



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 08:06 AM EDT

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

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

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

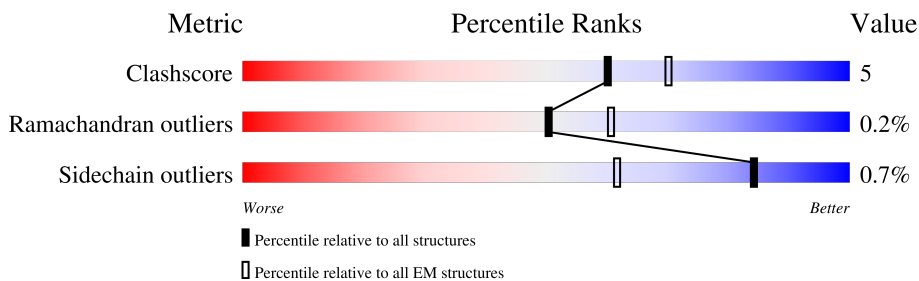
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 121272 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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

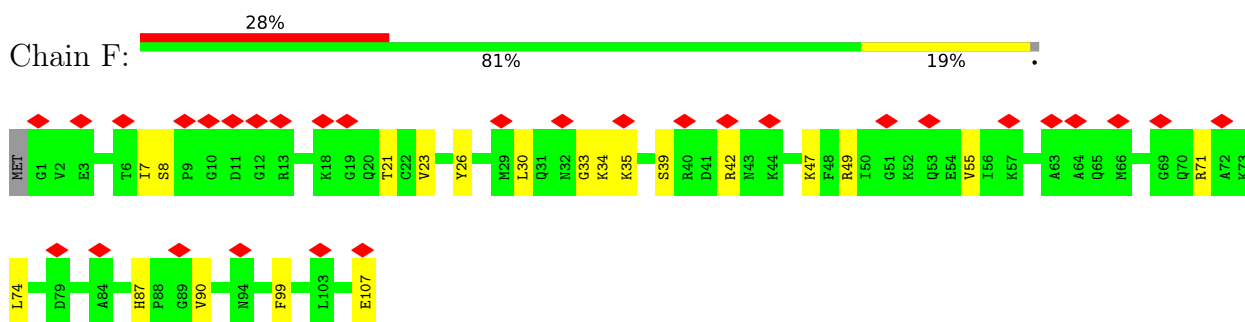
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

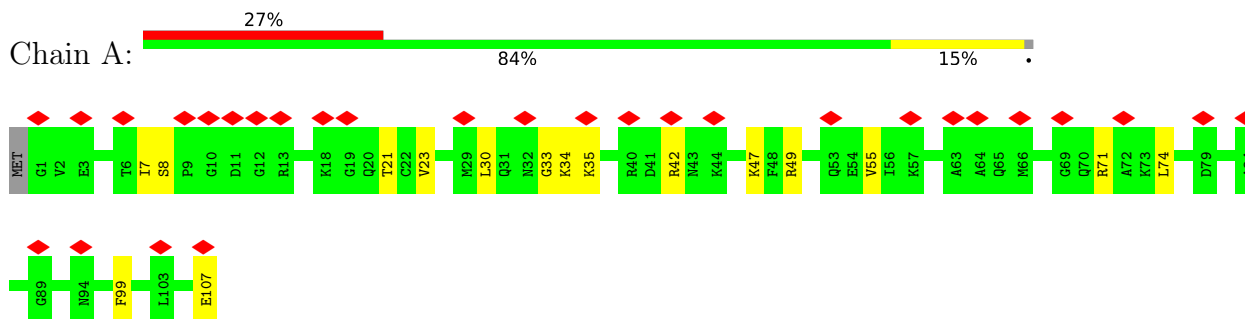
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

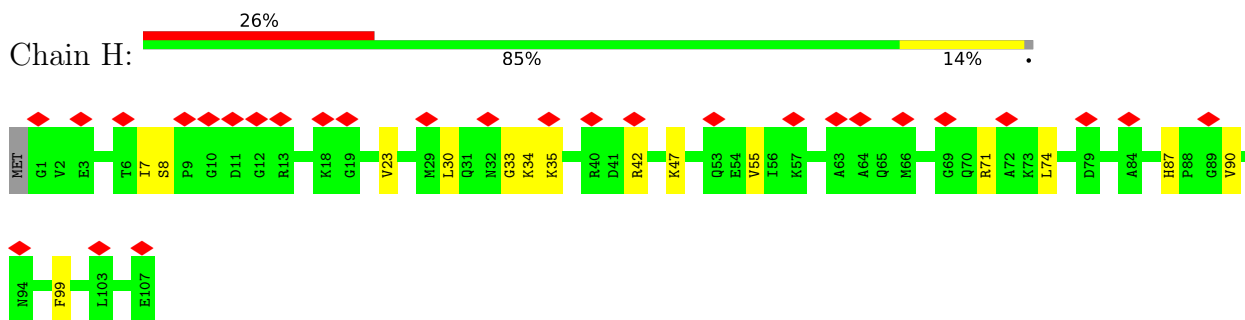
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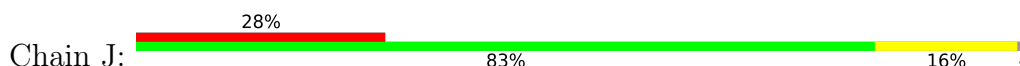
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

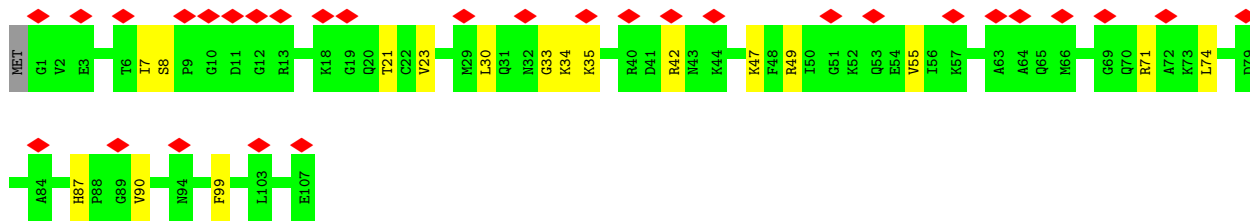


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

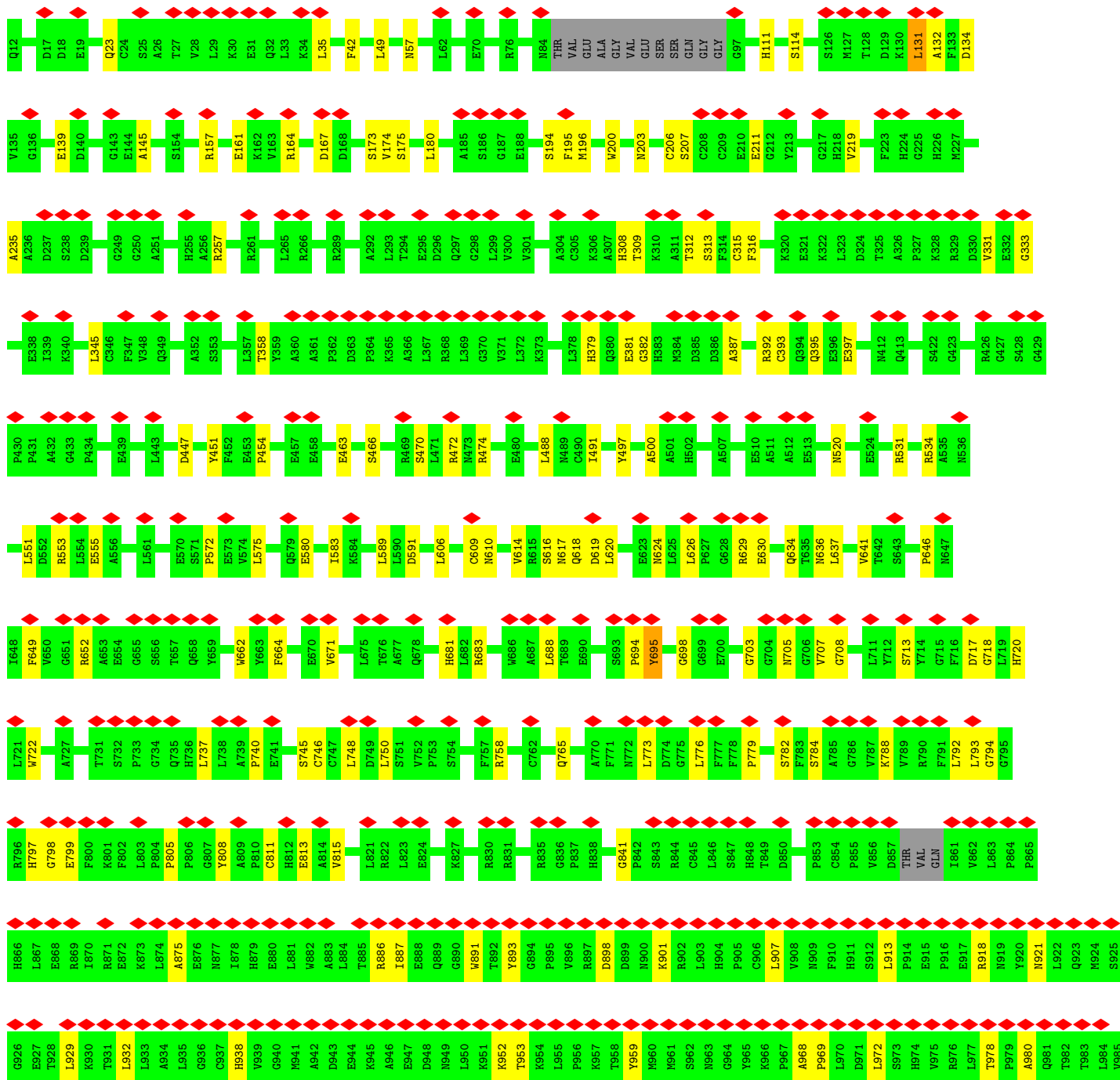
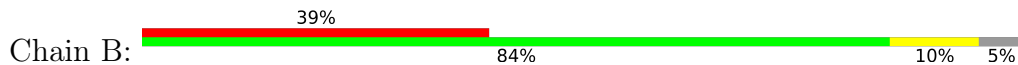


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



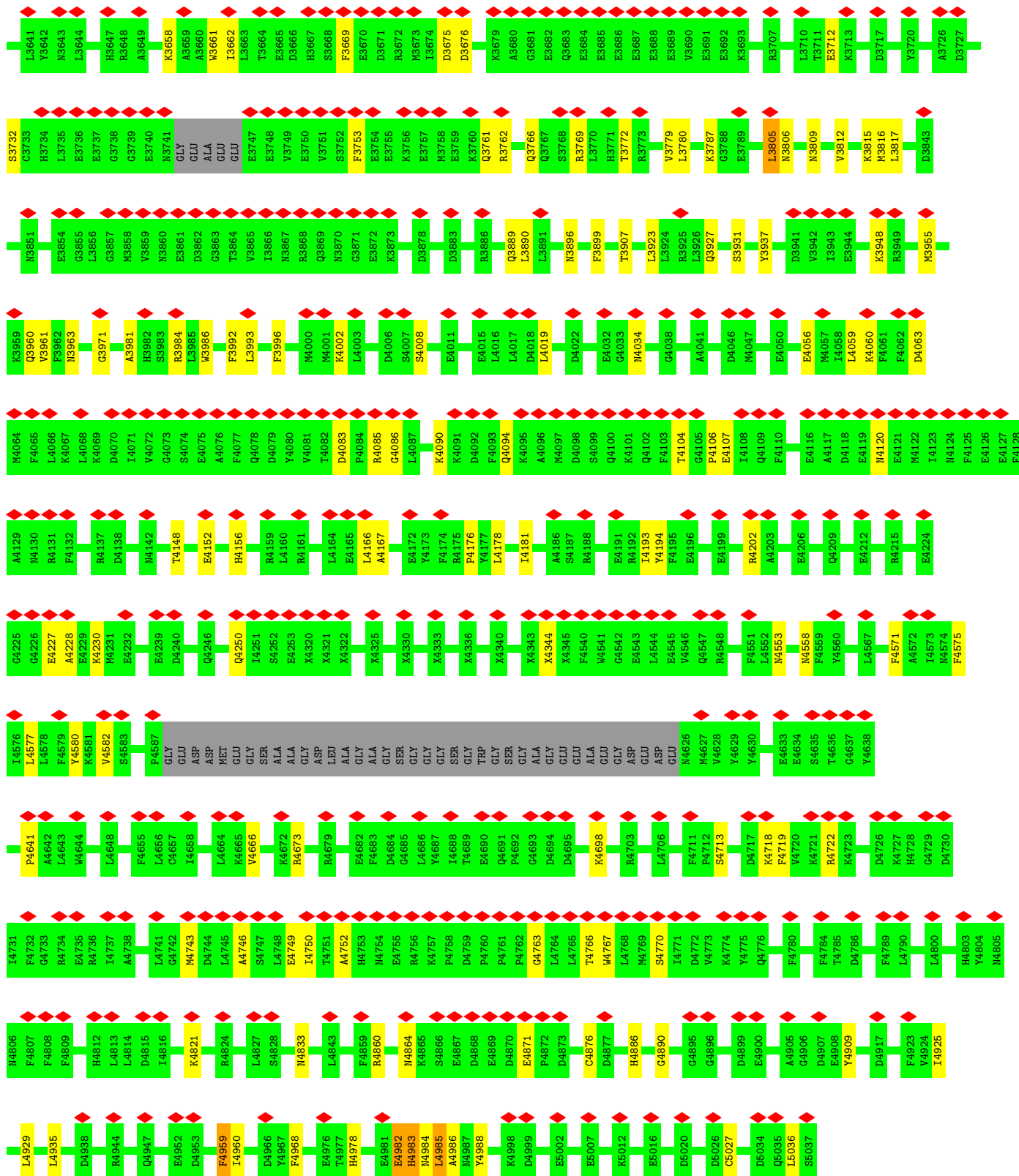


• Molecule 2: Ryanodine receptor 1

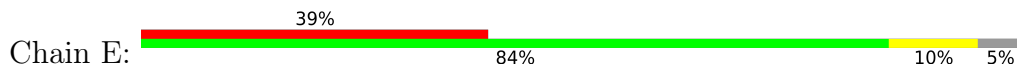




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X2423	X2432	X2435	X2436	X2437	X2438	X2439	X2440	X2441	X2442	X2448	X2454	X2455	X2463	X2464	X2465	X2466	X2469	X2472	X2473	X2474	X2475	X2476	X2477	X2478	X2479	X2487	X2488	X2489	X2490	X2523	X2524	X2529	X2532	X2536	X2537	X2538	X2562	X2563	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589																																																																							

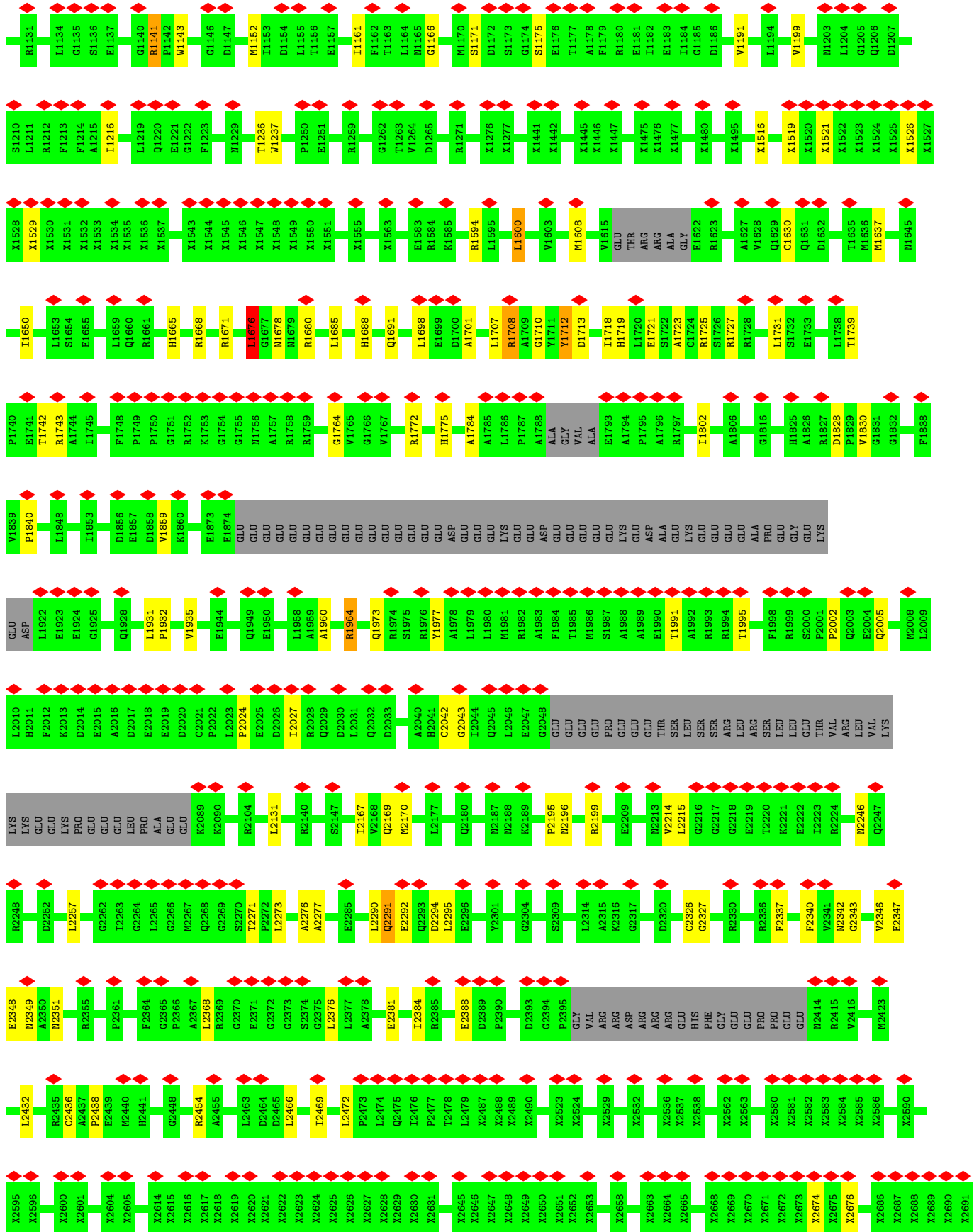


• Molecule 2: Ryanodine receptor 1



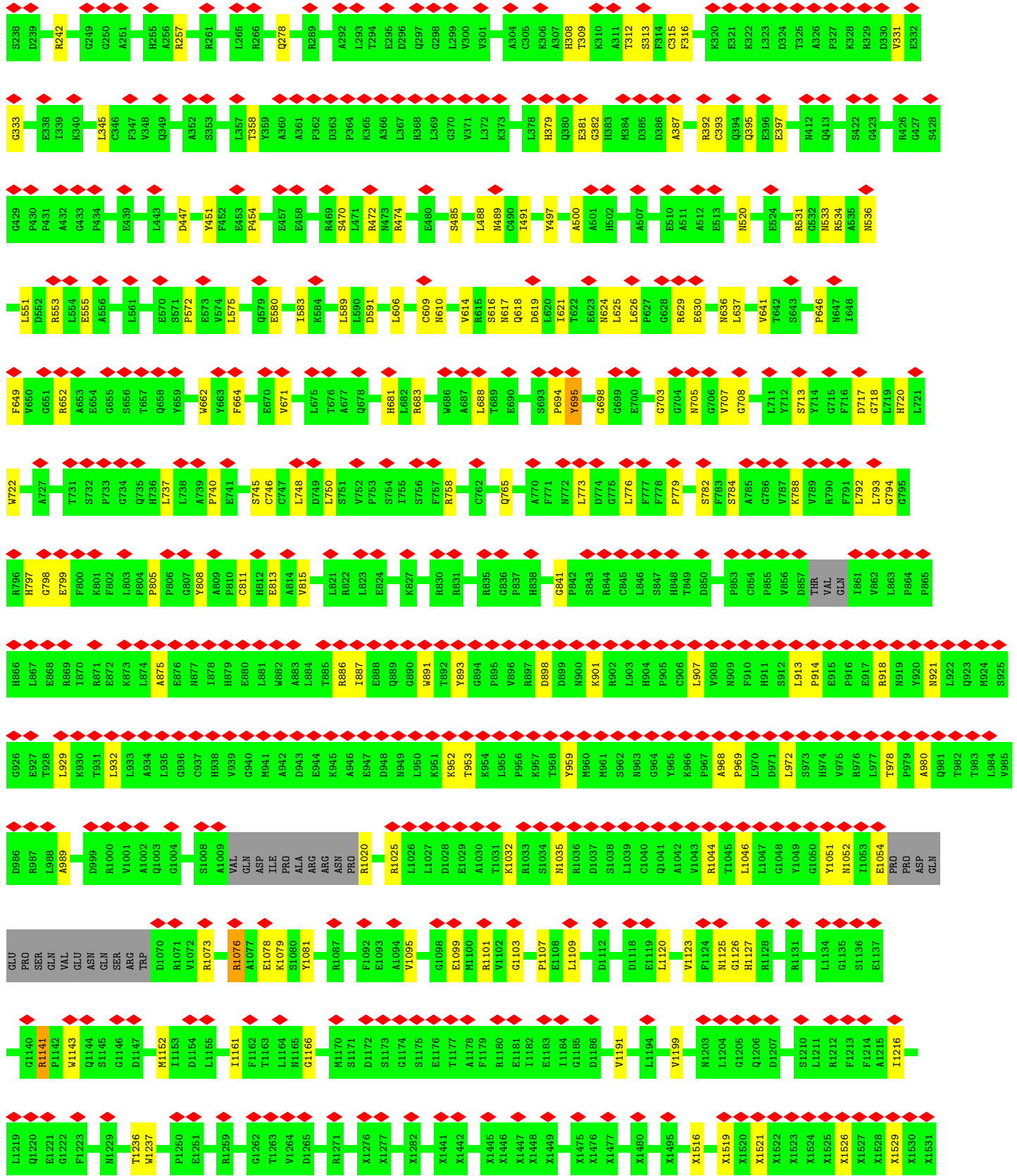






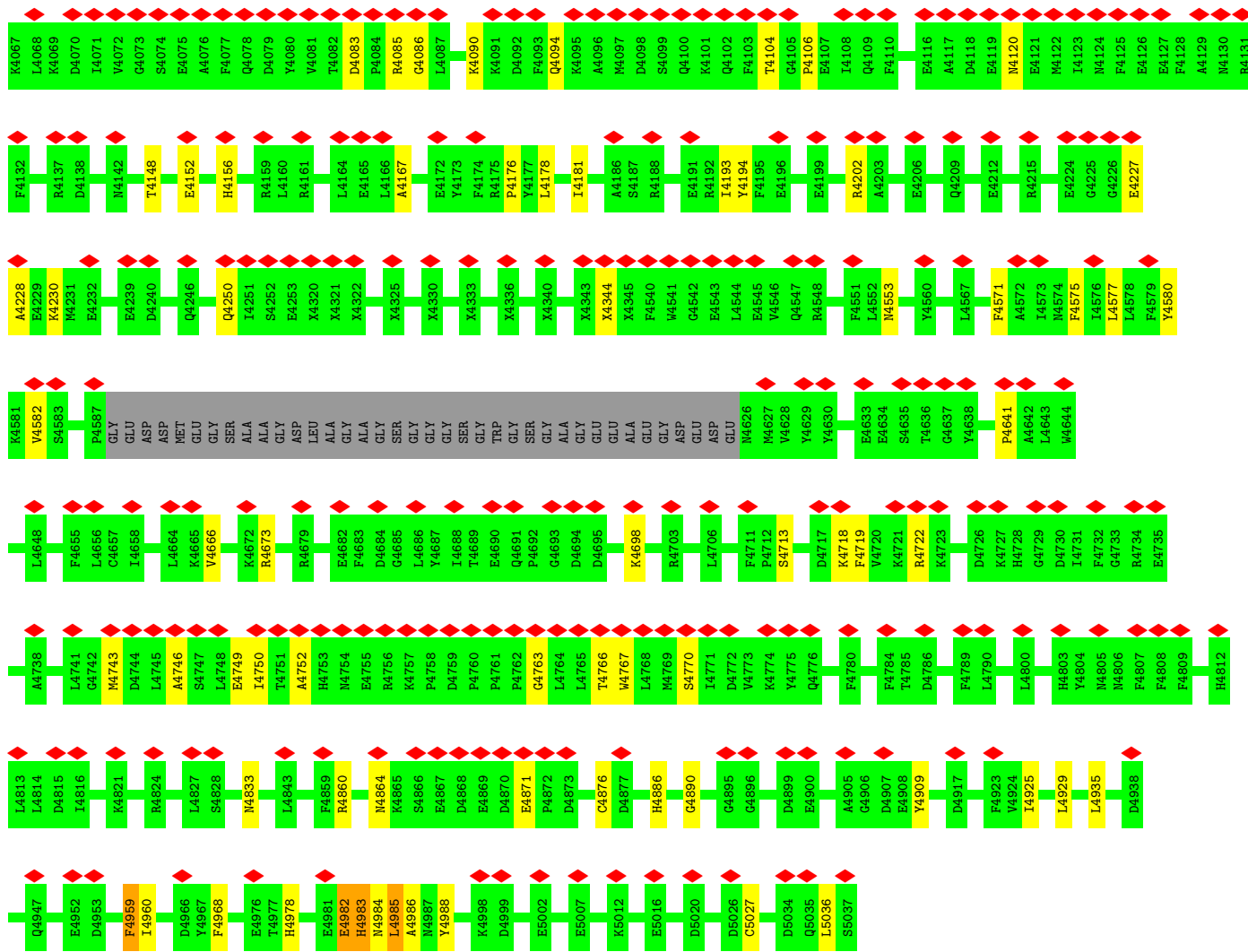




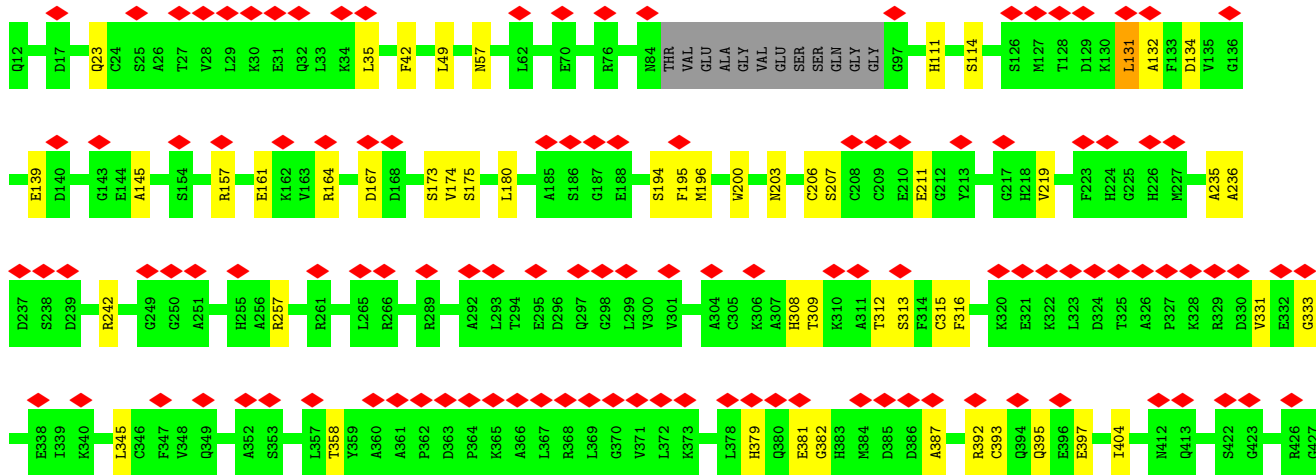
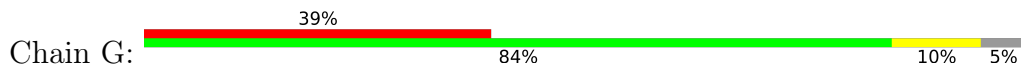


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G2343	V2346	E2347	E2348	N2349	A2350	N2351	R2355	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	A2378	E2381	L2384	R2385	E2388	D2389	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	R2415	V2416							
M2423	L2432	R2435	C2436	A2437	P2438	E2439	M2440	H2441	L2442	G2448	R2454	A2455	L2463	D2464	D2465	L2466	I2469	L2472	P2473	L2474	Q2475	L2476	P2477	L2478	L2479	X2487	X2488	X2489	X2490	X2523	X2524	X2529	X2532	X2536	X2537	X2538	X2562	X2563	X2580	X2581	X2582	X2583	X2584	X2585	X2586													
X2590	X2595	X2596	X2600	X2604	X2605	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2631	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2658	X2663	X2664	X2665	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2686	X2687	X2688	X2689	X2690										
X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	N2766	A2767	F2768	D2769	G2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	E2778	N2780
V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	F2793	N2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	T2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	N2816	L2817	A2818	N2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG

LYS	T2901	X2963	X3061	X3206	X3276	X3348	X3411	X3539	L3641	S3732	N3851	Q3960
ILE	H2902	X2964	X3062	X3207	X3277	X3349	X3412	X3540	G3733	G3733	E3854	Y3961
SER	P2903	X2968	X3063	X3208	X3278	X3350	X3413	X3541	H3734	H3734	G3855	F3962
GLN	L2904	X2969	X3134	X3209	X3279	X3351	X3414	X3542	L3644	L3735	G3856	N3963
ALA	L2905	X2970	X3135	X3210	X3280	X3352	X3415	X3543	L3644	L3736	G3857	G3971
GLN	V2906	X2971	X3136	X3211	X3281	X3353	X3416	X3544	H3647	E3737	M3858	A3981
THR	P2907	X2972	X3137	X3212	X3282	X3354	X3417	X3545	R3648	G3738	N3859	A3982
TYR	Y2908	X2973	X3138	X3213	X3283	X3355	X3421	X3546	R3649	G3739	N3860	S3983
ASP	D2909	X2974	X3139	X3214	X3284	X3356	X3422	X3547	K3650	E3740	N3861	L3984
PRO	D2910	X2975	X3140	X3215	X3285	X3357	X3423	X3548	K3651	G3741	E3862	L3985
ARG	T2911	X2976	X3141	X3216	X3286	X3358	X3433	X3549	A3652	GLU	R3863	K3986
GLU	L2912	X2977	X3142	X3217	X3287	X3359	X3434	X3550	W3661	ALA	T3864	L3987
GLY	T2913	X2978	X3143	X3218	X3288	X3360	X3435	X3551	L3662	GLU	V3865	L3988
	A2914	X2979	X3144	X3219	X3289	X3361	X3436	X3552	L3663	E3747	V3866	F3992
	E2915	X2980	X3145	X3220	X3290	X3362	X3439	X3553	T3664	E3748	T3867	L3993
	K2916	X2981	X3000	X3221	X3291	X3363	X3440	X3554	E3665	V3749	N3867	F3996
	E2917	X2982	X3001	X3222	X3292	X3364	X3441	X3555	D3666	E3750	R3868	M4000
	R2918	X2983	X3002	X3223	X3293	X3365	X3442	X3556	H3667	V3751	Q3869	M4001
	D2919	X2984	X3014	X3224	X3294	X3366	X3443	X3557	S3668	S3752	N3870	K4002
	R2920	X2985	X3015	X3225	X3295	X3367	X3444	X3558	F3669	F3753	G3871	L4003
	E2921	X2986	X3016	X3226	X3296	X3368	X3445	X3559	E3670	E3754	E3872	D4004
	K2922	X2987	X3017	X3227	X3297	X3369	X3446	X3560	D3671	E3755	K3873	A4007
	A2923	X2988	X3018	X3228	X3298	X3370	X3447	X3561	R3672	E3756	G3874	S4008
	Q2924	X2989	X3019	X3229	X3299	X3371	X3448	X3562	K3673	E3757	D3875	E4011
	E2925	X2990	X3020	X3230	X3300	X3372	X3449	X3563	B3674	M3758	D3883	E4015
	E2926	X2991	X3021	X3231	X3301	X3373	X3450	X3564	D3675	E3759	N3884	L4016
	L2927	X2992	X3022	X3232	X3302	X3374	X3451	X3565	D3676	K3760	R3885	L4017
	K2928	X2993	X3023	X3233	X3303	X3375	X3452	X3566	K3677	Q3761	Q3886	L4018
	F2929	X2994	X3024	X3234	X3304	X3376	X3453	X3567	A3680	R3762	L3889	D4019
	L2930	X2995	X3025	X3235	X3305	X3377	X3454	X3568	G3681	Q3766	L3890	L4019
	Q2931	X2996	X3026	X3236	X3306	X3378	X3455	X3569	E3682	E3767	N3891	D4022
	M2932	X2997	X3027	X3237	X3307	X3379	X3456	X3570	Q3683	S3768	N3896	E4032
	N2933	X2998	X3028	X3238	X3308	X3380	X3457	X3571	E3684	R3769	F3899	G4033
	E2934	X2999	X3029	X3239	X3309	X3381	X3458	X3572	E3685	L3770	F3900	M4034
	G2935	X3000	X3030	X3240	X3310	X3382	X3459	X3573	E3686	H3771	T3907	G4038
	Y2936	X3001	X3031	X3241	X3311	X3383	X3460	X3574	E3687	T3772	L3923	L4046
	A2936	X3002	X3032	X3242	X3312	X3384	X3461	X3575	E3688	R3773	L3924	M4047
	V2937	X3003	X3033	X3243	X3313	X3385	X3462	X3576	E3689	L3780	R3925	F4050
	T2938	X3004	X3034	X3244	X3314	X3386	X3463	X3577	E3690	K3781	L3926	E4056
	R2939	X3005	X3035	X3245	X3315	X3387	X3464	X3578	E3691	Q3788	Q3927	M4057
	Y2940	X3006	X3036	X3246	X3316	X3388	X3465	X3579	E3692	L3805	D3941	M4058
	X2941	X3007	X3037	X3247	X3317	X3389	X3466	X3580	R3707	N3806	V3942	L4059
	X2942	X3008	X3038	X3248	X3318	X3390	X3467	X3581	L3710	N3809	I3943	L4060
	X2943	X3009	X3039	X3249	X3319	X3391	X3468	X3582	T3711	V3812	E3944	F4061
	X2944	X3010	X3040	X3250	X3320	X3392	X3469	X3583	E3712	K3815	K3948	F4062
	X2945	X3011	X3041	X3251	X3321	X3393	X3470	X3584	K3713	M3816	R3949	D4063
	X2946	X3012	X3042	X3252	X3322	X3394	X3471	X3585	D3717	L3817	F4065	M4064
	X2947	X3013	X3043	X3253	X3323	X3395	X3472	X3586	X3526	X3592	L3955	F4065
	X2948	X3014	X3044	X3254	X3324	X3396	X3473	X3587	X3527	X3593	K3959	L4066
	X2949	X3015	X3045	X3255	X3325	X3397	X3474	X3588	X3528	X3594		
	X2950	X3016	X3046	X3256	X3326	X3398	X3475	X3589	X3529	X3595		
	X2951	X3017	X3047	X3257	X3327	X3399	X3476	X3590	X3530	X3596		
	X2952	X3018	X3048	X3258	X3328	X3400	X3477	X3591	X3531	X3597		
	X2953	X3019	X3049	X3259	X3329	X3401	X3478	X3592	X3532	X3598		
	X2954	X3020	X3050	X3260	X3330	X3402	X3479	X3593	X3533	X3599		
	X2955	X3021	X3051	X3261	X3331	X3403	X3480	X3594	X3534	X3600		
	X2956	X3022	X3052	X3262	X3332	X3404	X3481	X3595	X3535	X3601		
	X2957	X3023	X3053	X3263	X3333	X3405	X3482	X3596	X3536	X3602		
	X2958	X3024	X3054	X3264	X3334	X3406	X3483	X3597	X3537	X3603		
	X2959	X3025	X3055	X3265	X3335	X3407	X3484	X3598	X3538	X3604		
	X2960	X3026	X3056	X3266	X3336	X3408	X3485	X3599	X3539	X3605		
	X2961	X3027	X3057	X3267	X3337	X3409	X3486	X3600	X3540	X3606		
	X2962	X3028	X3058	X3268	X3338	X3410	X3487	X3601	X3541	X3607		
		X3029	X3059	X3269	X3339	X3411	X3488	X3602	X3542	X3608		
		X3030	X3060	X3270	X3340	X3412	X3489	X3603	X3543	X3609		
		X3031	X3061	X3271	X3341	X3413	X3490	X3604	X3544	X3610		
		X3032	X3062	X3272	X3342	X3414	X3491	X3605	X3545	X3611		
		X3033	X3063	X3273	X3343	X3415	X3492	X3606	X3546	X3612		
		X3034	X3064	X3274	X3344	X3416	X3493	X3607	X3547	X3613		
		X3035	X3065	X3275	X3345	X3417	X3494	X3608	X3548			
		X3036	X3066	X3276	X3346	X3418	X3495	X3609	X3549			
		X3037	X3067	X3277	X3347	X3419	X3496	X3610	X3550			
		X3038	X3068	X3278	X3348	X3420	X3497	X3611	X3551			
		X3039	X3069	X3279	X3349	X3421	X3498	X3612	X3552			
		X3040	X3070	X3280	X3350	X3422	X3499	X3613	X3553			
		X3041	X3071	X3281	X3351	X3423	X3500		X3554			
		X3042	X3072	X3282	X3352	X3424	X3501		X3555			
		X3043	X3073	X3283	X3353	X3425	X3502		X3556			
		X3044	X3074	X3284	X3354	X3426	X3503		X3557			
		X3045	X3075	X3285	X3355	X3427	X3504		X3558			
		X3046	X3076	X3286	X3356	X3428	X3505		X3559			
		X3047	X3077	X3287	X3357	X3429	X3506		X3560			
		X3048	X3078	X3288	X3358	X3430	X3507		X3561			
		X3049	X3079	X3289	X3359	X3431	X3508		X3562			
		X3050	X3080	X3290	X3360	X3432	X3509		X3563			
		X3051	X3081	X3291	X3361	X3433	X3510		X3564			
		X3052	X3082	X3292	X3362	X3434	X3511		X3565			
		X3053	X3083	X3293	X3363	X3435	X3512		X3566			
		X3054	X3084	X3294	X3364	X3436	X3513		X3567			
		X3055	X3085	X3295	X3365	X3437	X3514		X3568			
		X3056	X3086	X3296	X3366	X3438	X3515		X3569			
		X3057	X3087	X3297	X3367	X3439	X3516		X3570			
		X3058	X3088	X3298	X3368	X3440	X3517		X3571			
		X3059	X3089	X3299	X3369	X3441	X3518		X3572			
		X3060	X3090	X3300	X3370	X3442	X3519		X3573			
		X3061	X3091	X3301	X3371	X3443	X3520		X3574			
		X3062	X3092	X3302	X3372	X3444	X3521		X3575			
		X3063	X3093	X3303	X3373	X3445	X3522		X3576			
		X3064	X3094	X3304	X3374	X3446	X3523		X3577			
		X3065	X3095	X3305	X3375	X3447	X3524		X3578			
		X3066	X3096	X3306	X3376	X3448	X3525		X3579			
		X3067	X3097	X3307	X3377	X3449	X3526		X3580			
		X3068	X3098	X3308	X3378	X3450	X3527		X3581			
		X3069	X3099	X3309	X3379	X3451	X3528		X3582			
		X3070	X3100	X3310	X3380	X3452	X3529		X3583			
		X3071	X3101	X3311	X3381	X3453	X3530		X3584			
		X3072	X3102	X3312	X3382	X3454	X3531		X3585			
		X3073	X3103	X3313	X3383	X3455	X3532		X3586			
		X3074	X3104	X3314	X3384	X3456	X3533		X3587			
		X3075	X3105	X3315	X3385	X3457	X3534		X3588			
		X3076	X3106	X3316	X3386	X3458	X3535		X3589			
		X3077	X3107	X3317	X3387	X3459	X3536		X3590			
		X3078										

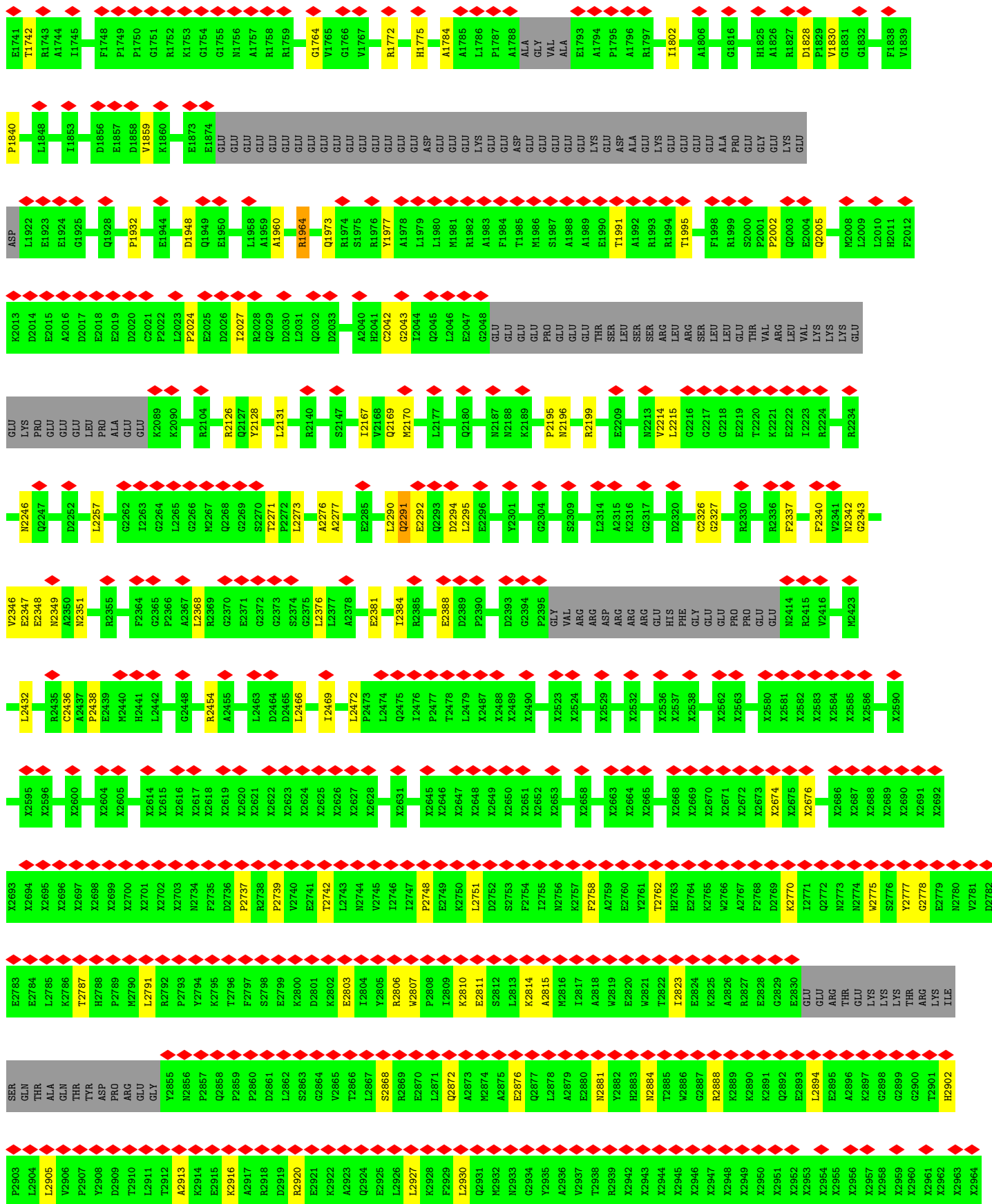


• Molecule 2: Ryanodine receptor 1













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.076	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ( $\text{\AA}$ )	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.31	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.55	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

All (4) bond length outliers are listed below:

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

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

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

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

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

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

## 5.2 Too-close contacts [i](#)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1040 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.51	0.76
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.51	0.76
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.51	0.75
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.51	0.74
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.57	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	47	81
2	E	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	47	81
2	G	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	47	81
2	I	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	47	81
All	All	13360/18096 (74%)	11956 (90%)	1376 (10%)	28 (0%)	50	81



5 of 28 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	84	90

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

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

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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

The worst 5 of 56 chain breaks are listed below:

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

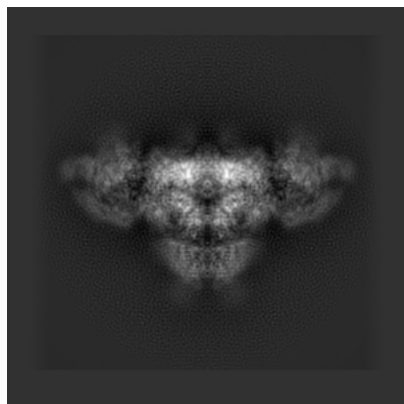
## 6 Map visualisation [i](#)

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

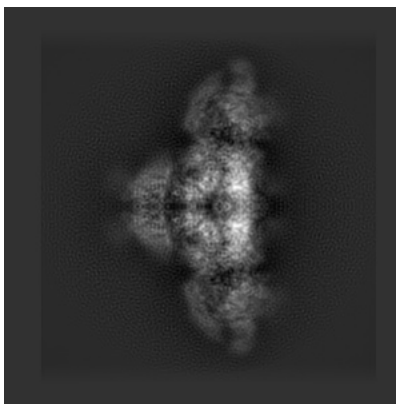
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

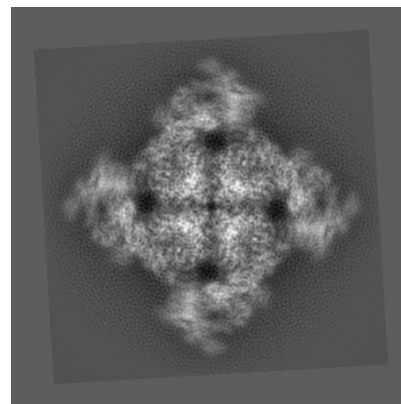
#### 6.1.1 Primary map



X

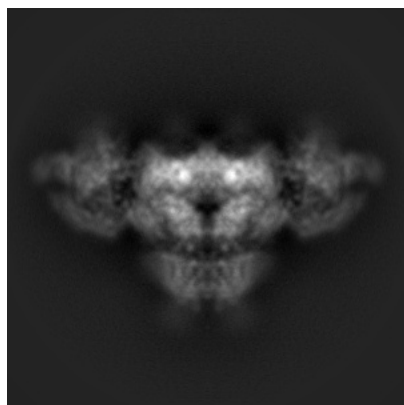


Y

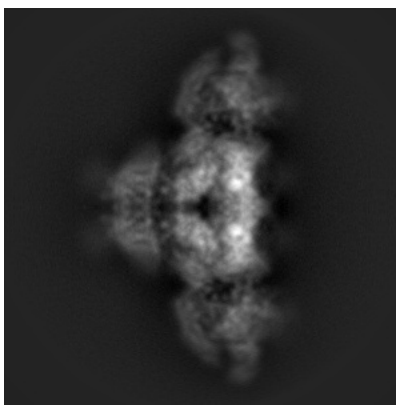


Z

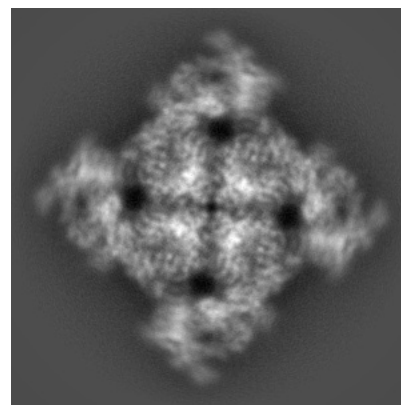
#### 6.1.2 Raw map



X



Y

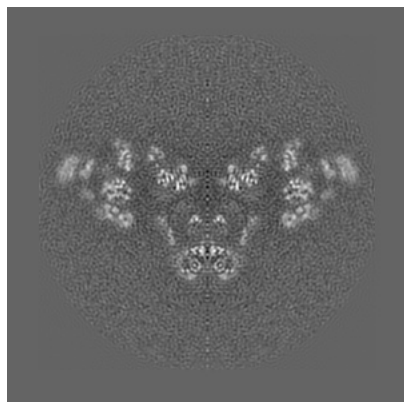


Z

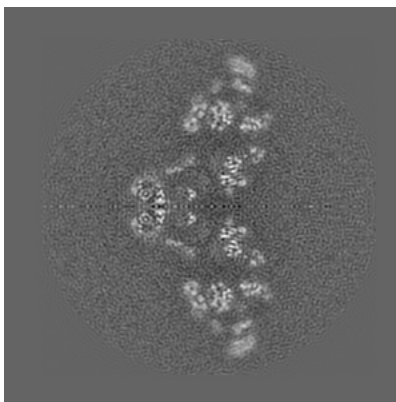
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

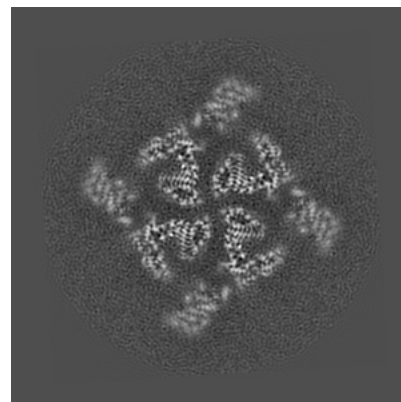
### 6.2.1 Primary map



X Index: 200

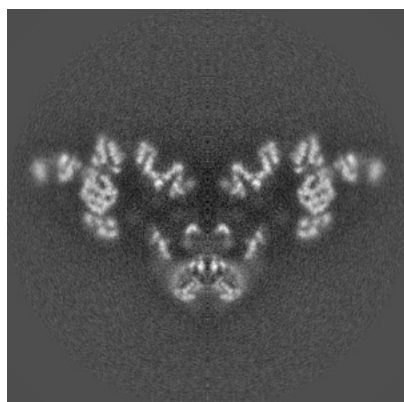


Y Index: 200

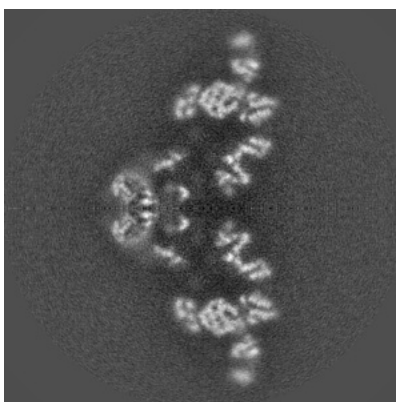


Z Index: 200

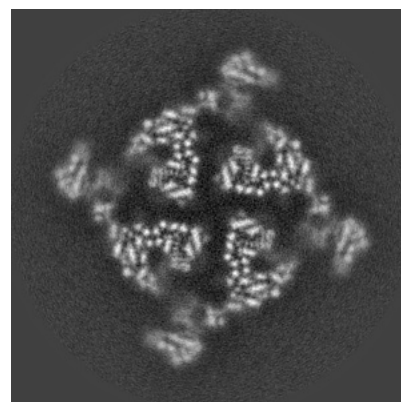
### 6.2.2 Raw map



X Index: 168



Y Index: 168

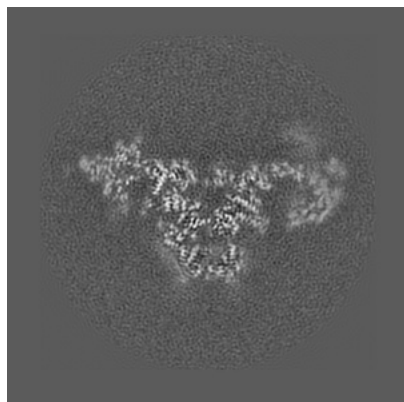


Z Index: 168

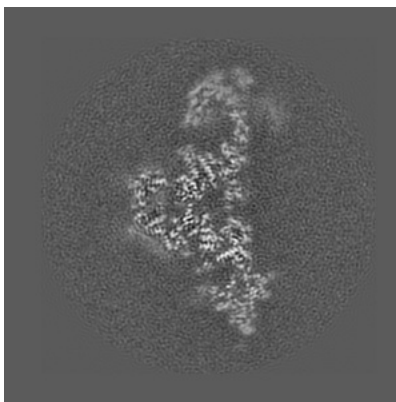
The images above show central slices of the map in three orthogonal directions.

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

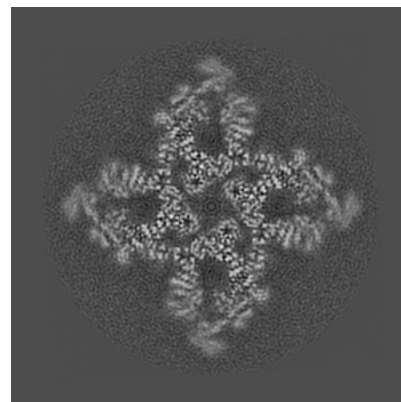
### 6.3.1 Primary map



X Index: 217

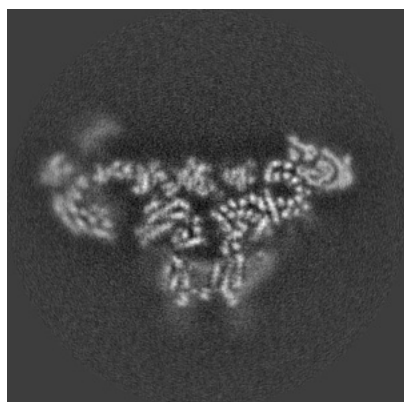


Y Index: 183

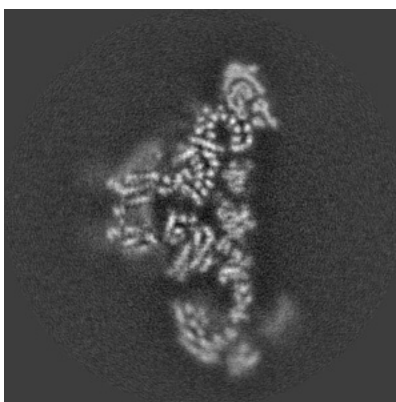


Z Index: 232

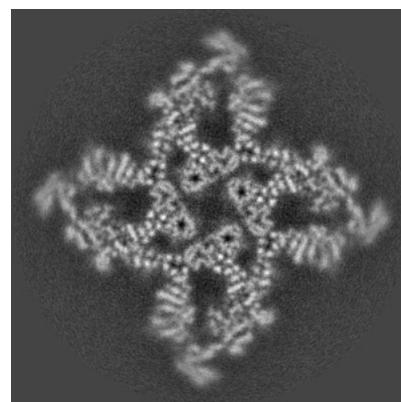
### 6.3.2 Raw map



X Index: 147



Y Index: 189

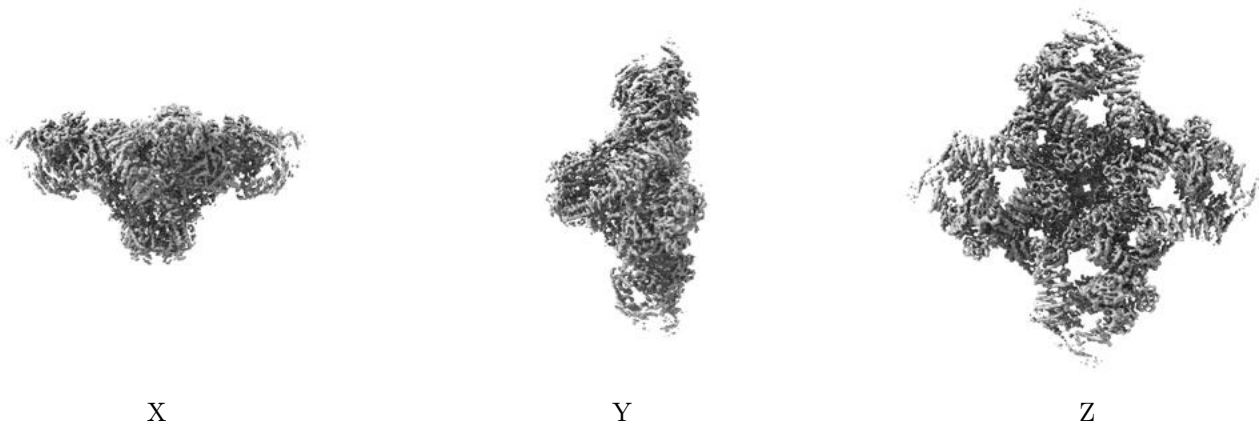


Z Index: 195

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

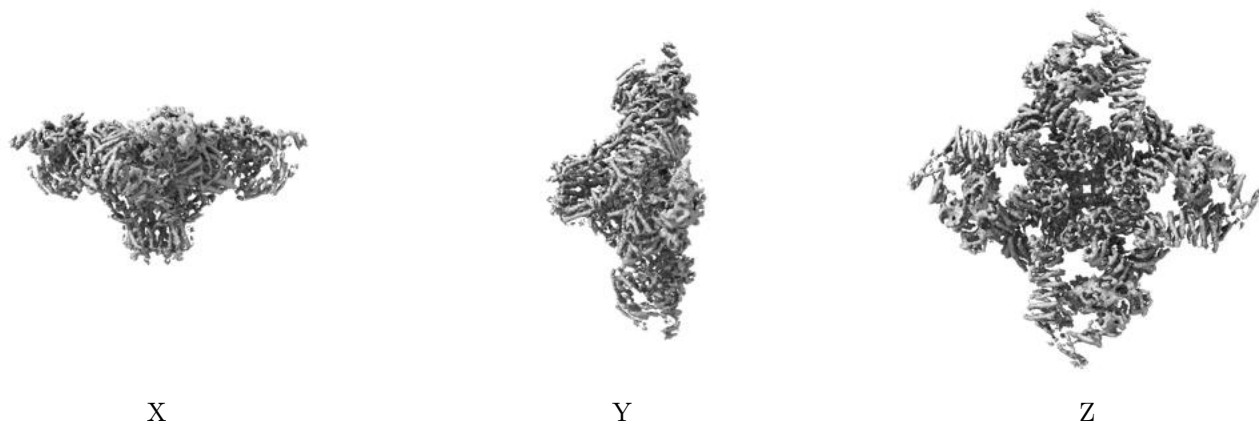
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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

### 6.4.2 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.

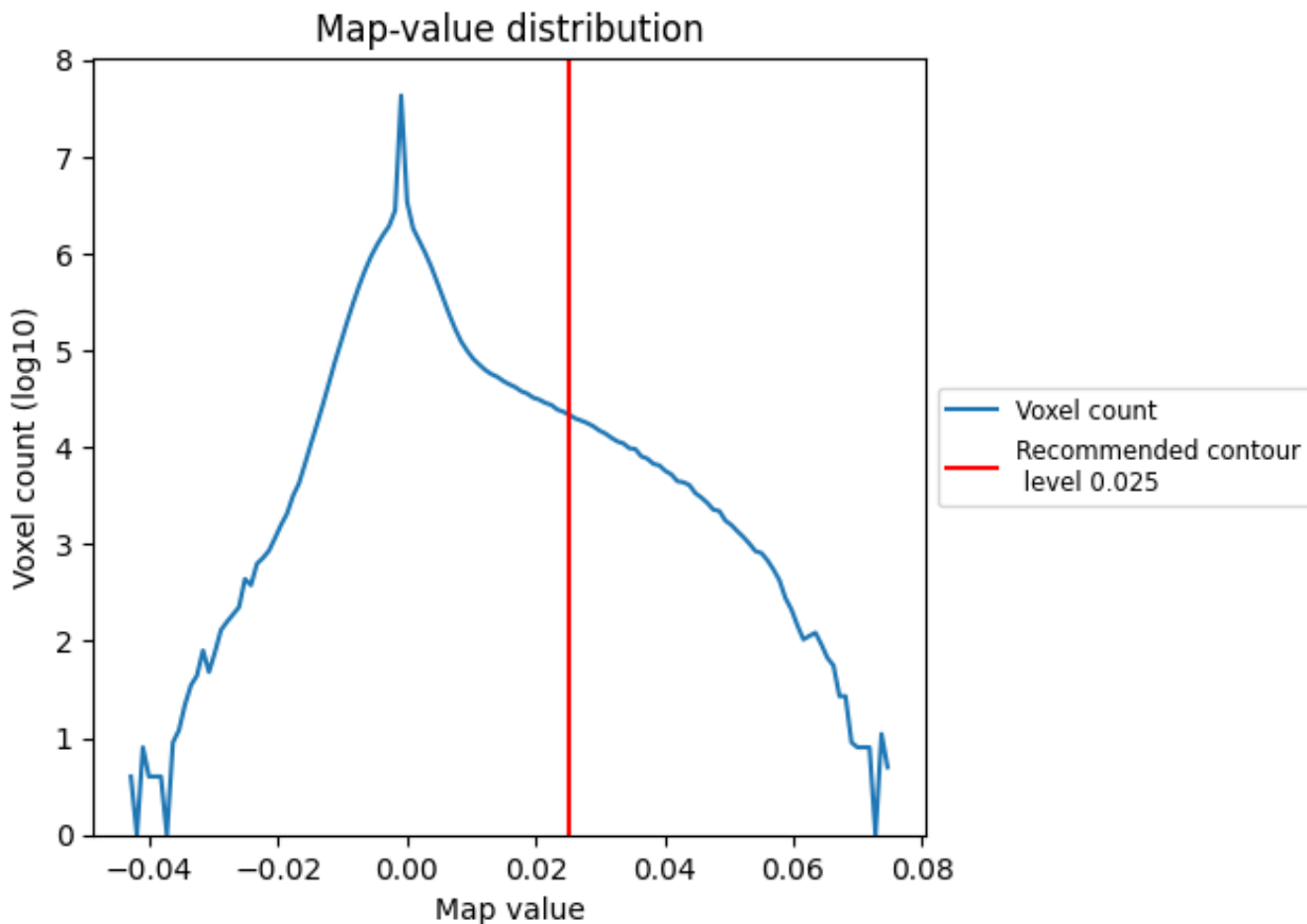
## 6.5 Mask visualisation [i](#)

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.

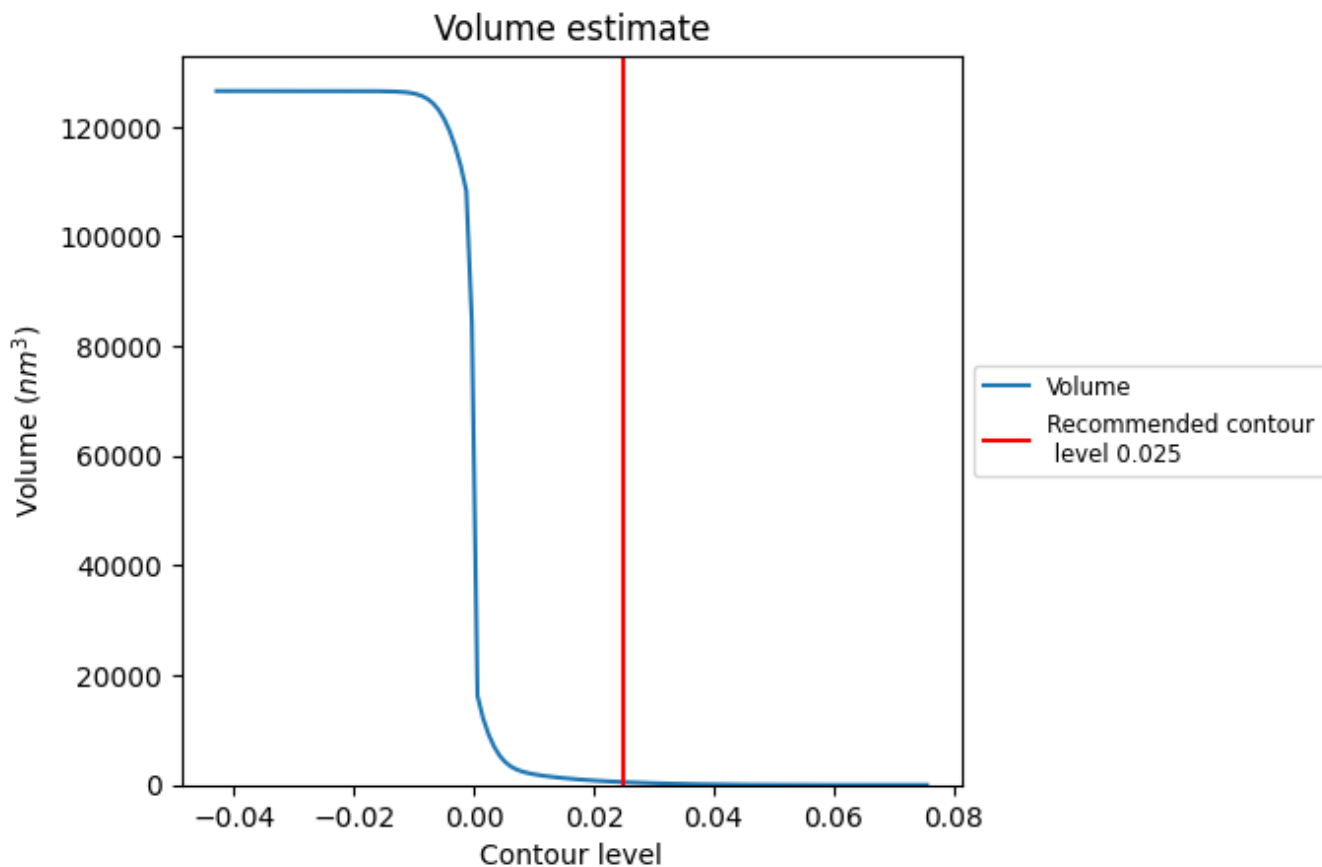
### 7.1 Map-value distribution [i](#)



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.



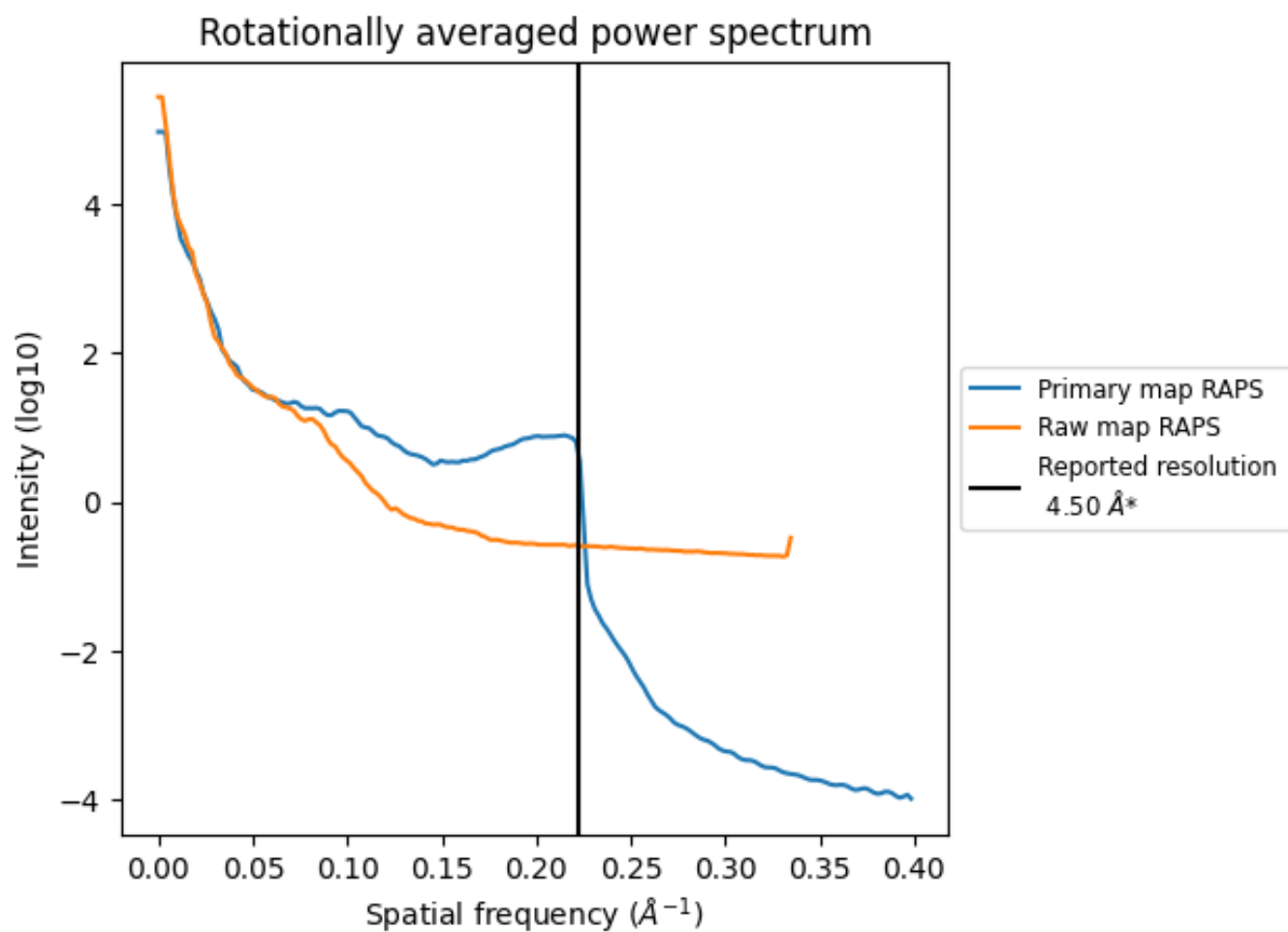
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 516  $\text{nm}^3$ ; this corresponds to an approximate mass of 466 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

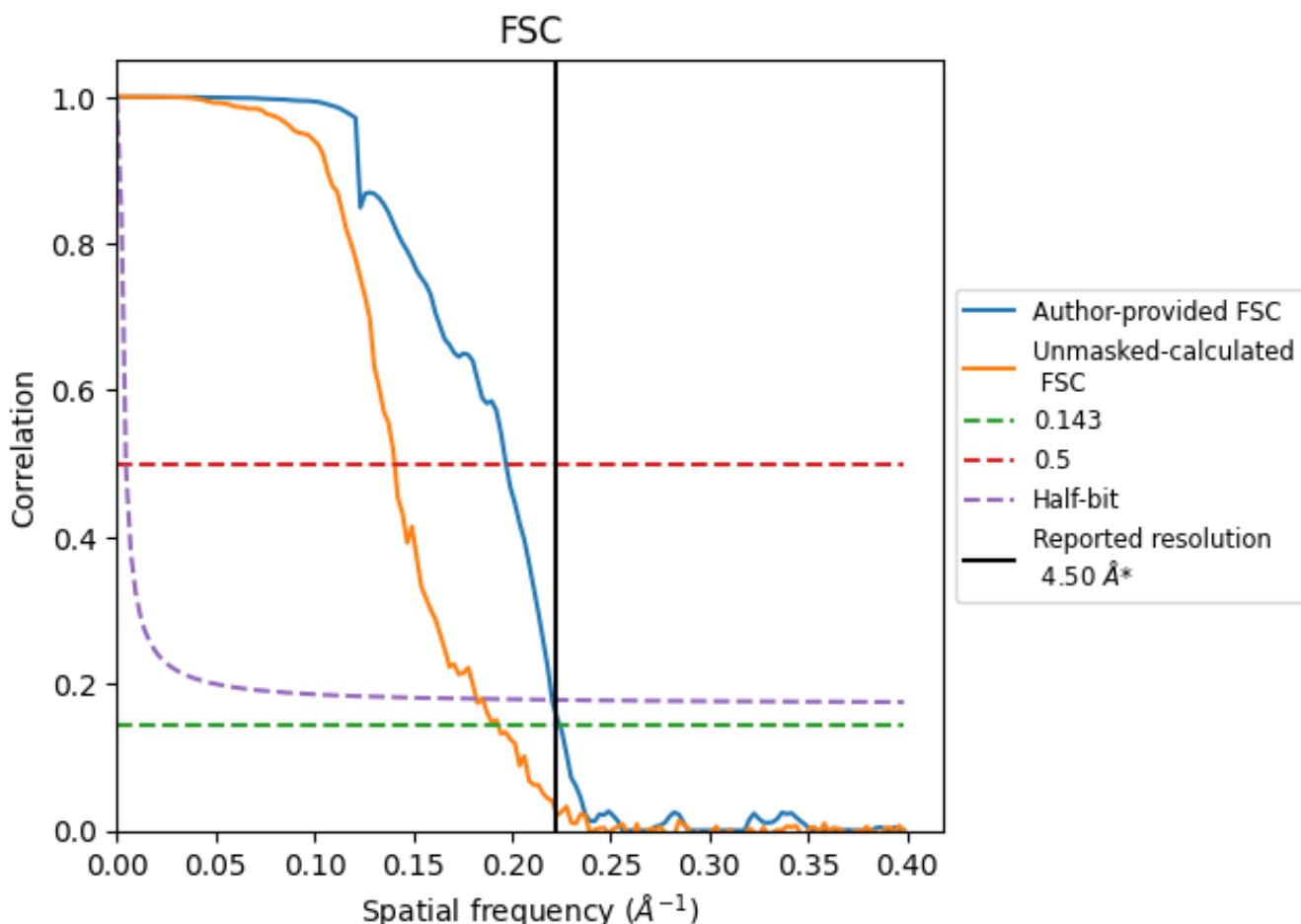


\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

## 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 0.222 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

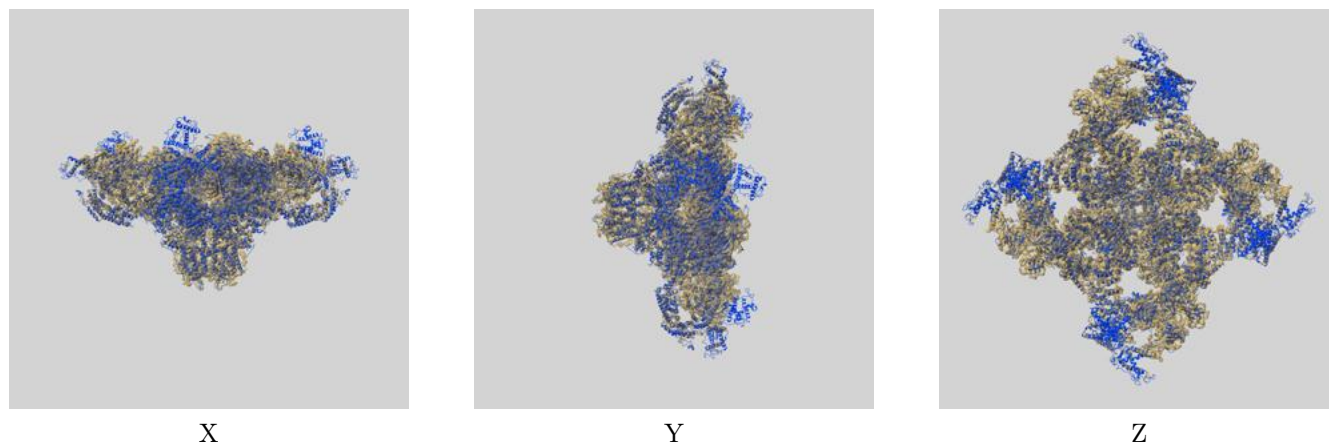
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	5.08	4.54
Unmasked-calculated*	5.18	7.11	5.49

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

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

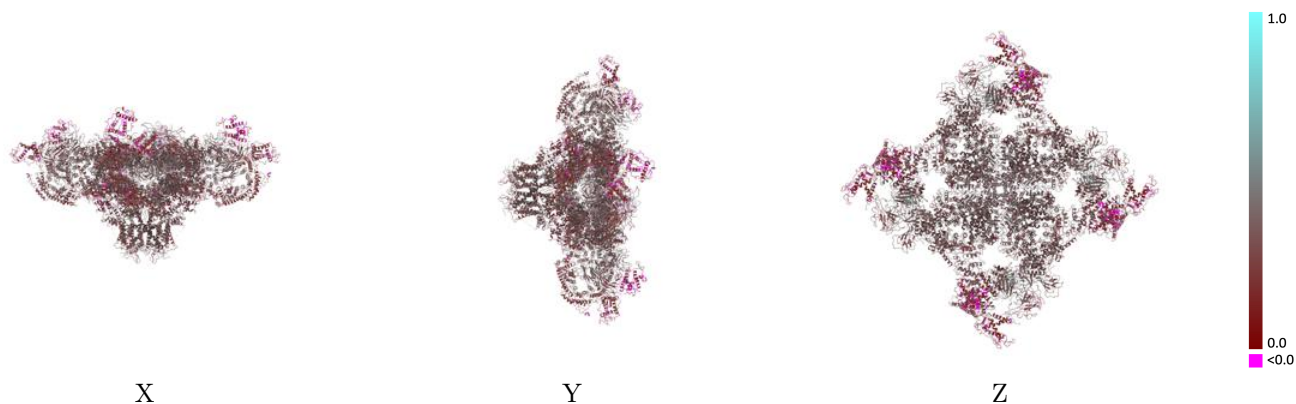
This section contains information regarding the fit between EMDB map EMD-8395 and PDB model 5TB4. Per-residue inclusion information can be found in section 3 on page 4.

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



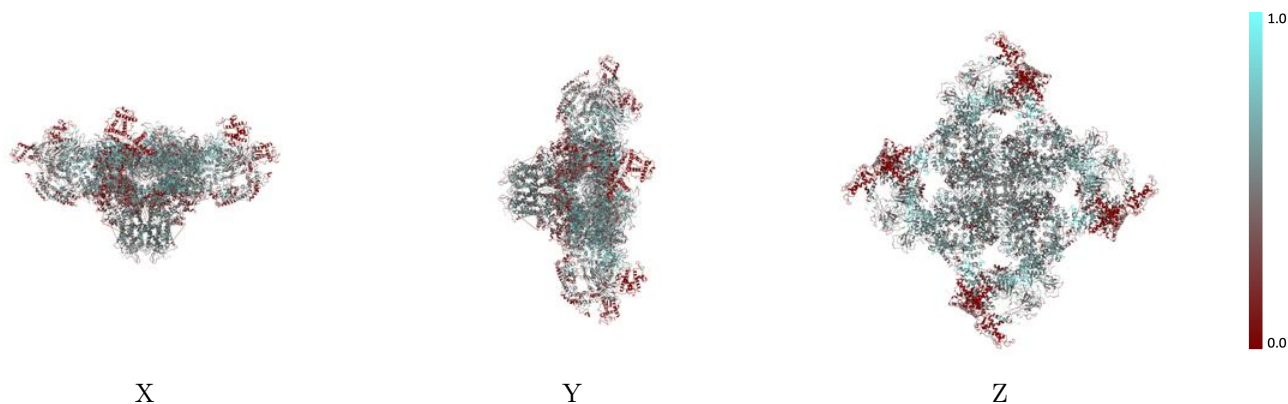
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



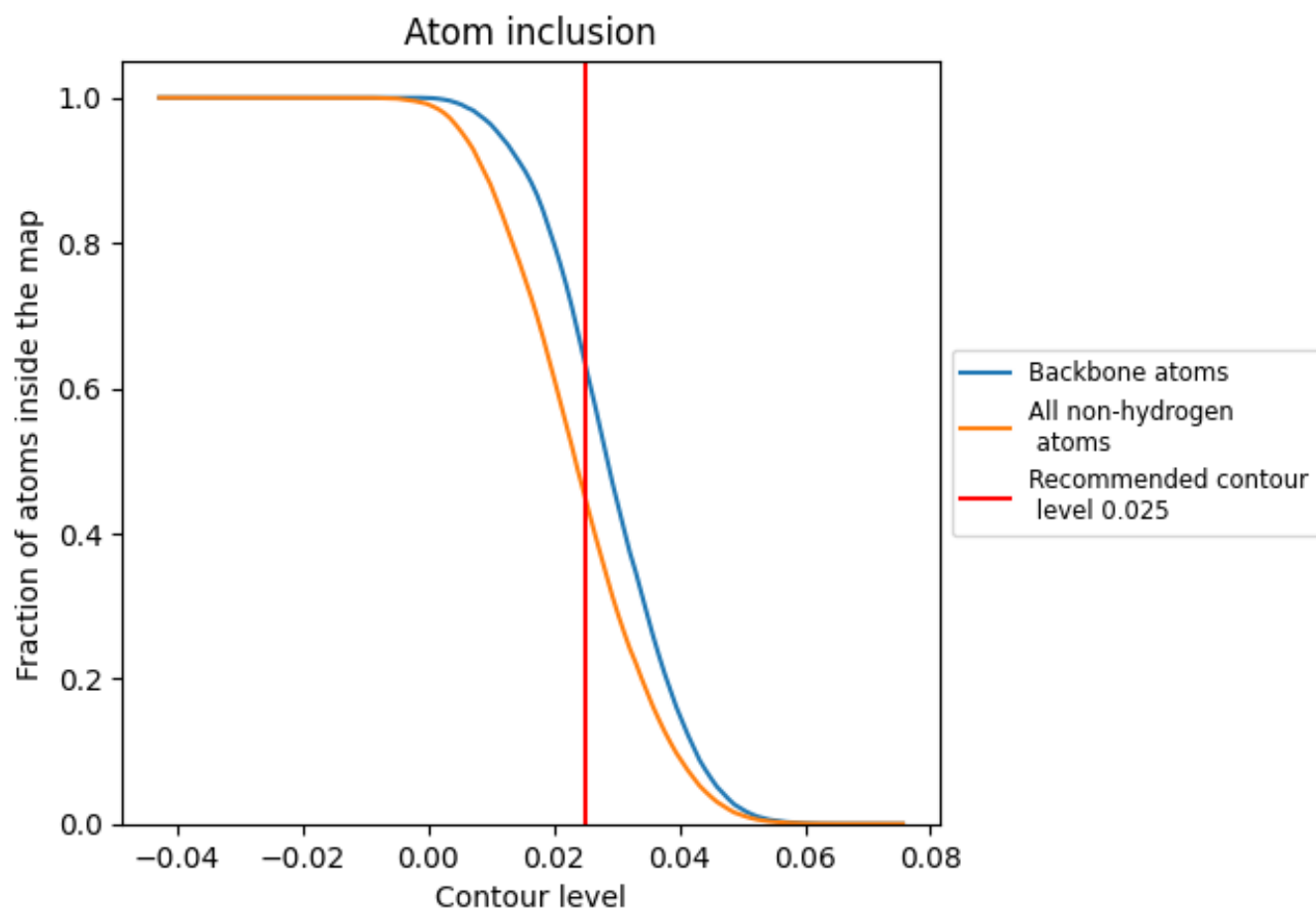
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.4477	■ 0.3170
A	■ 0.4814	■ 0.3380
B	■ 0.4468	■ 0.3160
E	■ 0.4467	■ 0.3160
F	■ 0.4739	■ 0.3420
G	■ 0.4470	■ 0.3160
H	■ 0.4789	■ 0.3410
I	■ 0.4469	■ 0.3160
J	■ 0.4801	■ 0.3400

