



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 05:38 PM UTC

PDB ID : 8SEP / pdb_00008sep
EMDB ID : EMD-40424
Title : Cryo-EM Structure of RyR1 + ADP
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.57 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

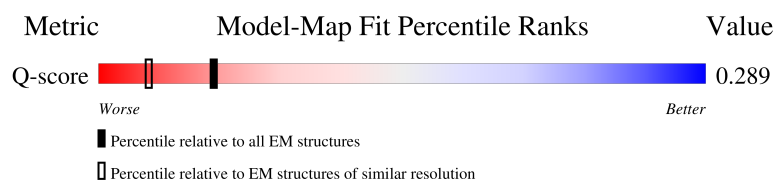
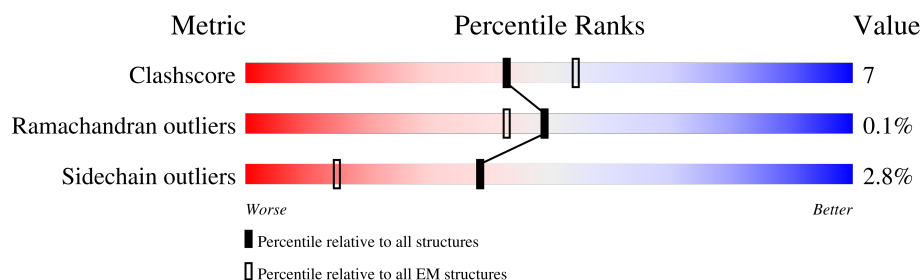
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 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	12682 (3.07 - 4.07)

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	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	350	22%8%69%
2	F	350	22%8%69%
2	G	350	23%8%69%
2	H	350	22%8%69%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 143100 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	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	B	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	C	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	D	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- # ADP

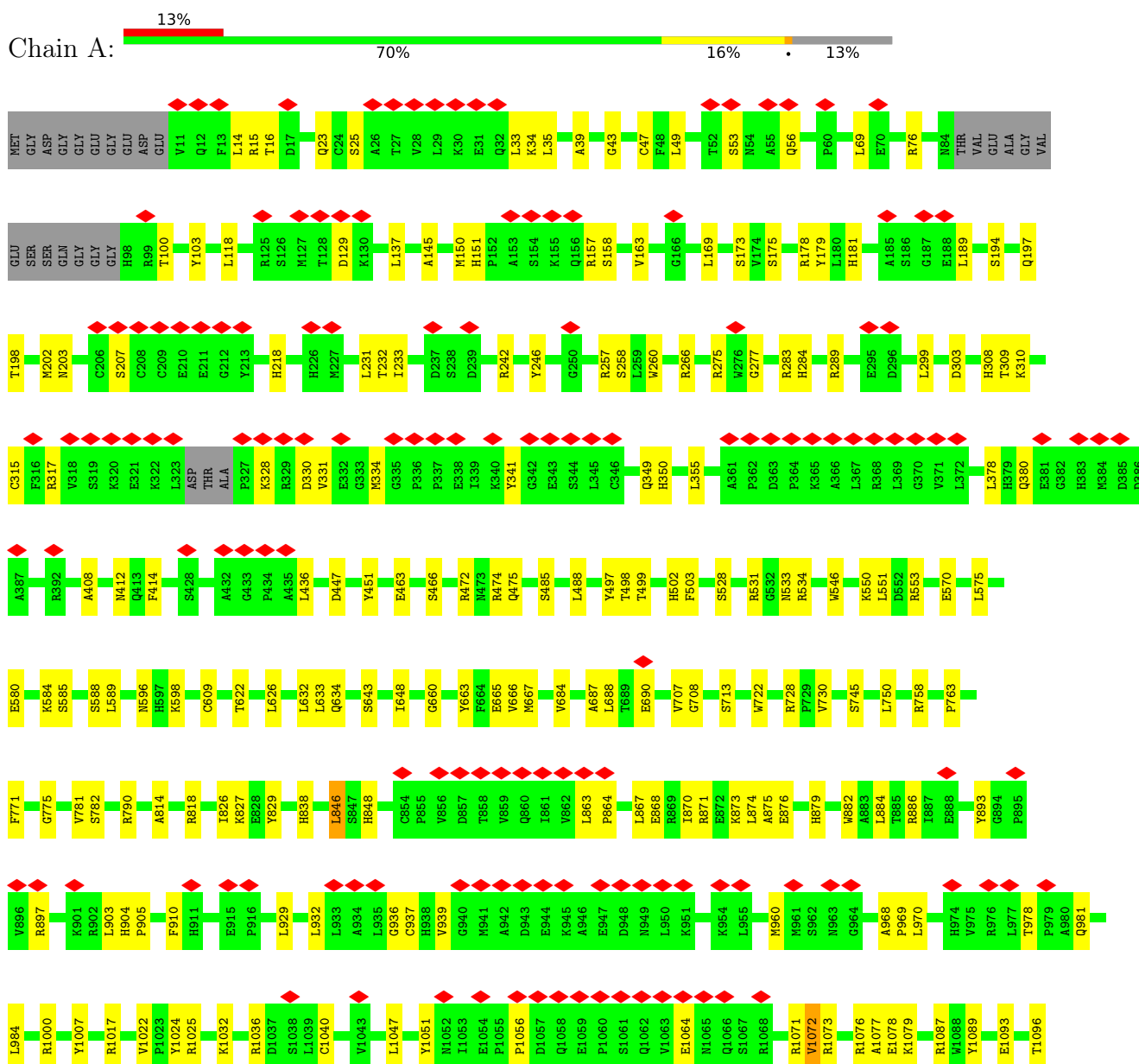
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

3 Residue-property plots

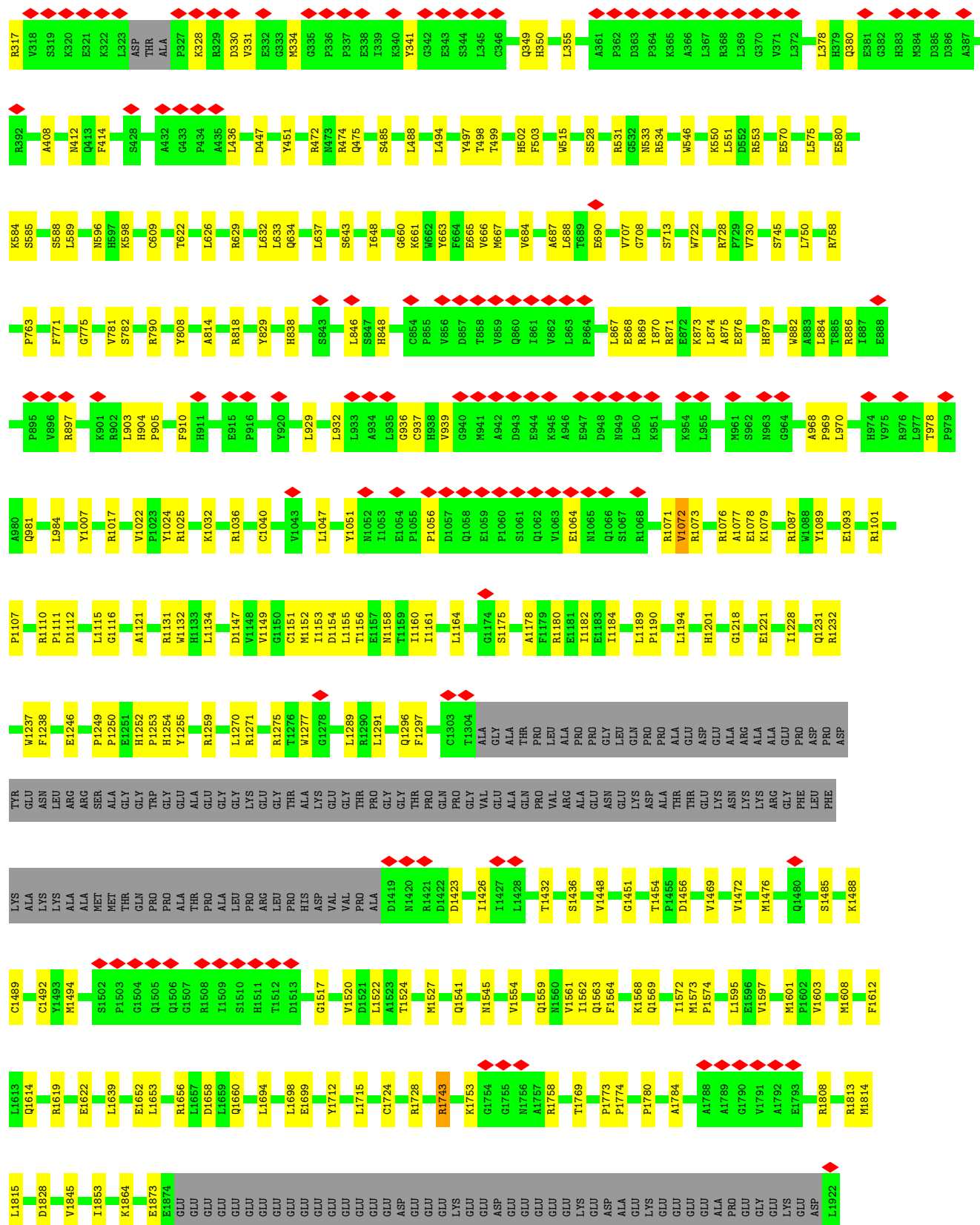
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



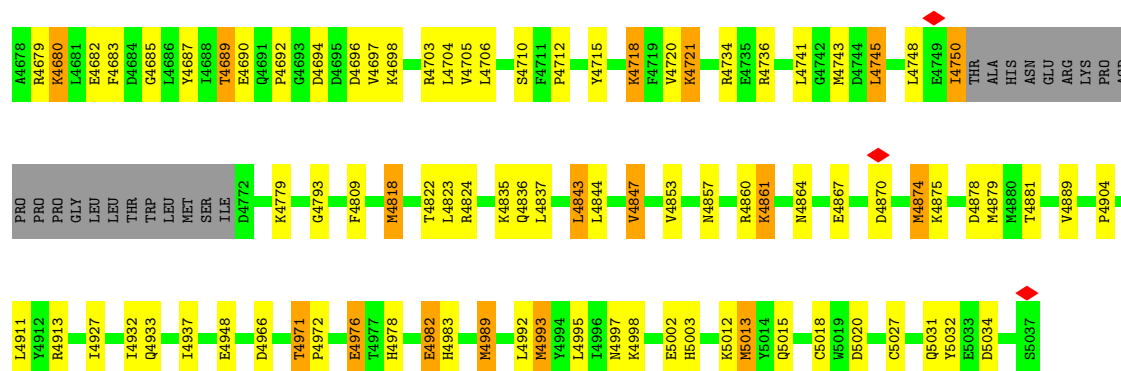


L3990	Q3766	R3637	G3561	K3477	R2448	H3146	G3028	A2936	E2876	M2816	W2755
L3891	Q3767	M3638	K3562	M3478	L3249	H3149	H3033	V2937	Q2877	L2817	W2756
F3899	R3768	L3641	V3563	A3479	M3250	H3150		T2938	L2878	A2818	K2757
L3924	H3770	M3652	E3564	LYS	S3259	Q3151	E3037	R2939	A2879	W2819	
S3929	T3772	E3655	G3565	ALA	I3270	Q3151	M3038	LEU	E2880	E2820	E2760
W3935	R3773	E3656	S3568	GLY	L3274	V3156	L3042	LYS	W2881	W2821	Y2761
W3935	M3782	A3659	Q3571	ASP	L3274	I3157	K3045	ASP	T2882	T2822	T2762
K3940	G3788	S3660	M3573	ALA	Y3280	V3161	L3046	MET	H2883	L2823	H2763
E3967	M3793	W3661	K3573	K3384	L2881	Q3162		GLY	N2884	E2824	E2764
L3980	G3801	L3662	L3579	A3386	P3282			L2946	N2885	K2825	K2765
R3984	D3676	L3663	R3582	E3387	W3285	N3160	L3049	D2947	W2886	A2826	W2766
L3805	A3680	E3681	E3583	E3388	E3290	V3183	V3050	T2948	A2767	R2827	A2767
N3809	G3682	E3682	E3584	E3389	A3291	E3184	R3051	S2949	K2888	E2828	F2768
V3812	Q3683	E3683	D3585	R3395	P3292	K3185	R3053	E2952	K2889	G2829	D2769
L3817	E3684	E3684	D3587	R3403	P3293	L3186	L3056	L2960	K2891	E2830	K2770
K3823	E3685	G3500	D3587	L3405	P3294	L3190	T3059	Q2962	Q2892	GLU	I2771
L3835	E3686	D3501	R3595	L3408	A3295	L3194	P3062	L2964	E2893	THR	Q2772
S3840	E3687	R3596	V3596	Y3409	L3296	L3197	V3065	R2965	L2894	GLU	W2774
V3841	E3688	L3603	L3603	L3413	A3298	A3204	L3068	W2966	E2895	LYS	W2775
L3842	E3689	Y3604	H3605	R3414	P3297	F3205	H3069	M2967	K2896	LYS	S2776
A3846	V3690	E3691	H3606	D3417	A3300	L3206	L3075	S2970	G2898	THR	Y2777
Q3850	E3692	E3692	E3607	N3418	P3302	E3207	L3076	Q2971	K2899	LYS	Q2778
M3858	D3696	Q3692	Q3603	L3424	P3303	L3210	A3077	E2978	G2900	ILE	E2779
V3859	C3733	D3696	T3609	E3433	C3304		R3078	A2979	T2901	GLN	W2780
N3860	E3736	E3736	E3610	E3434	S3309	Y3213		V2980	H2902	ALA	V2781
E3861	GLY	GLY	E3611	F3435	I3322	N3214	M3081	V2981	P2903	THR	D2782
D3862	GLY	GLY	F3612	R3436	I3323	A3215	K3082	S2982	L2904	GLN	E2783
G3863	ASN	ASN	K3613	E3453	N3325	C3216	S3083	S2983	L2905	THR	E2784
T3864	GLY	GLY	K3614	E3454	N3326	S3217	E3086	Q2984	V2906	TYR	L2785
V3865	GLY	GLY	K3615	E3454	N3327	V3218	L3087	R2985	P2907	PRO	K2786
L3866	GLY	GLY	K3616	N3457	G3328	T3220	R3093	V2986	D2908	GLY	H2787
N3867	GLY	GLY	K3617	F3458	L3327	T3221		R2987	D2909	GLY	H2788
N3868	ALA	ALA	A3618	V3459	I3329	K3222	M3106	E2987	T2910	Y2855	W2790
N3868	GLY	GLY	V3619	V3460	D3330	S3223	G3113	K2988	L2911	N2856	L2791
Q3869	GLY	GLY	W3620	Q3461	M3335	P3224	K3114	P2989	T2912	P2857	R2792
N3870	GLY	GLY	H3621	E3462	A3339	R3225	V3115	H2991	A2913	Q2858	F2793
N3870	V3749	V3749	K3622	L3464	V3340		S3116	E2992	K2914	P2859	Y2794
G3871	E3750	E3750	L3623	N3465	V3340	A3228	GLN	Q2993	E2915	D2861	K2795
E3872	V3751	V3751	L3624	N3466	I3346	L3229	ALA	F2997	K2916	L2862	T2796
K3873	S3752	S3752	L3625	N3467	I3346	L3230	ARG	F2997	A2917	S2863	F2797
V3874	F3753	F3753	K3626	S3468	R3348	G3231	THR		R2918	G2864	S2798
M3875	E3754	E3754	Q3627	S3468	R3349	L3232	VAL	I3001	D2919	E2799	S2798
N3876	E3755	E3755	Q3628	F3469	A3349	P3233	K3123	T3020	R2920	V2865	K2800
A3877	K3756	K3756	R3629	L3470	P3351	L3232		P3021	E2921	L2867	D2801
D3878	E3757	E3757	A3630	T3471	L3354	P3233	L3129	A3022	K2922	S2868	K2802
Q3889	K3760	K3760	A3631	A3472	L3354	E3258	Y3131	K3023	A2923	E2803	E2803
			V3632	D3473	F3358	K3239		V3024	Q2924	R2869	L2804
			V3633	S3474		V3246		L3025	E2925	E2870	Y2805
			A3634	K3475		D3247		G3026	L2926	L2871	R2806
			F3636	S3476					L2927	Q2872	W2807
									K2928	A2873	F2808
									F2929	M2874	L2809
									L2930	E2811	K2810
									Q2931	Q2872	E2812
									M2932		L2813
									N2933		K2814
									Q2934		A2815

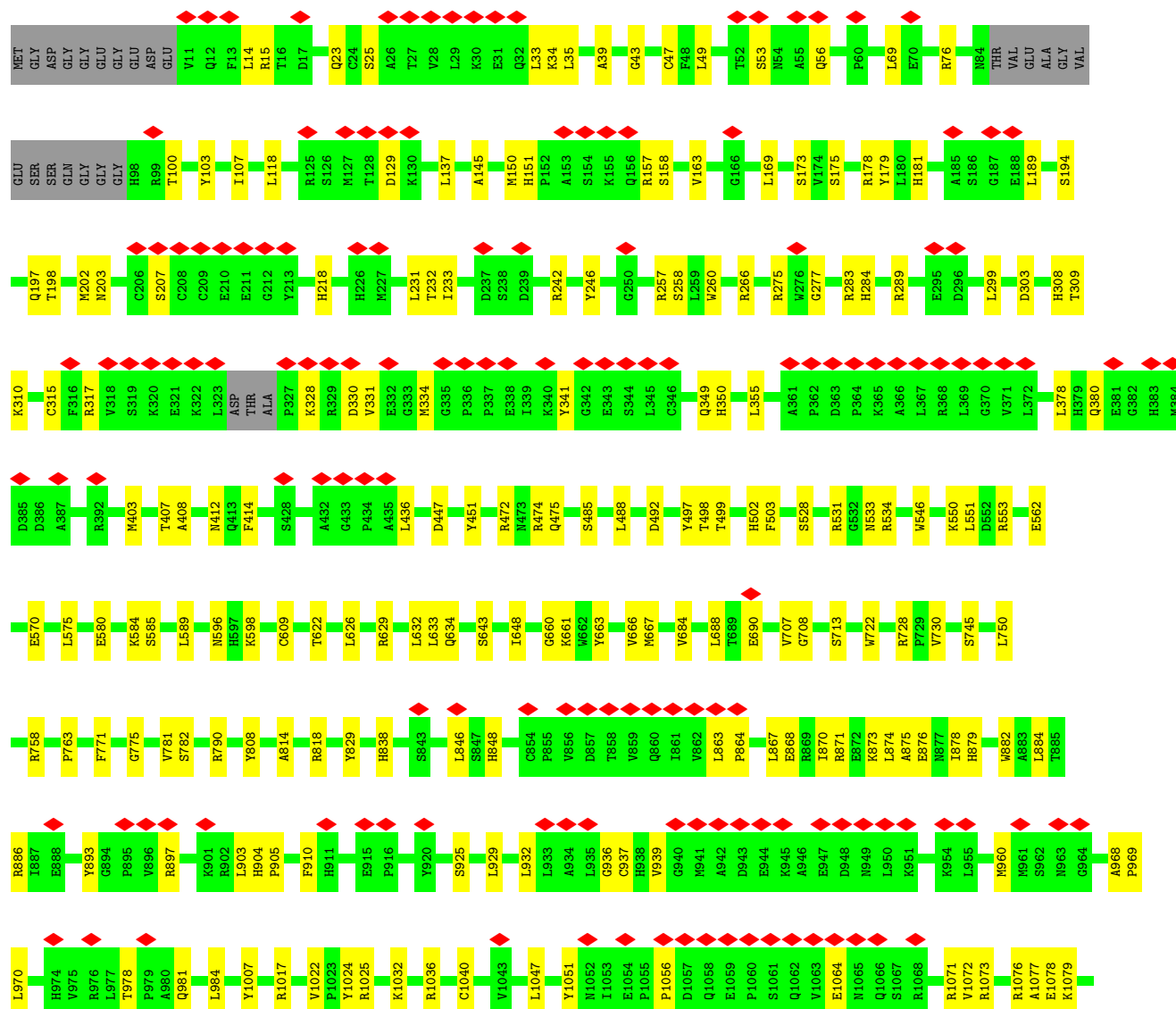


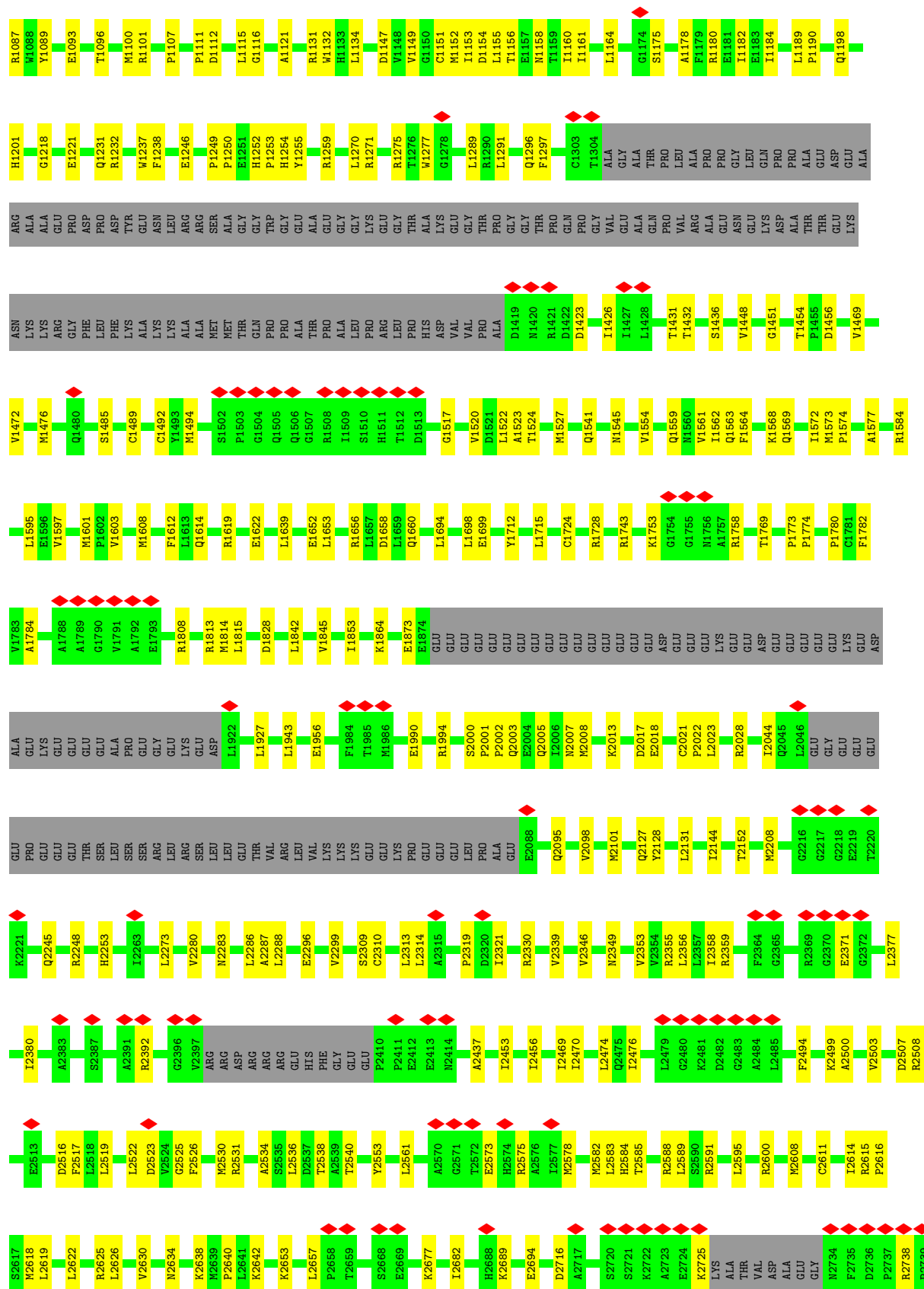






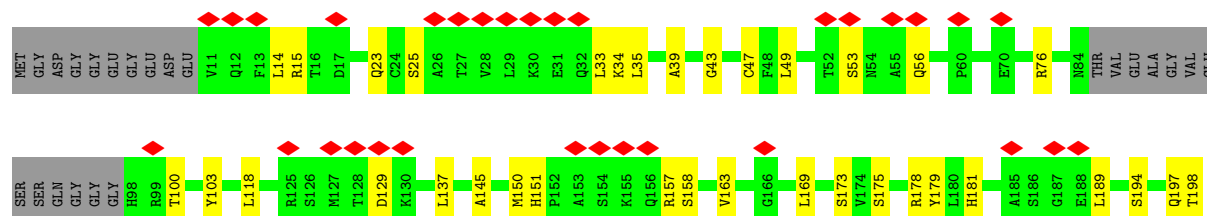
• Molecule 1: Ryanodine receptor 1

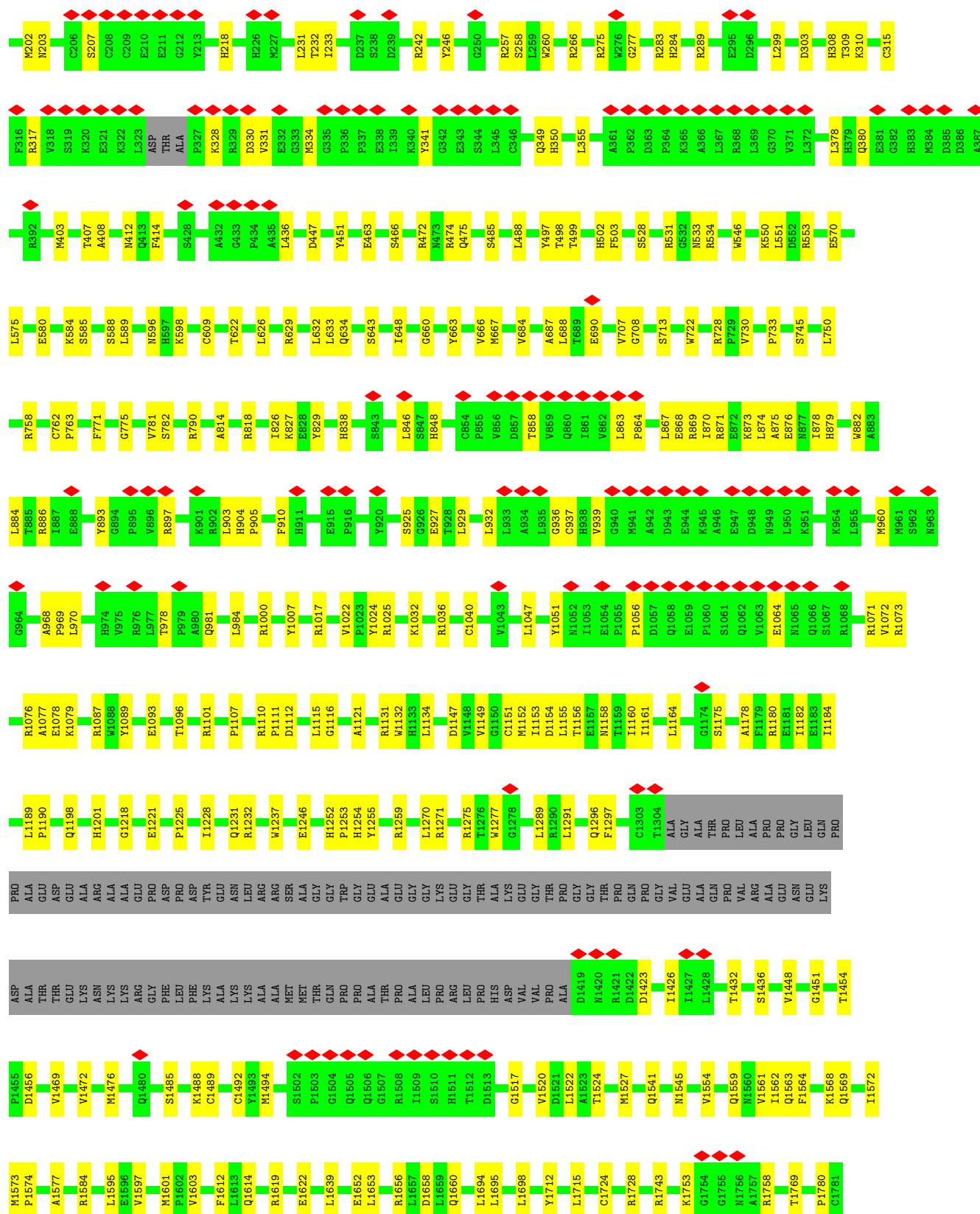




G3871	E3872	K3873	V3874	K3875	A3876	D3877	D3878	S3752	F3753	E3754	E3755	K3756	E3757	K3760	Q3766	Q3767	S3768	R3769	L3770	H3771	L3772	R3773	L3980	K3984	L3985	V3990	V3995	F3996	A3997	K3998	K3999	K4002	L4003	Q4009	I4010	E4011	A3846	Q3850	V3858	V3859	N3860	E3861	G3863	T3864	V3865	L3866	N3867	K3868	Q3869	N3870									
GLU	GLU	GLU	GLU	GLU	V3749	E3750	F3751	S3752	F3753	E3754	E3755	K3756	E3757	K3760	Q3766	Q3767	S3768	R3769	L3770	H3771	L3772	R3773	L3980	K3984	L3985	V3990	V3995	F3996	A3997	K3998	K3999	K4002	L4003	Q4009	I4010	E4011	A3846	Q3850	V3858	V3859	N3860	E3861	G3863	T3864	V3865	L3866	N3867	K3868	Q3869	N3870									
H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	H3638	L3641	M3652	E3655	A3659	A3660	V3661	L3662	L3663	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	D3696	G3703	E3736	GLY	GLY	GLU	ASN	GLY	GLY	GLU	ALA									
N3457	F3458	V3459	V3460	Q3461	N3462	E3463	N3464	N3465	N3466	M3467	R3468	F3469	L3470	T3471	D3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	ALA	GLY	ALA	GLN	SER	GLY	E3583	E3584	D3585	A3586	D3587	I3589	R3595	V3596	L3603	Y3604	H3605	L3606	E3607	Q3608	T3609	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620					
G3328	L3329	D3330	N3335	A3339	E3340	I3345	R3348	A3349	R3350	P3351	L3354	F3358	I3362	E3377	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	R3395	R3403	D3404	L3405	L3408	Y3409	I3413	R3414	D3417	N3418	L3424	E3433	L3434	F3435	R3436	R3453	E3454																		
V3218	Y3219	T3220	K3221	K3222	K3223	P3224	R3225	A3226	I3229	R3230	G3231	L3232	P3233	E3238	M3239	V3245	L3246	D3247	R3248	L3249	M3250	S3259	I3270	L3274	Y3280	L3281	P3282	W3285	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	I3322	K3323	V3324	M3325	N3326	L3327										
R3093	M3106	V3107	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	L3129	F3130	Y3131	H3146	Q3149	H3150	Q3151	V3156	I3157	V3161	Q3162	S3171	N3180	V3183	E3184	K3185	L3186	L3190	L3194	L3197	K3204	F3205	L3206	E3207	L3210	Y3213	N3214	A3215	C3216	S3217																
E2992	Q2993	F2997	I3001	N3007	T3011	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	N3033	E3037	M3038	L3042	K3045	L3046	L3049	V3050	R3051	H3052	R3053	L3056	T3059	P3062	V3065	L3068	H3069	L3075	D3076	A3077	R3078	M3081	K3082	S3083	E3086	I3087																			
E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	M2933	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	L2946	D2947	T2948	S2949	E2952	L2960	Q2961	Q2962	L2963	L2964	R2965	N2966	N2967	S2970	Q2971	I2974	E2978	A2979	V2980	L2981	S2982	S2983	V2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991						
D2861	L2862	S2863	Q2864	T2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	R2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	G2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920
D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	Y2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860			

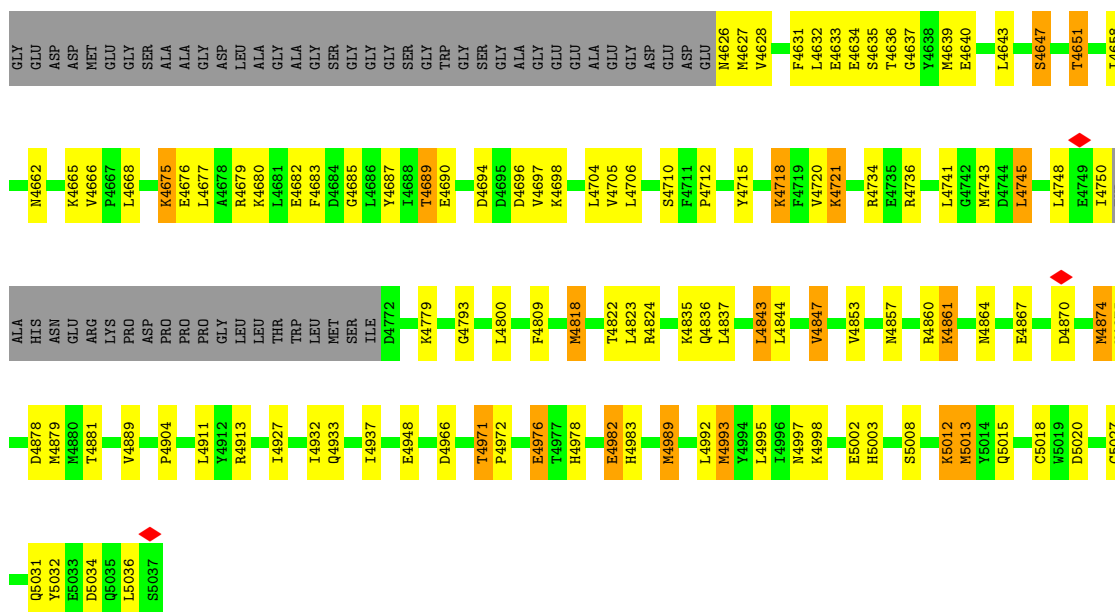
- Molecule 1: Ryanodine receptor 1



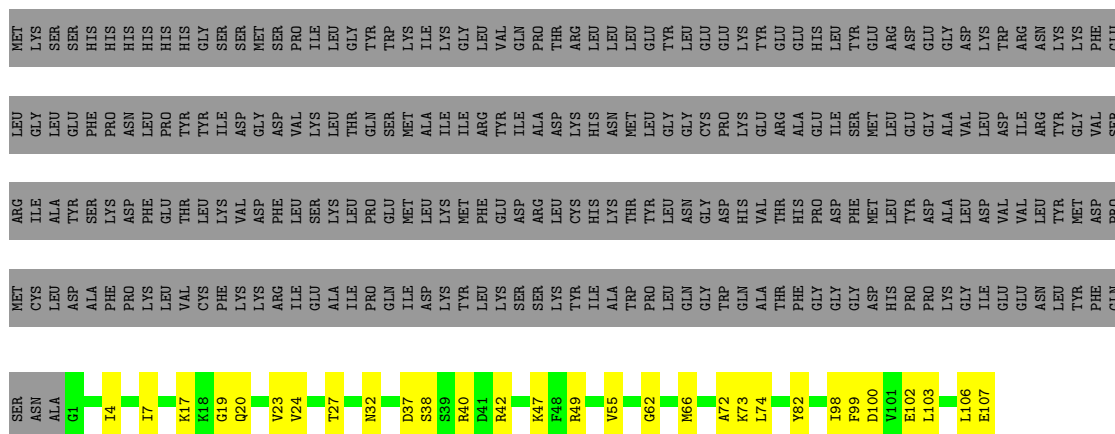




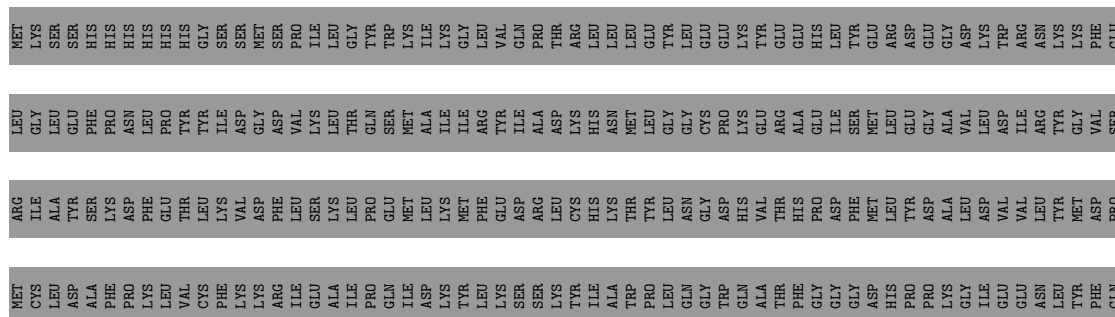
GLY	GLY	ARG	THR	GLU	MET	P4155	S4051	D3862	GLY	K3614	E3454	G3398	V3218
ALA	GLY	PRO	SER	ALA	GLY	E4155	GLY	G3863	S3615	S353	N3457	I3329	Y3219
LYS	ALA	GLY	ASP	ALA	GLU	E4156	ASN	T3864	K3616	M3534	F3458	D3330	T3220
VAL	ALA	ALA	VAL	ALA	ALA	E4158	GLY	V3865	K3617	K3537	V3459	M3335	T3221
PRO	GLY	GLY	HIS	LEU	GLY	E4172	GLU	I3866	A3618	T3538	Q3461	A3339	K3222
LEU	ALA	LEU	GLY	ALA	ALA	I4058	GLU	N3867	V3619	R3539	N3462	V3340	S3223
LEU	ALA	LEU	GLN	ALA	D4063	D4063	GLU	R3868	W3620	Y3540	E3463	P3224	P3224
ASP	PRO	ASP	PRO	LEU	M4064	M4064	GLU	Q3869	H3621	A3541	I3464	R3225	R3225
MET	GLY	MET	ALA	TRP	L4178	L4178	GLU	N3870	K3622	K3542	I3345	I3345	
GLY	GLY	GLY	GLY	ALA	G4179	G4179	GLY	N3871	L3623	K3543	N3465	A3228	A3228
VAL	ALA	VAL	ALA	ALA	R4180	R4180	ALA	K3871	L3624	E3548	R3467	R3229	I3229
VAL	VAL	VAL	VAL	ALA	I4181	I4181	ALA	E3872	S3750	V3549	A3349	I3230	I3230
THR	GLY	THR	GLY	GLY	E4182	E4182	GLY	K3873	S3625	W3549	P3351	G3231	G3231
PRO	ARG	PRO	ASP	ARG	I4183	I4183	ALA	V3874	F3752	R3550	F3469	L3232	L3232
ALA	ALA	ALA	ALA	ALA	M4184	M4184	ALA	M3875	F3753	E3551	L3470	P3233	P3233
PRO	GLY	PRO	GLY	GLY	S4074	S4074	GLY	D3878	E3754	N3555	T3471		
PRO	ALA	PRO	GLY	ALA	E4075	E4075	ALA	Q3888	K3756	N3556	A3472	E3238	E3238
PRO	ALA	PRO	ALA	ALA	D4079	D4079	GLY	Q3889	E3757	L3557	D3473	M3239	M3239
THR	GLY	THR	GLY	GLY	D4082	D4082	THR	L3888	E3757	H3558	S3474	I3362	
GLU	VAL	GLU	VAL	VAL	D4083	D4083	VAL	Q3889	K3760	R3559	K3475	E3377	
ALA	ALA	ALA	ALA	ALA			ALA	L3924	Q3766	L3559	S3476		
GLY	ALA	GLY	GLY	GLY	K4090	K4090	GLY	S3929	Q3767	Q3560	R3380	Y3245	Y3245
ALA	ALA	ALA	GLY	ALA	K4091	K4091	THR	S3929	S3768	G3561	L3381	I3246	I3246
LEU	THR	LEU	ASP	ALA	D4092	D4092	ALA	W3935	R3769	K3562	L3249	R3247	R3247
ALA	LEU	ALA	ALA	LEU	F4093	F4093	ARG	P4208	L3770	G3563	M3478	R3248	R3248
LEU	LEU	LEU	LEU	LEU	Q4209	Q4209	LEU	Q4209	H3771	V3563	M3479	M3250	M3250
ALA	ALA	ALA	GLY	LEU	D4094	D4094	ALA	K3940	R3772	E3564	LYS		
ALA	ALA	ALA	ALA	ALA	K4095	K4095	ALA	E3967	R3773	G3565	ALA	S3269	S3269
VAL	ALA	VAL	TRP	TRP	E4212	E4212	TRP	E3967	G3788	S3568	GLY	I3270	I3270
ASP	GLY	ASP	GLY	GLY	V4221	V4221	GLY	L3980	Q3801	W3572	ALA	L3274	L3274
ASP	SER	ASP	ALA	ALA	E4224	E4224	ALA	R3984	L3805	K3573	GLN		
GLY	GLY	GLY	ALA	ALA			ALA	L3985	N3809	R3579	ALA		
GLY	GLY	GLY	VAL	GLY	E4227	E4227	ALA	V3990	A3659	L3579	ASP	K3285	K3285
LEU	GLY	LEU	LEU	GLY	A4228	A4228	LEU	V3995	A3660	R3582	GLN		
LEU	GLY	LEU	LEU	GLY	E4229	E4229	GLY	V3996	W3661	E3583	GLU	E3290	E3290
VAL	VAL	VAL	VAL	VAL	K4230	K4230	VAL	A3997	I3662	E3584	ARG	A3291	A3291
PRO	ALA	PRO	SER	SER	M4231	M4231	SER	H3998	L3663	D3585	THR	P3292	P3292
GLY	GLY	GLY	TYR	TYR	I4242	I4242	ARG	M3999	D3676	A3586	LYS	P3293	P3293
GLY	GLY	GLY	ARG	ARG	F4243	F4243	ARG	P4106	K3823	D3587	LYS	P3294	P3294
GLY	GLY	GLY	ARG	ARG	E4244	E4244	ARG	E4107	L3835	D3587	LYS	A3295	A3295
PRO	ARG	PRO	ARG	ARG	P4254	P4254	ARG	I4108	L3842	I3592	LYS	P3297	P3297
PRO	VAL	PRO	VAL	VAL	GLY	GLY	VAL	Q4109	L3842	I3592	LYS	L3296	L3296
GLY	VAL	GLY	VAL	VAL	GLY	GLY	VAL	F4110	A3846	R3595	LYS	P3297	P3297
VAL	VAL	VAL	VAL	VAL	L4111	L4111	VAL	L4111	Q3850	V3596	LYS	A3298	A3298
LEU	LEU	LEU	LEU	LEU	L4112	L4112	LEU	L4112	R3851	E3607	LYS	Q3299	Q3299
ALA	ALA	ALA	ALA	ALA	S4115	S4115	ALA	K4014	Q3852	L3603	LYS	A3300	A3300
ALA	ALA	ALA	ALA	ALA	E4116	E4116	ALA	Q4009	K3852	H3605	LYS	P3301	P3301
ASP	ASP	ASP	ASP	ASP	A4117	A4117	ASP	I4010	L4013	R3606	LYS	P3302	P3302
GLY	GLY	GLY	GLY	GLY	D4119	D4119	GLY	E4011	L4013	E3607	LYS	P3303	P3303
GLY	GLY	GLY	GLY	GLY	E4119	E4119	GLY	Q4036	N3858	Q3608	LYS	C3304	C3304
PRO	PRO	PRO	THR	THR	D4119	D4119	PRO	M4039	V3859	T3609	LYS		
ASP	ASP	ASP	ALA	ALA	E4120	E4120	ASP	M4039	V3690	E3610	LYS		
ASN	ASN	ASN	ARG	ARG	E4121	E4121	ASN	Q4043	E3691	H3611	LYS		
					F4125	F4125			O3692	E3612	LYS		
					E4152	E4152			D3696	Y3613	LYS		
									C3733		LYS		
									E3736		LYS		
									GLU		LYS		

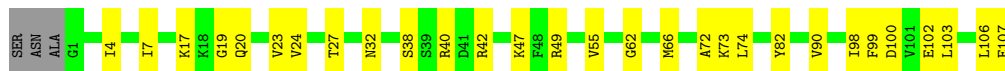


- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.602	Depositor
Minimum map value	-0.818	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.263	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	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, ADP

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	0.28	0/35746	0.62	7/48409 (0.0%)
1	B	0.28	0/35746	0.62	7/48409 (0.0%)
1	C	0.28	0/35746	0.62	8/48409 (0.0%)
1	D	0.28	0/35746	0.62	7/48409 (0.0%)
2	E	0.23	0/834	0.54	0/1123
2	F	0.23	0/834	0.54	0/1123
2	G	0.23	0/834	0.54	0/1123
2	H	0.23	0/834	0.54	0/1123
All	All	0.27	0/146320	0.62	29/198128 (0.0%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4581	LYS	CA-CB-CG	6.83	127.76	114.10
1	C	4581	LYS	CA-CB-CG	6.83	127.75	114.10
1	A	4581	LYS	CA-CB-CG	6.82	127.75	114.10
1	D	4581	LYS	CA-CB-CG	6.81	127.72	114.10
1	D	4184	MET	CA-C-N	-6.10	116.74	122.17

There are no chirality outliers.

There are no planarity outliers.

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	34929	0	34552	453	0
1	B	34929	0	34552	457	0
1	C	34929	0	34552	460	0
1	D	34929	0	34552	464	0
2	E	818	0	824	20	0
2	F	818	0	824	21	0
2	G	818	0	824	21	0
2	H	818	0	824	21	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	143100	0	141552	1879	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 7.

The worst 5 of 1879 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:B:2248:ARG:HB3	1:B:2286:LEU:HD11	1.72	0.71
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.72	0.71
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.72	0.71
1:D:2248:ARG:HB3	1:D:2286:LEU:HD11	1.72	0.71
1:A:2248:ARG:HB3	1:A:2286:LEU:HD11	1.72	0.71

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	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	B	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	C	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	D	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17844/21548 (83%)	17272 (97%)	560 (3%)	12 (0%)	49	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	A	4712	PRO
1	B	3615	SER
1	B	4712	PRO
1	C	3615	SER

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	A	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
1	B	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
1	C	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
1	D	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15584/18320 (85%)	15152 (97%)	432 (3%)	38 61

5 of 432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4193	ILE
1	C	4750	ILE
1	D	4835	LYS
1	C	4224	GLU
1	C	4640	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1541	GLN
1	C	4626	ASN
1	C	2127	GLN
1	C	3030	HIS
1	D	98	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	D	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)
3	ADP	C	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)
3	ADP	B	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)
3	ADP	A	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	5101	-	-	4/16/32/32	0/3/3/3
3	ADP	C	5101	-	-	4/16/32/32	0/3/3/3
3	ADP	B	5101	-	-	4/16/32/32	0/3/3/3
3	ADP	A	5101	-	-	4/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5101	ADP	C5-C4	4.36	1.46	1.39
3	D	5101	ADP	C5-C4	4.36	1.46	1.39
3	A	5101	ADP	C5-C4	4.36	1.46	1.39
3	B	5101	ADP	C5-C4	4.36	1.46	1.39
3	D	5101	ADP	C5-N7	-2.49	1.34	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5101	ADP	C5-C4-N3	-5.66	118.92	126.72
3	D	5101	ADP	C5-C4-N3	-5.66	118.92	126.72
3	A	5101	ADP	C5-C4-N3	-5.66	118.93	126.72
3	B	5101	ADP	C5-C4-N3	-5.66	118.93	126.72
3	C	5101	ADP	N3-C4-N9	4.67	135.11	127.17

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

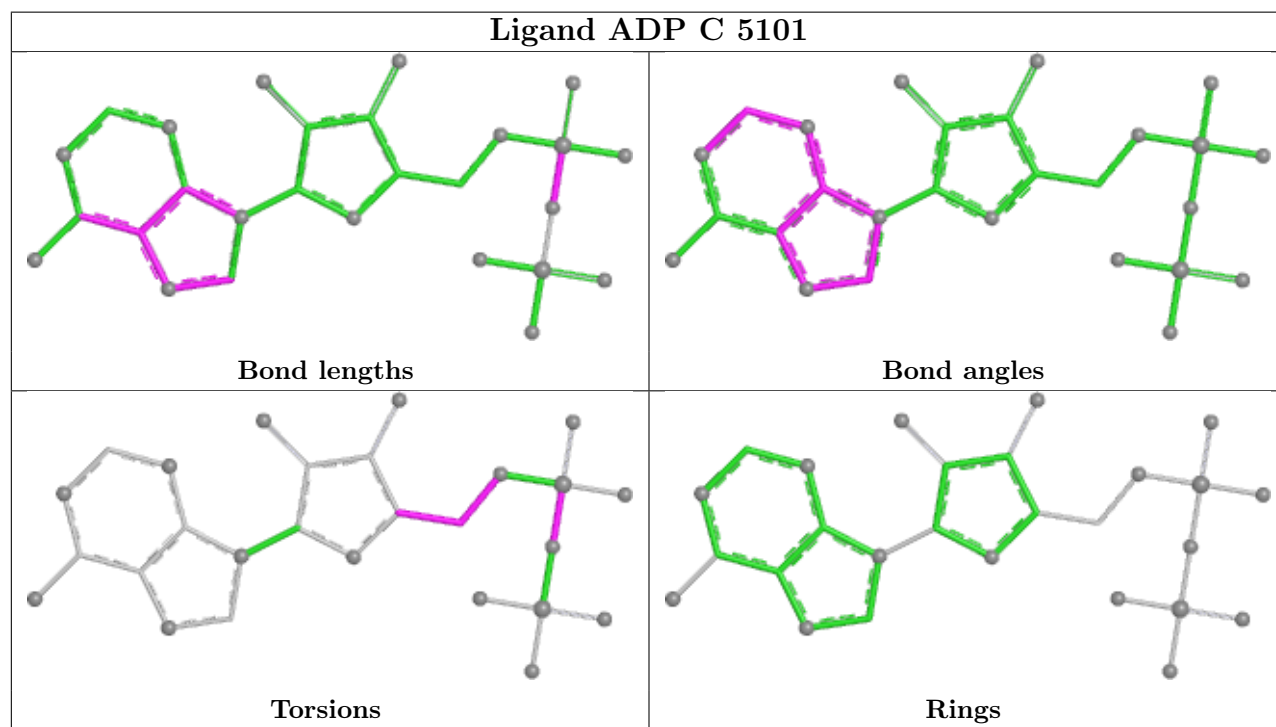
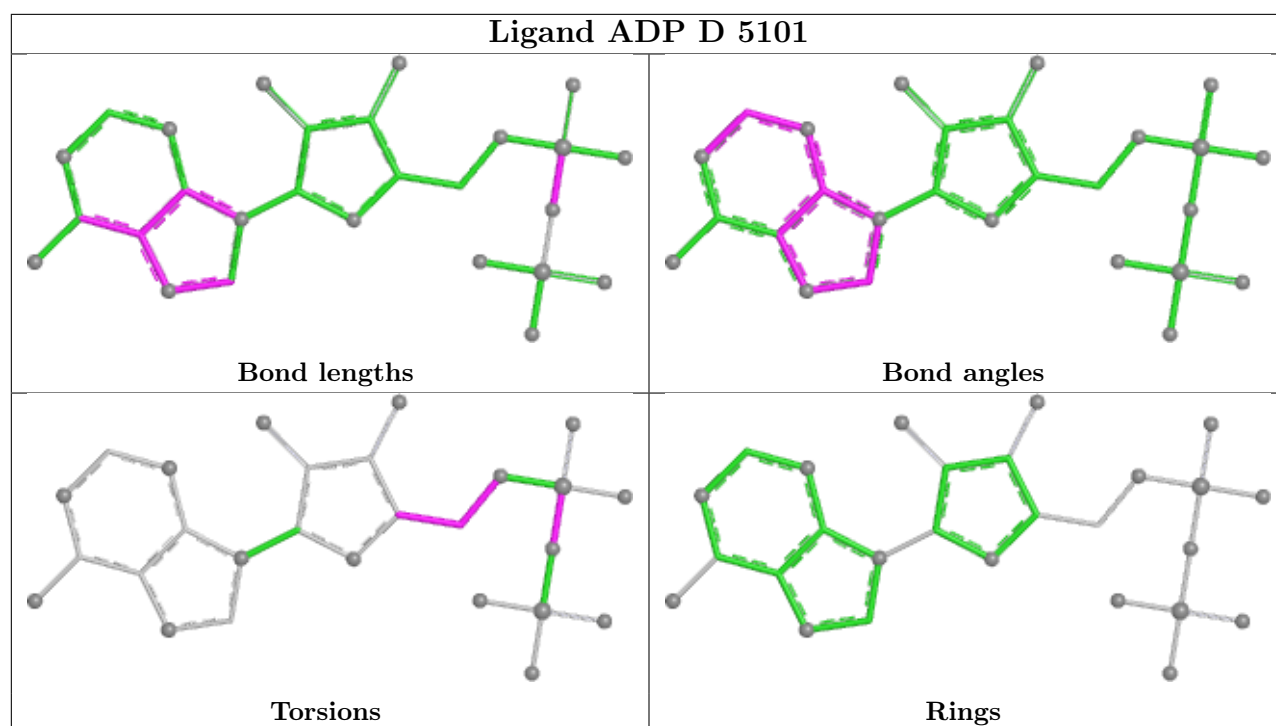
Mol	Chain	Res	Type	Atoms
3	A	5101	ADP	PB-O3A-PA-O5'
3	B	5101	ADP	PB-O3A-PA-O5'
3	C	5101	ADP	PB-O3A-PA-O5'
3	D	5101	ADP	PB-O3A-PA-O5'
3	A	5101	ADP	O4'-C4'-C5'-O5'

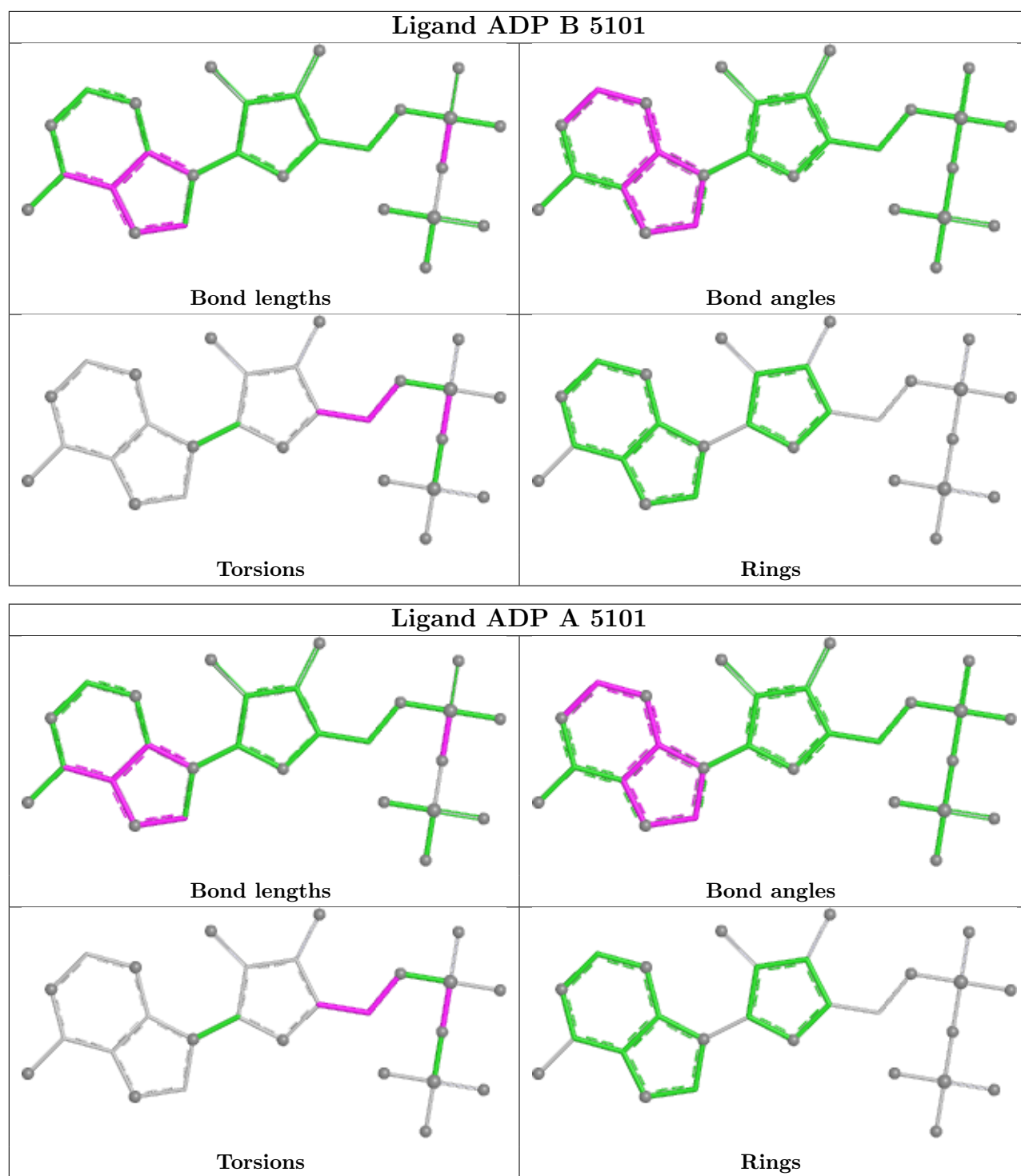
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5101	ADP	1	0
3	C	5101	ADP	1	0
3	B	5101	ADP	1	0
3	A	5101	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

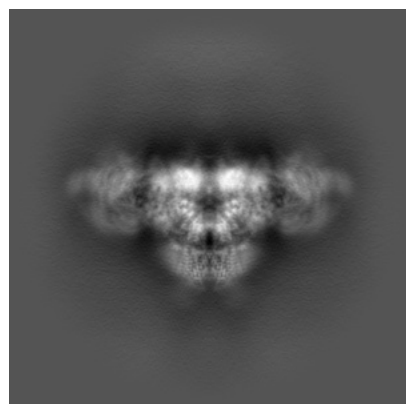
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40424. These allow visual inspection of the internal detail of the map and identification of artifacts.

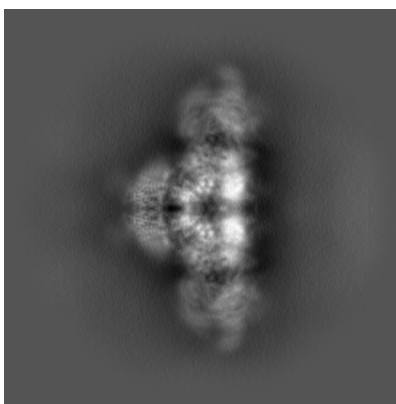
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

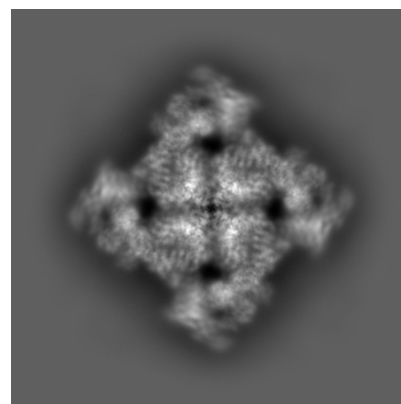
6.1.1 Primary map



X

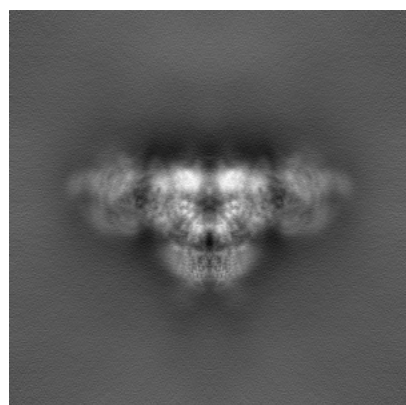


Y

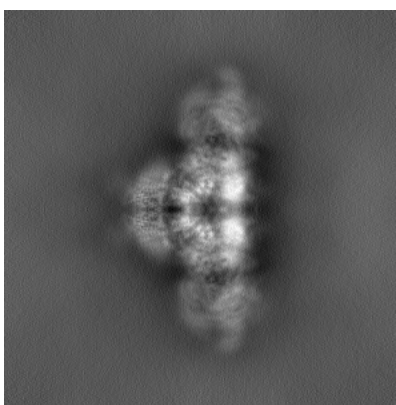


Z

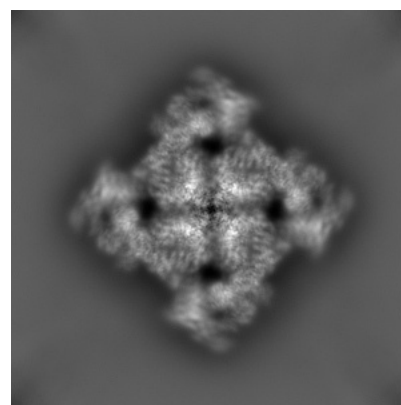
6.1.2 Raw map



X



Y

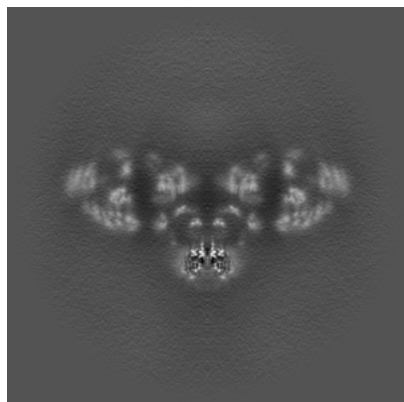


Z

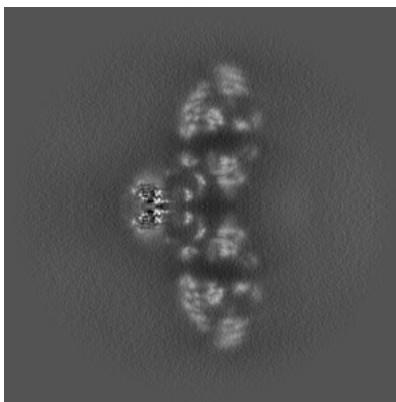
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

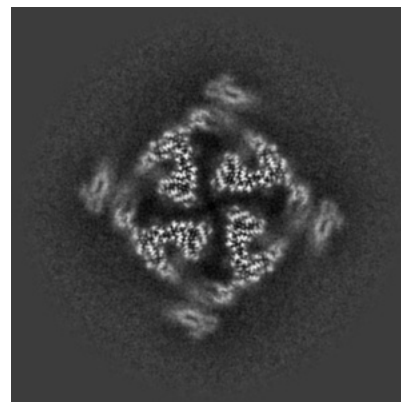
6.2.1 Primary map



X Index: 200

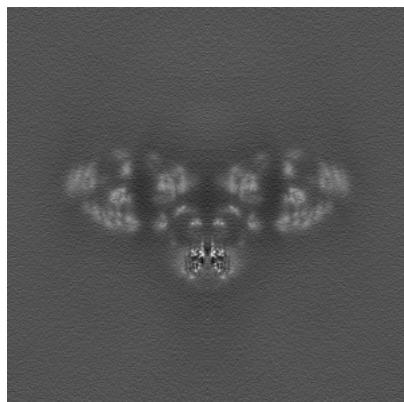


Y Index: 200

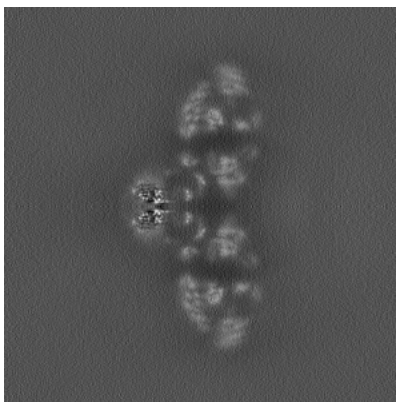


Z Index: 200

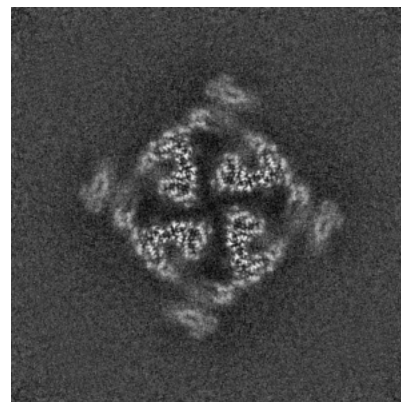
6.2.2 Raw map



X Index: 200



Y Index: 200

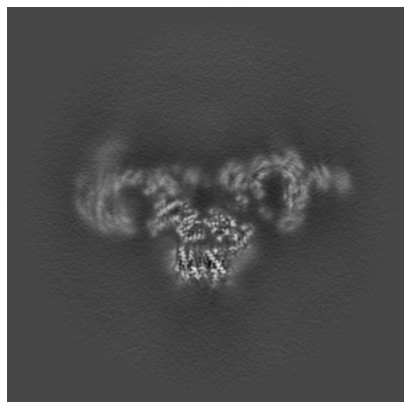


Z Index: 200

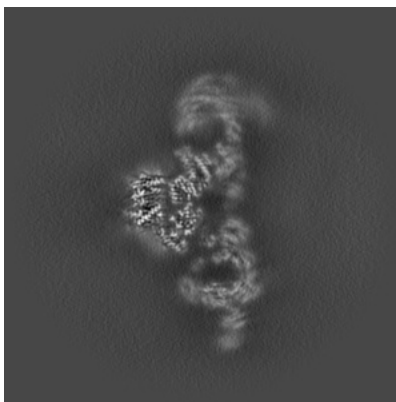
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

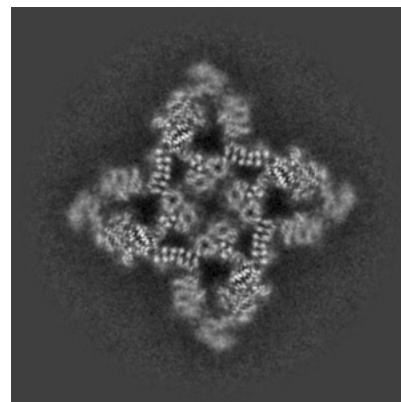
6.3.1 Primary map



X Index: 186

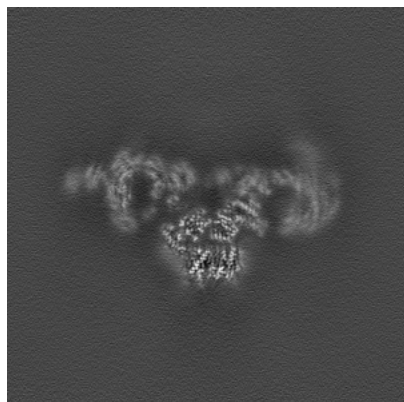


Y Index: 186

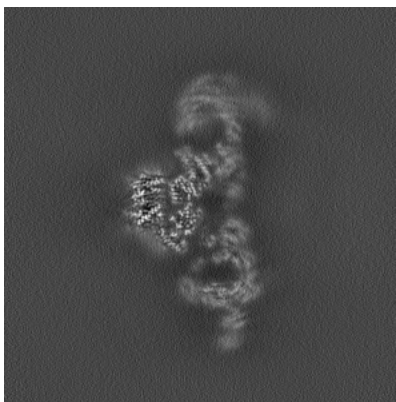


Z Index: 223

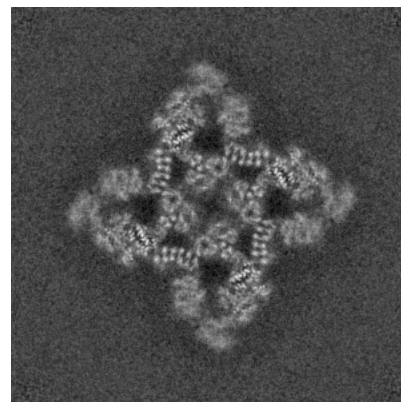
6.3.2 Raw map



X Index: 214



Y Index: 186

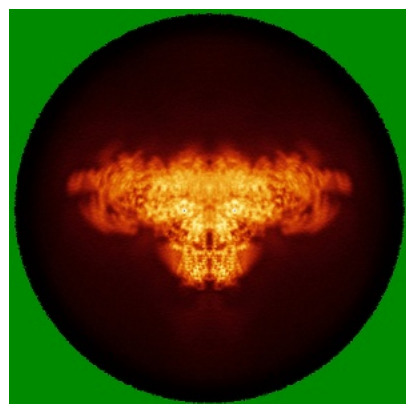


Z Index: 223

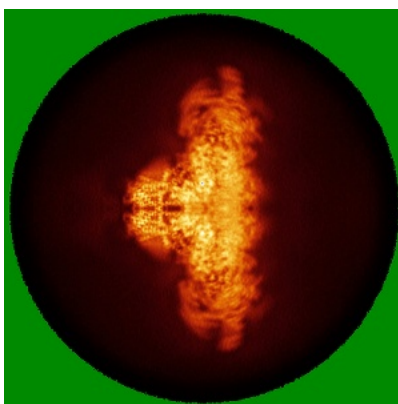
The images above show the largest variance slices of the map in three orthogonal directions.

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

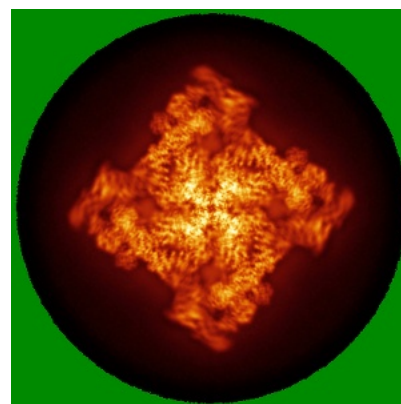
6.4.1 Primary map



X

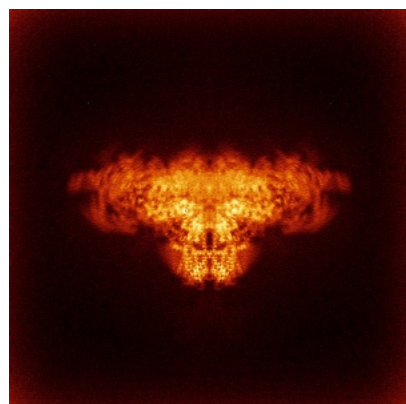


Y

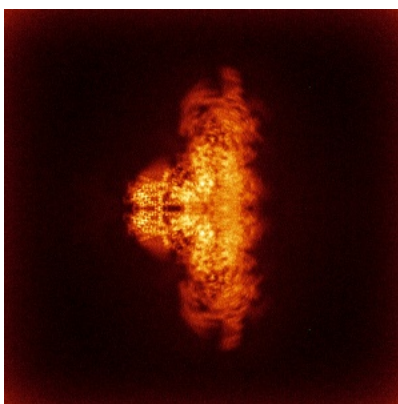


Z

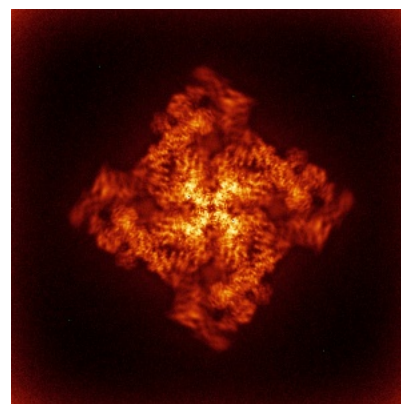
6.4.2 Raw map



X



Y

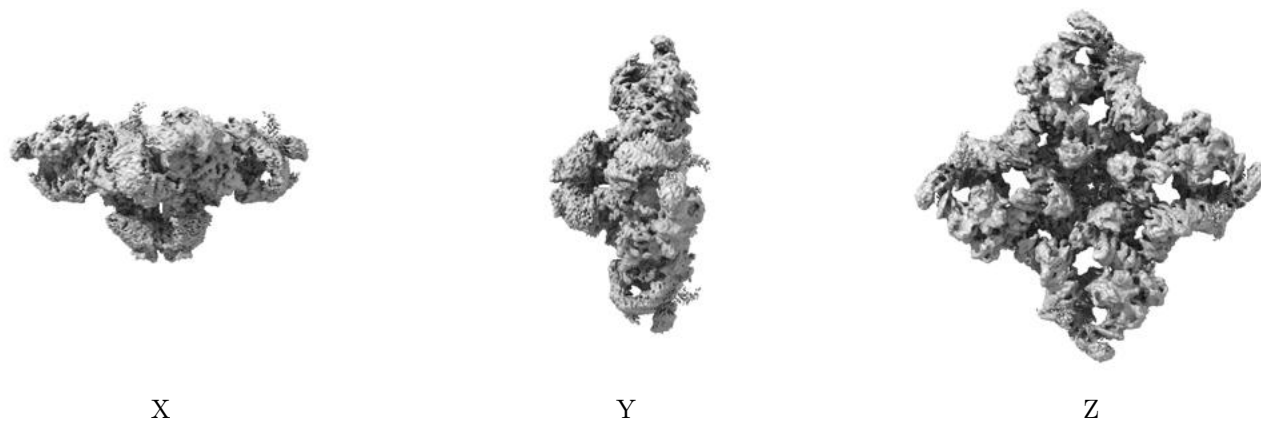


Z

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

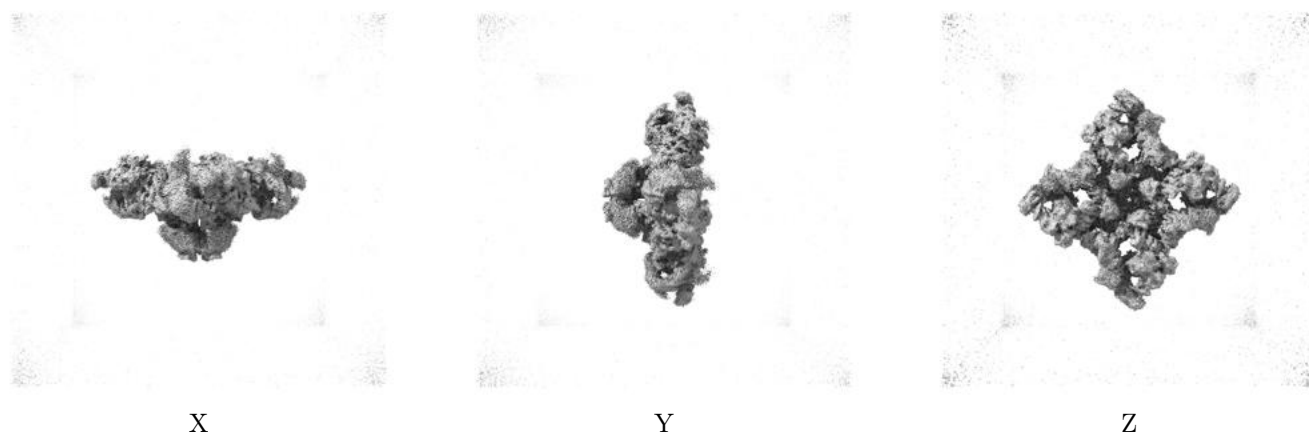
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

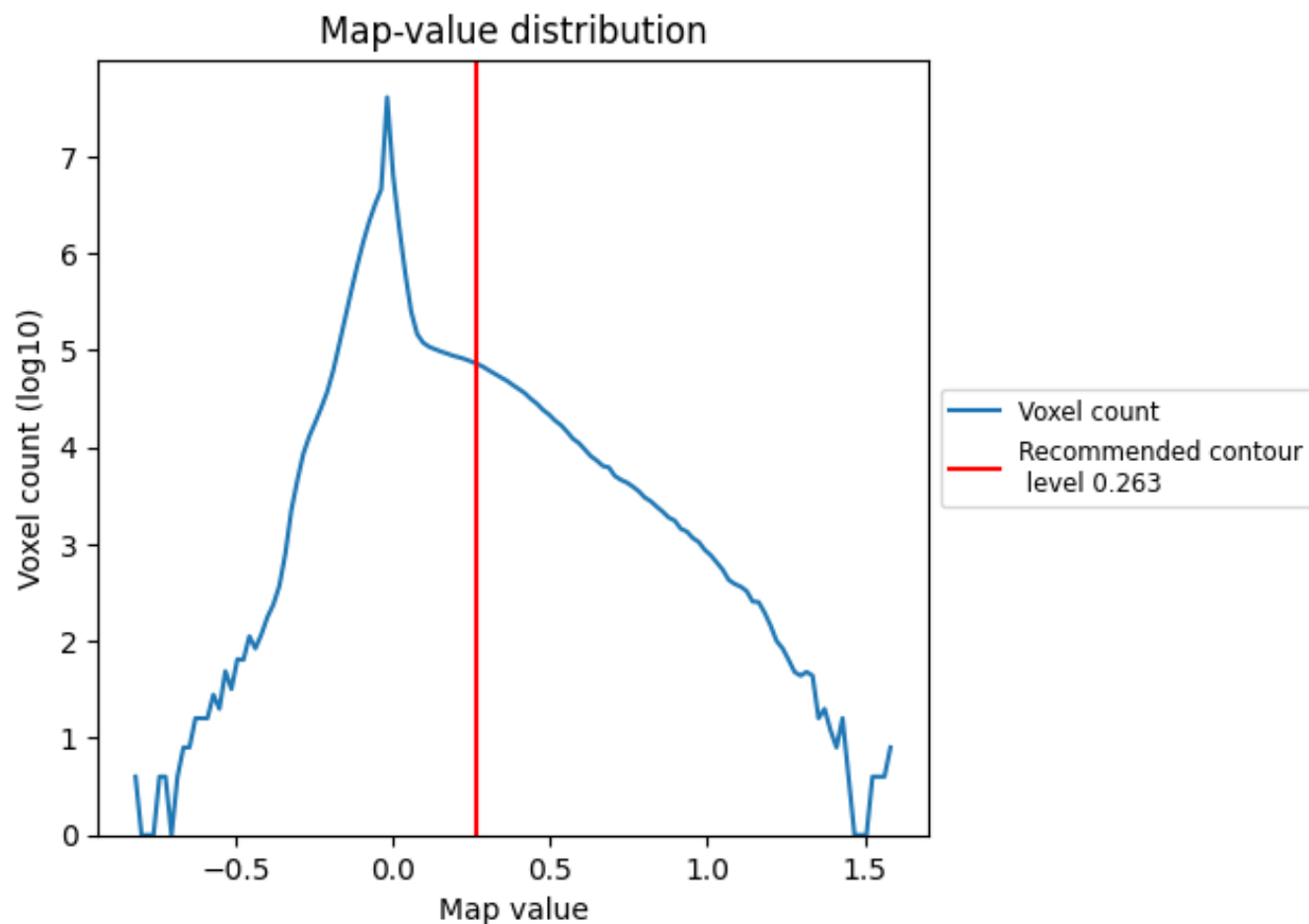
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

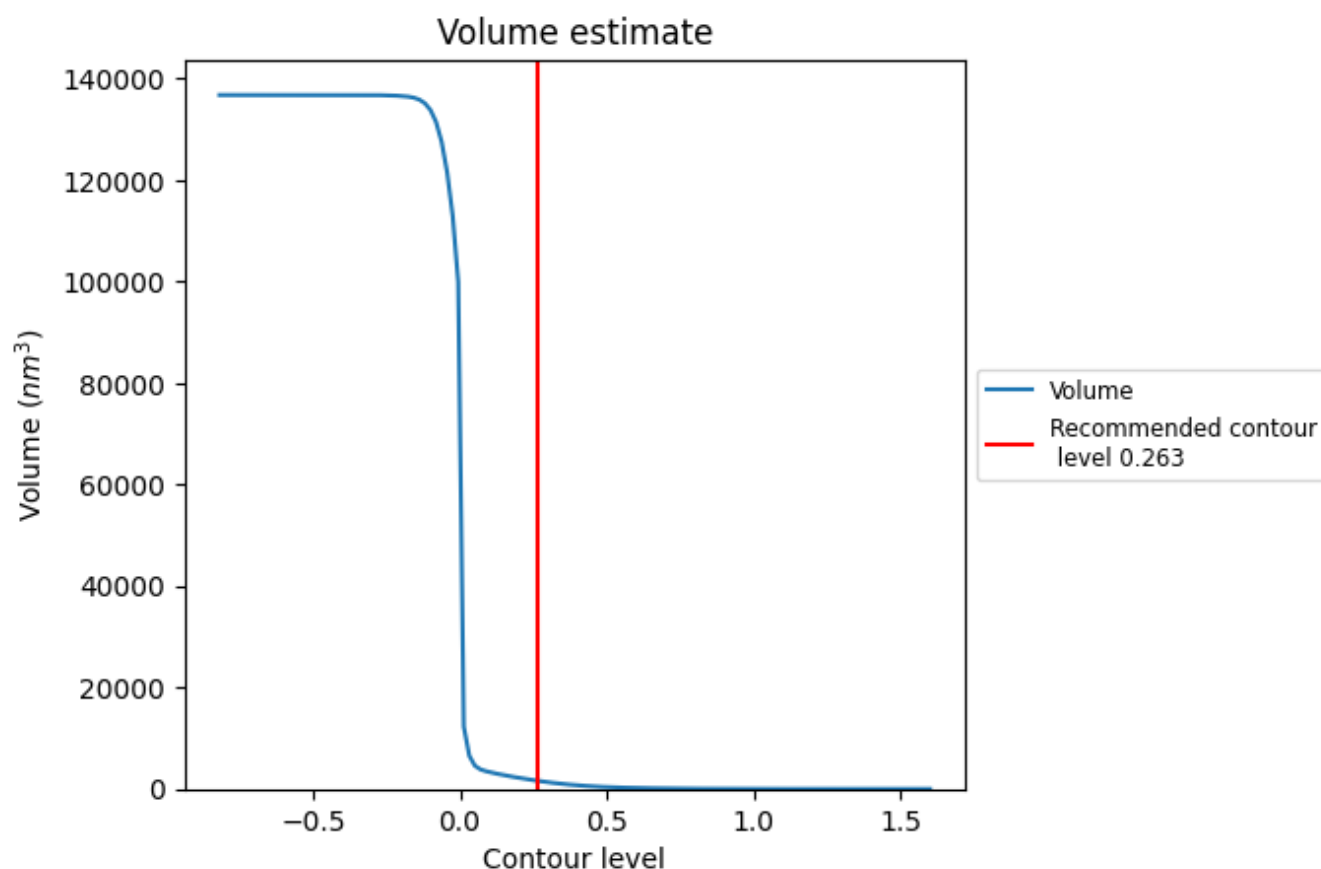
This section contains the results of statistical analysis of the map.

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.

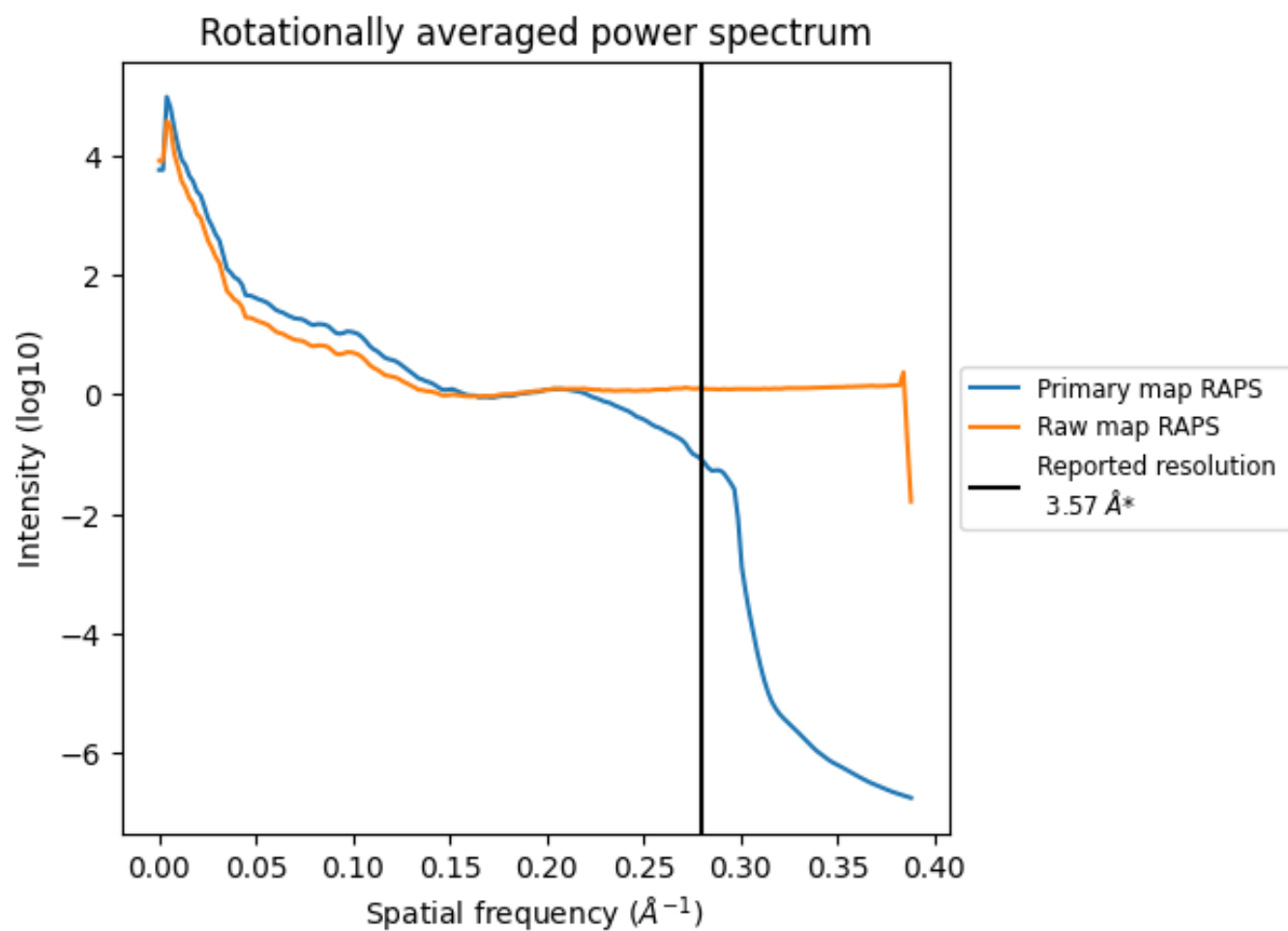
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1622 nm³; this corresponds to an approximate mass of 1465 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 ⓘ

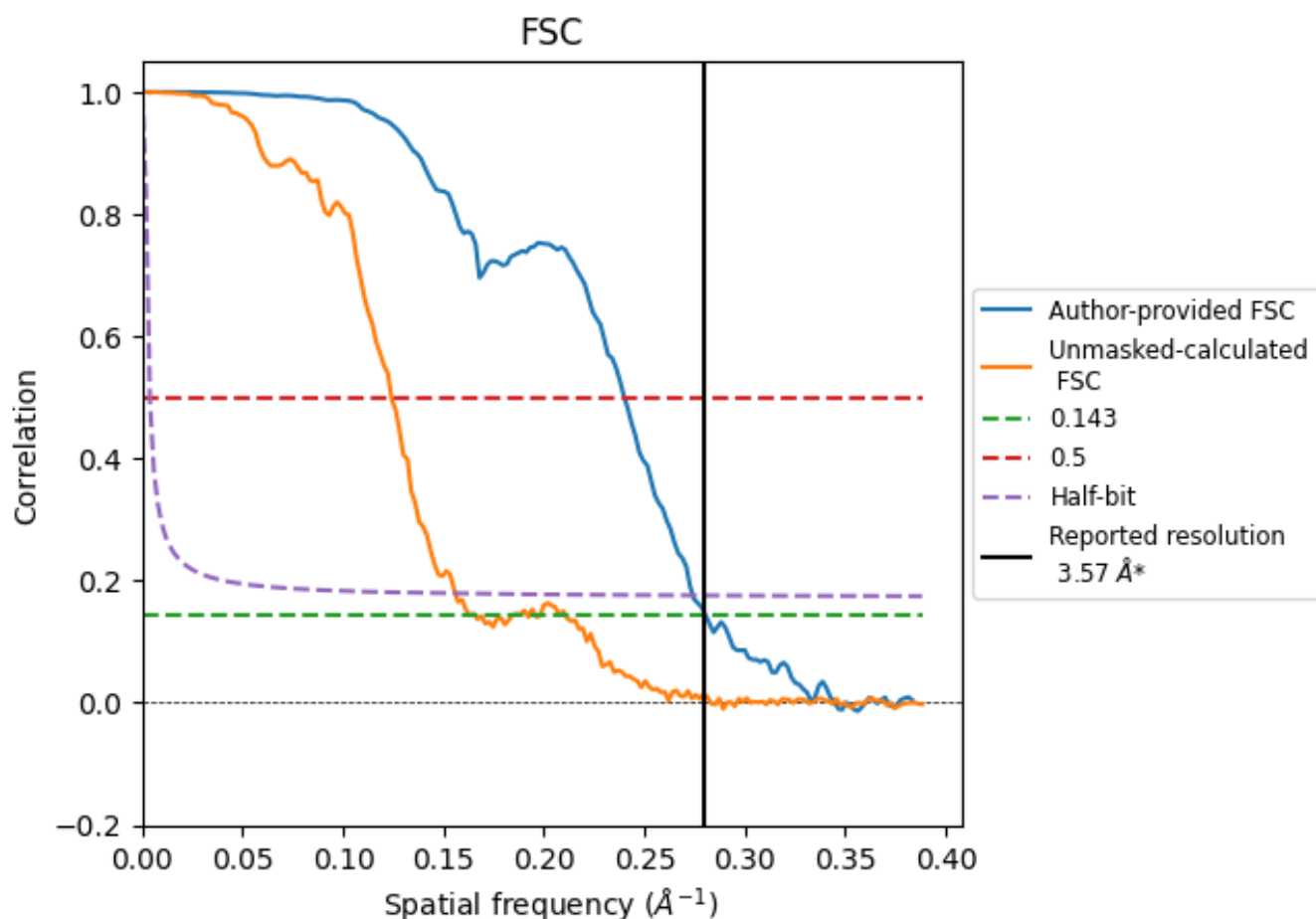


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

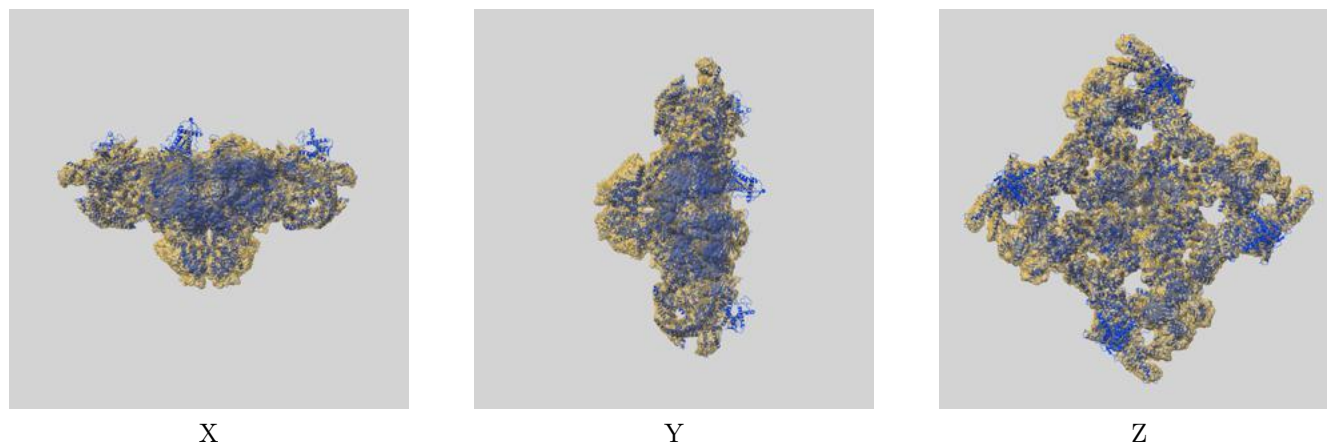
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.17	3.65
Unmasked-calculated*	6.04	8.06	6.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.04 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

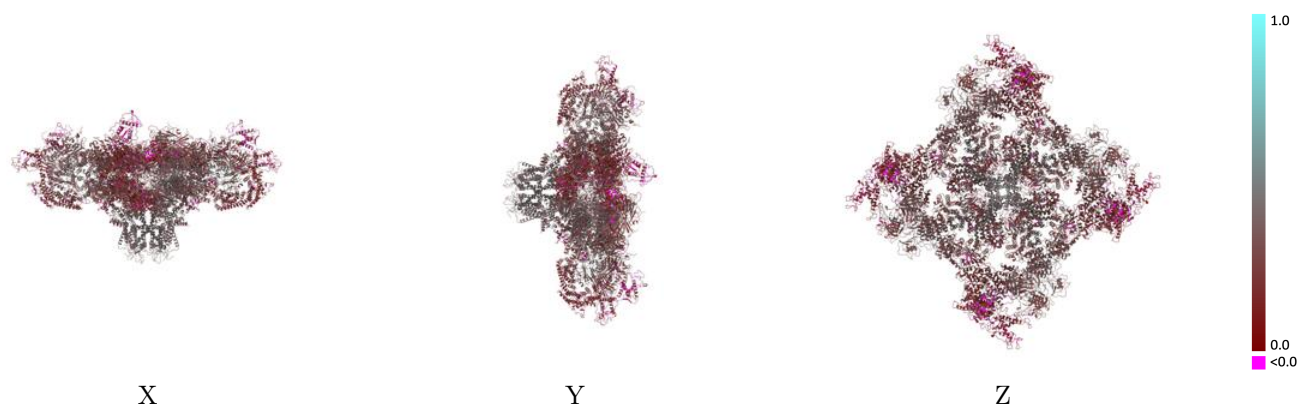
This section contains information regarding the fit between EMDB map EMD-40424 and PDB model 8SEP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



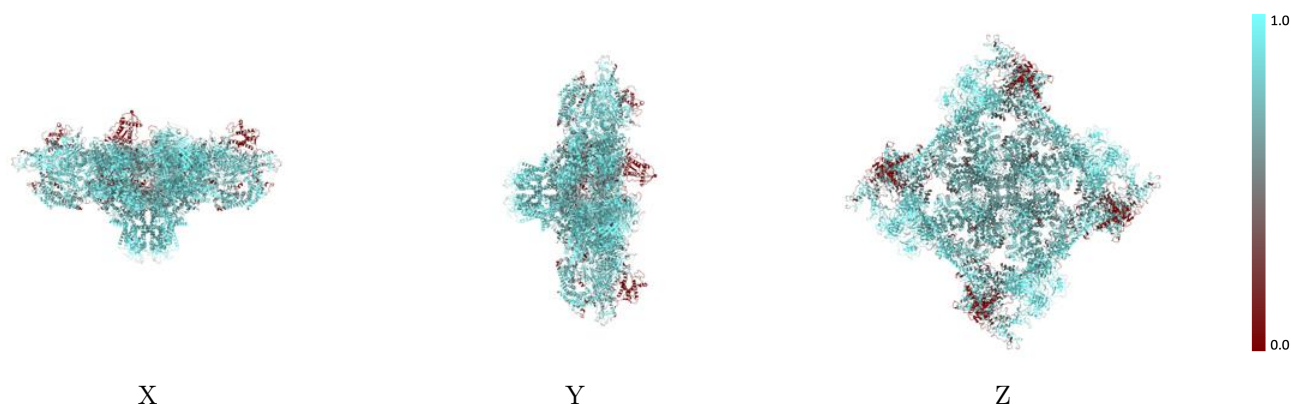
The images above show the 3D surface view of the map at the recommended contour level 0.263 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



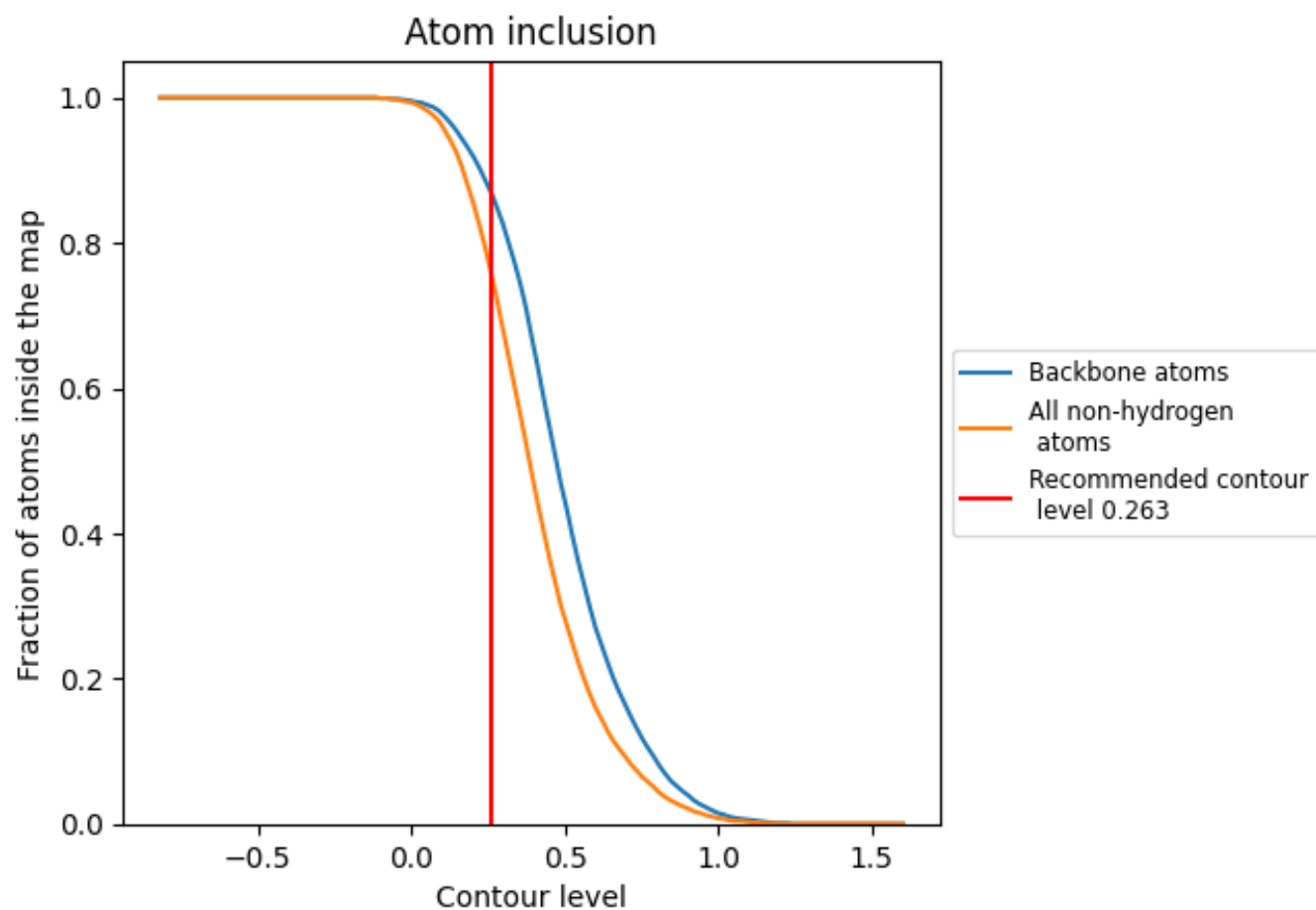
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.263).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.2890
A	0.7480	0.2870
B	0.7490	0.2880
C	0.7490	0.2880
D	0.7490	0.2880
E	0.9160	0.3620
F	0.9160	0.3620
G	0.9160	0.3620
H	0.9160	0.3620

1.0

0.0

<0.0