



wwPDB EM Validation Summary Report ⓘ

Mar 2, 2024 – 09:33 AM EST

PDB ID : 5TB2
EMDB ID : EMD-8393
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-11
Resolution : 4.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

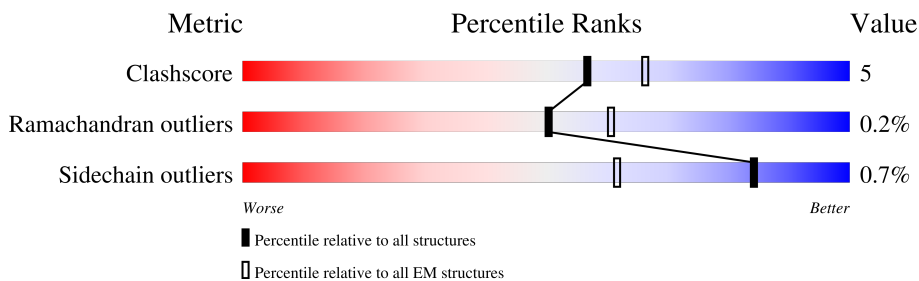
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	I	4194	29499	18686	5228	5428	157	0	0
2	E	4194	29499	18686	5228	5428	157	0	0
2	G	4194	29499	18686	5228	5428	157	0	0

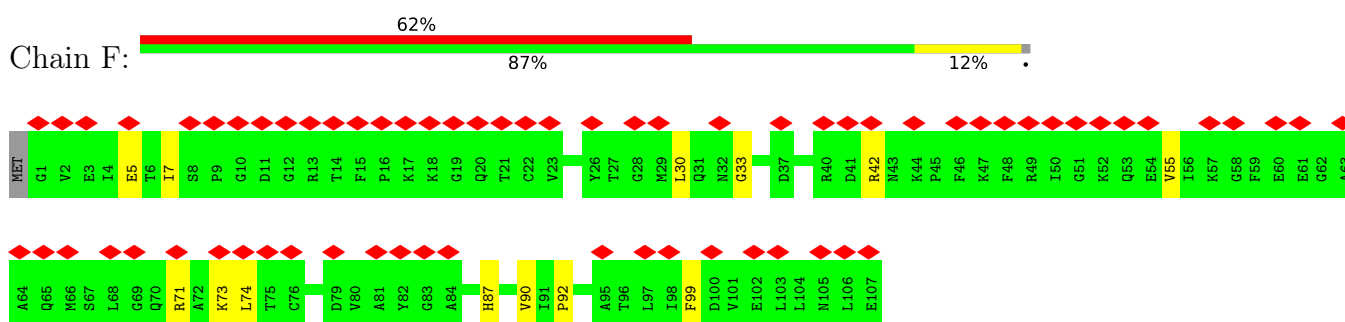
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

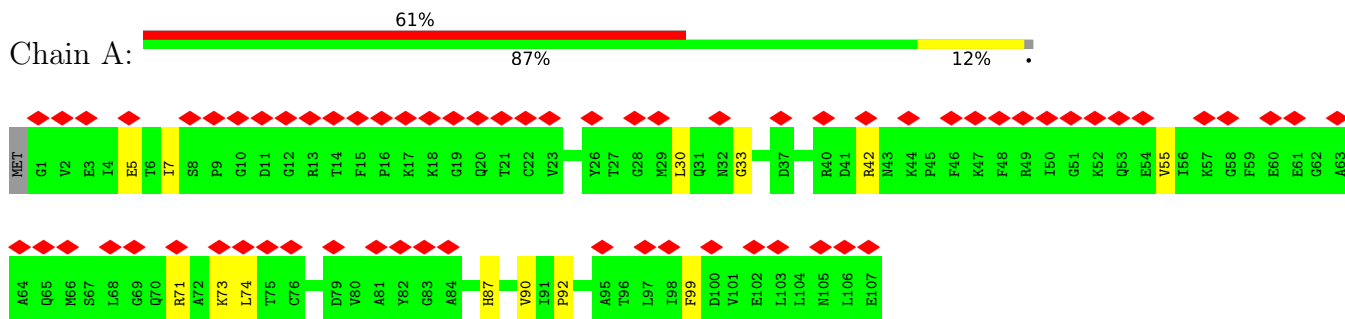
3 Residue-property plots [i](#)

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.

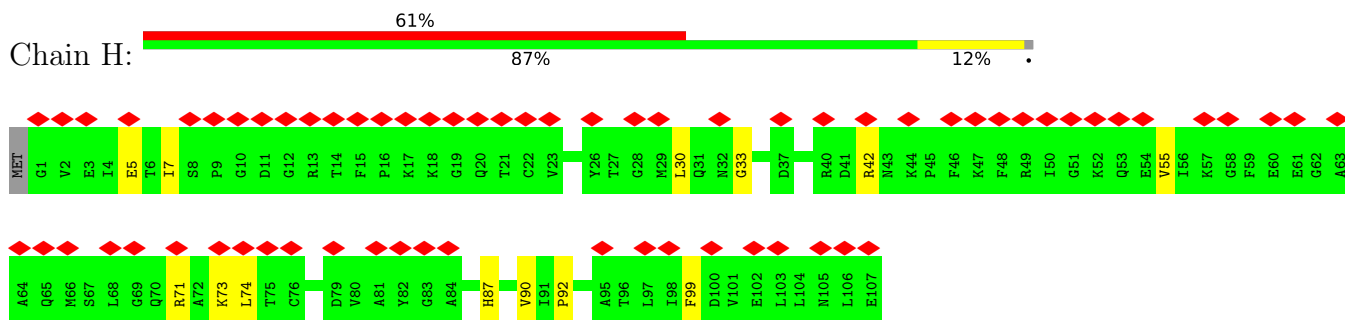
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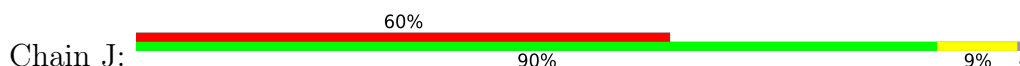
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



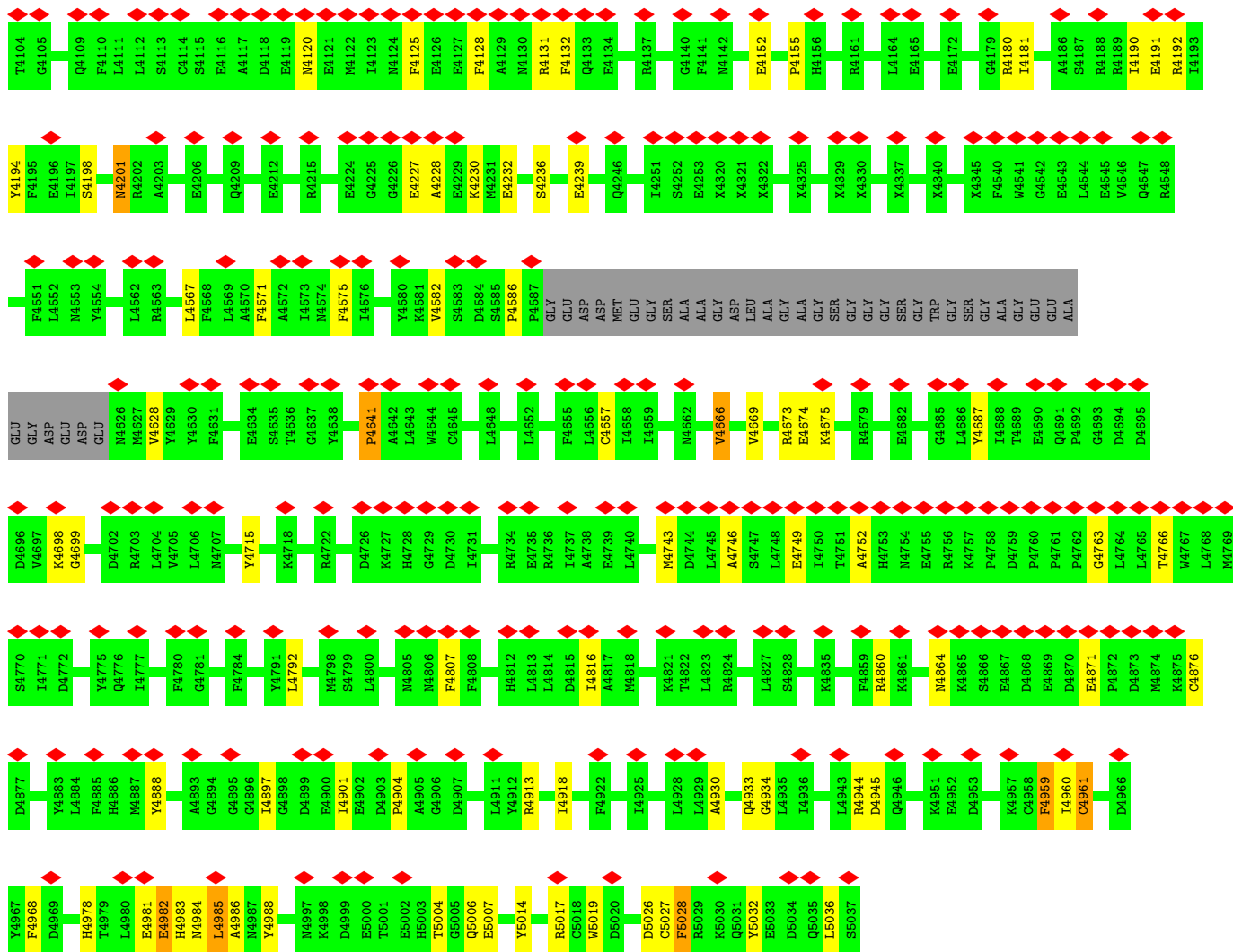
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



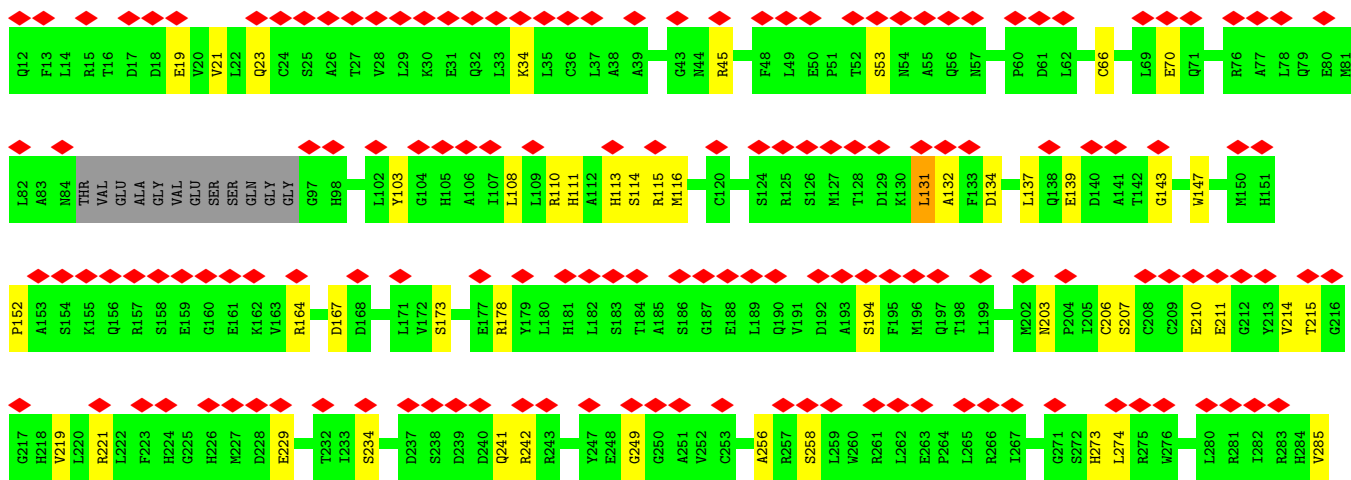
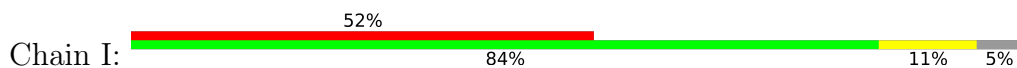
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

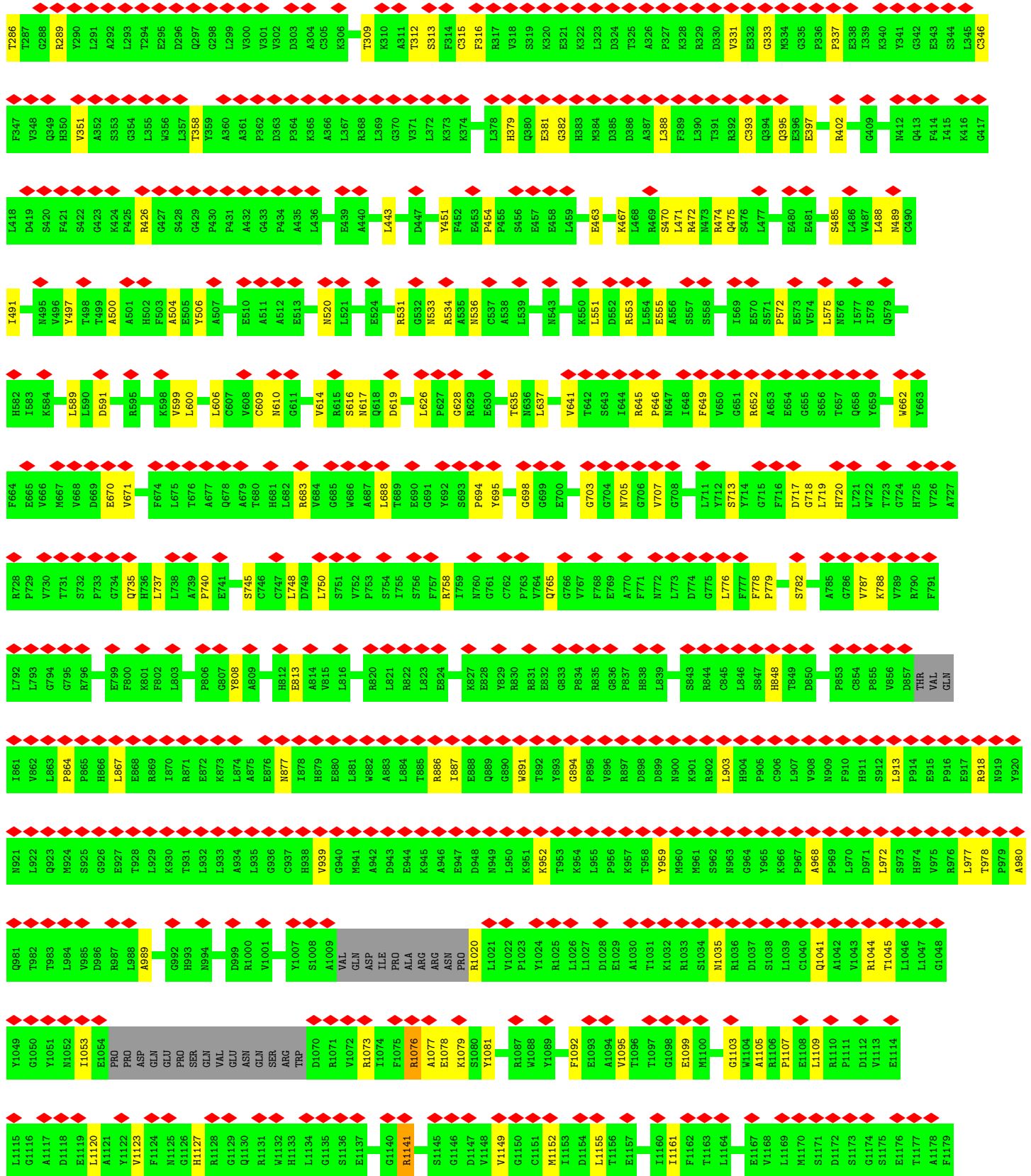


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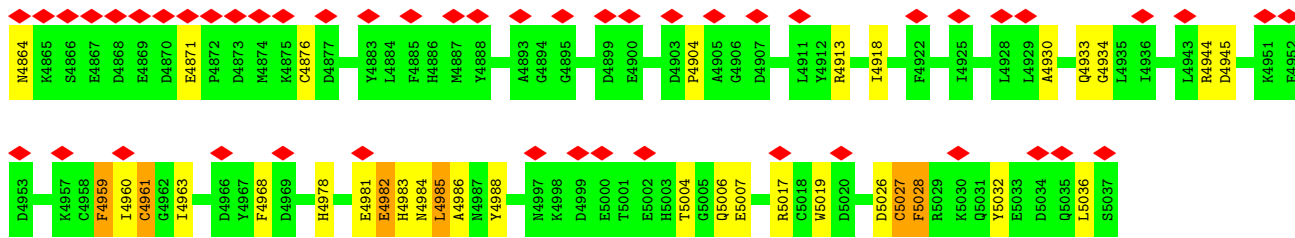
• Molecule 2: Ryanodine receptor 1



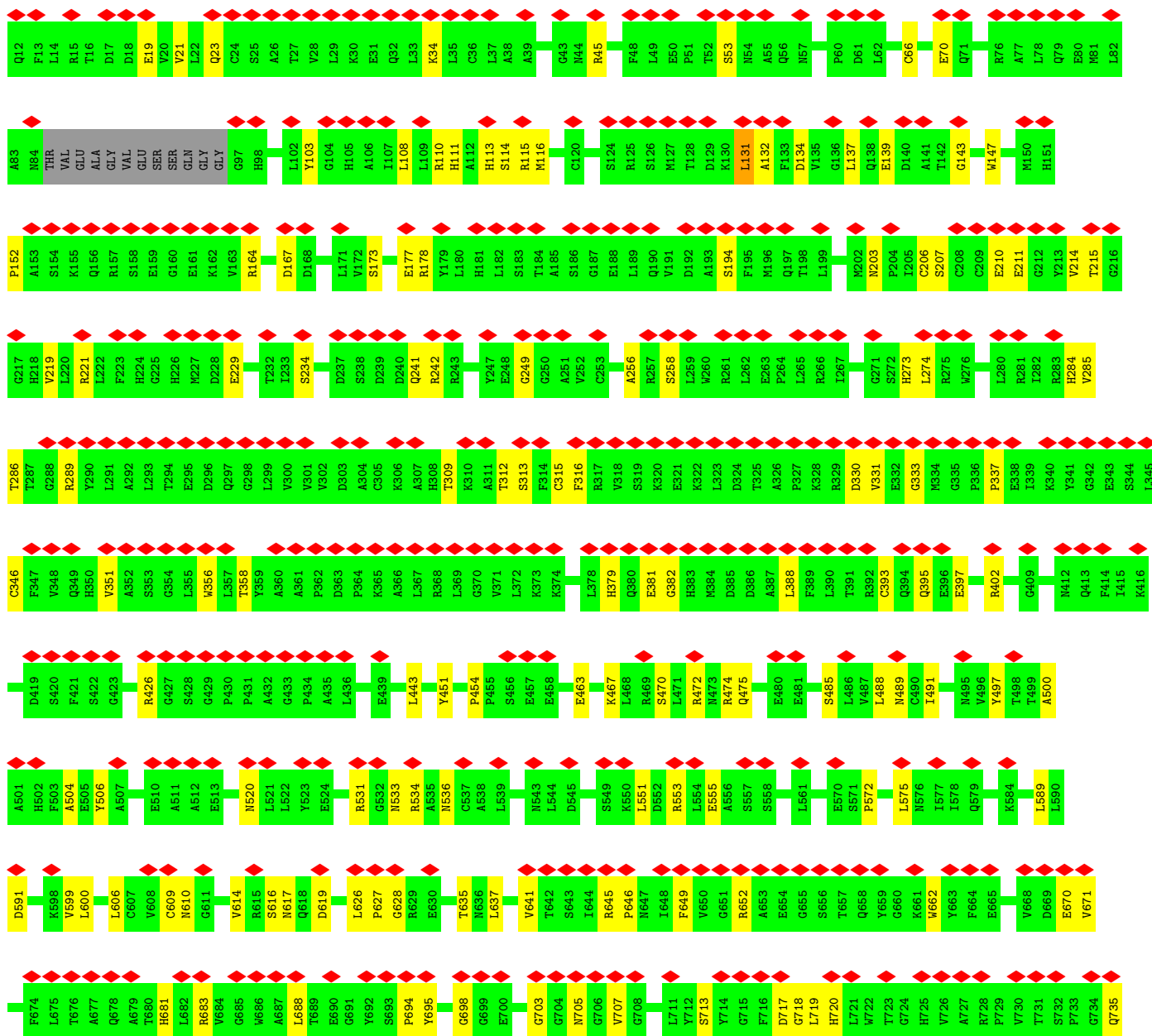
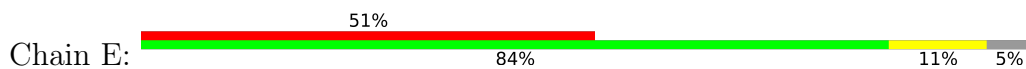


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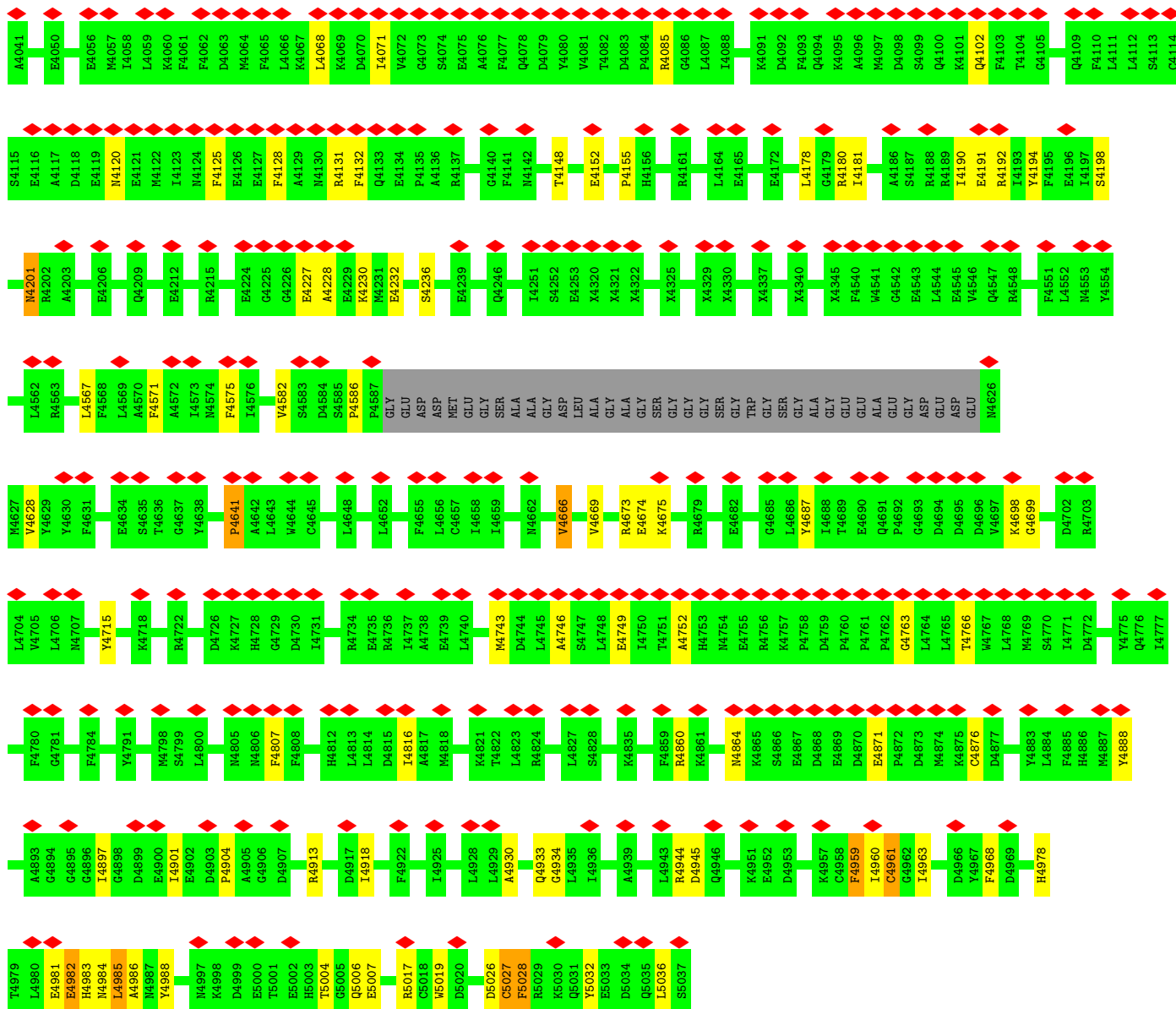


• Molecule 2: Ryanodine receptor 1

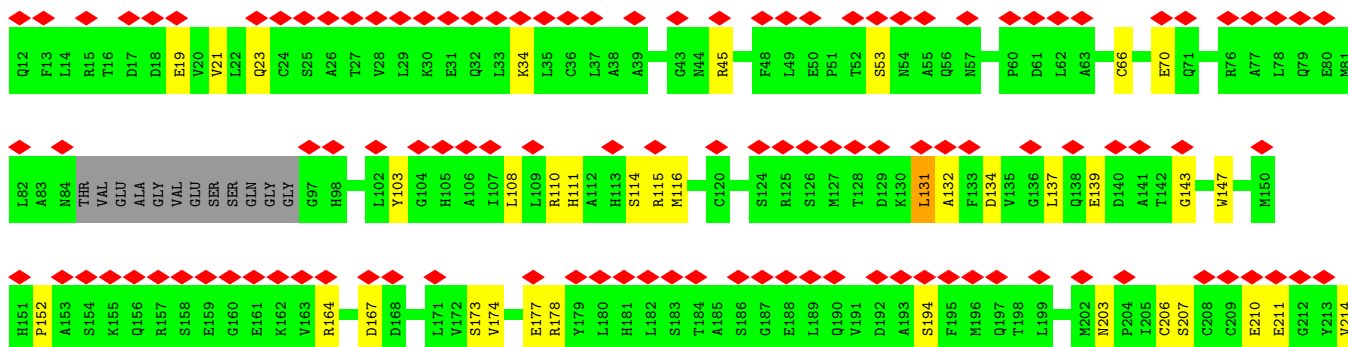
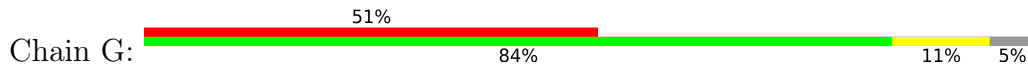


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GLU	A1962	L2023	Q2092	T2220	L2307	G2373	G2448	X2534	X2632	X2696	K2786	ALA
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LYS	A1982	GLU	E2150	N2260	R2331	D2393	Q2476	X2580	X2653	V2745	V2745	
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		GLU	M2189	A2278	L2397	R2457	X2560	X2586	X2717			
		GLU	M2189	A2278	L2398	R2458	X2561	X2586	X2718			
		GLU	M2189	A2278	L2399	R2459	X2562	X2586	X2719			
		GLU	M2189	A2278	L2400	R2460	X2563	X2586	X2720			
		GLU	M2189	A2278	L2401	R2461	X2564	X2586	X2721			
		GLU	M2189	A2278	L2402	R2462	X2565	X2586	X2722			
		GLU	M2189	A2278	L2403	R2463	X2566	X2586	X2723			
		GLU	M2189	A2278	L2404	R2464	X2567	X2586	X2724			
		GLU	M2189	A2278	L2405	R2465	X2568	X2586	X2725			
		GLU	M2189	A2278	L2406	R2466	X2569	X2586	X2726			
		GLU	M2189	A2278	L2407	R2467	X2570	X2586	X2727			
		GLU	M2189	A2278	L2408	R2468	X2571	X2586	X2728			
		GLU	M2189	A2278	L2409	R2469	X2572	X2586	X2729			
		GLU	M2189	A2278	L2410	R2470	X2573	X2586	X2730			
		GLU	M2189	A2278	L2411	R2471	X2574	X2586	X2731			
		GLU	M2189	A2278	L2412	R2472	X2575	X2586	X2732			
		GLU	M2189	A2278	L2413	R2473	X2576	X2586	X2733			
		GLU	M2189	A2278	L2414	R2474	X2577	X2586	X2734			
		GLU	M2189	A2278	L2415	R2475	X2578	X2586	X2735			
		GLU	M2189	A2278	L2416	R2476	X2579	X2586	X2736			
		GLU	M2189	A2278	L2417	R2477	X2580	X2586	X2737			
		GLU	M2189	A2278	L2418	R2478	X2581	X2586	X2738			
		GLU	M2189	A2278	L2419	R2479	X2582	X2586	X2739			
		GLU	M2189	A2278	L2420	R2480	X2583	X2586	X2740			
		GLU	M2189	A2278	L2421	R2481	X2584	X2586	X2741			
		GLU	M2189	A2278	L2422	R2482	X2585	X2586	X2742			
		GLU	M2189	A2278	L2423	R2483	X2586	X2586	X2743			
		GLU	M2189	A2278	L2424	R2484	X2587	X2586	X2744			
		GLU	M2189	A2278	L2425	R2485	X2588	X2586	X2745			
		GLU	M2189	A2278	L2426	R2486	X2589	X2586	X2746			
		GLU	M2189	A2278	L2427	R2487	X2590	X2586	X2747			
		GLU	M2189	A2278	L2428	R2488	X2591	X2586	X2748			
		GLU	M2189	A2278	L2429	R2489	X2592	X2586	X2749			
		GLU	M2189	A2278	L2430	R2490	X2593	X2586	X2750			
		GLU	M2189	A2278	L2431	R2491	X2594	X2586	X2751			
		GLU										

L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	R2914	E2915	A2916	A2917	R2918	D2919	R2920	E2921	R2922	A2923	Q2924	E2925	L2926	L2927	R2928	R2929	L2930	Q2931	R2932	H2933	G2934	V2935	A2936	V2937	T2938	R2939	A2942	L2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2966																																																																						
X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047																																																				
X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3101	X3102	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185
X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	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	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316																																																																			
X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3420	X3421	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3441	X3442	X3443	X3444	X3445	X3447																																																																					
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X3448	X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3463	X3464	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556																																																																								
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M3651	M3652	F3653	K3658	A3659	A3660	M3661	L3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	D3675	D3676	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	P3690	E3691	E3692	K3693	R3707	E3712	K3713	S3714	K3715	E3718	D3719	P3720	M3723	A3724	P3725	K3731	S3732	C3733	H3734	L3735	P3639	E3736	E3737	G3738																																																																												
G3739	E3740	M3741	GLY	ALA	GLU	E3747	E3748	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	E3759	K3760	Q3761	R3762	L3763	Q3766	R3769	T3772	R3773	V3779	L3780	K3787	S3803	L3804	L3805	N3809	A3810	E3811	K3815	M3816	L3817	K3821	D3822	Q3830	Q3833	H3734	L3842	D3843	R3849	L3923	L3924	R3925	E3928	S3929	D3932	Y3937	S3938	G3939	K3940	D3941	V3942																																																																						
R3849	Q3850	E3854	G3855	L3856	G3857	M3858	R3859	N3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873	R3874	M3875	A3876	D3877	D3878	E3879	T3772	R3773	V3779	L3780	K3787	S3803	L3804	L3805	N3809	A3810	E3811	K3815	M3816	L3817	K3821	D3822	Q3830	Q3833	H3734	L3842	D3843	R3849	L3923	L3924	R3925	E3928	S3929	D3932	Y3937	S3938	G3939	K3940	D3941	V3942																																																																		
L3943	E3944	E3945	Q3946	G3947	K3948	R3949	N3950	K3953	V3961	F3962	N3963	R3970	Q3978	S3979	L3980	A3981	H3982	L3985	L3993	F3996	A3997	M4000	M4001	K4002	L4003	A4004	Q4005	L4006	S4007	S4008	Q4009	L4010	E4011	L4012	L4013	L4014	E4015	D4018	L4019	D4022	L4031	E4032	G4033	M4034	V4035	G4038																																																																																	

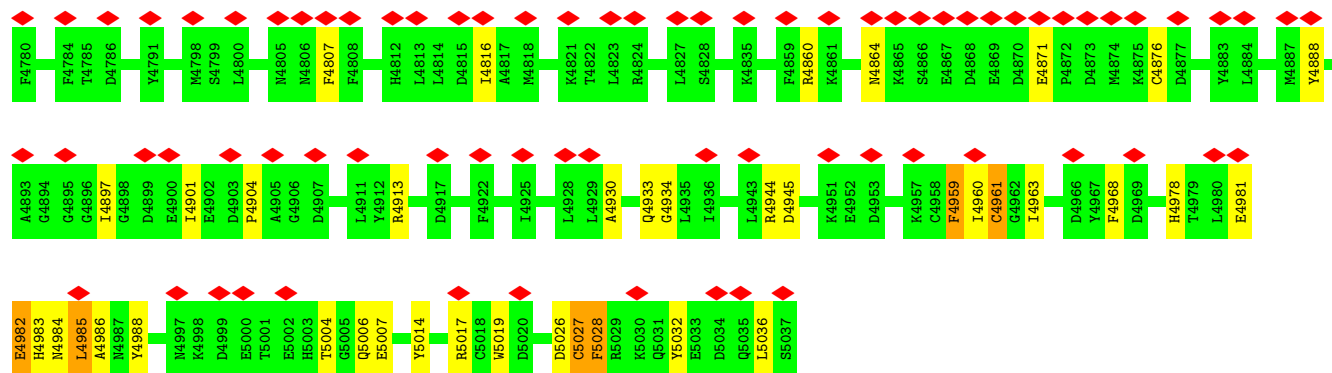


● Molecule 2: Ryanodine receptor 1



PRO	D986	G926	E799	G734	D669	L589	T499	I415	S344	H984	T215
ASP	R987	E927	F800	Q735	E670	L590	A500	K416	L345	V285	G216
GLN	L988	T928	K801	H736	V671	D591	A501	D419	C346	T286	G217
PRO	A989	L929	F802	L737	V672	K998	H502	S420	F347	G288	H218
SER	G992	K930	P806	L738	F674	V599	F503	S421	V348	R289	V219
GLN	H993	A739	G807	A739	L675	L600	A504	F421	Q349	R290	L220
VAL	H994	P740	T676	P740	L676	L606	E505	S422	H350	Y291	R221
GLU	H994	E741	A677	E741	L677	L607	Y506	G423	R351	L292	L222
ASN	D999	S745	A809	S745	Q678	C607	A507	G424	A292	A292	F223
GLN	Y1007	C746	H812	C746	Q679	V608	E510	R426	L293	L293	H224
SER	A1009	C747	E813	C747	A679	C609	E511	G427	S353	G225	G225
ARG	VAL	L748	E814	L748	L682	N610	A512	S428	G354	T294	H226
GLN	GLN	L750	A814	L750	R683	G611	E513	G429	L355	D296	M227
ASP	GLN	S751	A815	S751	V684	V614	N520	P430	L357	Q297	D228
ILE	ASP	W752	L816	W752	G685	R615	L521	P431	T358	G298	E229
PRO	PRO	F753	L817	F753	S616	N617	L522	A432	Y359	L299	T232
ALA	ARG	S754	R820	S754	N618	Q618	Y523	G433	A360	V300	I233
ARG	ARG	W755	L821	W755	D619	D619	E524	P434	A361	V301	S234
ASN	PRO	F756	E690	F756	L626	L626	R531	A435	P362	D303	D237
PRO	PRO	R757	E691	R757	P627	P627	G532	L436	P364	A304	S238
PRO	PRO	R758	E692	R758	G628	G628	N533	E439	K365	K306	D239
PRO	PRO	W760	E693	W760	R629	R629	N534	L443	A366	A307	Q240
PRO	PRO	G761	E694	G761	E630	E630	A535	L444	L367	H308	R242
PRO	PRO	F763	E695	F763	T635	T635	N536	Y451	R368	T309	R243
PRO	PRO	W764	G698	W764	C537	C537	C537	P454	L369	K310	Y247
PRO	PRO	Q765	G699	Q765	A538	A538	L539	P455	G370	A311	Y248
PRO	PRO	G766	E700	G766	L637	L637	L539	S456	V371	T312	E248
PRO	PRO	W767	G703	W767	V641	V641	N543	S457	L372	G249	G249
PRO	PRO	F768	G704	F768	T642	T642	L544	E458	K373	F314	G250
PRO	PRO	E769	G705	E769	S643	S643	D545	E459	F315	C315	A251
PRO	PRO	R835	N705	R835	R644	R644	D545	E463	F316	F316	V252
PRO	PRO	P837	G706	P837	R645	R645	S549	K467	R378	R317	C253
PRO	PRO	H838	G707	H838	W707	W707	K550	L468	H379	V318	A256
PRO	PRO	L839	G708	L839	N647	N647	D552	R469	Q380	S319	R257
PRO	PRO	S843	L711	S843	T648	T648	L554	S470	E381	K320	S258
PRO	PRO	R844	Y112	R844	F649	F649	L554	L471	G382	E321	L259
PRO	PRO	C845	S713	C845	V650	V650	E555	M473	H583	K322	W260
PRO	PRO	L846	Y114	L846	R652	R652	A556	R474	D385	D324	R261
PRO	PRO	S847	G715	S847	A653	A653	S557	Q475	D386	T325	L262
PRO	PRO	H848	F716	H848	G654	G654	S558	E480	A326	A326	E263
PRO	PRO	T849	D717	T849	E655	E655	L561	E481	A387	P327	P264
PRO	PRO	D850	G718	D850	G656	G656	L561	E482	L388	P327	P264
PRO	PRO	P853	L719	P853	S656	S656	E570	S485	F389	K328	L265
PRO	PRO	C854	H720	C854	T657	T657	S571	L486	L390	R329	R266
PRO	PRO	R855	W722	R855	Q658	Q658	P572	V487	T391	R329	I267
PRO	PRO	V856	T723	V856	Y659	Y659	L575	L488	R392	D330	L267
PRO	PRO	D857	G724	D857	G660	G660	N576	M489	C393	V331	G271
PRO	PRO	THR	H725	THR	W662	W662	N576	C490	Q394	E332	S272
PRO	PRO	VAL	W726	VAL	Y663	Y663	I577	I491	Q395	G333	H273
PRO	PRO	GLN	A727	GLN	F664	F664	I578	V496	E596	M334	L274
PRO	PRO	I861	R728	I861	Q579	Q579	Q579	M495	E597	G335	R275
PRO	PRO	V862	P729	V862	V666	V666	K584	Y497	E597	P336	W276
PRO	PRO	L863	W730	L863	M667	M667	K584	T498	R402	P337	L280
PRO	PRO	P864	I731	P864	V668	V668	K584	T498	G409	E338	R281
PRO	PRO	F865	S732	F865	V668	V668	K584	T498	M412	I339	I282
PRO	PRO	L866	T733	L866	V668	V668	K584	T498	Q413	R340	R283
PRO	PRO	R867	S732	R867	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	E868	T733	E868	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	R869	S733	R869	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L870	T734	L870	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	H871	S734	H871	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	E872	T735	E872	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	K873	S735	K873	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L874	T736	L874	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	A875	S736	A875	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	E876	T737	E876	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	N877	S737	N877	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L878	T738	L878	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	H879	S738	H879	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	E880	T739	E880	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L881	S739	L881	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	W882	T740	W882	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	A883	S740	A883	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L884	T741	L884	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	T885	S741	T885	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	R886	T742	R886	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	I887	S742	I887	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	E888	T743	E888	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	Q889	S743	Q889	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	G890	T744	G890	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	W891	S744	W891	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	T892	T745	T892	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	Y893	S745	Y893	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	G894	T746	G894	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	P895	S746	P895	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	V896	T747	V896	V668	V668	K584	T498	F414	G342	R283
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PRO	PRO	D898	T748	D898	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	Y899	S748	Y899	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	M960	T749	M960	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	K961	S749	K961	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	S962	T750	S962	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	D1037	S750	D1037	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	S1038	T751	S1038	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L1039	S751	L1039	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	C1040	T752	C1040	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	Q1041	S752	Q1041	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	A1042	T753	A1042	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	Y1043	S753	Y1043	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	R1044	T754	R1044	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	T1045	S754	T1045	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L1046	T755	L1046	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	L1047	S755	L1047	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	G1048	T756	G1048	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	Y1049	S756	Y1049	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	F1050	T757	F1050	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	W1123	S757	W1123	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	V1124	T758	V1124	V668	V668	K584	T498	F414	G342	R283
PRO	PRO	M1125	S758	M1125	V668	V668	K584	T498	F414	G342	R283

X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3420	X3421	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3441	X3442	X3443	X3447																																																																																																																																																																																											
X3449	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3463	X3464	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3553	X3554	X3555	X3557																																																																																																																																																																																												
X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3597	X3598	X3599	X3600	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	X3639	X3640	X3641	X3642	X3643	X3644	X3648																																																																																																																																																																																											
N3651	N3652	F3653	K3658	A3659	A3660	K3661	L3662	L3663	T3664	E3665	D3666	H3667	F3668	F3669	D3675	D3676	K3679	G3680	G3681	E3682	E3684	E3685	E3686	E3687	E3688	E3689	G3690	E3691	E3692	K3693	E3712	K3713	S3714	K3715	E3718	D3719	Y3720	M3723	A3724	Y3725	A3726	D3727	K3731	S3732	C3733	H3734	L3735	T3639	L3736	E3737	G3738	G3739																																																																																																																																																																																													
E3740	N3741	GLY	GLU	ALA	GLU	E3747	E3748	E3749	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	E3759	K3760	G3681	Q3761	R3762	L3763	Q3766	R3769	T3772	R3773	V3779	L3780	K3787	S3803	I3804	L3805	N3809	A3810	E3811	K3815	M3816	L3817	K3821	D3822	Q3830	Q3833	L3842	D3843	R3849																																																																																																																																																																																																		
Q3850	E3854	G3855	M3856	G3857	K3858	V3859	K3860	E3861	L3862	G3863	T3864	V3865	L3866	N3867	L3868	N3869	K3870	G3871	R3872	K3873	V3874	K3875	A3876	D3877	K3878	E3879	Q3882	R3886	Q3889	E3893	N3896	F3899	Q3906	T3907	L3923	L3924	R3925	E3928	S3929	D3932	Y3937	S3938	G3939	K3940	D3941	V3942	L3943																																																																																																																																																																																																		
E3944	E3945	Q3946	G3947	K3948	R3949	N3950	K3953	V3961	E3962	N3963	Q3970	Q3978	S3979	L3980	A3981	H3982	L3985	L3989	F3996	A3997	M4000	M4001	K4002	L4003	A4004	Q4005	D4006	S4007	S4008	Q4009	I4010	E4011	L4012	L4013	K4014	E4015	D4018	L4019	D4022	L4031	G4033	M4034	V4035	G4038	A4041																																																																																																																																																																																																				
E4050	E4056	M4057	L4058	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	I4071	V4072	G4073	S4074	A4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4087	L4088	K4091	D4092	F4093	Q4094	K4095	A4096	M4097	D4098	S4099	Q4100	K4101	Q4102	G4103	M4104	Q4105	Q4109	F4110	L4111	L4112	S4113	S4115																																																																																																																																																																																											
E4116	A4117	D4118	E4119	M4120	M4121	M4122	I4123	M4124	F4125	E4126	E4127	F4128	A4129	M4130	R4131	F4132	Q4133	E4134	P4135	A4136	R4137	G4140	F4141	M4142	E4152	P4155	H4156	R4151	L4164	E4185	E4172	Y4177	L4178	G4179	R4180	I4181	A4186	S4187	R4188	R4189	E4190	E4191	R4192	I4193	Y4194	F4195	E4196	I4197	S4198	M4201																																																																																																																																																																																															
R4202	A4203	E4206	Q4209	E4212	R4215	E4224	G4225	G4226	E4227	A4228	K4229	K4230	M4231	E4232	S4236	E4239	E4244	M4245	Q4246	I4251	S4252	E4253	X4250	X4321	X4322	X4325	X4329	X4330	X4337	X4340	X4345	F4340	M4341	G4342	E4343	L4344	L4345	E4345	F4346	Q4347	M4348	F4351	L4352	I4357	L4358	L4359	L4360	L4361	L4362	L4363	L4364	L4365	L4366	L4367	L4368	L4369	L4370	L4371	L4372	L4373	L4374	L4375	L4376	L4377	L4378	L4379	L4380	L4381	L4382	L4383	L4384	L4385	L4386	L4387	L4388	L4389	L4390	L4391	L4392	L4393	L4394	L4395	L4396	L4397	L4398	L4399	L4400	L4401	L4402	L4403	L4404	L4405	L4406	L4407	L4408	L4409	L4410	L4411	L4412	L4413	L4414	L4415	L4416	L4417	L4418	L4419	L4420	L4421	L4422	L4423	L4424	L4425	L4426	L4427	L4428	L4429	L4430	L4431	L4432	L4433	L4434	L4435	L4436	L4437	L4438	L4439	L4440	L4441	L4442	L4443	L4444	L4445	L4446	L4447	L4448	L4449	L4450	L4451	L4452	H4453	L4454	L4455	L4456	L4457	L4458	L4459	L4460	L4461	L4462	G4463	D4464	L4465	L4466	L4467	L4468	L4469	L4470	L4471	L4472	L4473	L4474	L4475	L4476	L4477	L4478	L4479	L4480	L4481	L4482	L4483	L4484	L4485	L4486	L4487	L4488	L4489	L4490	L4491	L4492	L4493	L4494	L4495	L4496	L4497	L4498	L4499	L4500	L4501	L4502	L4503	L4504	L4505	L4506	L4507	L4508	L4509	L4510	L4511	L4512	L4513	L4514	L4515	L4516	L4517	L4518	L4519	L4520	L4521	L4522	L4523	L4524	L4525	L4526	L4527	L4528	L4529	L4530	L4531	L4532	L4533	L4534	L4535	L4536	L4537	L4538	L4539	L4540	L4541	L4542	L4543	L4544	L4545	L4546	L4547	L4548	L4549	L4550	L4551	L4552	L4553	L4554
L4562	R4563	L4567	F4568	L4569	A4570	F4571	A4572	I4573	M4574	F4575	L4576	Y4582	S4583	D4584	S4585	P4586	L4587	GLY	GLU	ASP	ASP	MET	GLY	SER	ALA	ALA	GLY	ASP	LEU	ALA	GLY	ALA	GLY	SER	GLY	GLY	SER	GLY	GLY	TRP	GLY	SER	GLY	ALA	GLY	GLU	GLU	ALA	GLY	ASP	ASP	GLU	ASP	GLU	M4626																																																																																																																																																																																										
M4627	V4628	Y4629	Y4630	F4631	E4634	S4635	T4636	G4637	Y4638	P4641	A4642	L4643	M4644	C4645	L4648	L4652	F4655	L4656	C4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																			
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691	P4692	C4693	D4694	D4695	D4696	V4697	K4698	G4699	D4702	R4703																																																																																																																																																																																																				
L4704	V4705	L4706	M4707	Y4715	K4718	R4722	D4726	K4727	H4728	C4729	D4730	L4731	F4732	R4734	E4735	R4736	L4656	L4657	I4658	I4659	M4662	V4666	V4669	R4673	E4674	K4675	R4679	E4682	C4685	L4686	Y4687	I4688	T4689	E4690	Q4691																																																																																																																																																																																																														



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	0.068	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	33/142628 (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
2	B	0	17
2	E	0	17
2	G	0	16
2	I	0	16
All	All	0	66

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	G	131	LEU	CA-CB-CG	8.35	134.51	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.48	115.30
2	E	131	LEU	CA-CB-CG	8.33	134.46	115.30

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1676	LEU	CA-CB-CG	6.33	129.86	115.30

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	312	THR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	8	0
1	F	818	0	824	8	0
1	H	818	0	824	8	0
1	J	818	0	824	5	0
2	B	29499	0	24751	284	0
2	E	29499	0	24751	290	0
2	G	29499	0	24751	288	0
2	I	29499	0	24751	286	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
All	All	121272	0	102300	1147	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 1147 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:I:4190:ILE:CD1	2:I:5026:ASP:OD2	1.76	1.33
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	1.77	1.33
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	1.77	1.32
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	1.76	1.31
2:B:4190:ILE:HD11	2:B:5026:ASP:OD2	1.31	1.26

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%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	335 (10%)	8 (0%)	47	81
2	E	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	47	81
2	G	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	336 (10%)	8 (0%)	47	81
All	All	13360/18096 (74%)	11941 (89%)	1387 (10%)	32 (0%)	50	81

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	I	5028	PHE
2	E	5028	PHE
2	G	5028	PHE
2	B	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%)	2474 (99%)	19 (1%)	81	89
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	84	90

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	131	LEU
2	G	4120	ASN
2	G	553	ARG
2	G	3762	ARG
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4120	ASN
2	G	3781	GLN
2	E	520	ASN
2	G	3766	GLN
2	G	4553	ASN

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	I	14
2	E	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	73.35
1	I	4345:UNK	C	4540:PHE	N	73.35
1	E	4345:UNK	C	4540:PHE	N	73.35
1	G	4345:UNK	C	4540:PHE	N	73.35

Continued on next page...

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	45.90

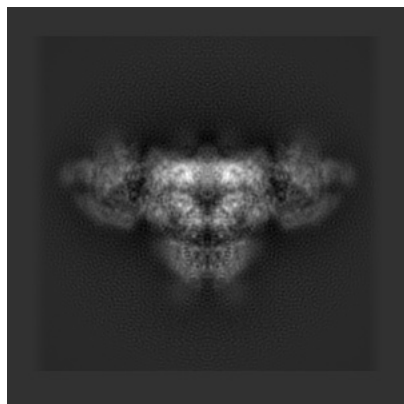
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8393. These allow visual inspection of the internal detail of the map and identification of artifacts.

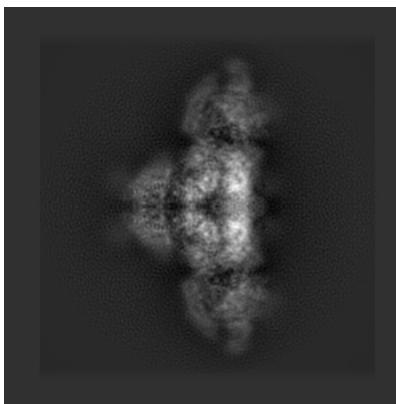
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

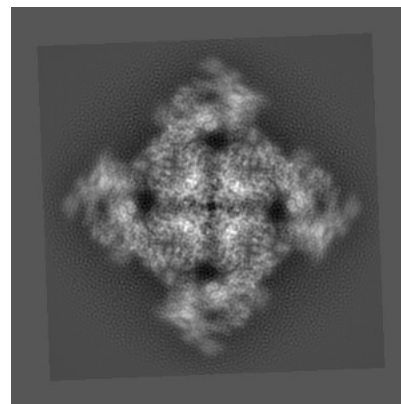
6.1.1 Primary map



X

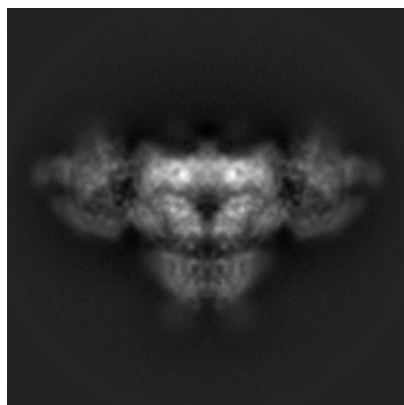


Y

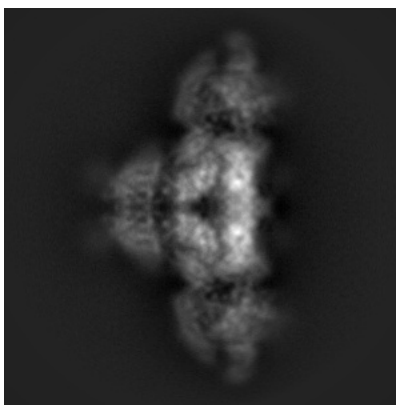


Z

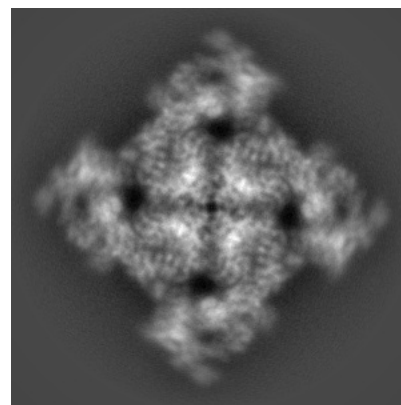
6.1.2 Raw map



X



Y

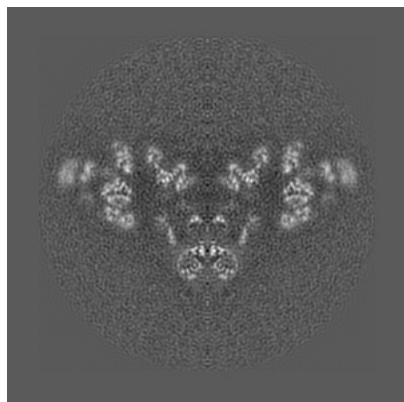


Z

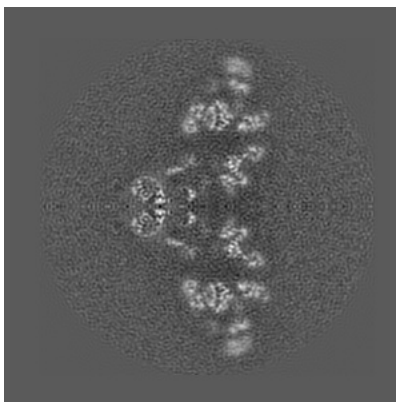
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

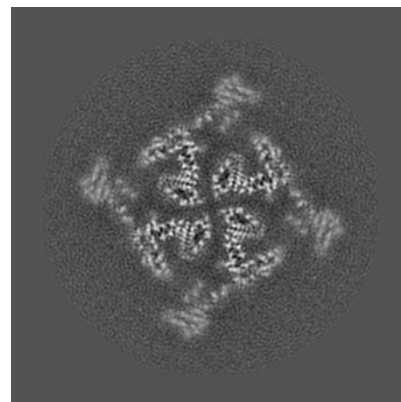
6.2.1 Primary map



X Index: 200

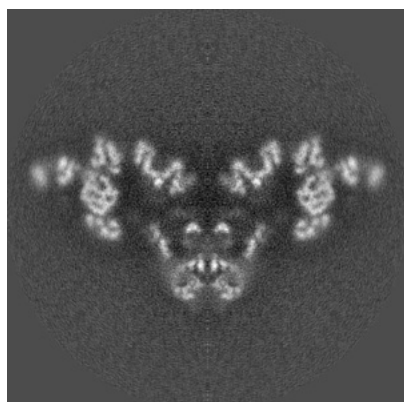


Y Index: 200

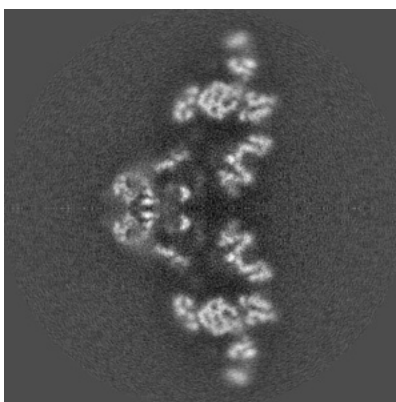


Z Index: 200

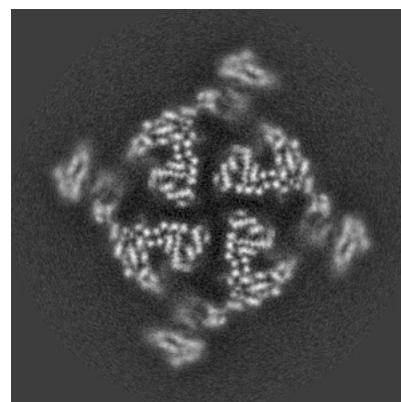
6.2.2 Raw map



X Index: 168



Y Index: 168

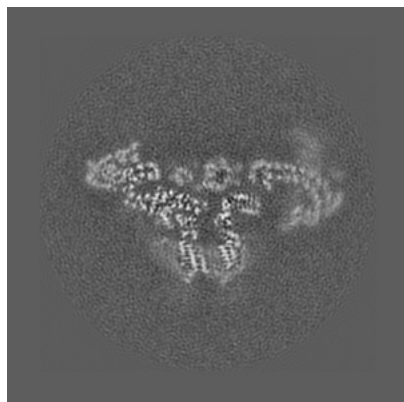


Z Index: 168

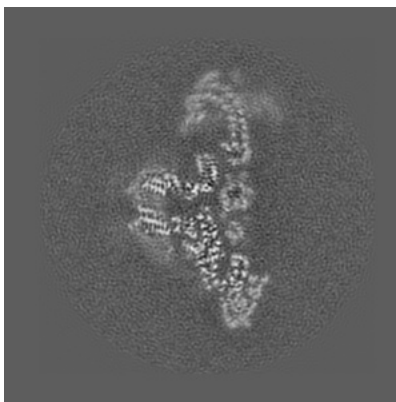
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

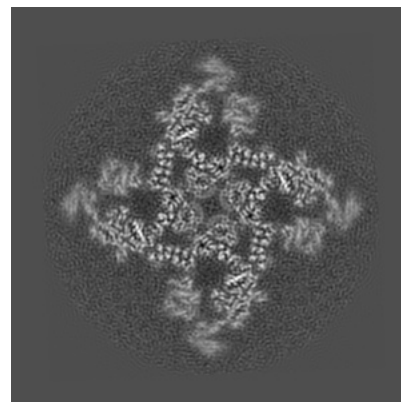
6.3.1 Primary map



X Index: 224

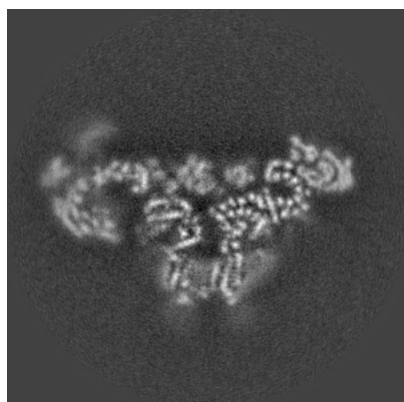


Y Index: 176

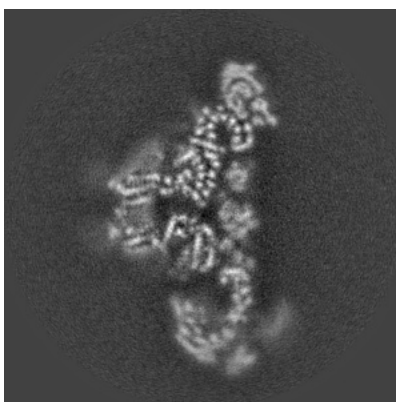


Z Index: 228

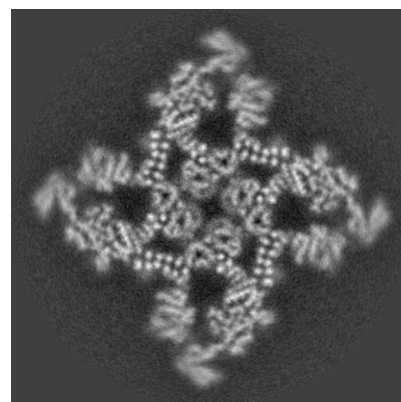
6.3.2 Raw map



X Index: 146



Y Index: 190

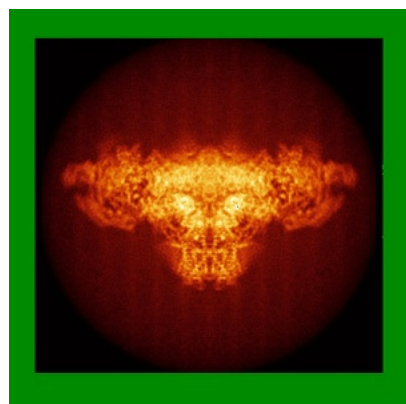


Z Index: 193

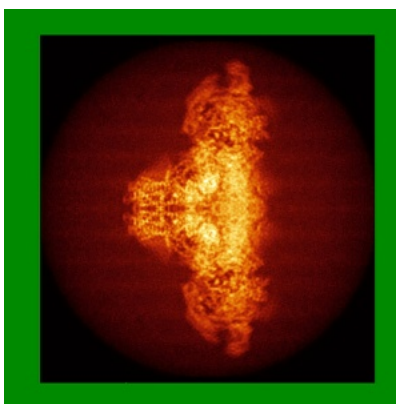
The images above show the largest variance slices of the map in three orthogonal directions.

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

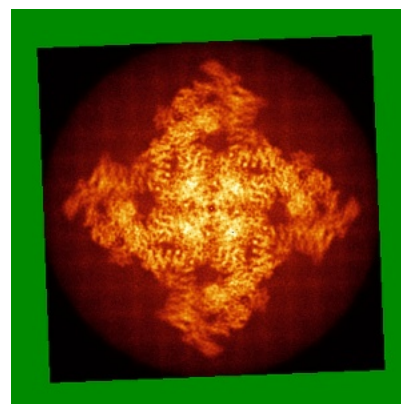
6.4.1 Primary map



X

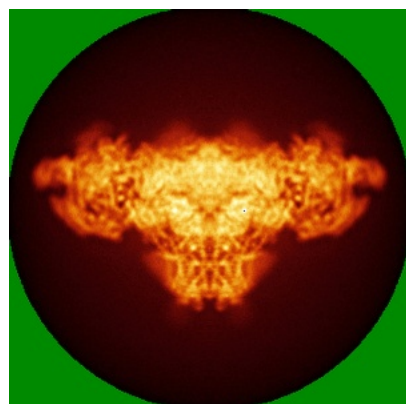


Y

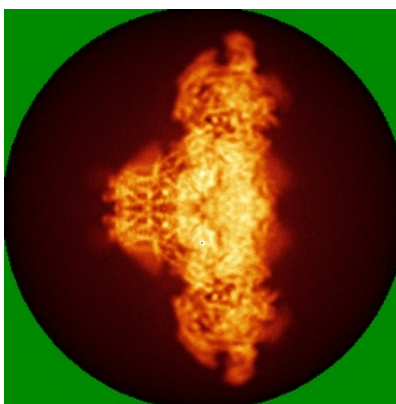


Z

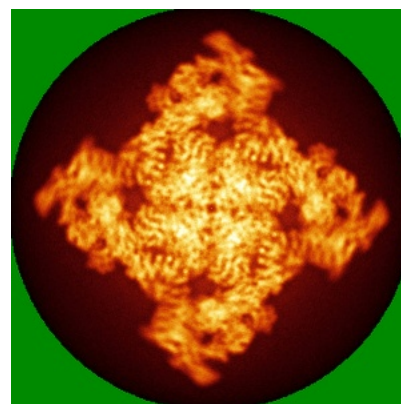
6.4.2 Raw map



X



Y

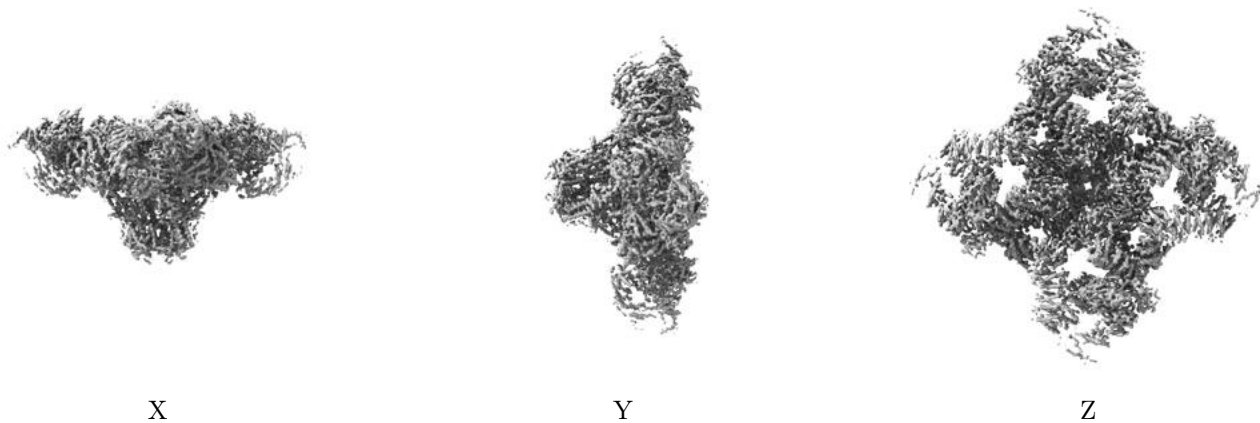


Z

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.

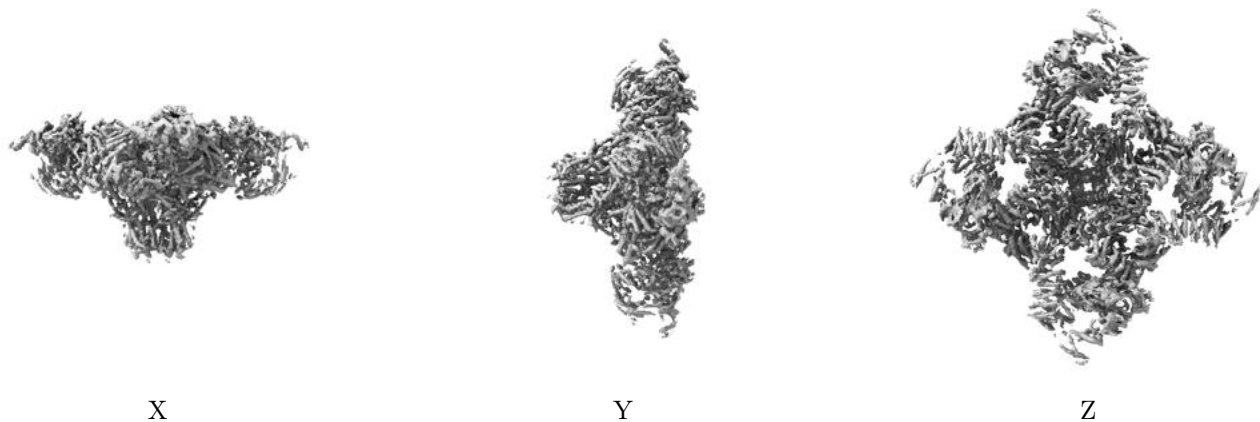
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

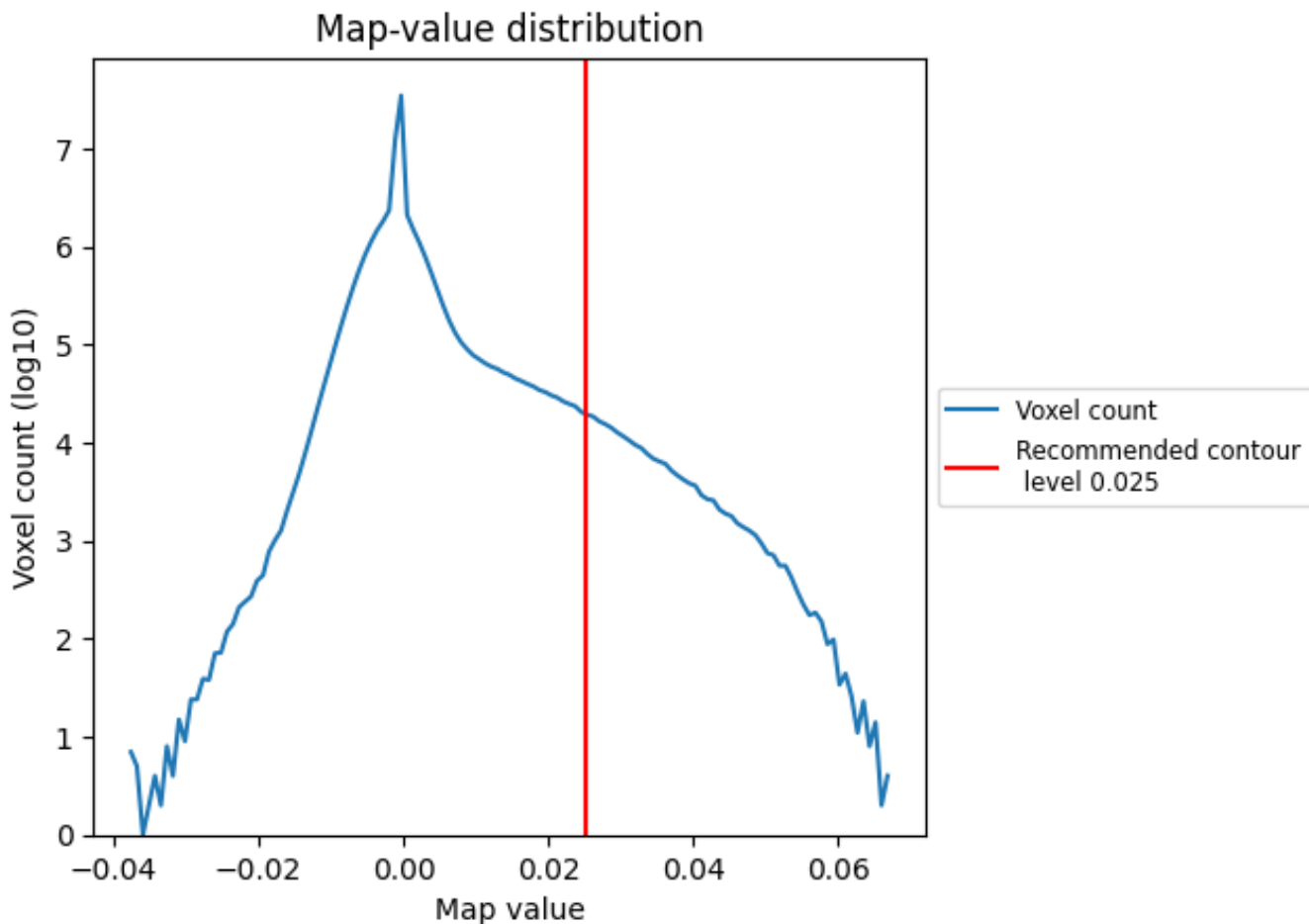
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

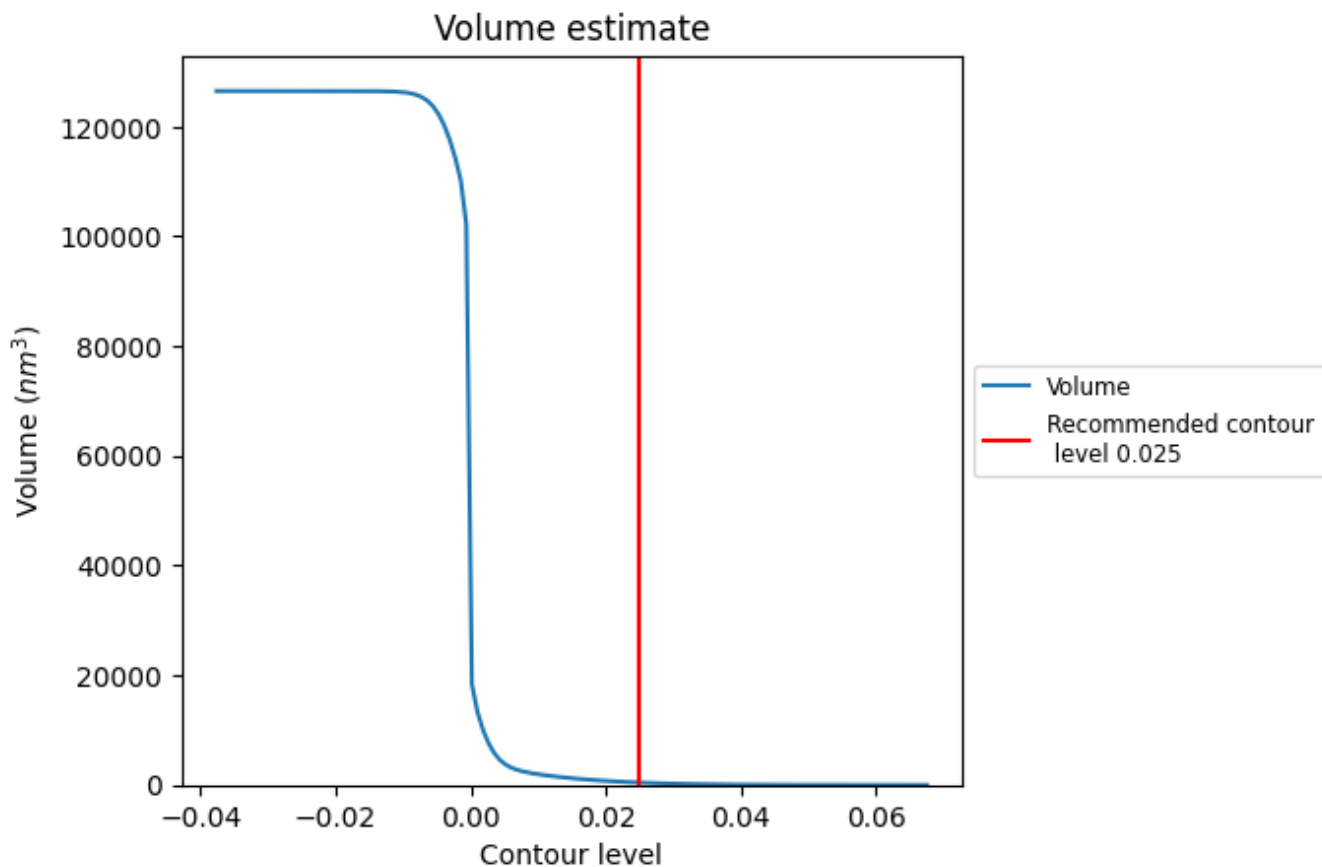
This section contains the results of statistical analysis of the map.

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.

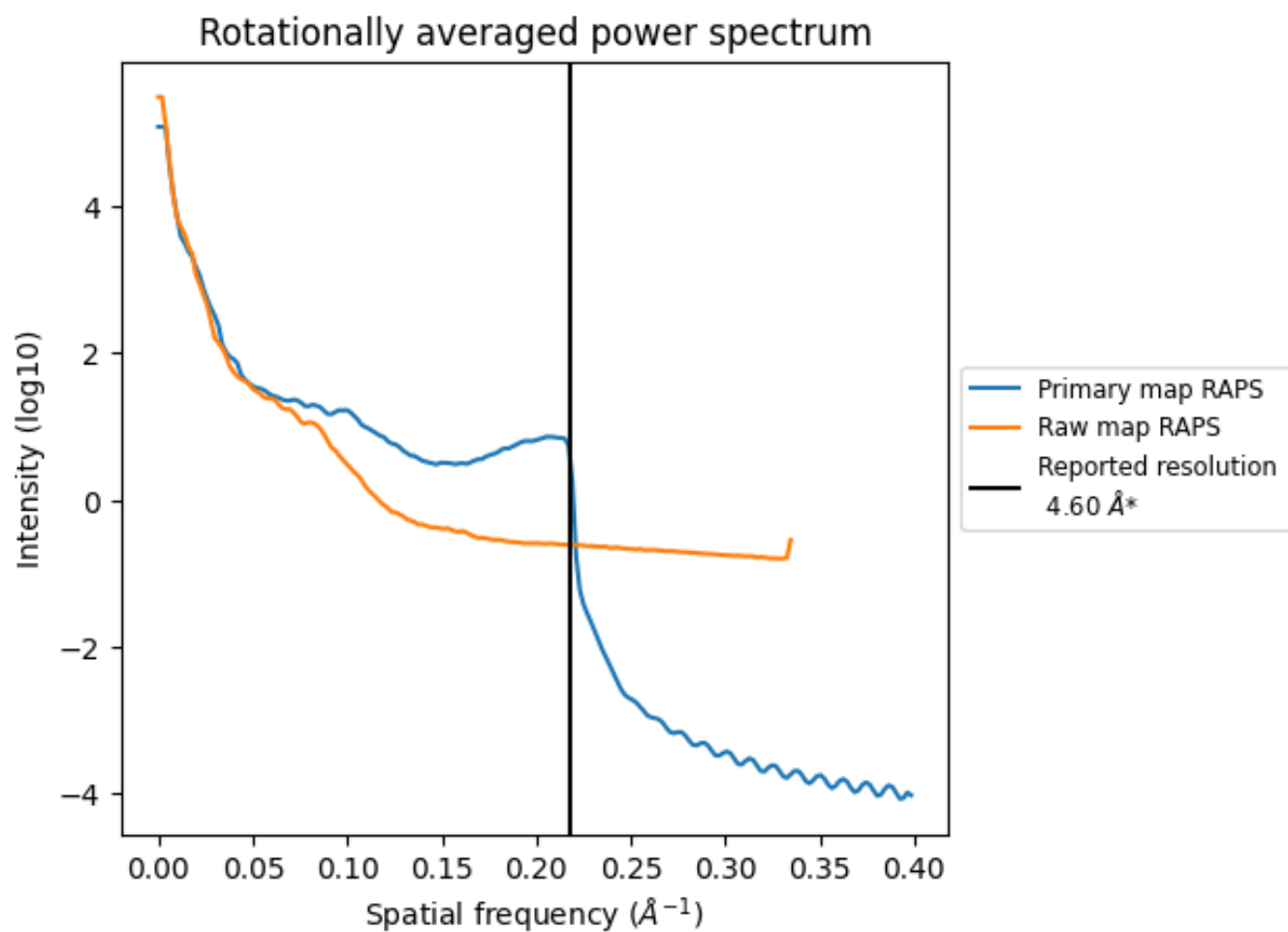
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm^3 ; this corresponds to an approximate mass of 390 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

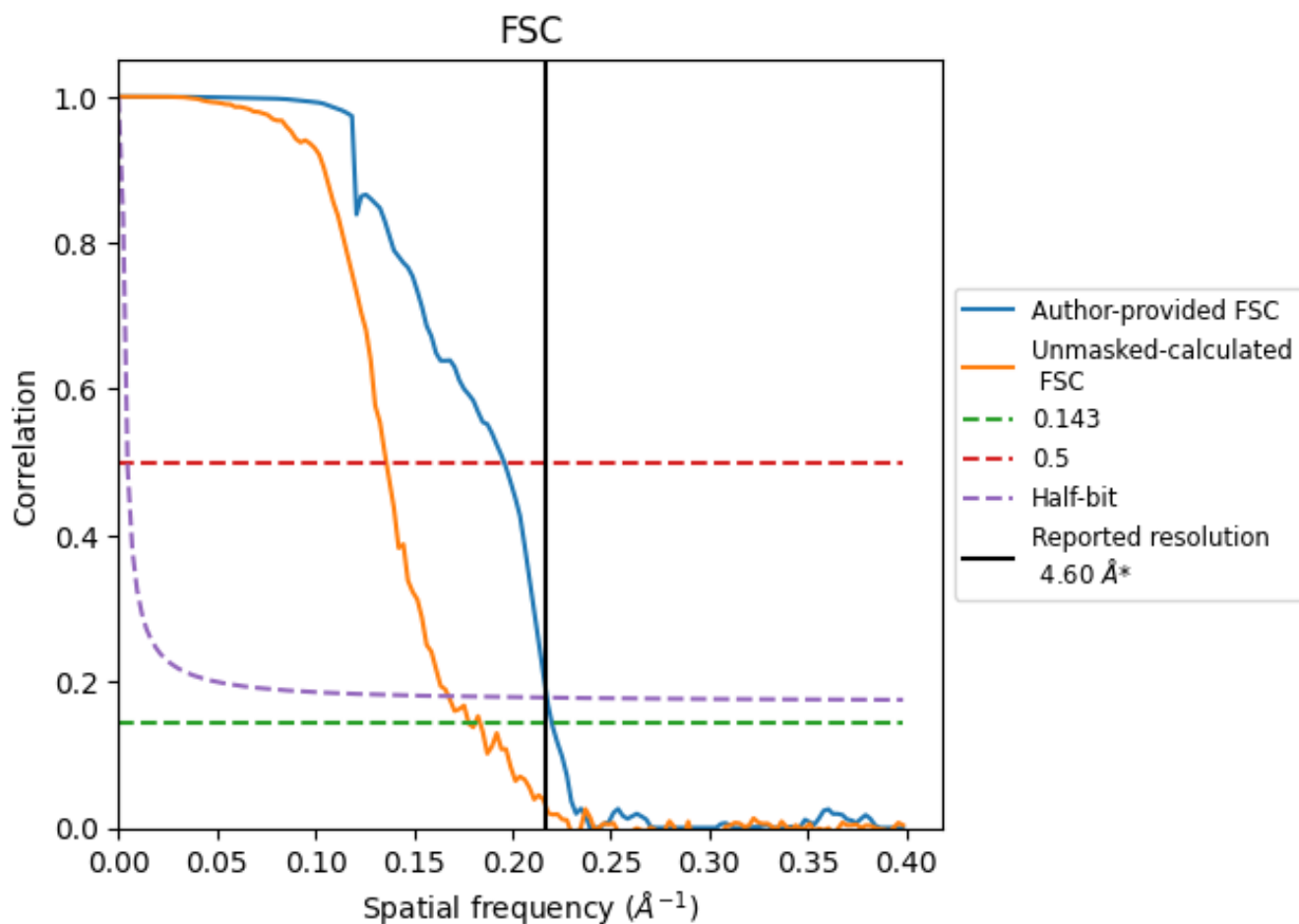


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates

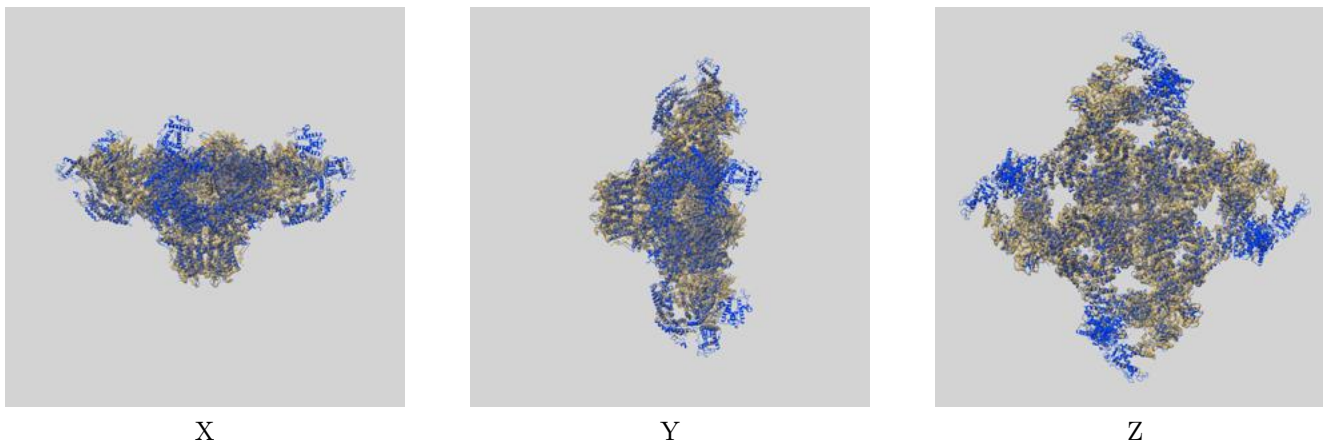
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.54	5.11	4.60
Unmasked-calculated*	5.62	7.35	5.97

*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 5.62 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

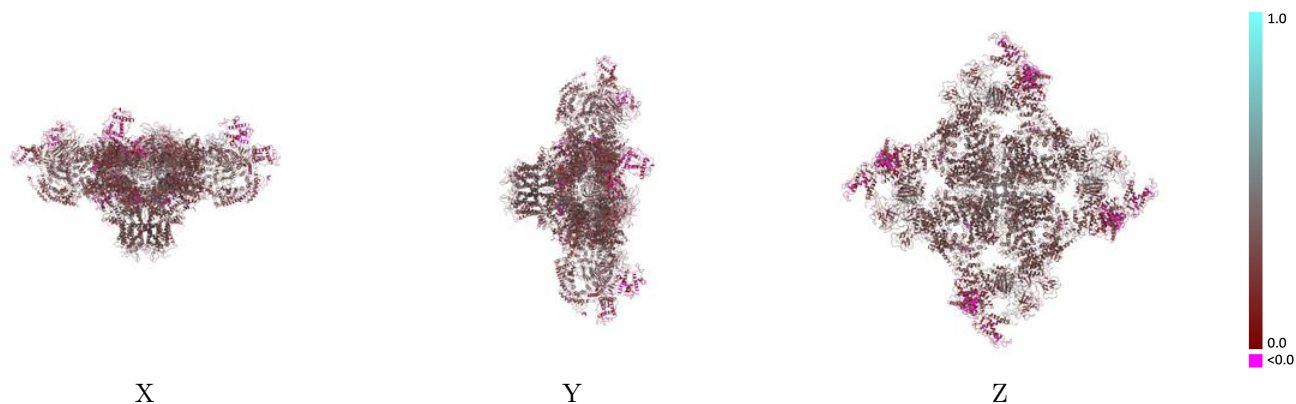
This section contains information regarding the fit between EMDB map EMD-8393 and PDB model 5TB2. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



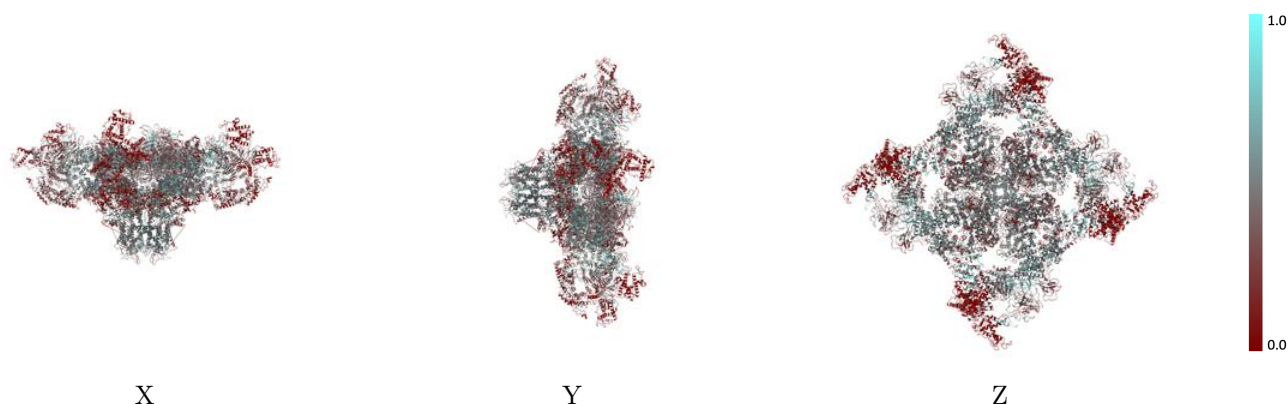
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



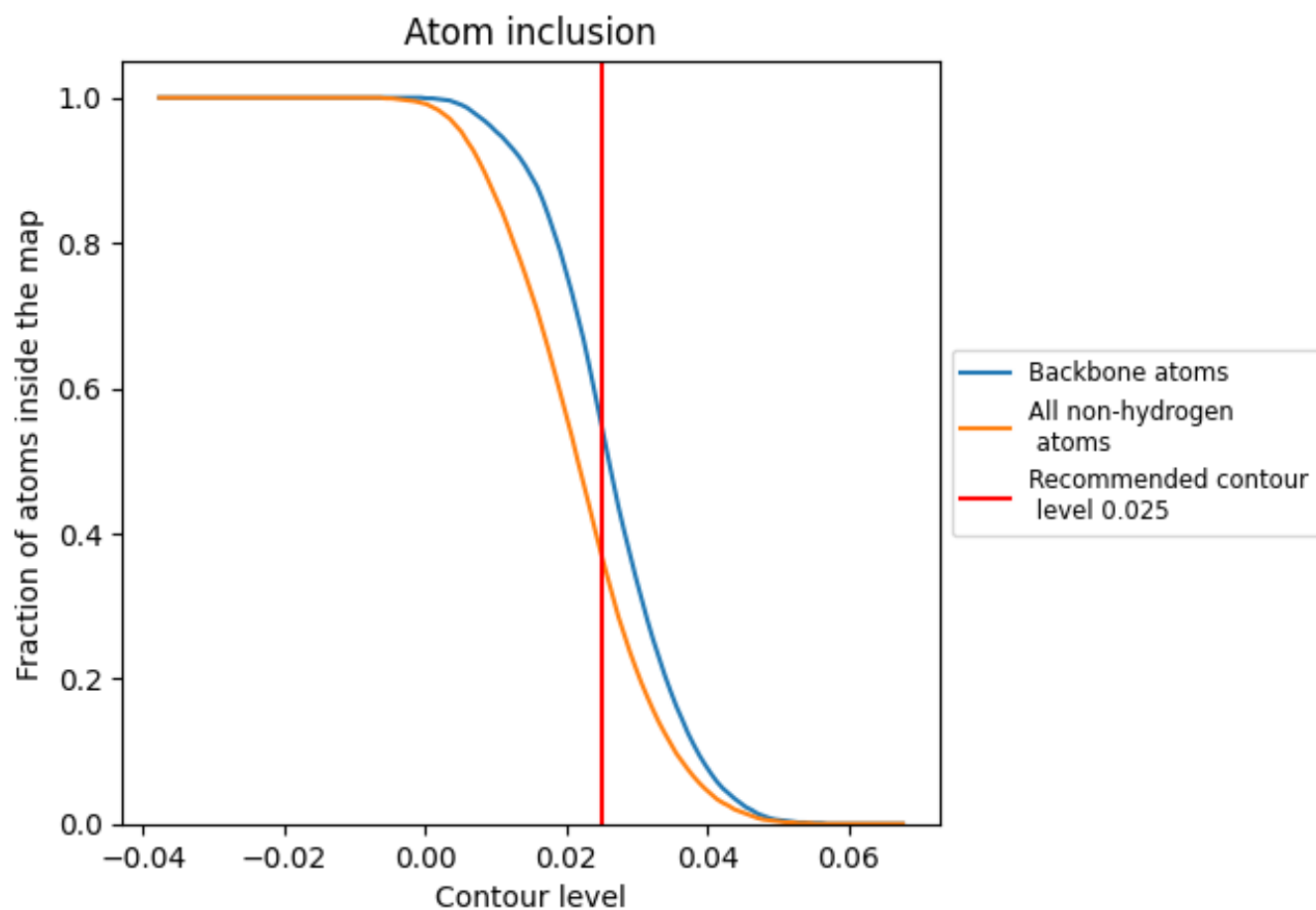
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 55% of all backbone atoms, 37% 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	0.3690	0.2880
A	0.3500	0.3000
B	0.3700	0.2880
E	0.3690	0.2880
F	0.3440	0.3030
G	0.3700	0.2880
H	0.3490	0.3040
I	0.3700	0.2870
J	0.3500	0.3030

