLU	K1864
K2827	X2742	X2657	X2459		Q2199	GLU		GLU	M1865
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K2829	X2744	X2659	X2459		Q2199	GLU		GLU	
K2830	X2745	X2660	X2459		Q2199	GLU		GLU	
K2831	X2746	X2661	X2459		Q2199	GLU		GLU	
K2832	X2747	X2662	X2459		Q2199	GLU		GLU	
K2833	X2748	X2663	X2459		Q2199	GLU		GLU	
K2834	X2749	X2664	X2459		Q2199	GLU		GLU	
K2835	X2750	X2665	X2459		Q2199	GLU		GLU	
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K2837	X2752	X2667	X2459		Q2199	GLU		GLU	
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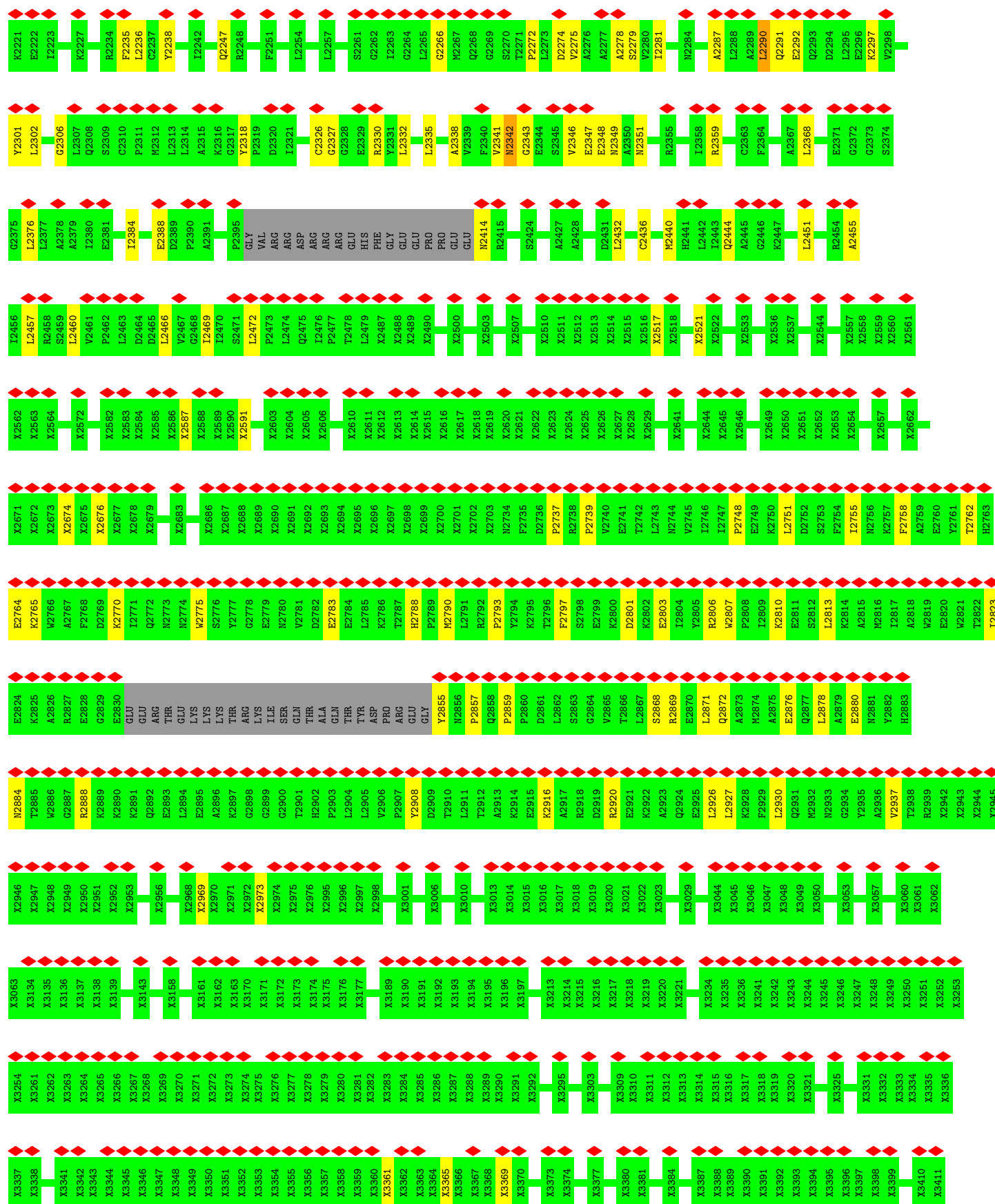


• Molecule 1: Ryanodine receptor 1

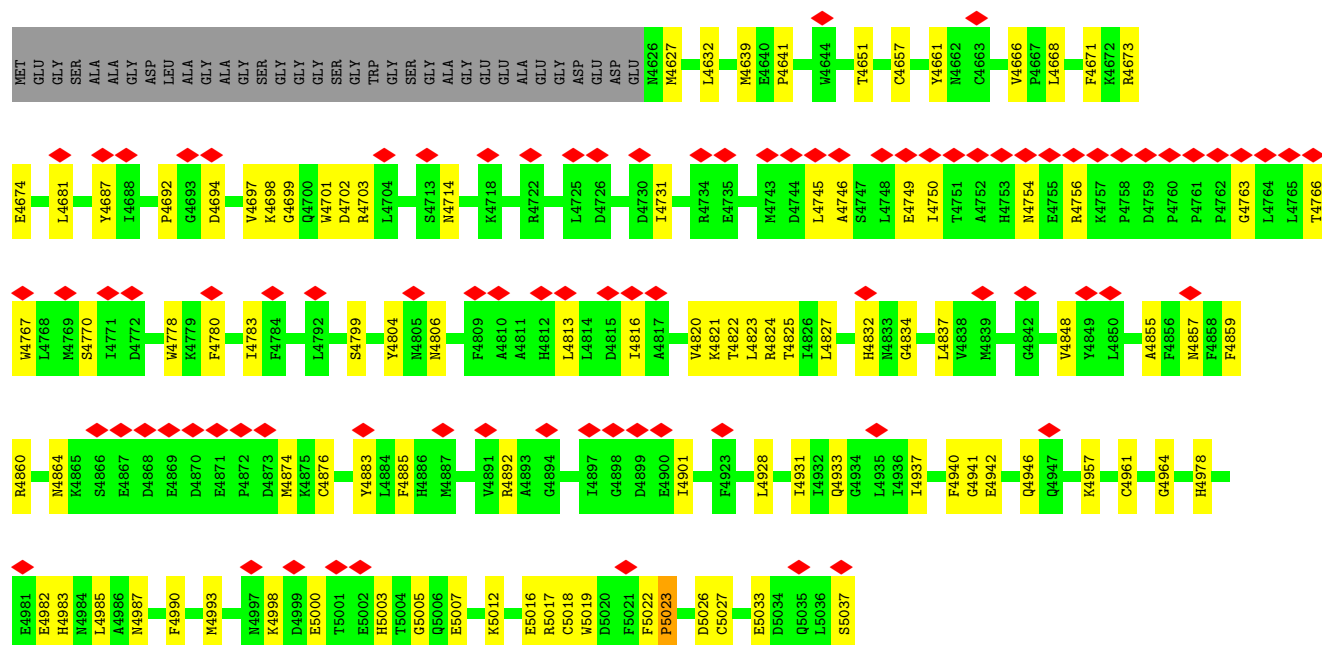




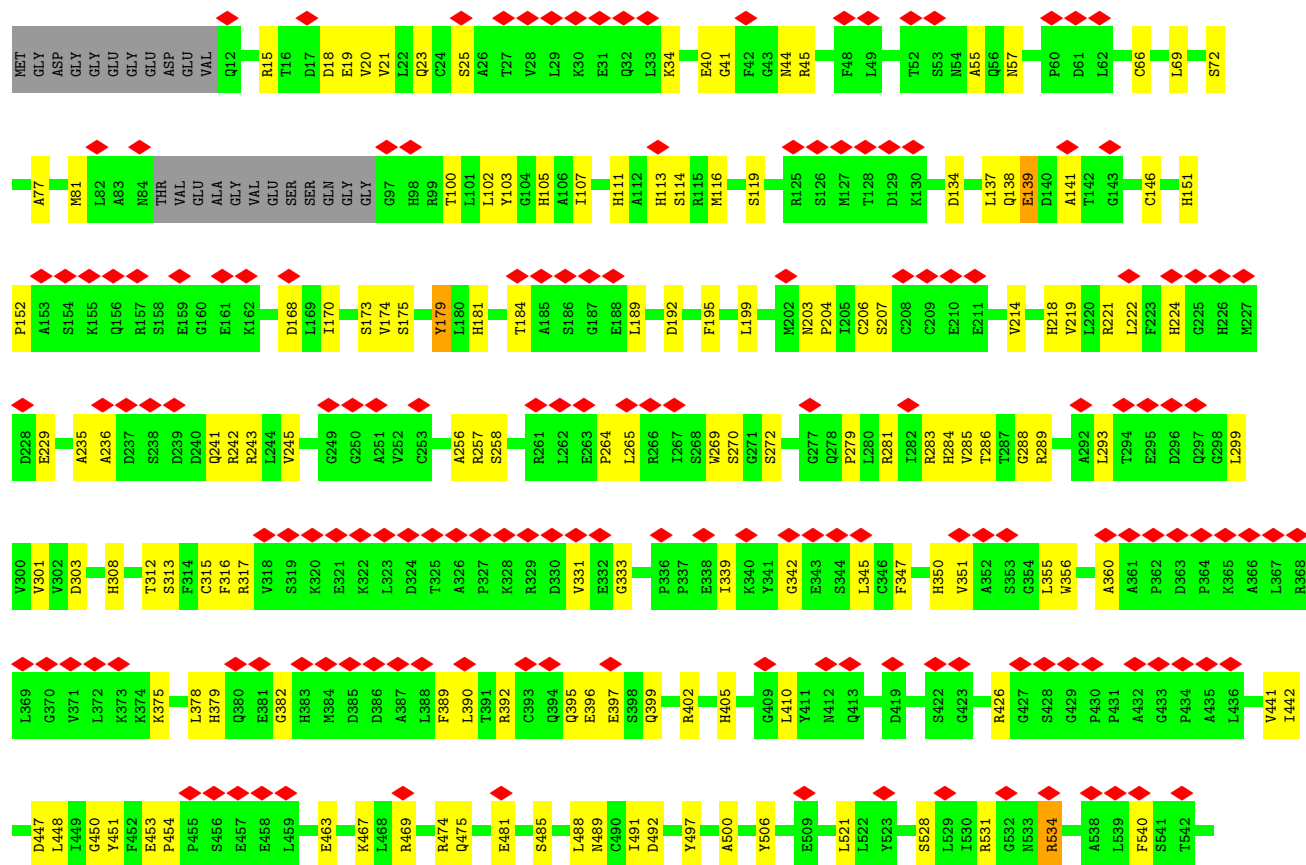


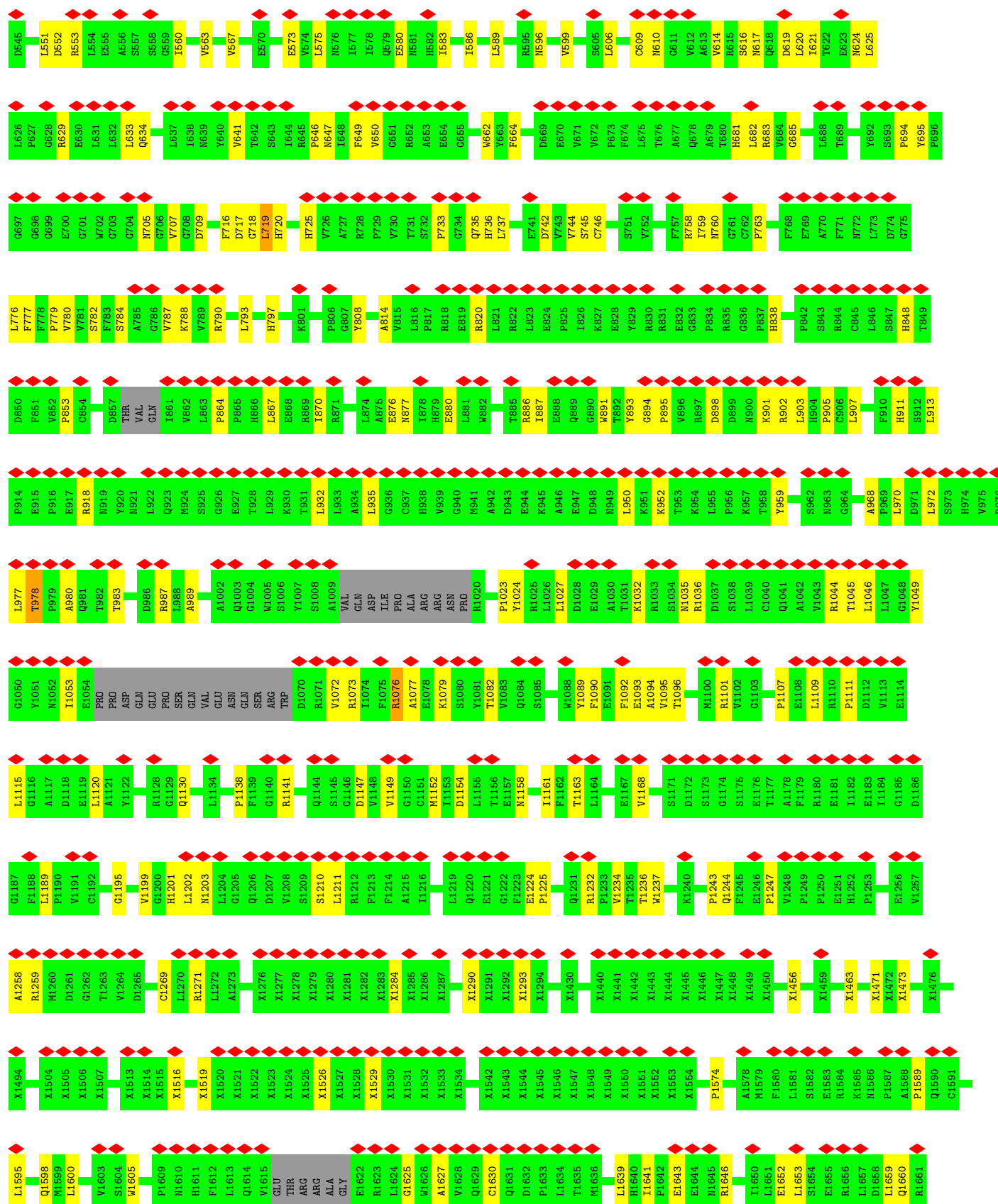


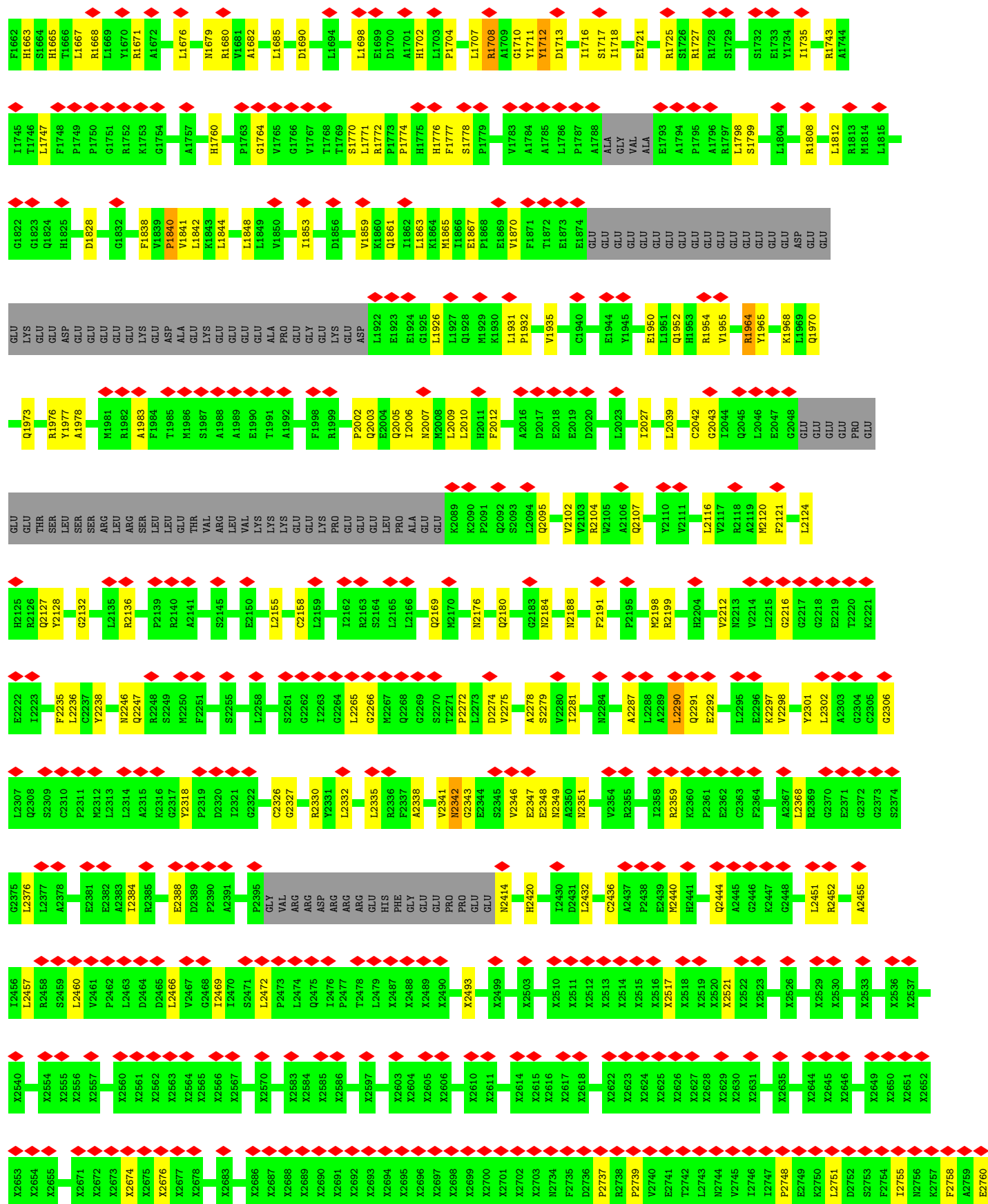




• Molecule 1: Ryanodine receptor 1

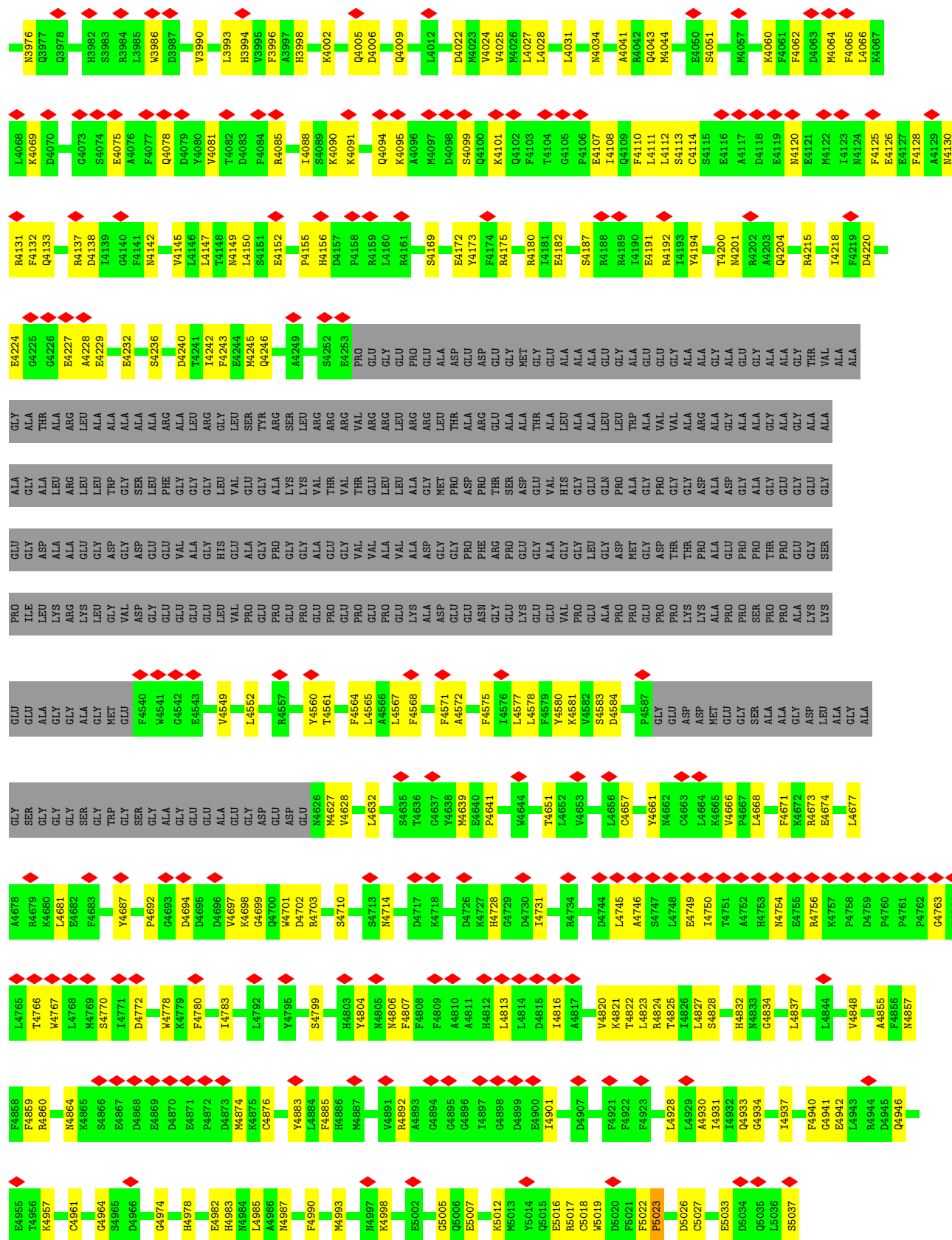




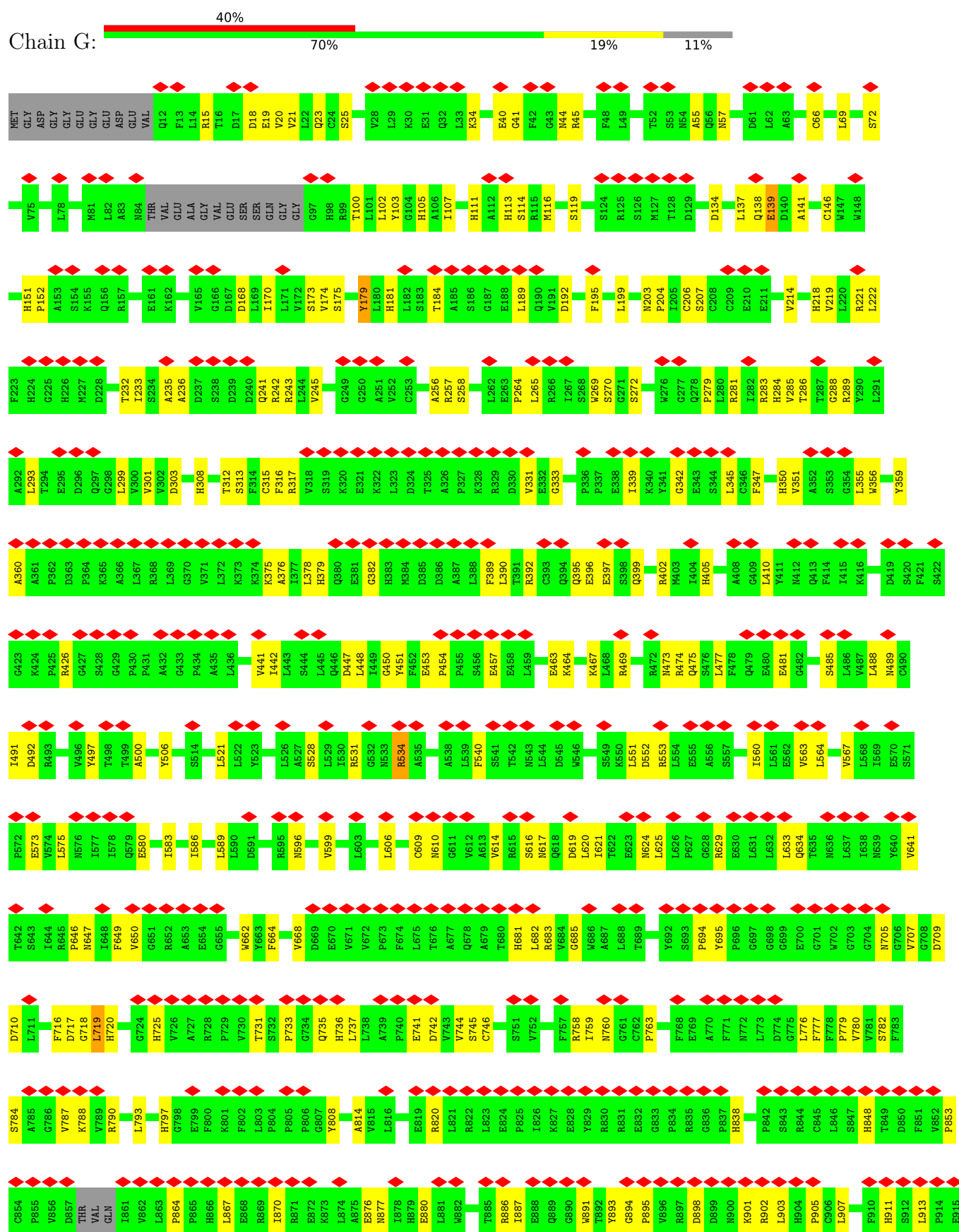




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X3314	X3317	X3318	X3319	X3320	X3323	X3327	X3330	X3331	X3336	X3336	X3337	X3338	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3365	X3369	X3372	X3373	X3376	X3380	X3383	X3386	X3387	X3390	X3391														
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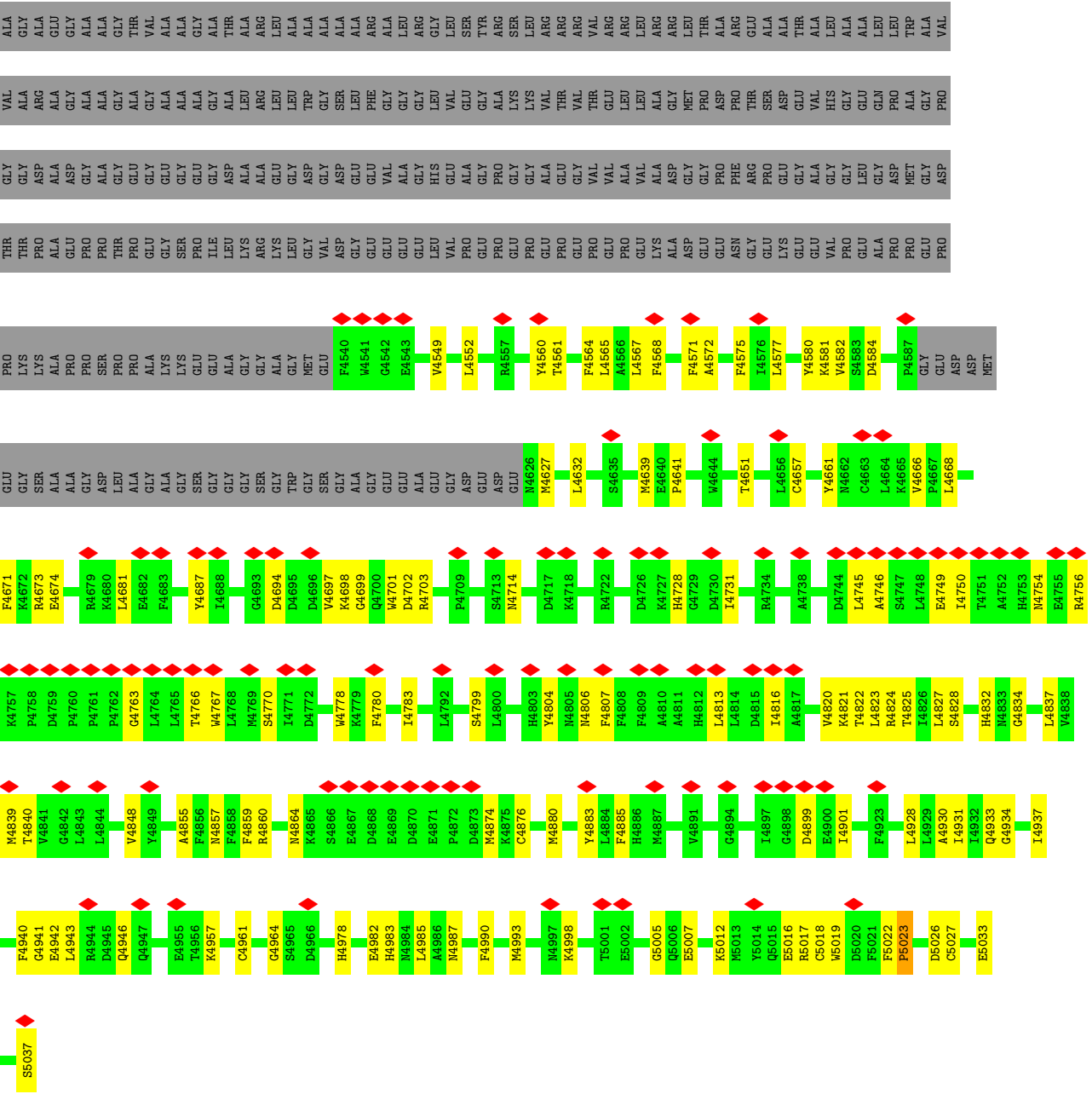
- Molecule 1: Ryanodine receptor 1



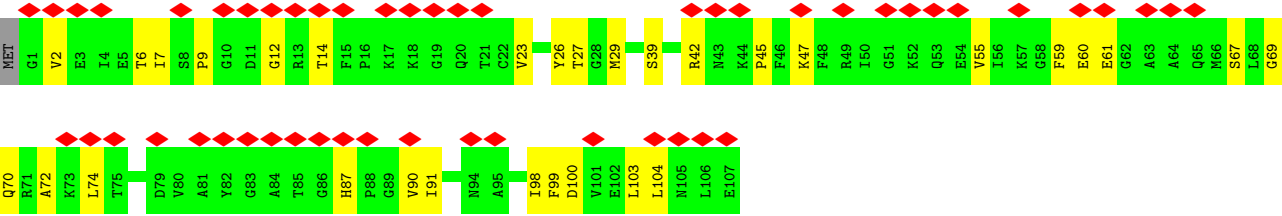




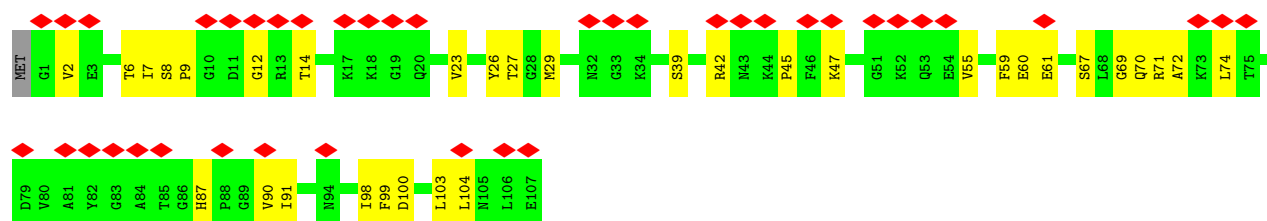
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Q4204	M4122	F4061	L3965	F3885	N3816	S3732	E3655	X3542	X3395	X3316	X3218	X3029
N4205	N4123	F4062	C3971	L3888	L3817	H3734	S3656	X3546	X3396	X3317	X3219	X3045
E4206	N4124	D4063	F3972	Q8889	D3818	L3735	T3657	X3552	X3397	X3318	X3220	X3046
R4215	F4125	M4064	C3973	L3890	Y3819	E3736	K3658	X3556	X3398	X3319	X3221	X3047
E4218	E4126	F4065	N3976	L3891	L3820	E3737	V3661	X3560	X3411	X3320	X3234	X3048
F4219	F4128	L4066	H3982	C3892	K3821	G3738	L3662	X3561	X3412	X3321	X3235	X3049
D4220	N4129	K4067	S3983	E3893	D3822	G3739	L3663	X3562	X3413	X3330	X3236	X3050
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G4225	R4131	K4069	R3985	N3897	Q3830	GLY	E3665	X3567	X3415	X3334	X3242	X3060
Q4226	F4132	I4070	L3986	D3898	GLU	ALA	E3666	X3568	X3419	X3335	X3243	X3061
A4228	Q4133	V4072	W3986	F3899	L3832	GLU	H3667	X3569	X3423	X3336	X3244	X3062
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S4236	D4138	E4075	G3991	Q3906	Q3837	E3748	T3674	X3572	X3426	X3341	X3247	X3135
D4240	N4142	F4076	F3992	T3910	S3840	V3749	D3675	X3576	X3427	X3342	X3248	X3136
F4243	V4143	Q4078	L3993	T3911	L3842	E3750	D3676	X3577	X3428	X3343	X3249	X3137
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E4253	N4148	D4083	K4002	L3926	E3848	E3755	E3684	X3585	X3433	X3348	X3254	X3142
PRO	F4149	P4084	Q4005	Q3927	E3849	E3757	E3685	X3586	X3434	X3349	X3255	X3170
GLY	N4150	R4085	D4006	E3928	Q3850	M3758	E3686	X3587	X3435	X3350	X3256	X3171
GLY	P4155	I4088	S4007	S3929	N3851	E3759	E3687	X3588	X3461	X3351	X3257	X3172
PRO	R4157	K4090	D4008	S3930	K3852	E3760	E3688	X3589	X3462	X3352	X3258	X3173
ALA	Q4094	Q4095	L4019	Y3935	E3854	R3762	V3690	X3590	X3463	X3353	X3259	X3174
ASP	K4096	M4023	D4022	Y3936	Q3855	R3769	E3691	X3591	X3464	X3354	X3270	X3175
GLU	N4097	V4024	M4026	Y3937	L3856	H3770	E3692	X3605	X3465	X3355	X3271	X3176
ASP	D4098	V4025	M4026	S3938	Q3857	T3772	K3693	X3606	X3466	X3356	X3272	X3177
GLU	S4099	L4027	K3940	G3939	N3858	R3773	H3704	X3607	X3467	X3357	X3273	X3178
GLU	K4100	L4028	D3941	K3940	N3860	E3776	R3707	X3608	X3468	X3358	X3274	X3179
GLY	Q4102	L4031	V3942	V3942	E3861	A3776	L3708	X3609	X3469	X3359	X3275	X3180
GLY	F4103	F4103	Q3945	Q3945	D3862	L3780	L3710	X3610	X3520	X3360	X3276	X3189
GLY	T4104	G4105	M4034	Q3946	Q3863	M3782	T3711	X3611	X3521	X3361	X3277	X3190
ALA	P4106	P4106	A4041	R3949	V3865	E3712	E3712	X3612	X3522	X3362	X3278	X3191
ALA	E4107	E4092	Q4043	N3950	L3866	S3714	K3713	X3613	X3523	X3363	X3279	X3192
GLY	I4108	M4044	F3951	F3951	N3867	K3715	L3716	X3614	X3524	X3364	X3280	X3193
ALA	Q4109	L4048	H3955	H3955	R3868	K3717	G3788	X3615	X3525	X3365	X3281	X3194
GLU	F4110	L4049	K3959	K3959	Q3869	L3718	E3789	X3616	X3526	X3366	X3282	X3195
GLU	L4112	L4112	Q4050	Q4050	N3870	D3717	D3718	X3641	X3527	X3367	X3283	X3196
GLY	S4115	S4115	V3961	V3961	C3871	D3719	D3719	Y3642	X3528	X3368	X3284	X3197
E4116	E4116	E4116	F3962	F3962	E3872	V3720	V3720	N3643	X3529	X3369	X3285	X3198
D4117	D4117	D4117			K3723	Y3642	Y3642	X3643	X3530	X3370	X3286	X3199
E4118	E4118	E4118			A3724	T3646	T3646	X3644	X3531	X3371	X3287	X3200
E4119	E4119	E4119			A3726	H3647	H3647	X3645	X3532	X3372	X3288	X3213
					D3727	R3648	R3648		X3533	X3373	X3289	X3214
									X3534	X3374	X3290	X3215
									X3535	X3375	X3291	
										X3376	X3292	
										X3377	X3293	
										X3378	X3294	
										X3379	X3295	
										X3380	X3296	
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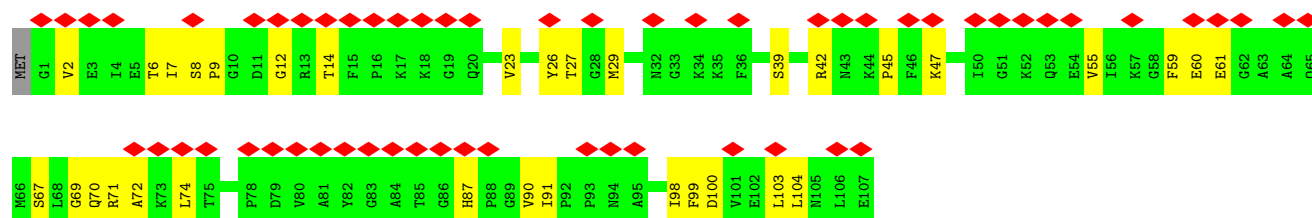
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



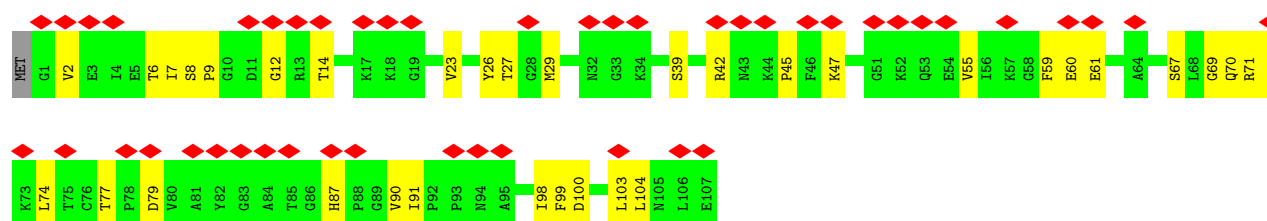
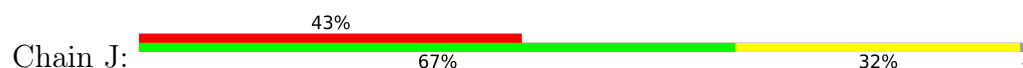
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.535	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.166	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	B	0.35	0/25428	0.59	6/34534 (0.0%)
1	E	0.35	0/25428	0.59	6/34534 (0.0%)
1	G	0.35	0/25428	0.59	6/34534 (0.0%)
1	I	0.35	0/25428	0.59	6/34534 (0.0%)
2	A	0.35	0/834	0.61	0/1123
2	F	0.35	0/834	0.61	0/1123
2	H	0.35	0/834	0.61	0/1123
2	J	0.35	0/834	0.61	0/1123
All	All	0.35	0/105048	0.59	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	B	0	22
1	E	0	22
1	G	0	22
1	I	0	22
All	All	0	88

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1667	LEU	CA-CB-CG	6.67	130.64	115.30
1	B	1667	LEU	CA-CB-CG	6.66	130.62	115.30
1	G	1667	LEU	CA-CB-CG	6.64	130.56	115.30
1	I	1667	LEU	CA-CB-CG	6.62	130.53	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	977	LEU	CA-CB-CG	5.60	128.18	115.30

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	GLU	Peptide
1	B	179	TYR	Peptide
1	B	552	ASP	Peptide
1	B	694	PRO	Peptide
1	B	808	TYR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	29369	0	24717	498	0
1	E	29369	0	24716	494	0
1	G	29369	0	24717	506	0
1	I	29369	0	24717	497	0
2	A	818	0	824	19	0
2	F	818	0	824	19	0
2	H	818	0	824	19	0
2	J	818	0	824	20	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102163	2047	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 9.

The worst 5 of 2047 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:2318:TYR:HH	1:G:2414:ASN:N	1.80	0.79
1:I:2318:TYR:HH	1:I:2414:ASN:N	1.80	0.79
1:E:2318:TYR:HH	1:E:2414:ASN:N	1.81	0.79
1:B:2318:TYR:HH	1:B:2414:ASN:N	1.81	0.79
1:E:179:TYR:OH	1:G:2359:ARG:NH1	2.18	0.76

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	B	3235/4687 (69%)	2875 (89%)	355 (11%)	5 (0%)	47	81
1	E	3235/4687 (69%)	2874 (89%)	356 (11%)	5 (0%)	47	81
1	G	3235/4687 (69%)	2876 (89%)	354 (11%)	5 (0%)	47	81
1	I	3235/4687 (69%)	2876 (89%)	354 (11%)	5 (0%)	47	81
2	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
All	All	13360/19180 (70%)	11877 (89%)	1463 (11%)	20 (0%)	54	85

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1708	ARG
1	E	1708	ARG
1	I	1708	ARG
1	G	1708	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1932	PRO

### 5.3.2 Protein sidechains ⓘ

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	B	2493/3209 (78%)	2478 (99%)	15 (1%)	86	92
1	E	2493/3209 (78%)	2478 (99%)	15 (1%)	86	92
1	G	2493/3209 (78%)	2478 (99%)	15 (1%)	86	92
1	I	2493/3209 (78%)	2478 (99%)	15 (1%)	86	92
2	A	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	J	88/89 (99%)	88 (100%)	0	100	100
All	All	10324/13192 (78%)	10264 (99%)	60 (1%)	86	92

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4137	ARG
1	G	4034	ASN
1	I	1964	ARG
1	G	3896	ASN
1	G	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	4102	GLN
1	G	1973	GLN
1	I	4156	HIS
1	G	405	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	3946	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 8 ligands modelled in this entry, 8 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	E	12
1	B	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Number of breaks
1	I	12
1	G	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3613:UNK	C	3639:THR	N	45.91
1	B	3613:UNK	C	3639:THR	N	45.70
1	I	3613:UNK	C	3639:THR	N	45.65
1	G	3613:UNK	C	3639:THR	N	45.46
1	I	3163:UNK	C	3170:UNK	N	16.67

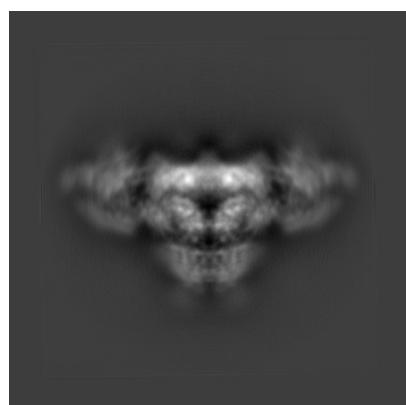
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20486. These allow visual inspection of the internal detail of the map and identification of artifacts.

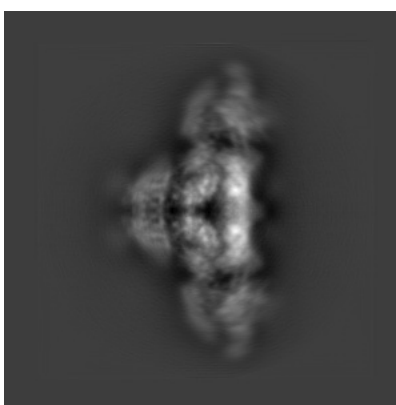
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

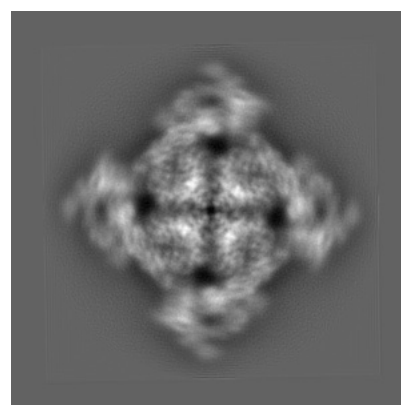
#### 6.1.1 Primary map



X



Y

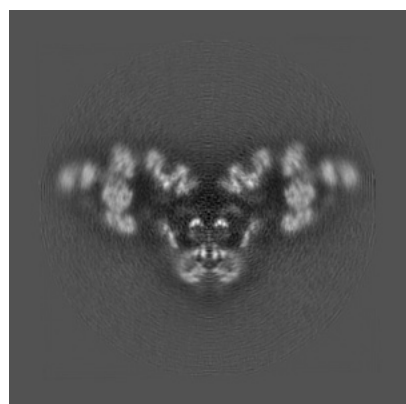


Z

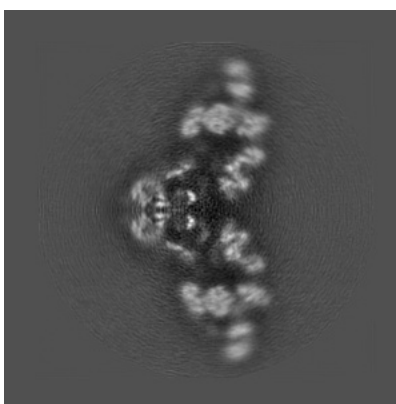
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

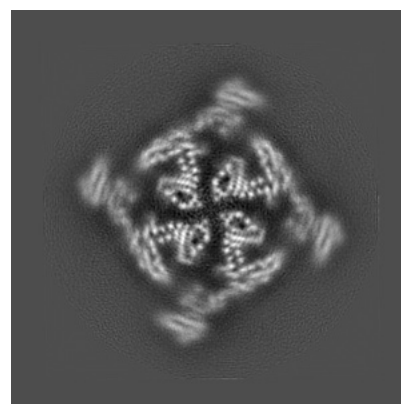
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



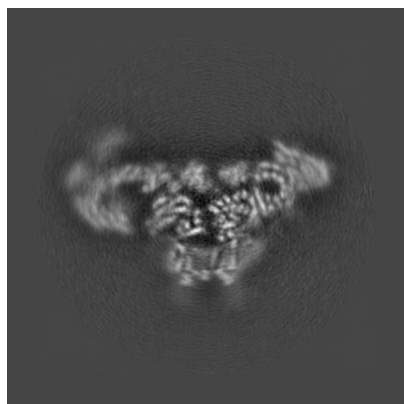
Z Index: 200



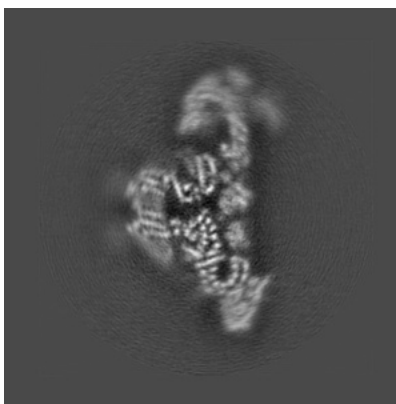
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

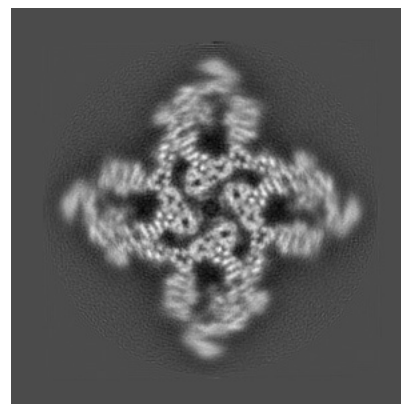
### 6.3.1 Primary map



X Index: 179



Y Index: 177



Z Index: 231

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

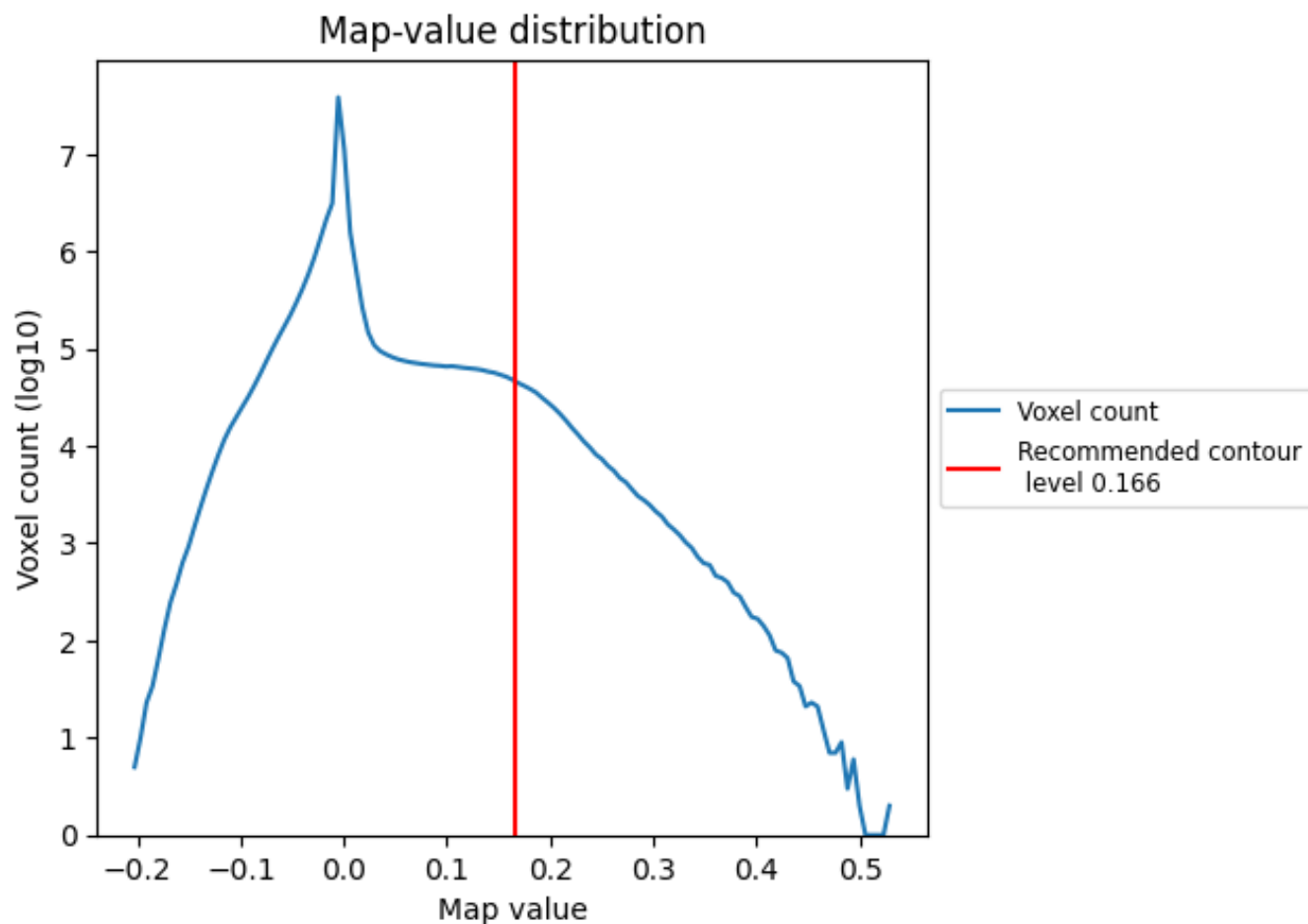
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

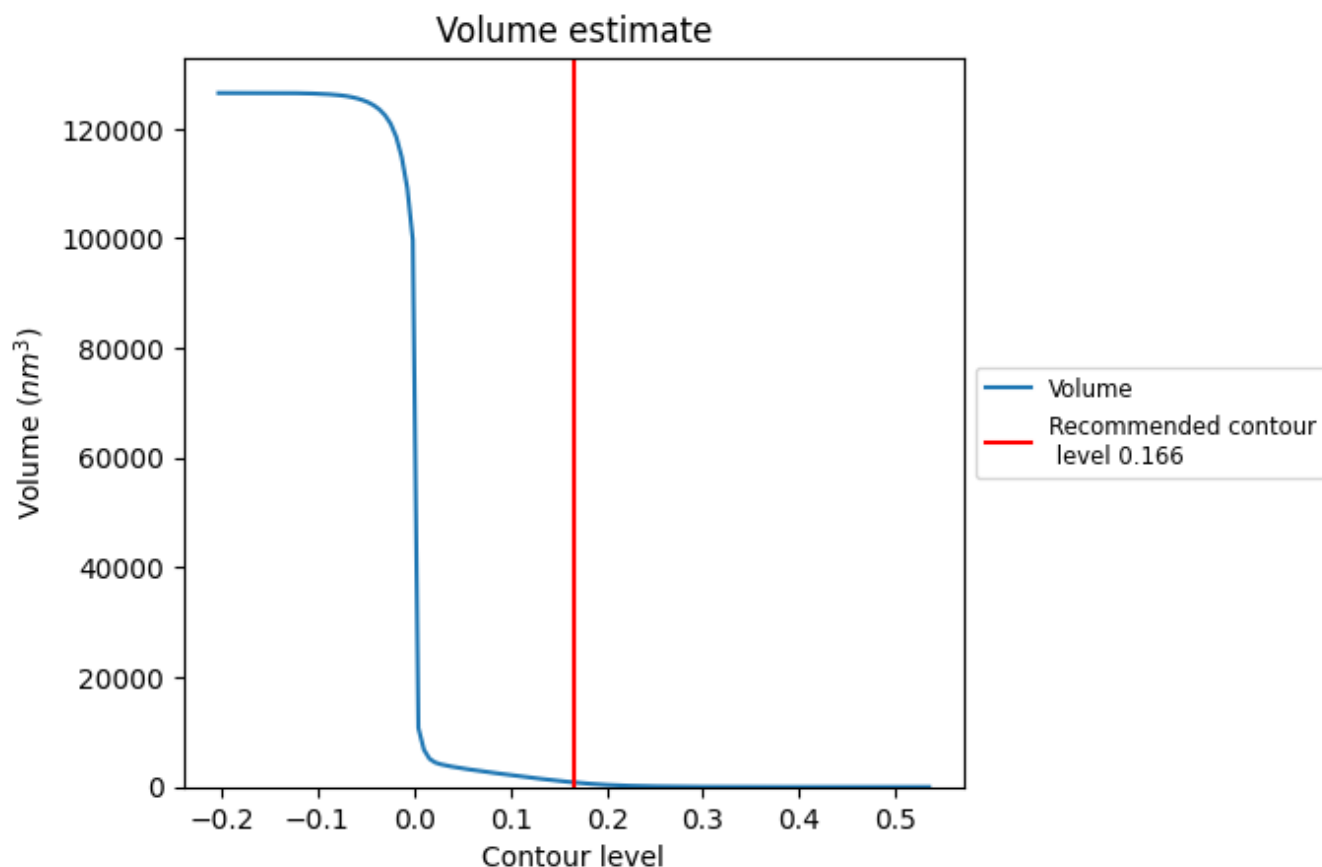
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

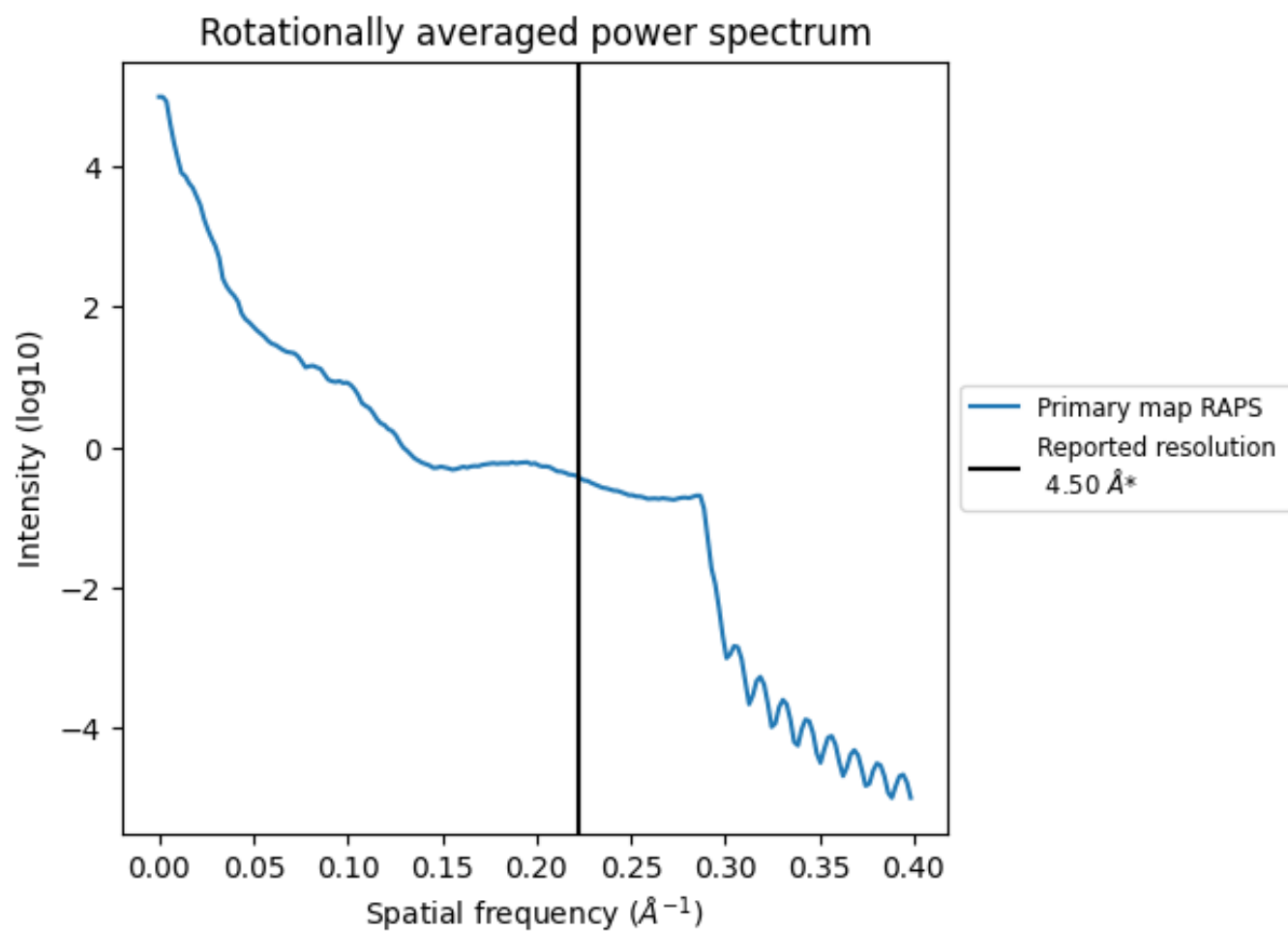
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm<sup>3</sup>; this corresponds to an approximate mass of 750 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

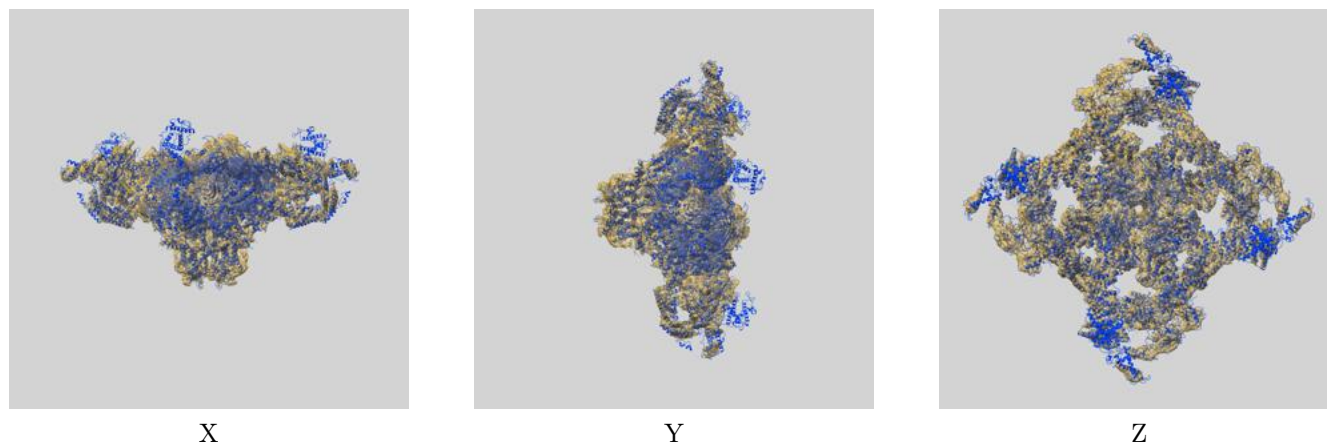
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

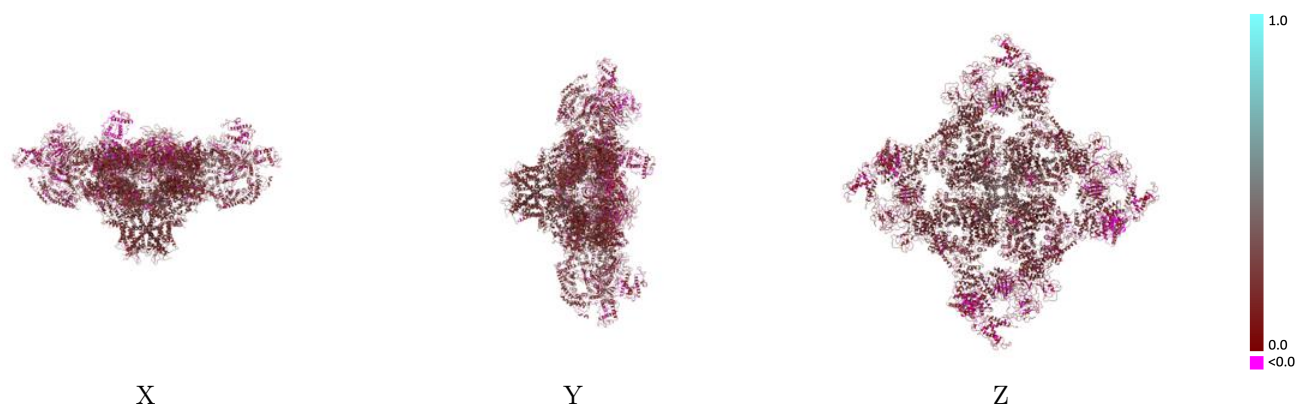
This section contains information regarding the fit between EMDB map EMD-20486 and PDB model 6PV6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



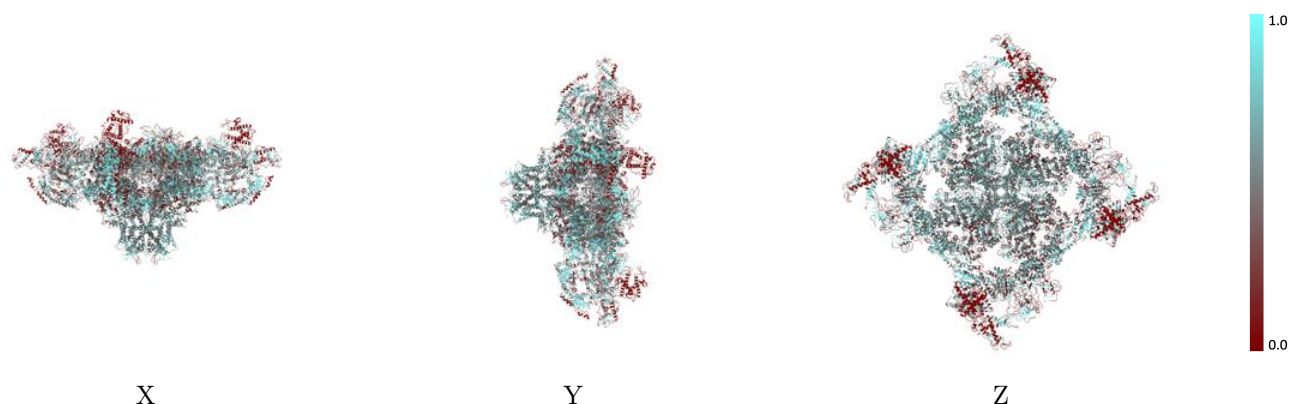
The images above show the 3D surface view of the map at the recommended contour level 0.166 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to 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.

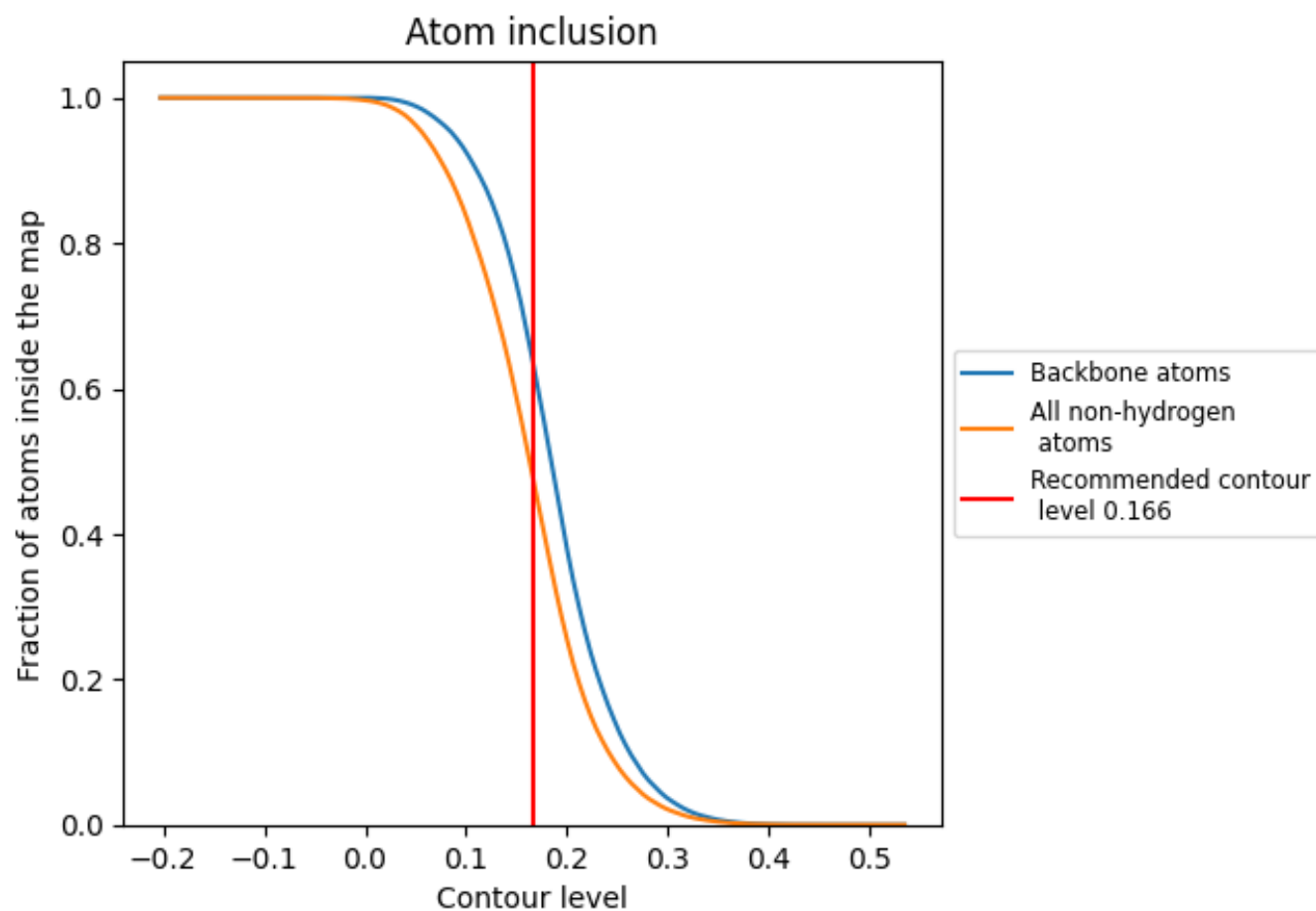
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.166).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.166) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4791	<div></div> 0.1800
A	<div></div> 0.4851	<div></div> 0.1850
B	<div></div> 0.4972	<div></div> 0.1950
E	<div></div> 0.4766	<div></div> 0.1780
F	<div></div> 0.4268	<div></div> 0.1320
G	<div></div> 0.4624	<div></div> 0.1660
H	<div></div> 0.4107	<div></div> 0.1400
I	<div></div> 0.4837	<div></div> 0.1860
J	<div></div> 0.4702	<div></div> 0.1810

1.0

0.0

<0.0