



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 01:18 AM UTC

PDB ID : 6PV6 / pdb_00006pv6
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

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

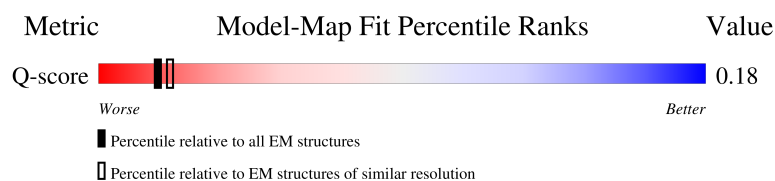
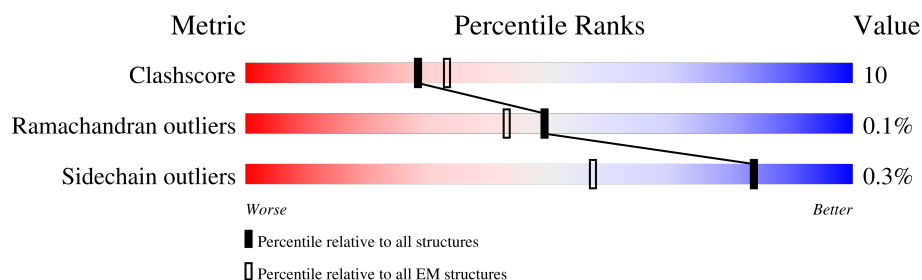
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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 $\leq 5\%$. 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	33% 70% 19% 11%
1	E	4687	37% 70% 19% 11%
1	G	4687	40% 70% 19% 11%
1	I	4687	36% 70% 19% 11%

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Mol	Chain	Length	Quality of chain
2	A	108	37%67%31%..
2	F	108	47%69%30%.
2	H	108	54%69%30%..
2	J	108	43%69%30%..

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest")

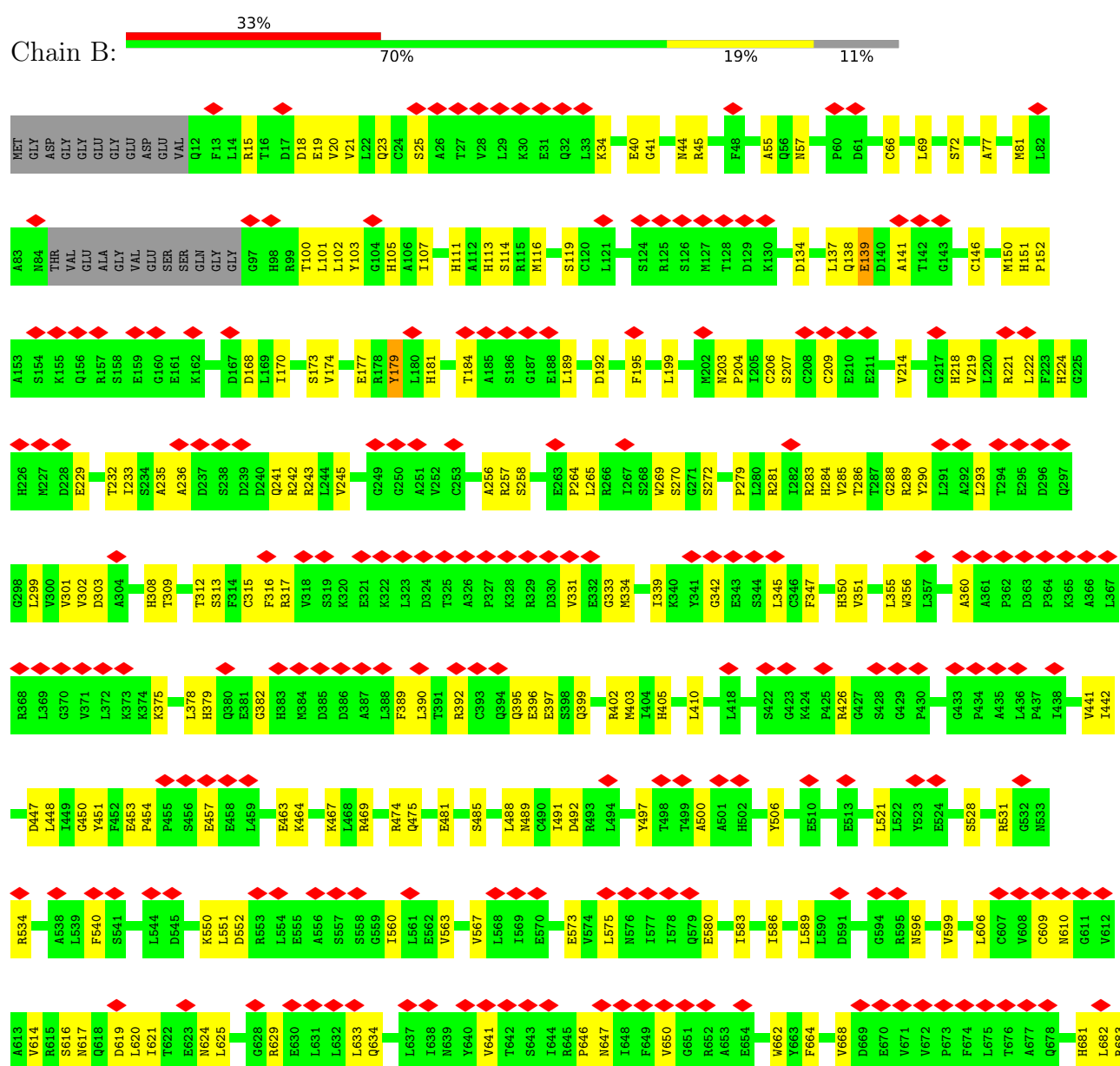
by depositor).

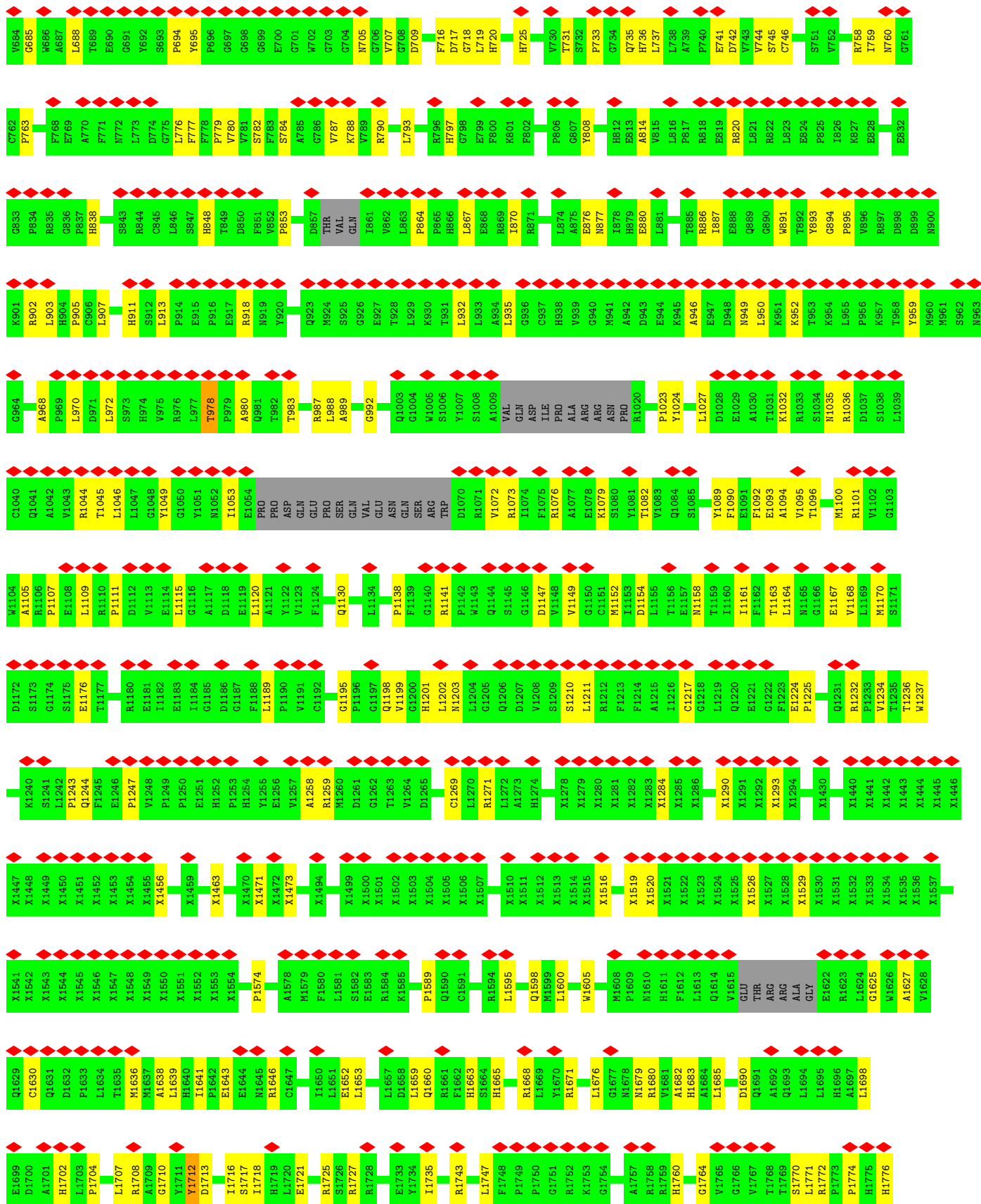
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

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.

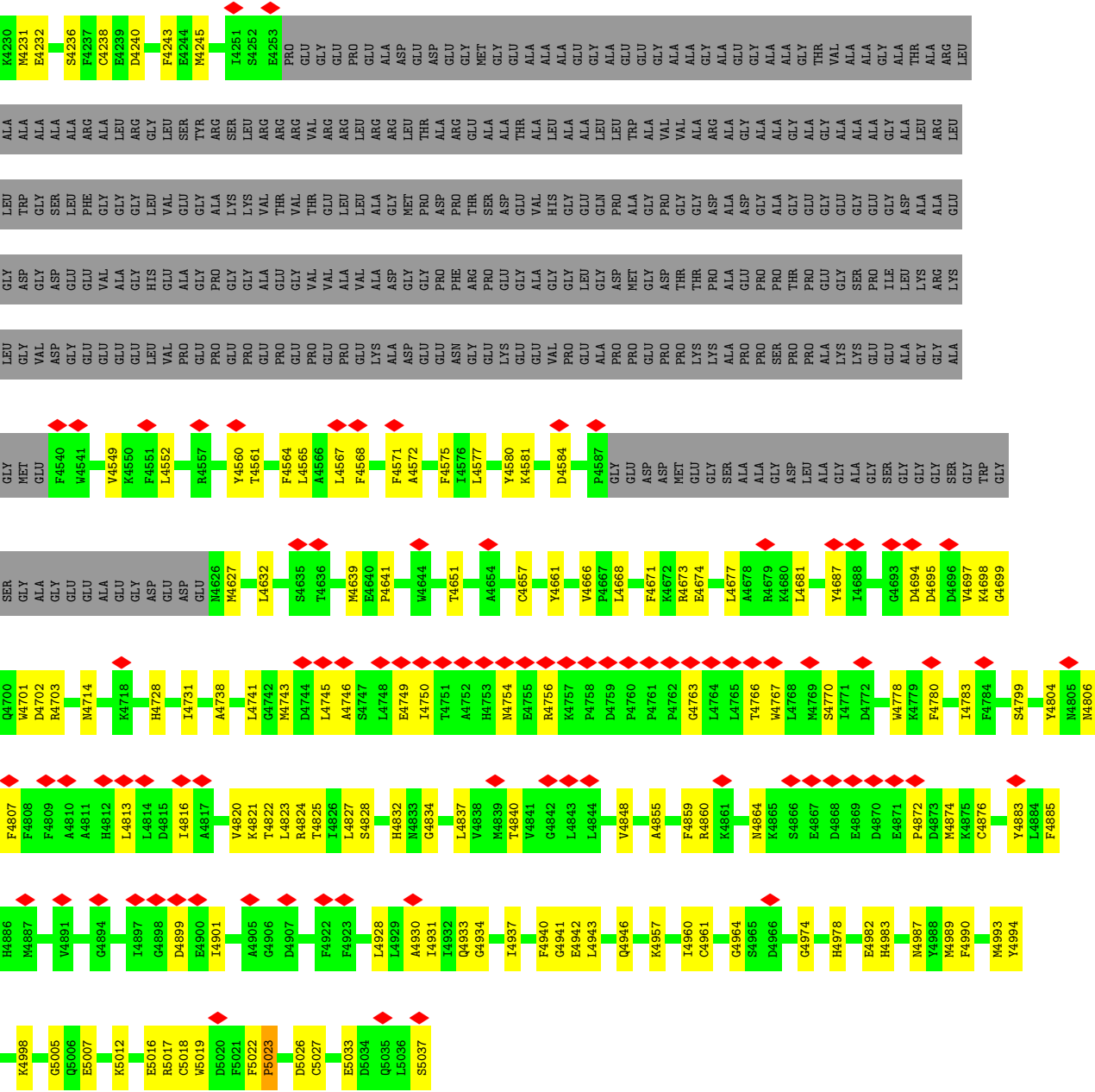
• Molecule 1: Ryanodine receptor 1



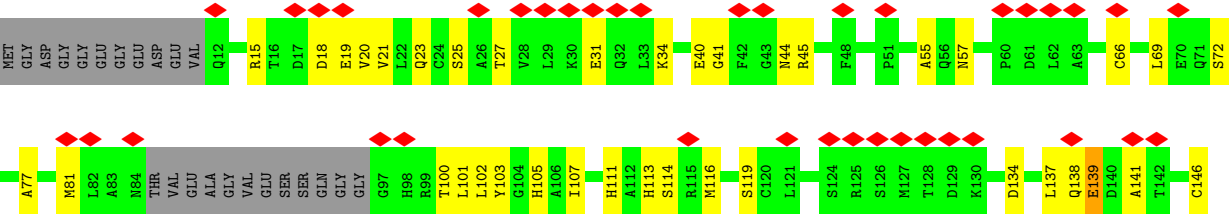




F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3251	X3140	X2956	F4065	R3949	T3864	L3770	E3687	X3576	X3428	X3343	X3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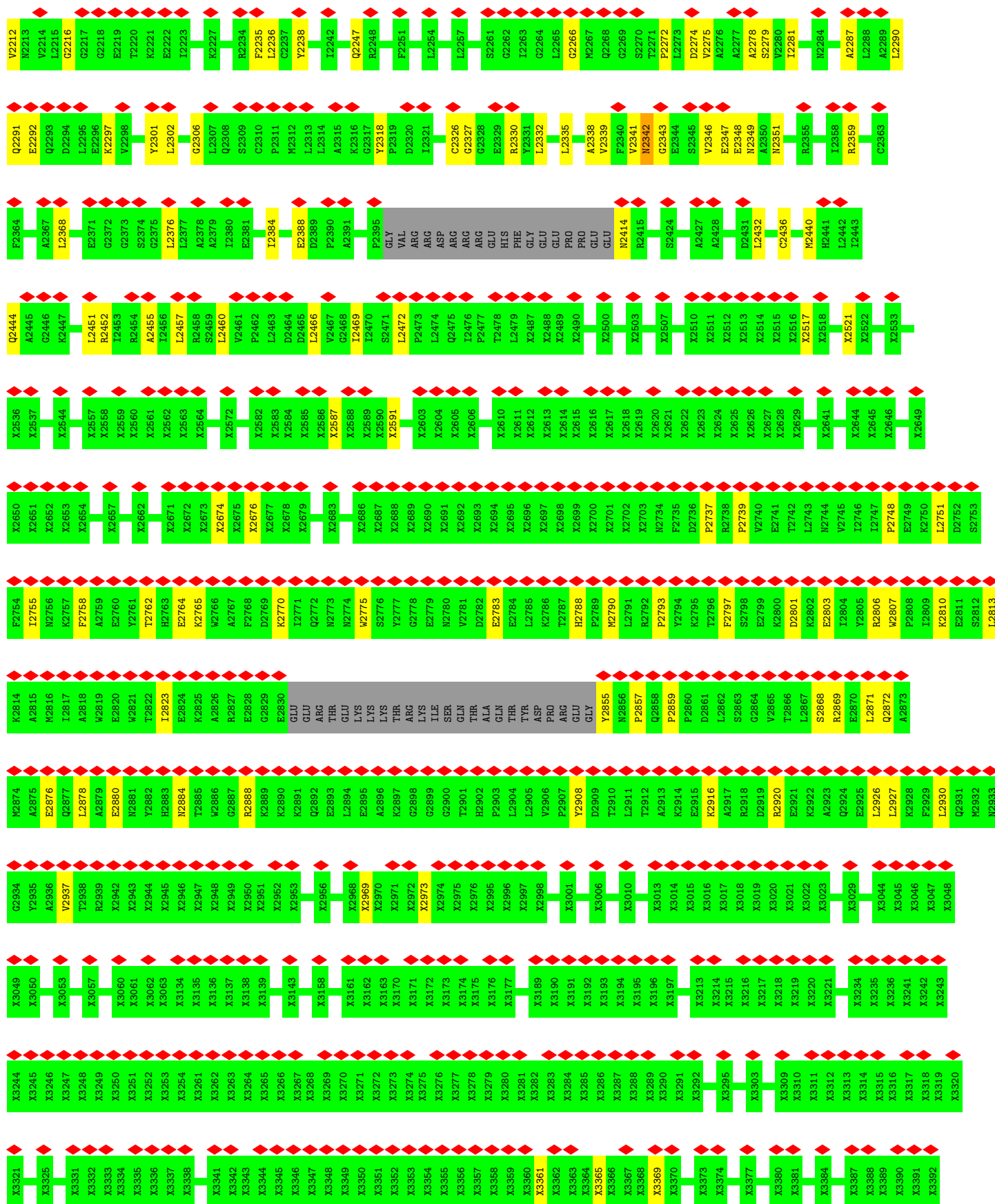


● Molecule 1: Ryanodine receptor 1

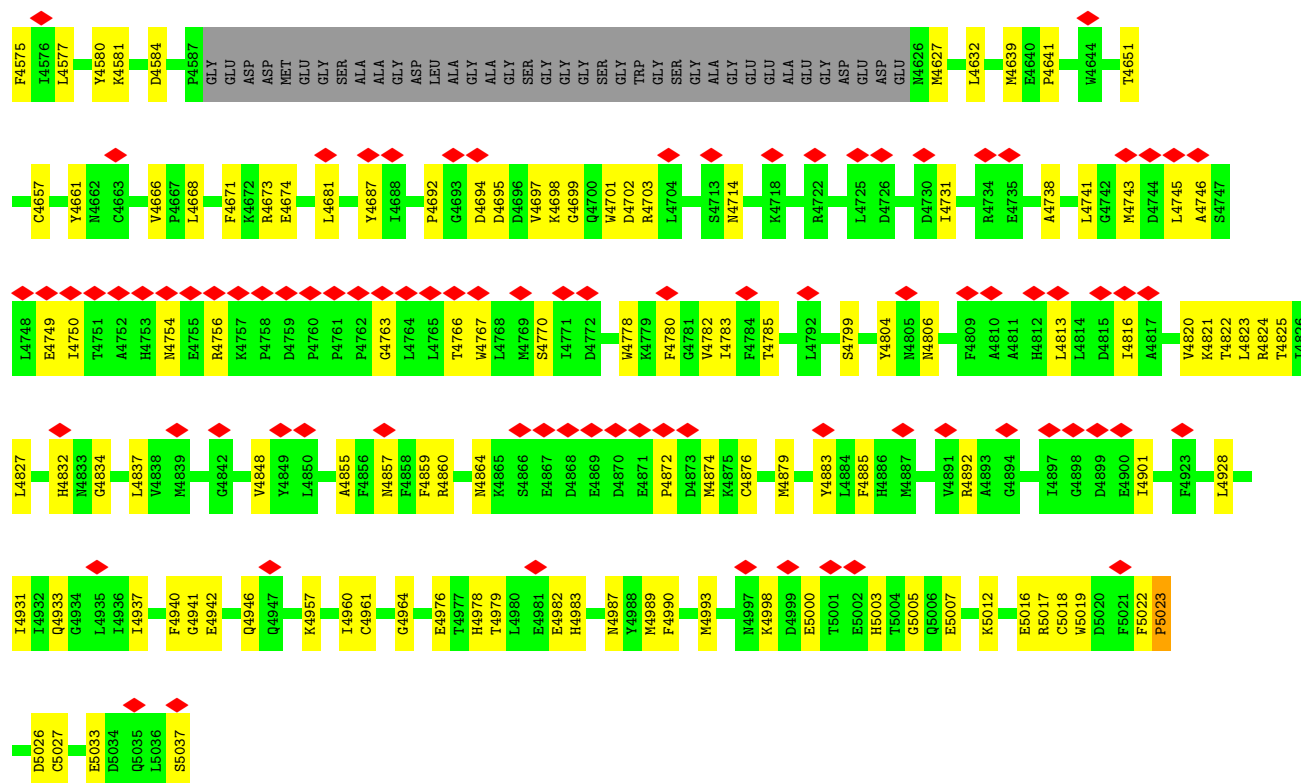




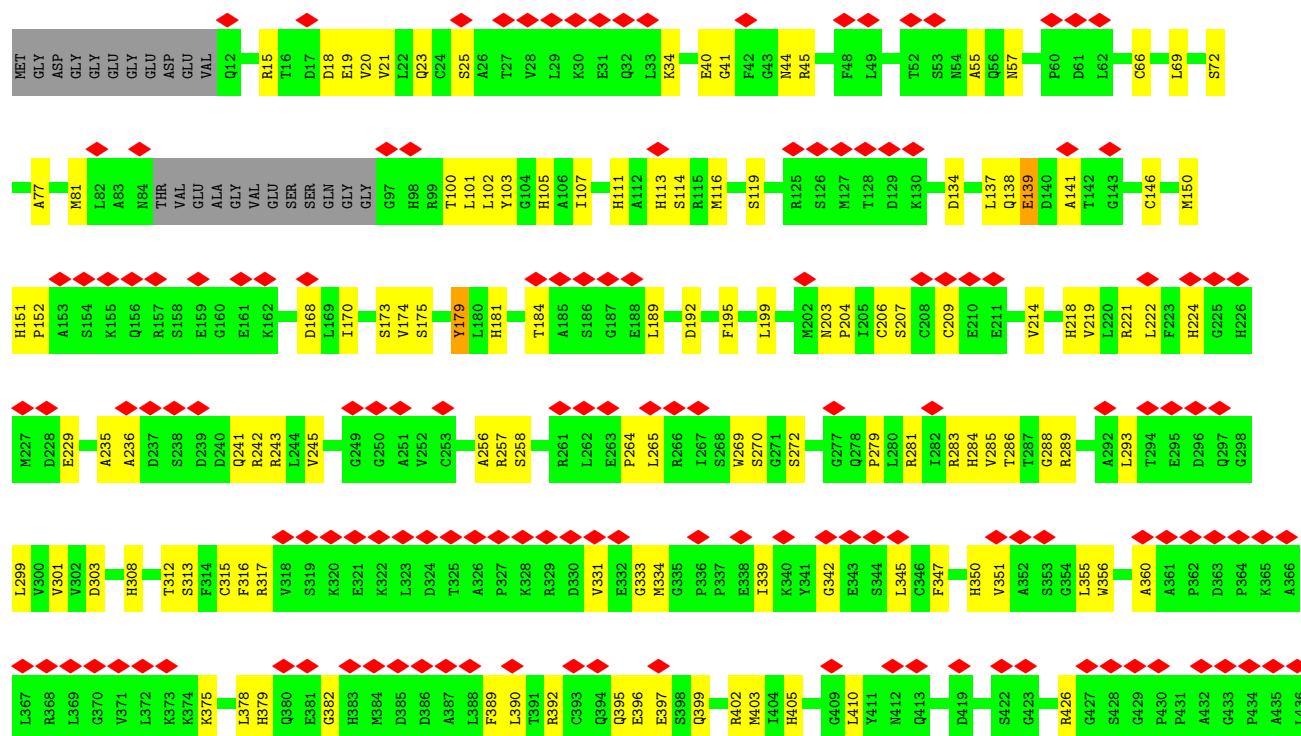


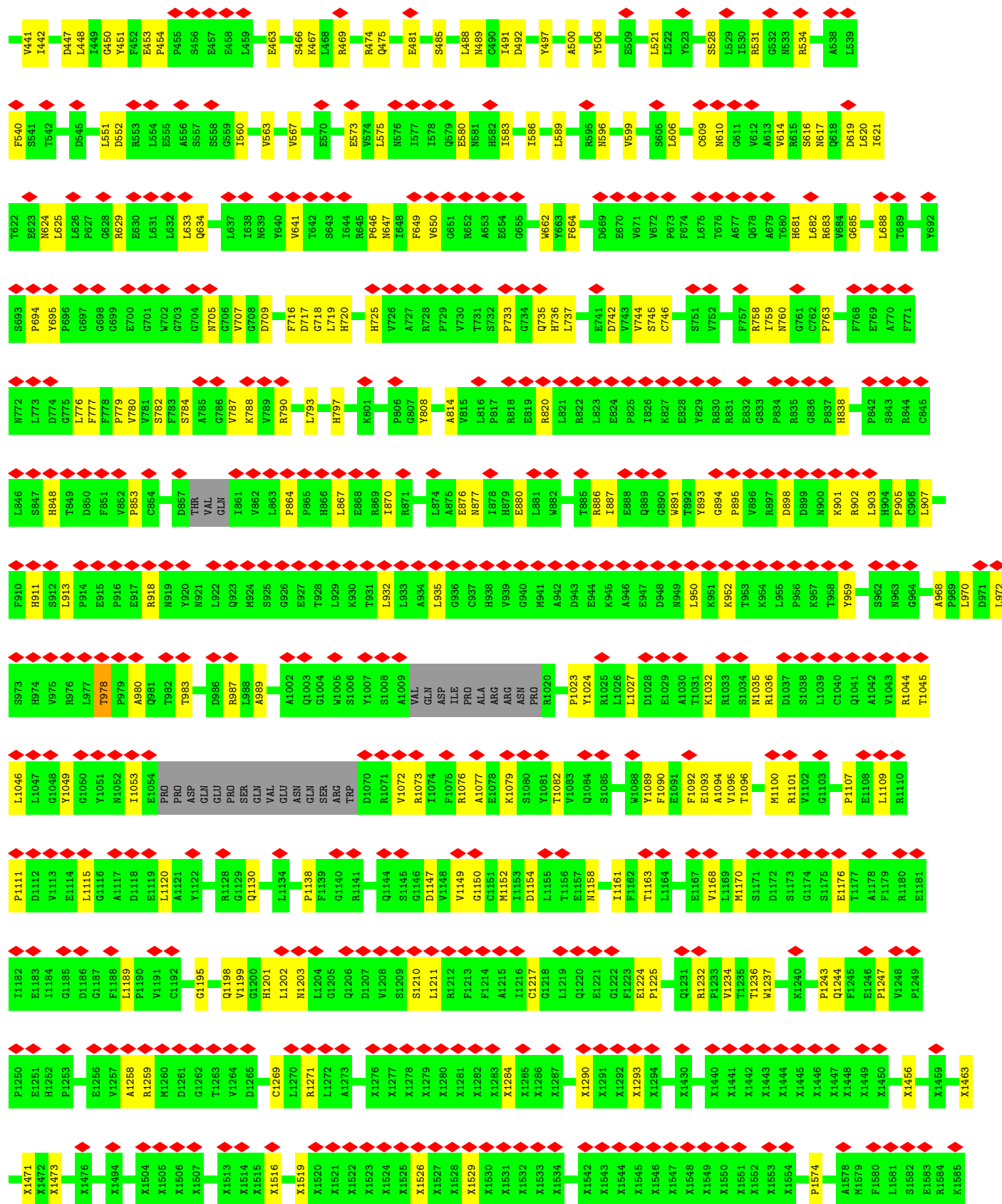


[illegible]



• Molecule 1: Ryanodine receptor 1

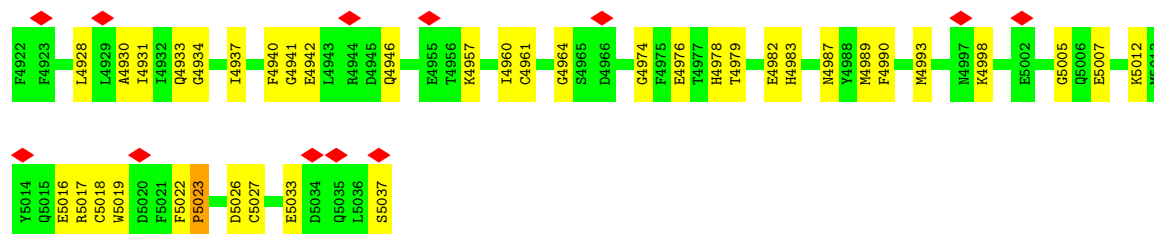




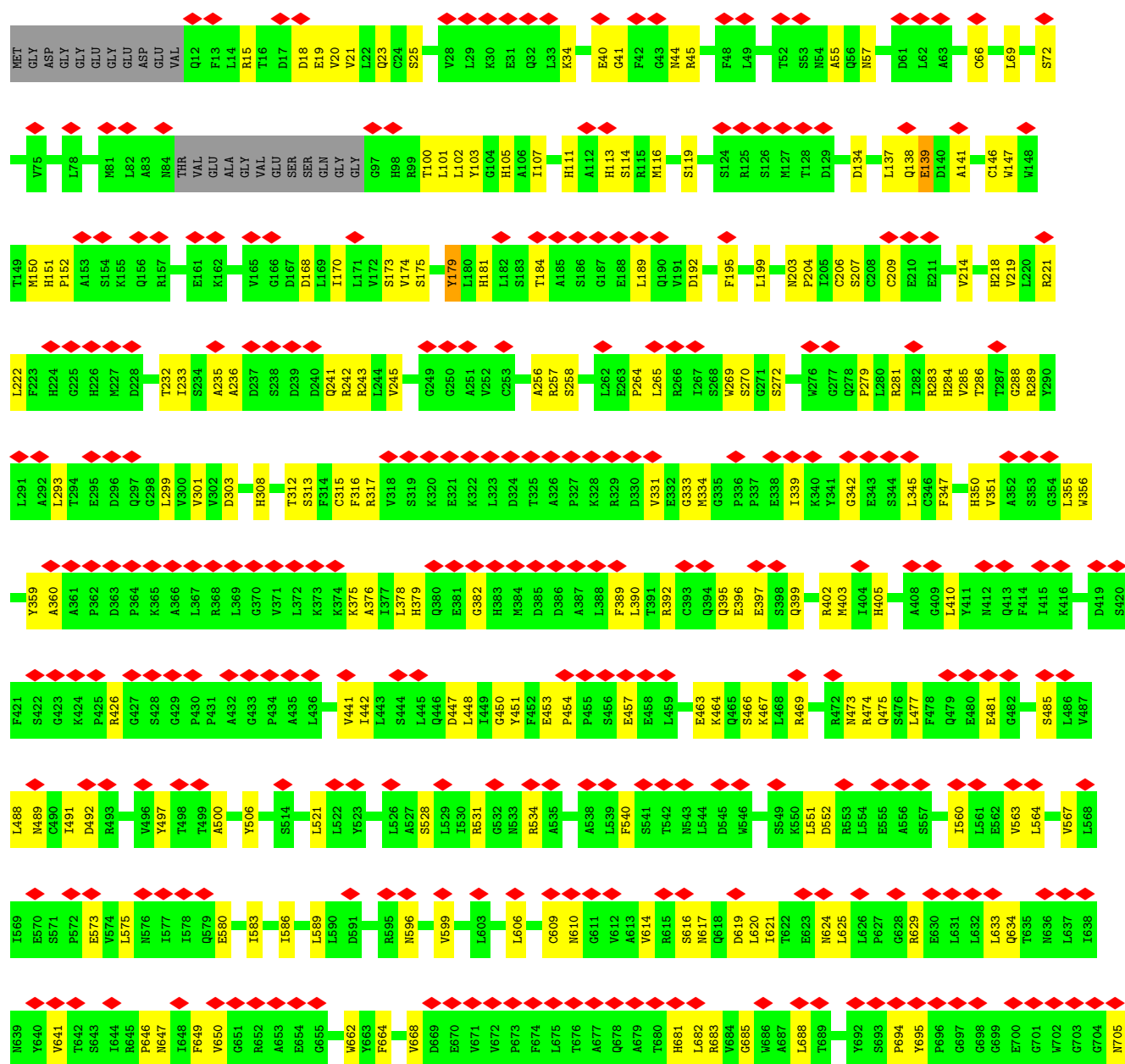
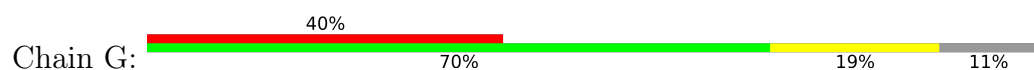


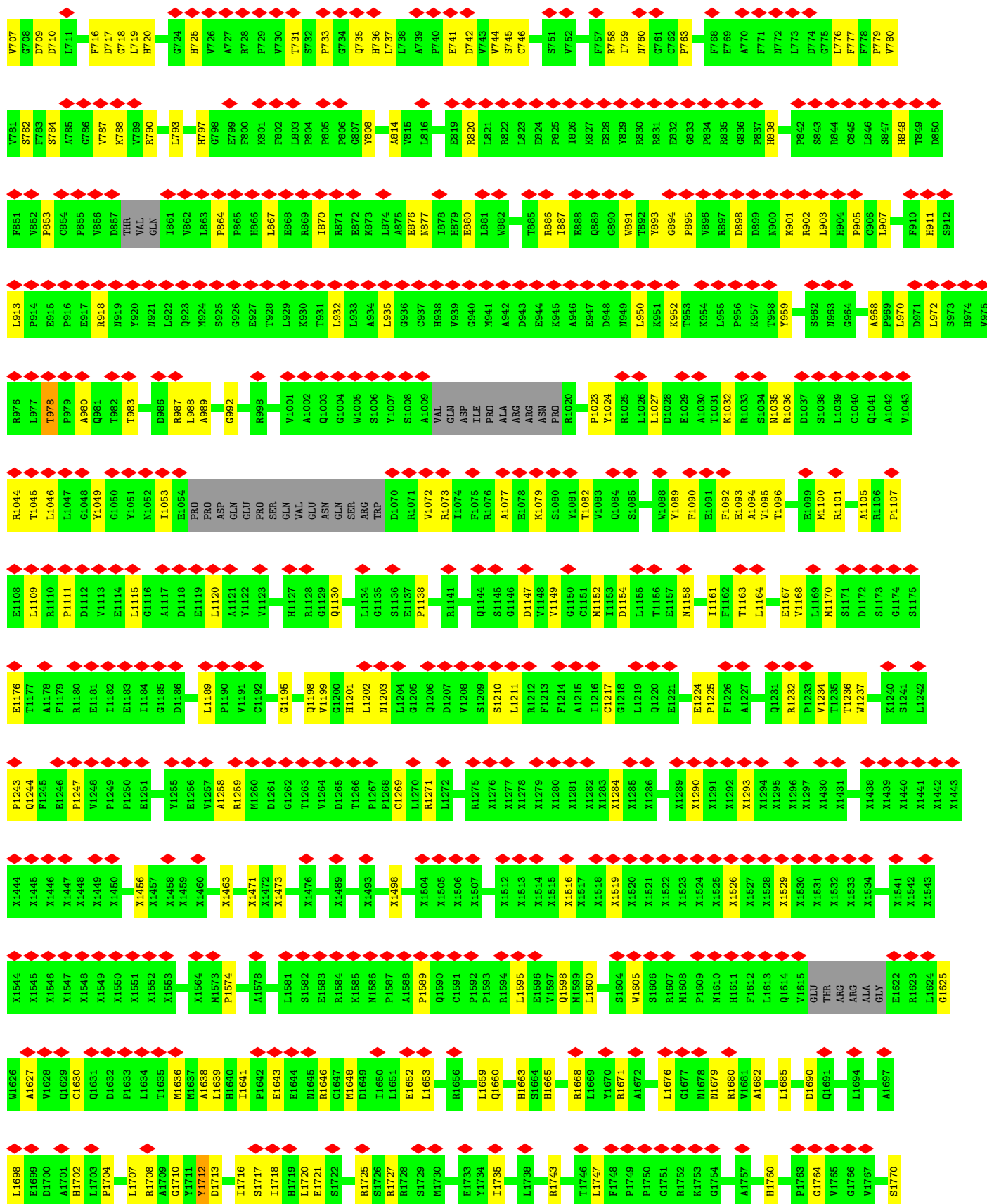






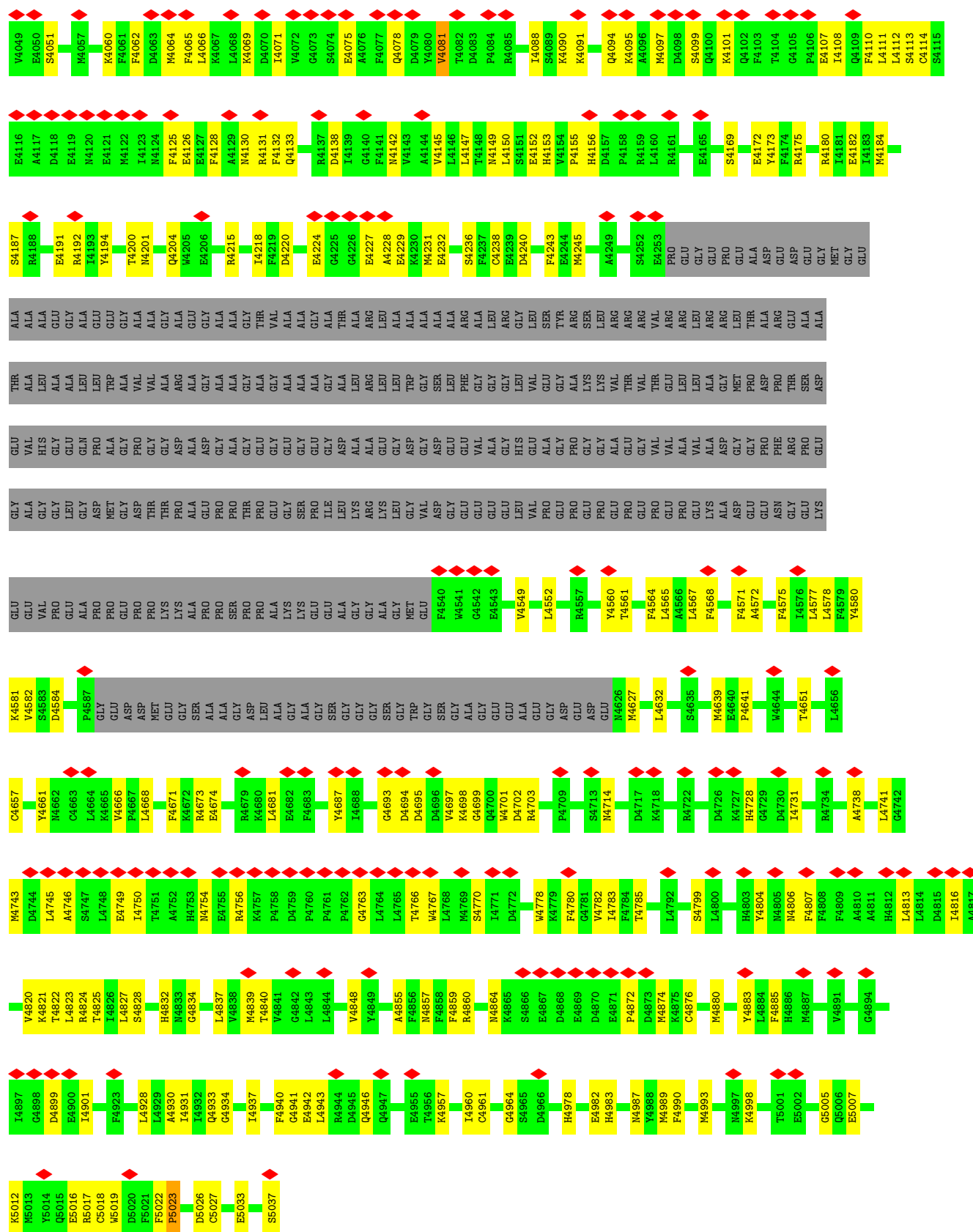
• Molecule 1: Ryanodine receptor 1

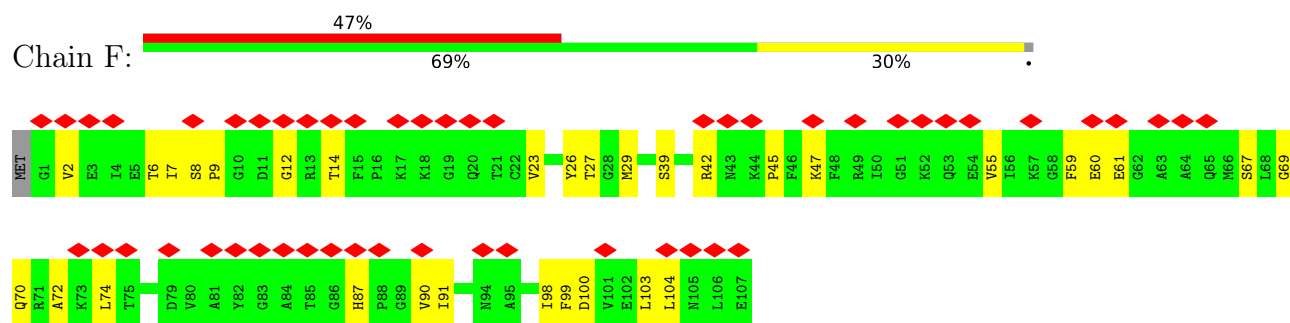




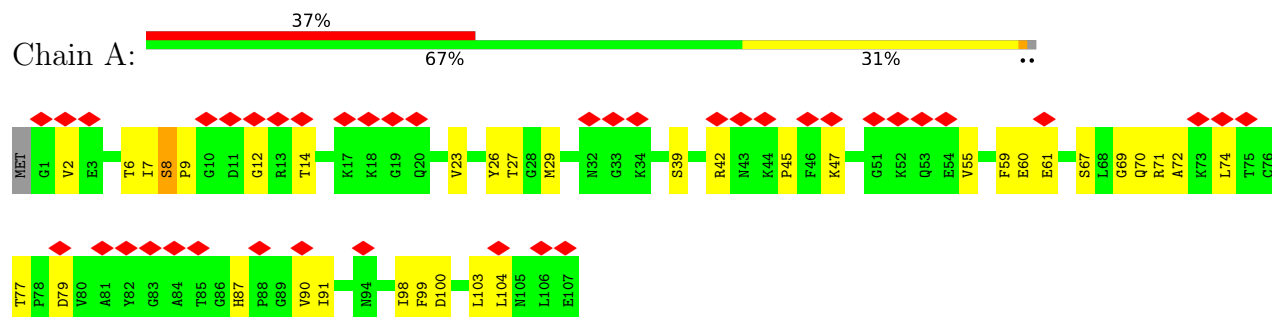


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L3798	K3799	L3805	G3808	N3809	V3812	K3816	L3817	D3818	Y3819	L3820	K3821	D3822	F3829	D3830	T3832	Q3833	K3836	Q3837	S3840	Y3841	L3842	D3843	L3844	N3845	E3848	R3849	Q3850	N3851	K3852	A3853	E3854	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873																
M3723	A3724	Y3725	A3726	D3727	A3730	K3731	S3732	C3733	H3734	L3735	E3736	E3737	Q3738	Q3739	E3740	N3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	S3758	E3759	K3760	Q3761	R3762	R3769	L3770	H3771	T3772	R3773	A3776	L3780	Q3781	M3782	I3783	S3784	A3785	C3786	K3787	G3788	E3789	T3790													
N3643	T3646	H3647	R3648	F3653	L3654	E3655	S3656	Y3657	K3658	A3659	A3660	W3661	L3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	I3674	D3675	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	H3704	R3707	T3708	A3709	L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720														
K3531	K3532	K3533	K3534	K3535	K3538	K3539	K3542	K3546	K3552	K3556	K3560	K3561	K3562	K3563	K3564	K3565	K3566	K3567	K3568	K3569	K3570	K3571	K3572	K3576	K3577	K3578	K3579	K3580	K3581	K3582	K3583	K3584	K3585	K3586	K3587	K3588	K3589	K3590	K3591	K3605	K3606	K3607	K3608	K3609	K3610	K3611	K3612	K3613	L3641	Y3642																
X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3411	X3412	X3413	X3414	X3415	X3419	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3520	X3521	X3524	X3525	X3528	X3529	X3530														
X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3330	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	X3361	X3362	X3363	X3364	X3365	X3369	X3373	X3374	X3377	X3381	X3386	X3395													
X3200	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3256	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	X3295										
X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3029	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3158	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3186	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197															
A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	R2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2961	X2964	X2965	X2968	X2971	X2972	X2975	X2976	X2995	V2996	P2997	Y2998	D2999	T2910	L2911	A2913	K2914	E2915												
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	R2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	A2913	K2914	E2915									
F2797	S2798	E2799	K2800	D2801	K2802	E2803	T2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	W2816	L2817	A2818	K2819	E2820	K2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	GLY	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856						

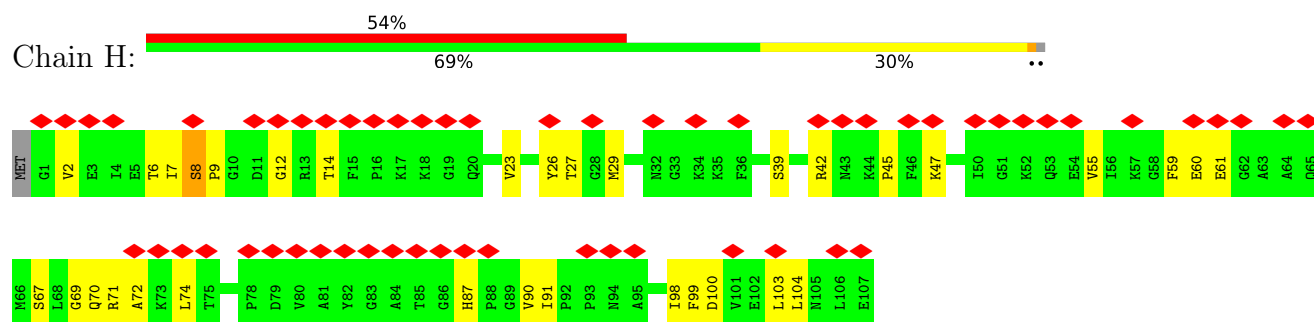




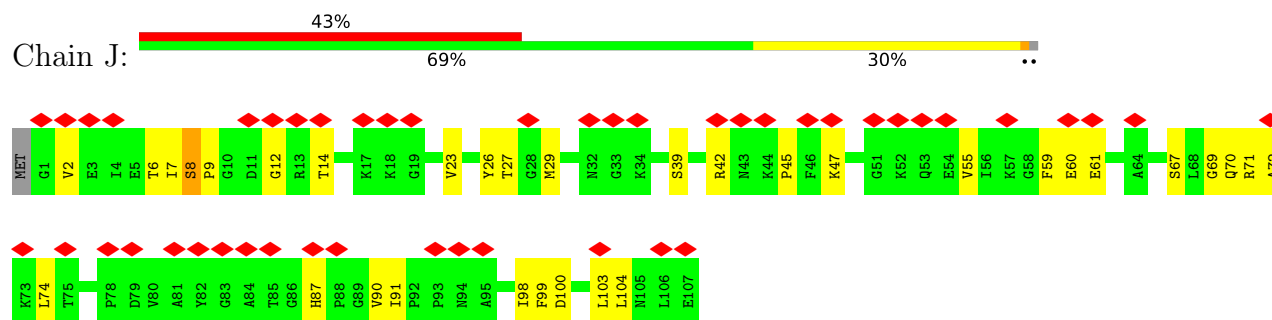
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• 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

5.1 Standard geometry

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	0.30	0/25428	0.66	13/34534 (0.0%)
1	E	0.30	0/25428	0.66	11/34534 (0.0%)
1	G	0.30	0/25428	0.66	15/34534 (0.0%)
1	I	0.30	0/25428	0.66	13/34534 (0.0%)
2	A	0.27	0/834	0.62	1/1123 (0.1%)
2	F	0.27	0/834	0.63	1/1123 (0.1%)
2	H	0.27	0/834	0.62	1/1123 (0.1%)
2	J	0.27	0/834	0.62	1/1123 (0.1%)
All	All	0.30	0/105048	0.66	56/142628 (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 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4153	HIS	CA-C-N	-7.64	116.68	123.33
1	B	4153	HIS	C-N-CA	-7.64	116.68	123.33
1	E	4153	HIS	CA-C-N	-7.57	116.74	123.33
1	E	4153	HIS	C-N-CA	-7.57	116.74	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4153	HIS	CA-C-N	-7.56	116.75	123.33

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	514	0
1	E	29369	0	24716	515	0
1	G	29369	0	24717	527	0
1	I	29369	0	24717	516	0
2	A	818	0	824	20	0
2	F	818	0	824	19	0
2	H	818	0	824	19	0
2	J	818	0	824	19	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	2122	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 10.

The worst 5 of 2122 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%)	43	77
1	E	3235/4687 (69%)	2874 (89%)	356 (11%)	5 (0%)	43	77
1	G	3235/4687 (69%)	2876 (89%)	354 (11%)	5 (0%)	43	77
1	I	3235/4687 (69%)	2876 (89%)	354 (11%)	5 (0%)	43	77
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%)	49	83

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

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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%)	2485 (100%)	8 (0%)	86	84
1	E	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
1	G	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
1	I	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
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%)	10292 (100%)	32 (0%)	84	84

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3663	LEU
1	G	3770	LEU
1	E	3663	LEU
1	E	2339	VAL
1	G	3805	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 235 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	105	HIS
1	G	4553	ASN
1	I	2127	GLN
1	G	4142	ASN

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Mol	Chain	Res	Type
1	G	1970	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 oligosaccharides 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

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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

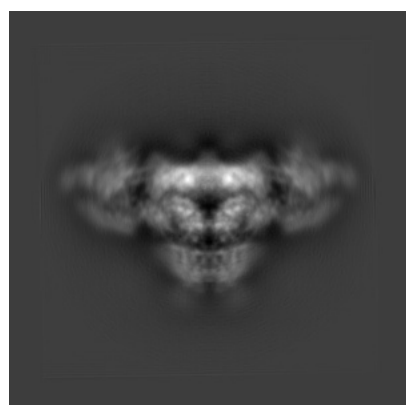
6 Map visualisation [i](#)

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.

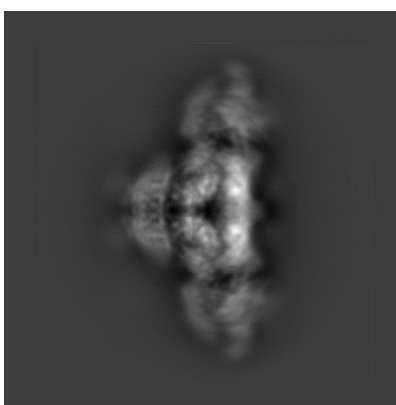
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

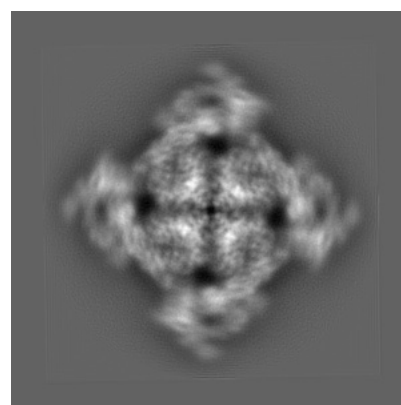
6.1.1 Primary map



X



Y

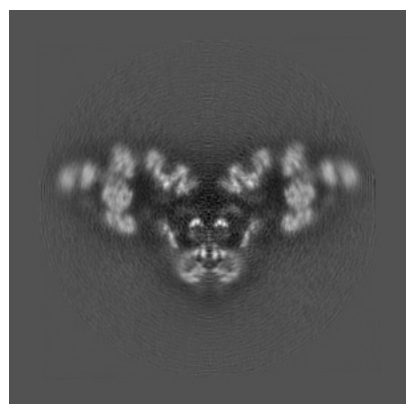


Z

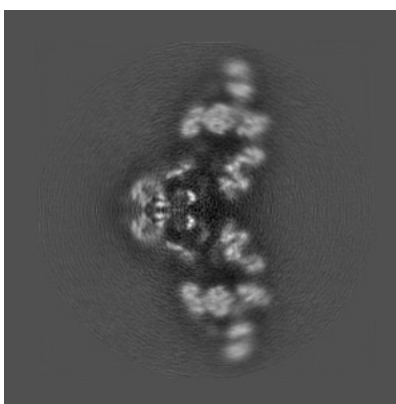
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

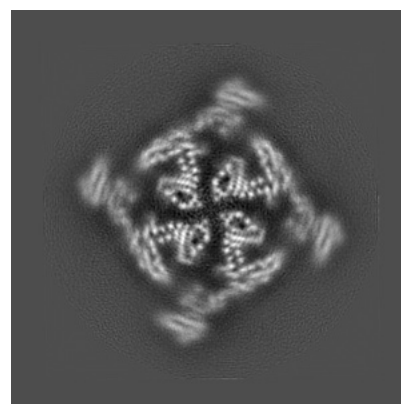
6.2.1 Primary map



X Index: 200



Y Index: 200

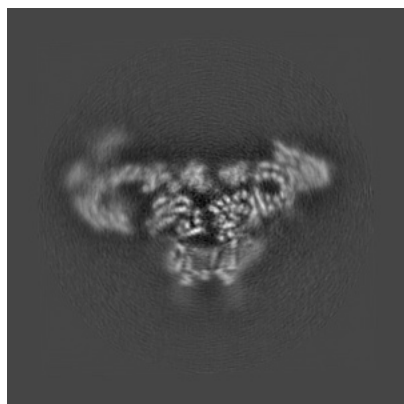


Z Index: 200

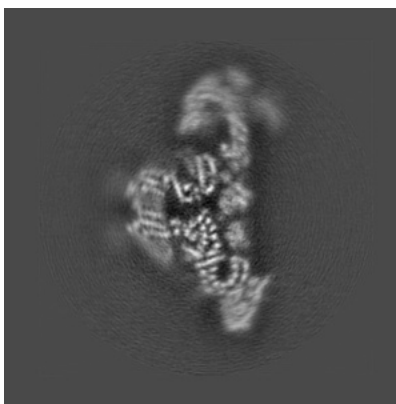
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

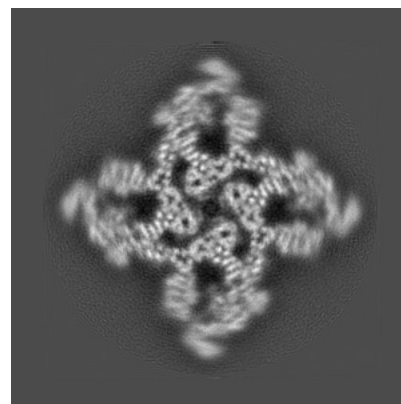
6.3.1 Primary map



X Index: 179



Y Index: 177



Z Index: 231

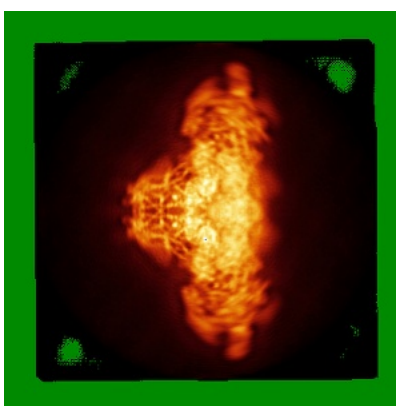
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

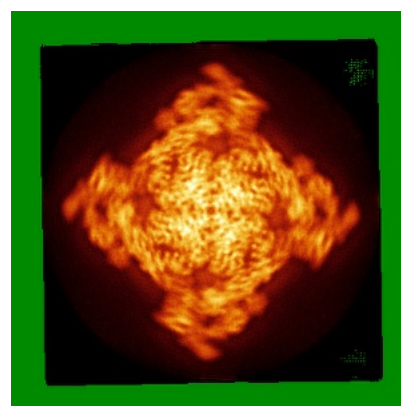
6.4.1 Primary map



X



Y

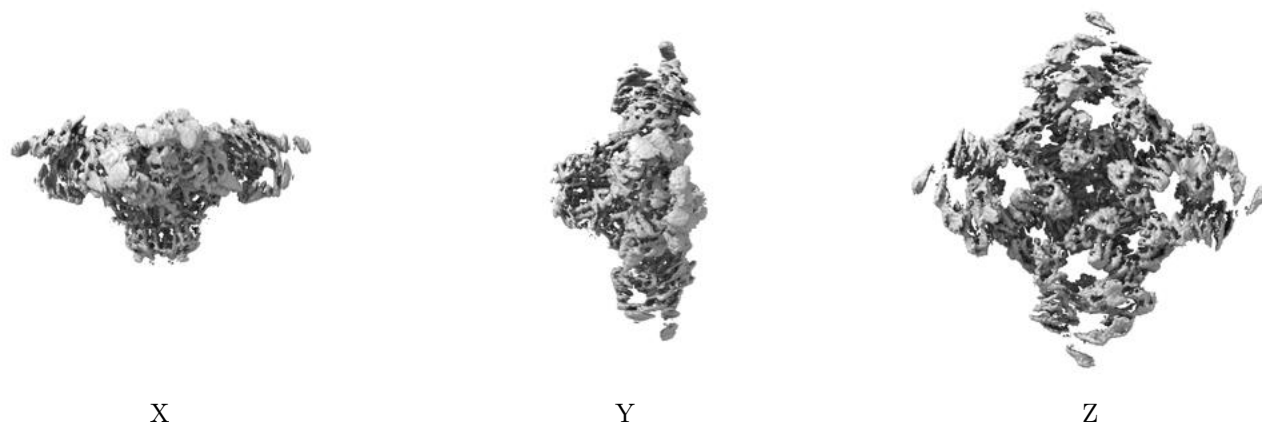


Z

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



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.

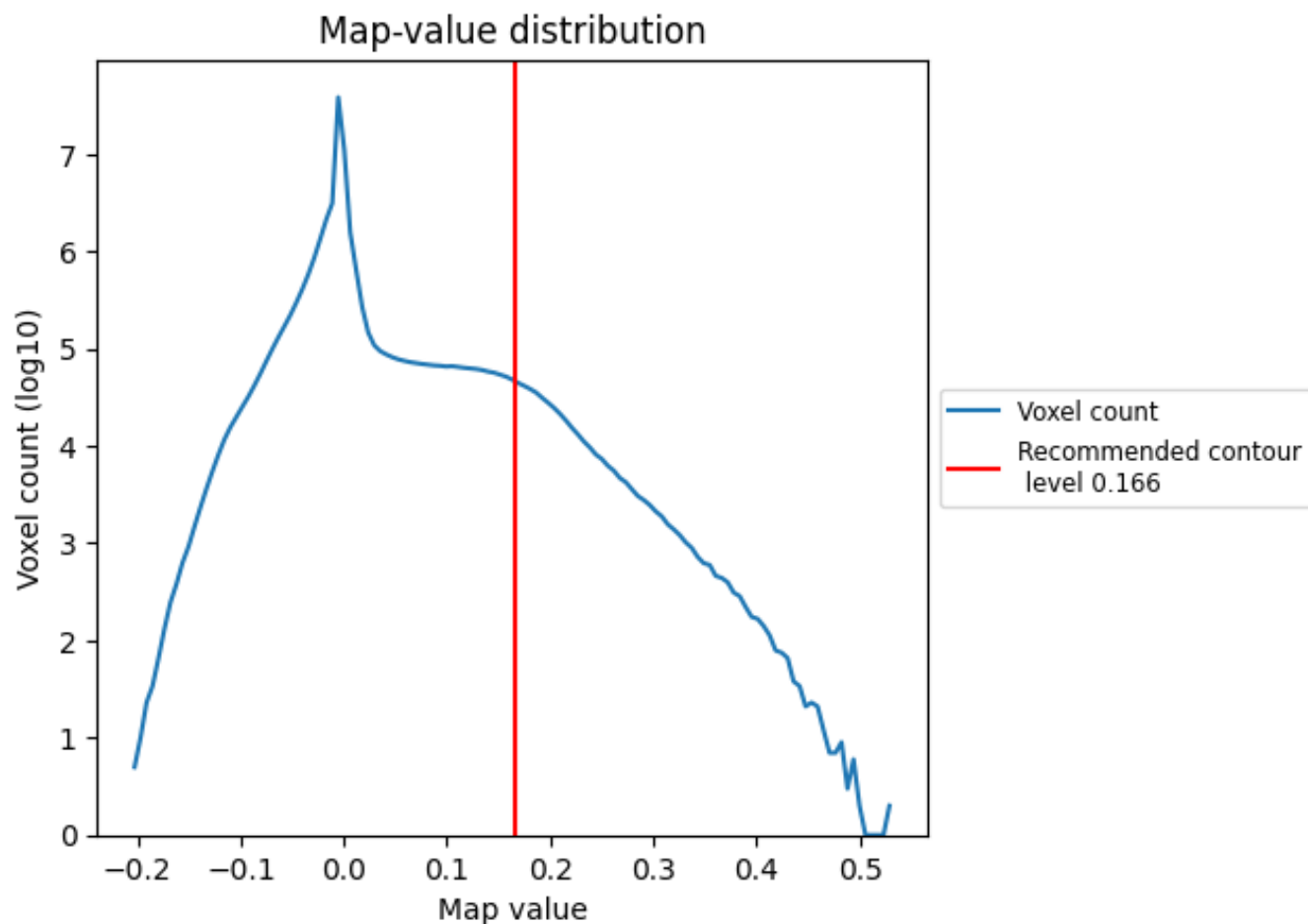
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

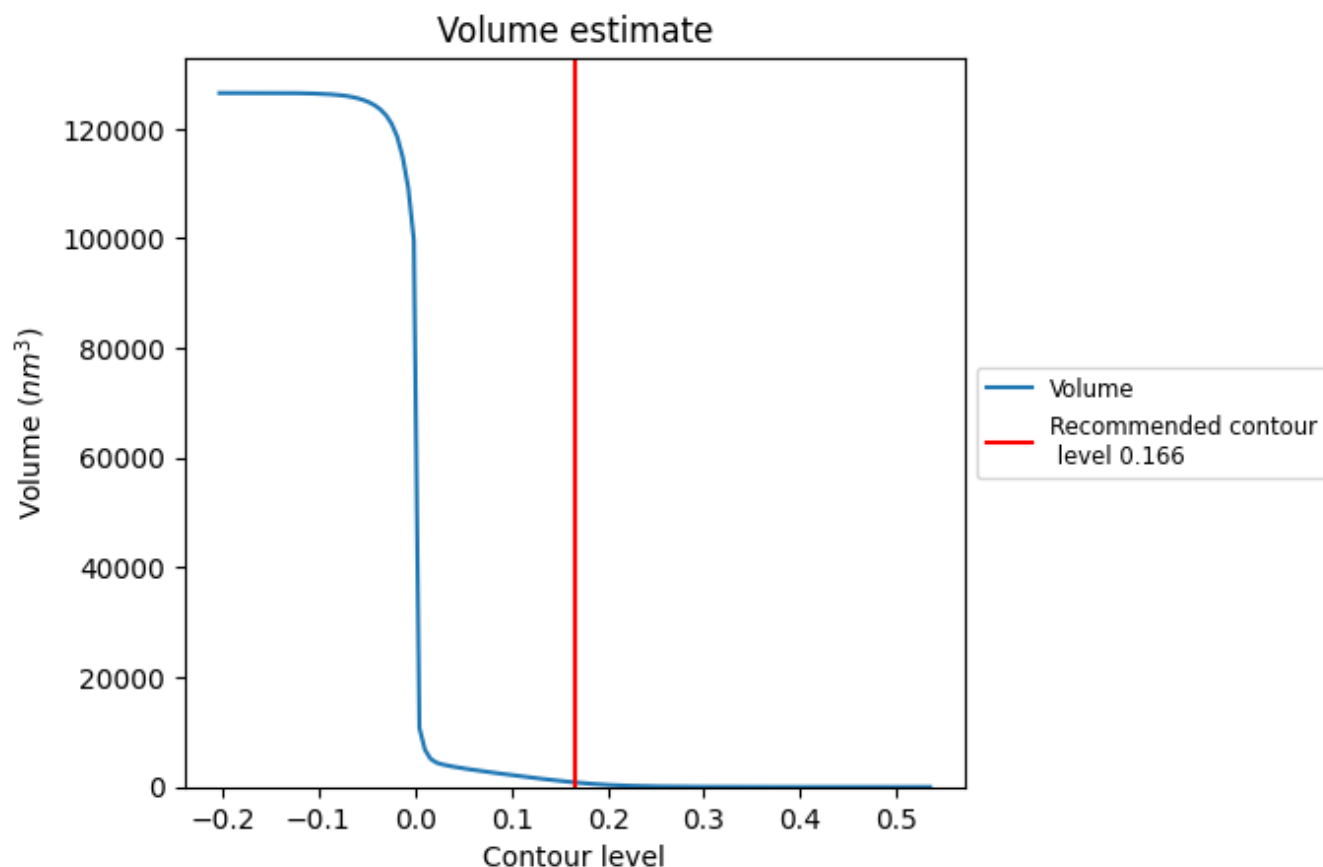
This section contains the results of statistical analysis of the map.

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.

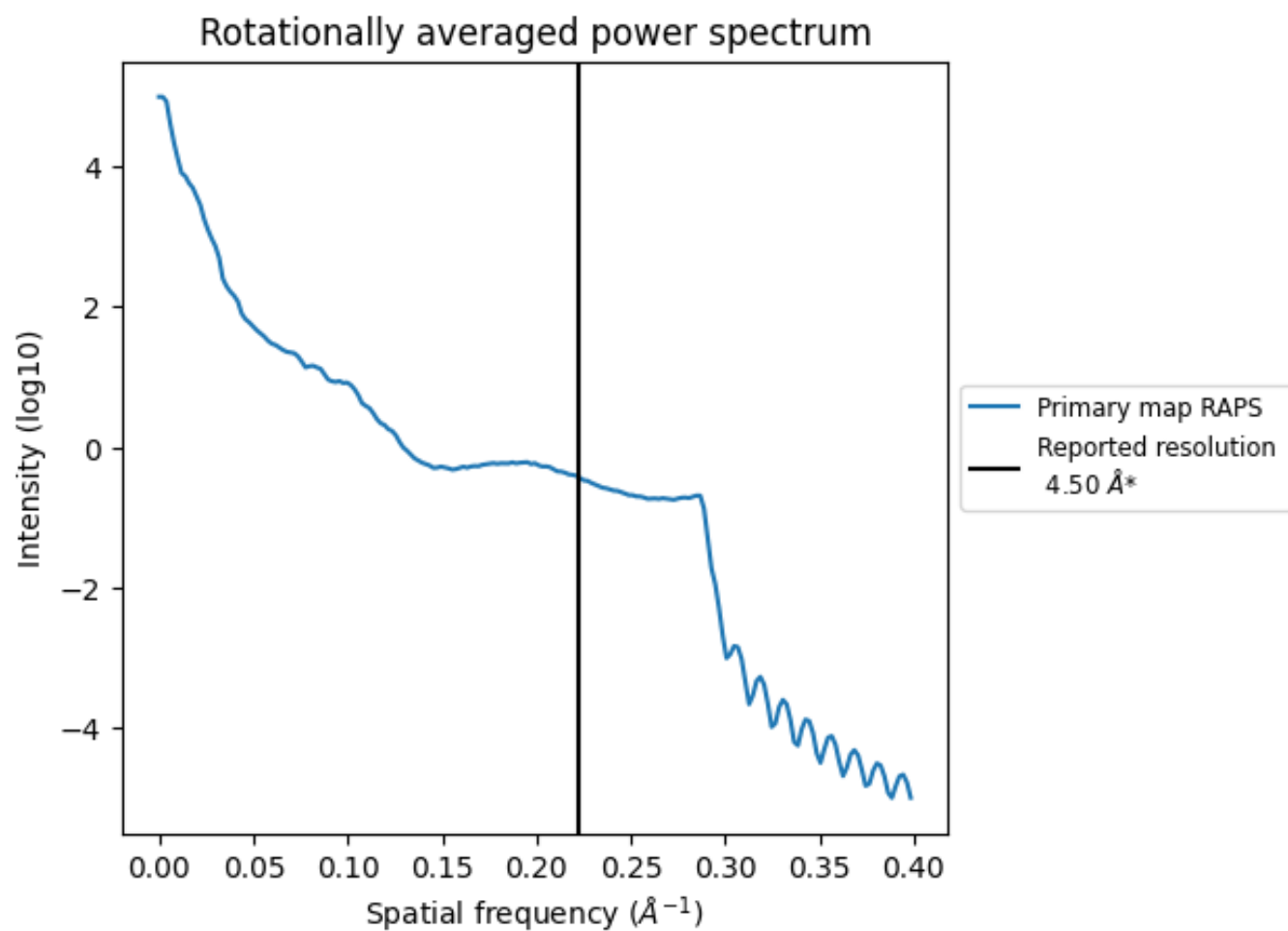
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm³; 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⁻¹

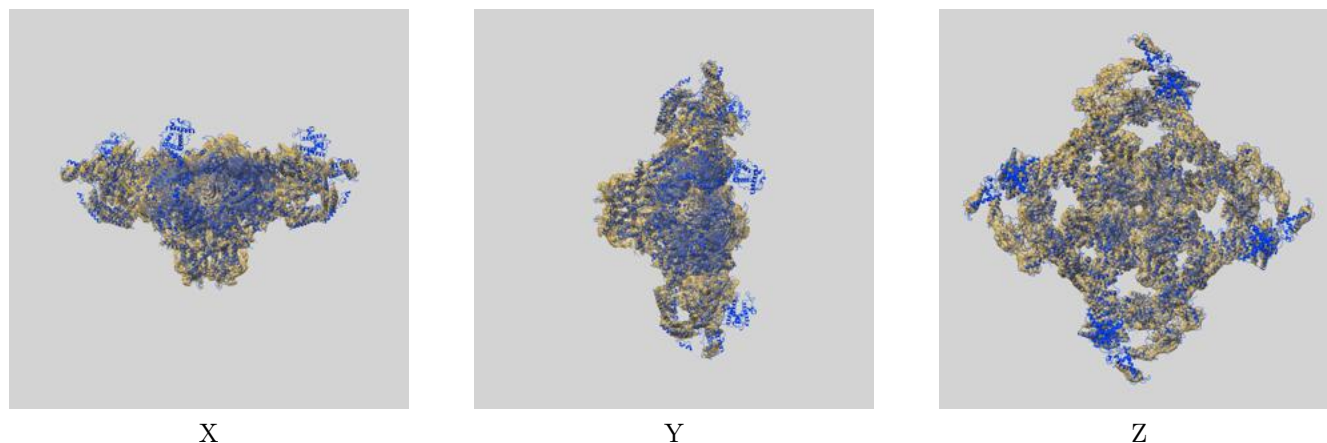
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

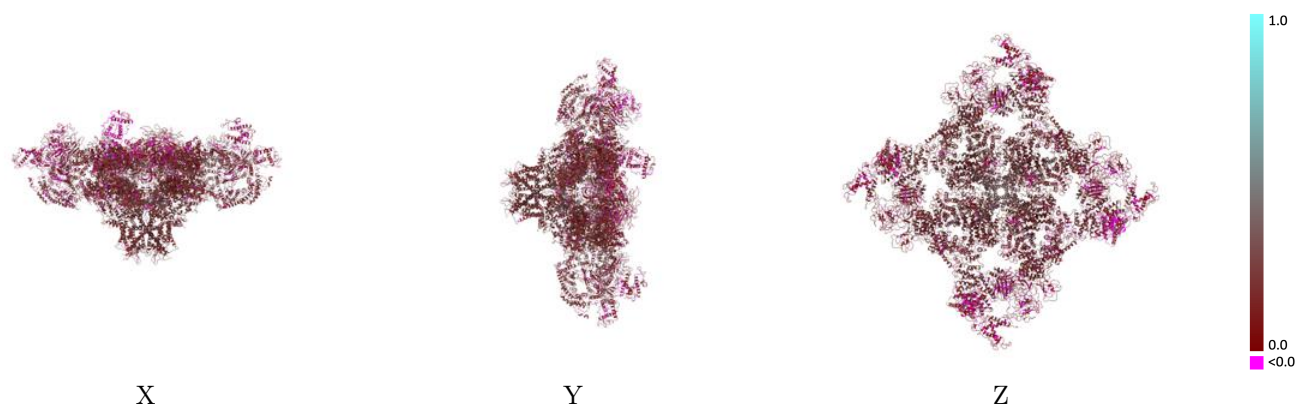
This section contains information regarding the fit between EMDB map EMD-20486 and PDB model 6PV6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



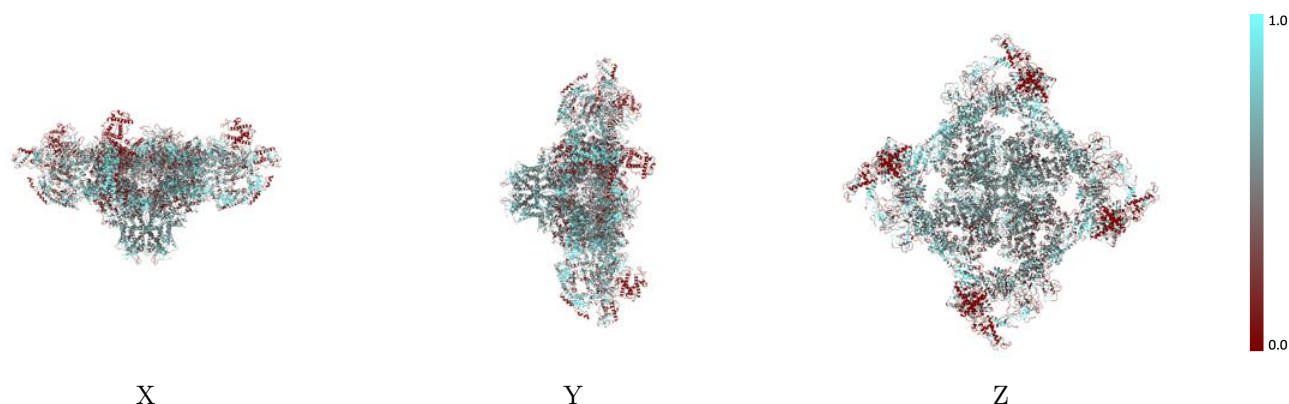
The images above show the 3D surface view of the map at the recommended contour level 0.166 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



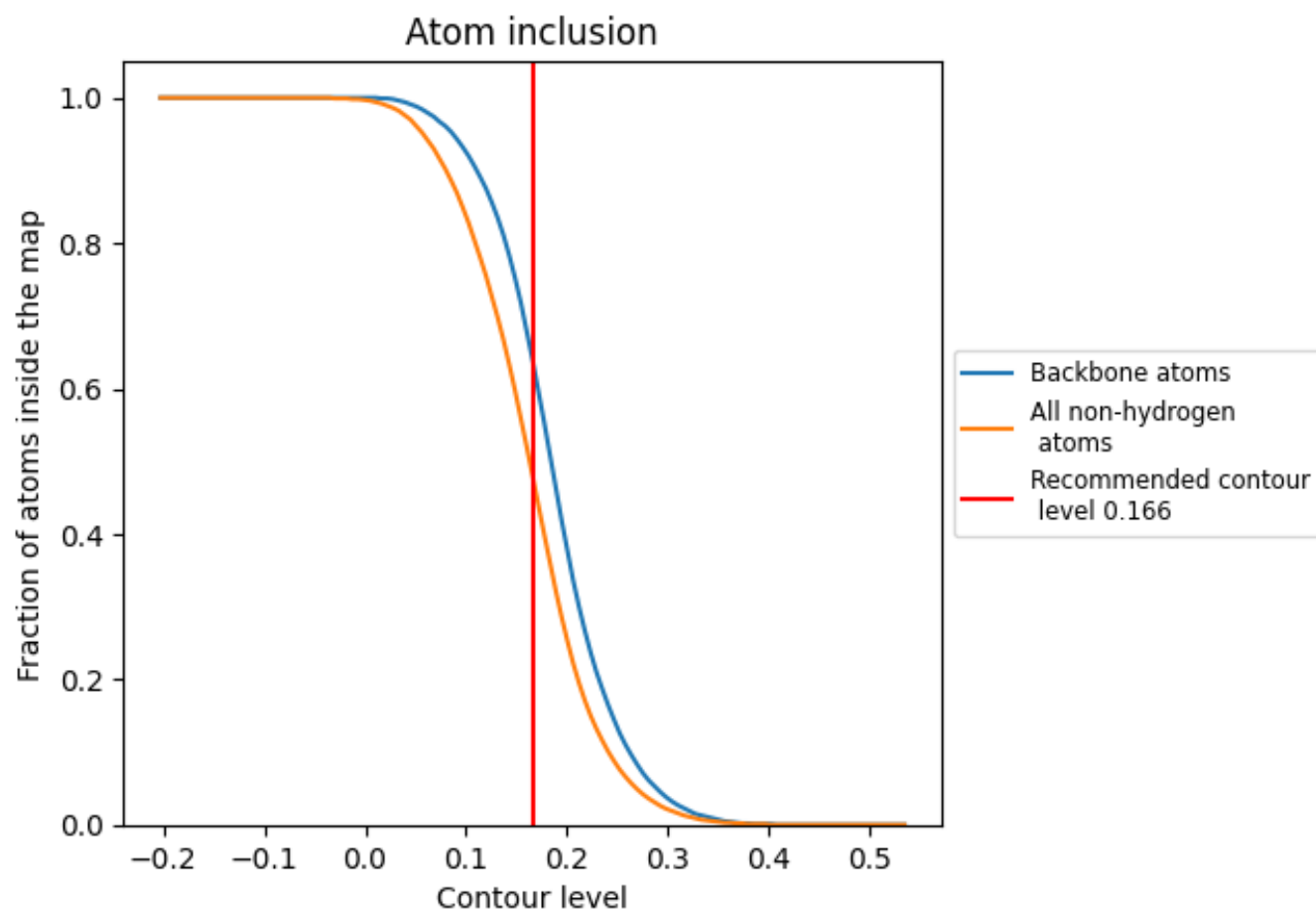
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.4790	0.1800
A	0.4850	0.1850
B	0.4970	0.1950
E	0.4770	0.1780
F	0.4270	0.1320
G	0.4620	0.1660
H	0.4110	0.1400
I	0.4840	0.1860
J	0.4700	0.1810

1.0

0.0

<0.0