



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 09:42 PM UTC

PDB ID : 8SEN / pdb\_00008sen  
EMDB ID : EMD-40422  
Title : Cryo-EM Structure of RyR1  
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.  
Deposited on : 2023-04-10  
Resolution : 3.49 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:

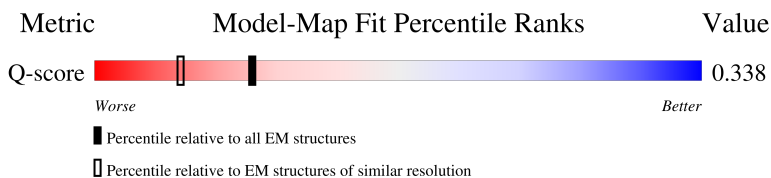
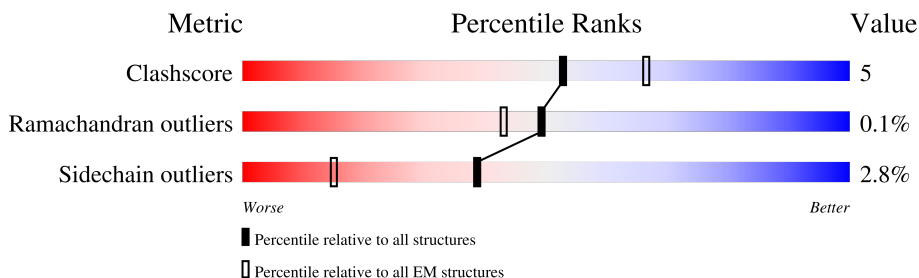
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.49 Å.

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







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 ( 2.99 - 3.99 )

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	5037	<p>16% (Poor fit), 73% (0-1 outliers), 14% (2 outliers), 13% (3+ outliers)</p>
1	B	5037	<p>16% (Poor fit), 73% (0-1 outliers), 14% (2 outliers), 13% (3+ outliers)</p>
1	C	5037	<p>16% (Poor fit), 73% (0-1 outliers), 14% (2 outliers), 13% (3+ outliers)</p>
1	D	5037	<p>16% (Poor fit), 73% (0-1 outliers), 14% (2 outliers), 13% (3+ outliers)</p>

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Mol	Chain	Length	Quality of chain
2	E	350	 24% 6% 69%
2	F	350	 24% 7% 69%
2	G	350	 24% 6% 69%
2	H	350	 24% 7% 69%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 142960 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		
1	B	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		
1	C	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		
1	D	4378	Total	C	N	O	S	9	0
			34921	22217	6025	6443	236		

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

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

There are 100 discrepancies between the modelled and reference sequences:

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

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

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

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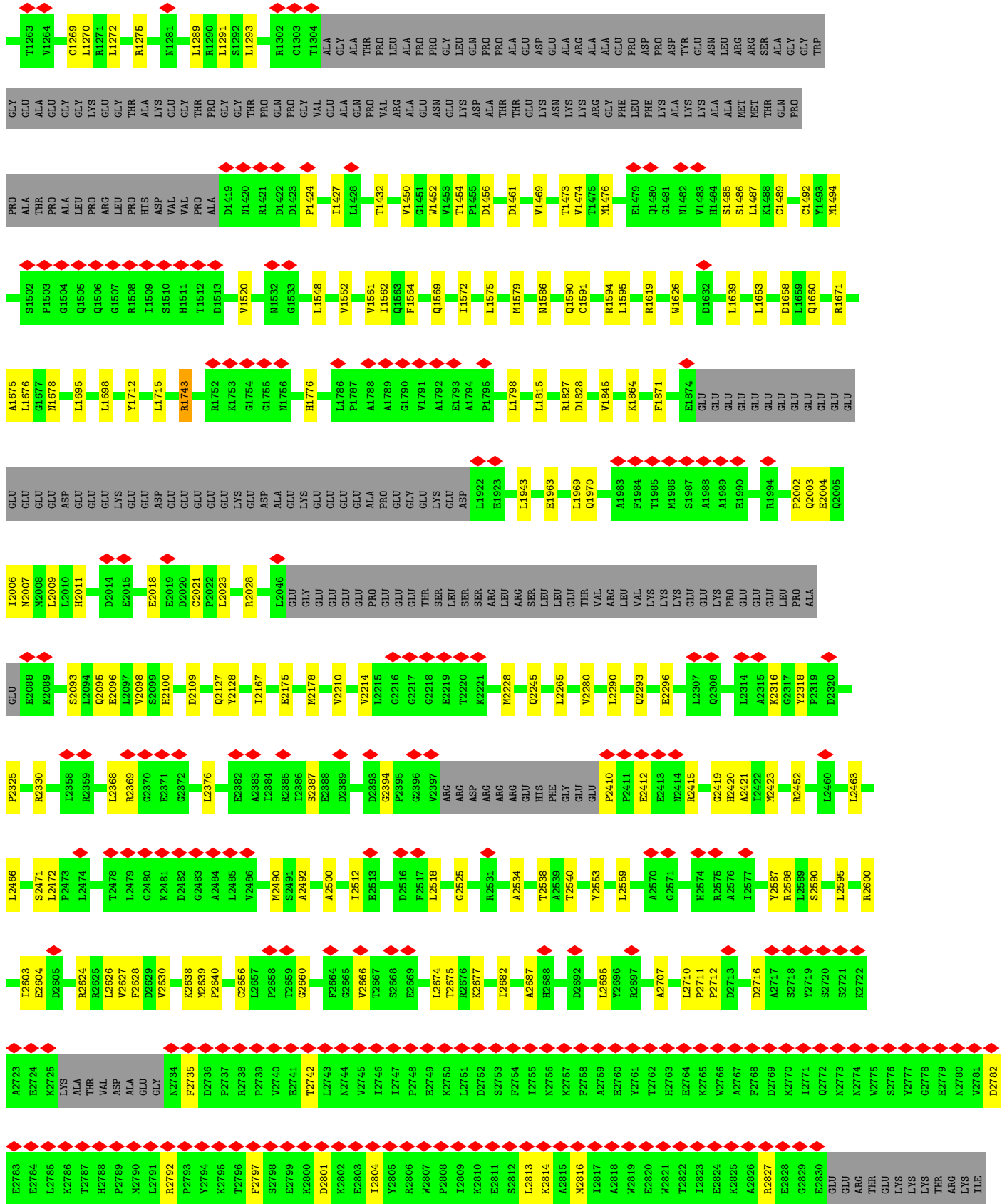
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

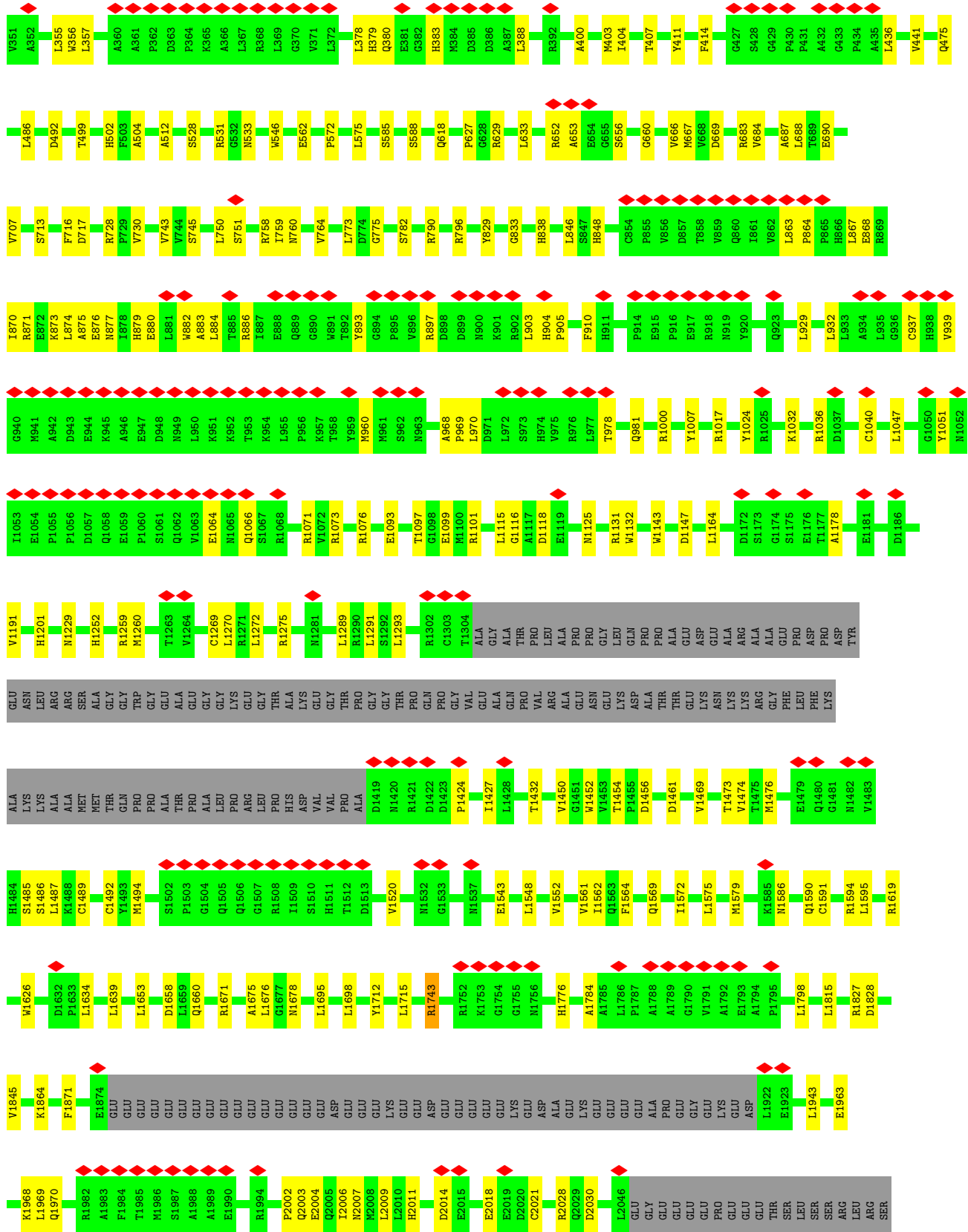
Mol	Chain	Residues	Atoms	AltConf
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3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

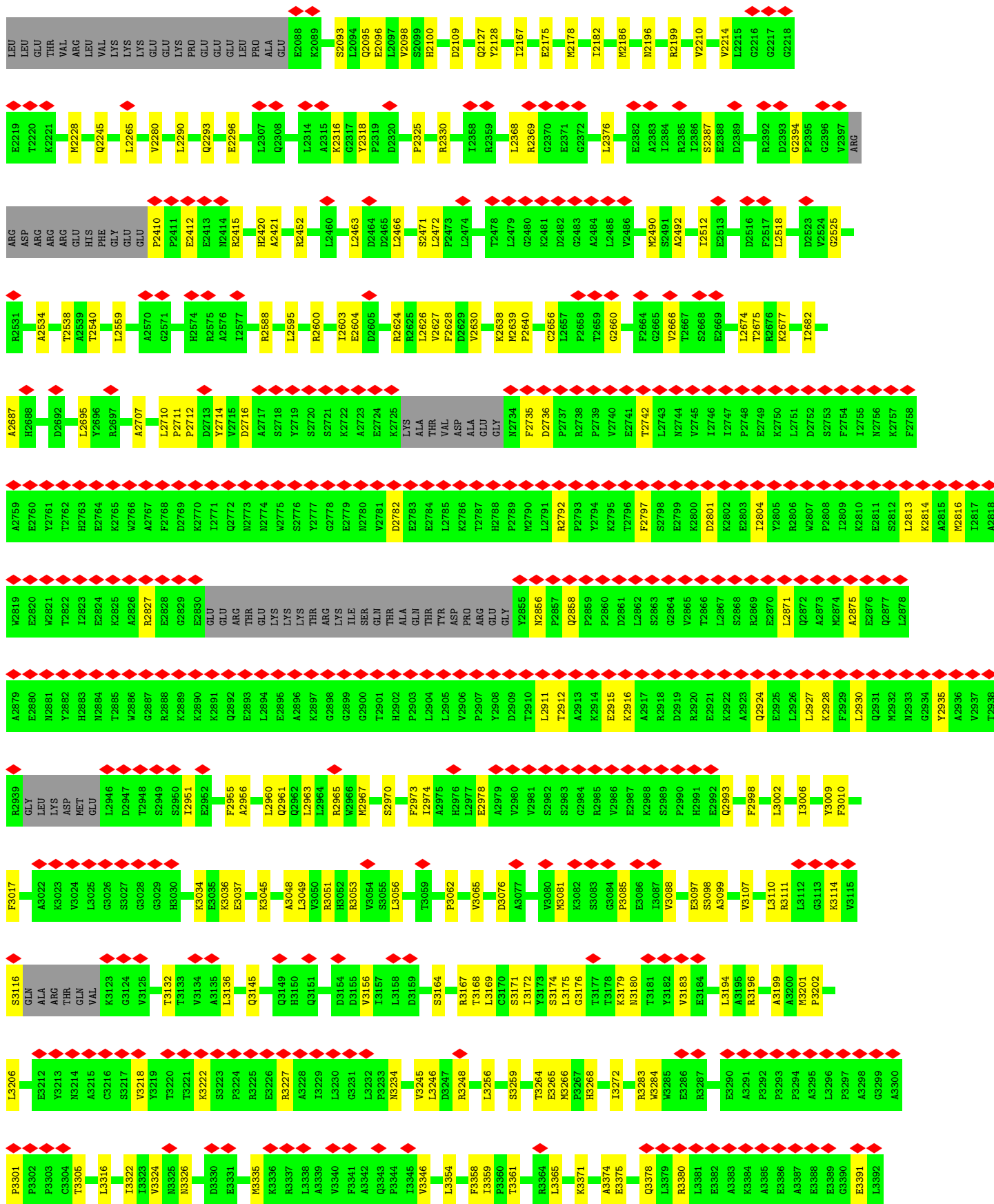




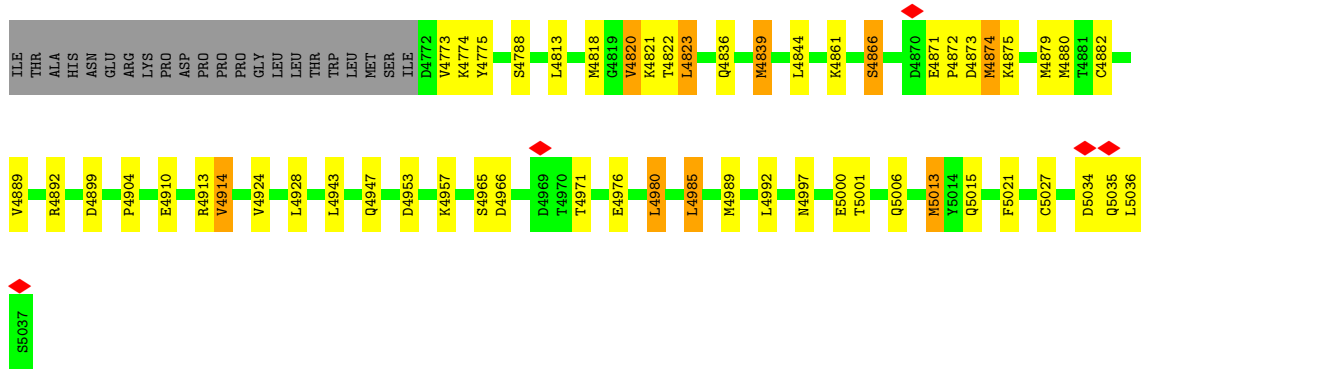
SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	Y2856	Y2857	Y2858	Y2859	Y2860	Y2861	Y2862	Y2863	Y2864	Y2865	Y2866	Y2867	Y2868	Y2869	Y2870	Y2871	Y2872	Y2873	Y2874	Y2875	Y2876	Y2877	Y2878	Y2879	Y2880	Y2881	Y2882	Y2883	Y2884	Y2885	Y2886	Y2887	Y2888	Y2889	Y2890	Y2891	Y2892	Y2893	Y2894	Y2895	Y2896	Y2897	Y2898	Y2899	Y2900	Y2901
P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	L2946	D2947	T2948	S2949	K2950	L2951	E2952	A2956	L2960	Q2961	Q2962	L2963	L2964	G2965	V2966			
M2967	R3052	R3053	V3054	S3055	L3056	T3059	P3062	V3065	D3076	A3077	V3080	K3081	K3082	S3083	G3084	P3085	S2989	P2990	I3087	A2923	E2992	Q2993	F2997	F2998	I3001	L3002	I3006	Y3009	F3010	F3017	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	K3034	E3035	K3036	E3037	K3045	A3048	L3049	R3051											
H3052	R3053	V3054	S3055	L3056	T3059	P3062	V3065	D3076	A3077	V3080	K3081	K3082	S3083	G3084	P3085	S2989	P2990	I3087	A2923	E2992	Q2993	F2997	F2998	I3001	L3002	I3006	Y3009	F3010	F3017	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	K3034	E3035	K3036	E3037	K3045	A3048	L3049	R3051												
D3154	D3155	I3156	I3157	L3158	D3159	S3164	R3167	T3168	L3169	C3170	S1171	L3172	S3173	L3174	L3175	G3176	T3177	T3178	K3179	P3085	E3086	I3087	V3088	E3087	S3088	A3099	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	S3027	V3125	T3132	T3133	V3134	A3135	L3136	Q3145	Q3149	H3150	Q3151					
D3154	D3155	I3156	I3157	L3158	D3159	S3164	R3167	T3168	L3169	C3170	S1171	L3172	S3173	L3174	L3175	G3176	T3177	T3178	K3179	P3085	E3086	I3087	V3088	E3087	S3088	A3099	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	S3027	V3125	T3132	T3133	V3134	A3135	L3136	Q3145	Q3149	H3150	Q3151					
R3247	R3248	L3249	L3256	T3264	E3265	P3266	P3267	H3268	I3272	L3277	K3284	W3285	E3286	R3287	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	G3300	F3301	P3302	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	P3223	R3225	E3226	R3227	A3228	K3036	I3229	L3230	G3231	L3232	P3233	N3234	V3245	L3246							
V3346	S3347	L3354	F3356	I3359	T3361	R3364	L3365	K3371	A3374	E3375	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	R3403	L3408	R3414	D3417	R3420	L3424	N3430	E3433	L3434	F3435	R3436	M3437	F3442																
H3449	M3450	R3453	V3459	V3460	Q3461	M3462	F3463	T3464	M3465	M3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	S3504	V3505	Q3506	T3507	V3511	T3520	M3524						
T3528	I3533	H3534	K3537	A3541	L3542	K3543	D3544	T3545	E3548	M3555	N3556	L3557	H3558	L3559	G3561	K3562	V3563	E3564	G3565	M3573	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	T3592	V3593	R3594	R3595	V3596	H3605	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	H3621												
K3622	L3623	L3624	S3625	K3626	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	Y3642	R3648	M3652	E3655	A3659	L3663	D3676	G3681	E3682	G3683	Q3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	K3694	P3695	H3699	F3705	T3708	E3736	GLU	GLY	GLY	ASN													
GLY	GLU	ALA	GLU	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	S3768	R3769	L3770	H3771	T3772	R3773	G3801	L3805	L3817	K3821	D3822	K3823	L3835	S3840	V3841	L3842	K3852	G3857	K3858	V3859	K3860	E3861	D3862	G3863	T3864	V3865	L3866	N3867	K3868	Q3869	N3870	K3871	E3872	K3873	V3874									
M3875	A3876	D3877	F3880	L3891	F3899	Q3900	N3901	R3904	S3929	Y3937	D3941	E3945	K3948	R3949	Y3968	N3976	M4001	K4002	D4006	L4017	M4044	F4061	K4067	L4068	D4070	I4071	G4073	S4074	E4075	A4076	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	I4088																				
S4089	K4090	K4091	D4092	F4093	Q4094	K4095	M4097	D4098	S4099	K4101	D4102	F4103	G4105	F4106	I4108	Q4109	F4110	L4111	L4112	E4115	A4117	D4118	E4119	E4121	F4122	N4123	N4124	F4125	A4129	P4135	D4138	F4141	N4142	L4146	P4155	R4161	E4165	R4180	I4181	E4196	I4197	S4198																



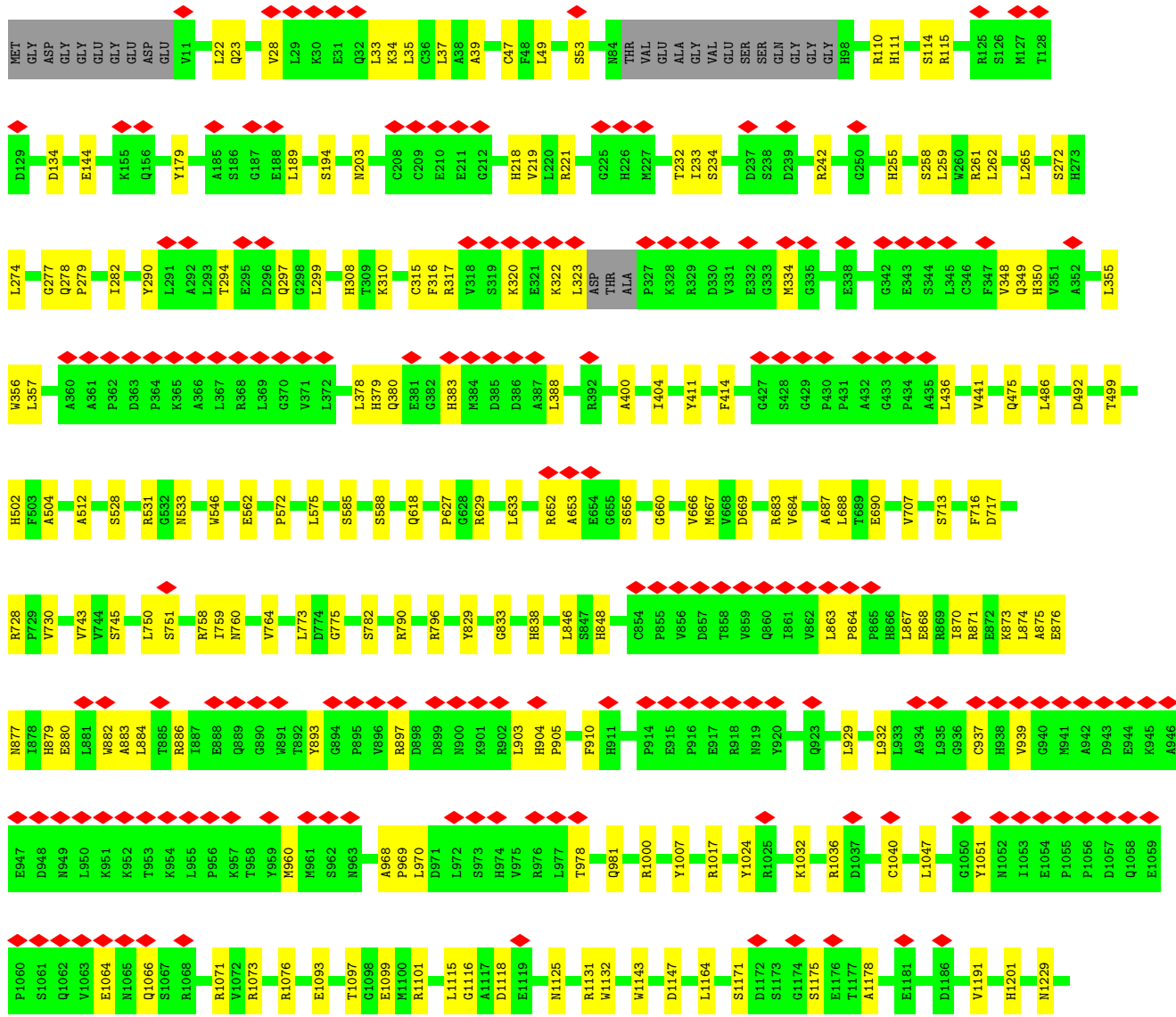
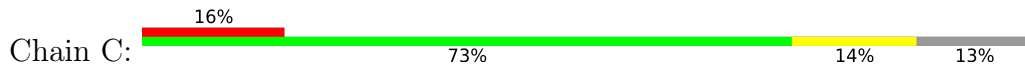


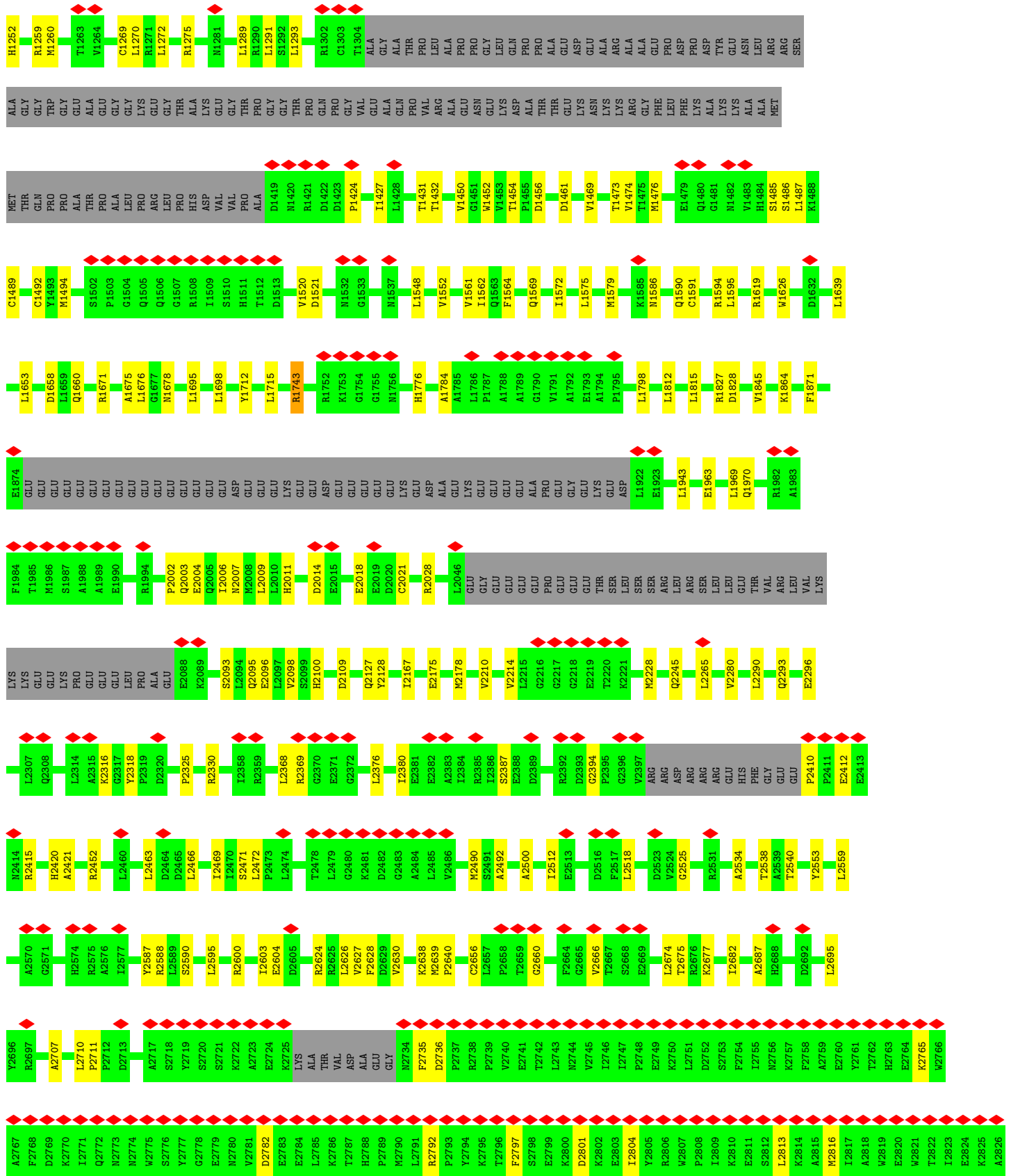




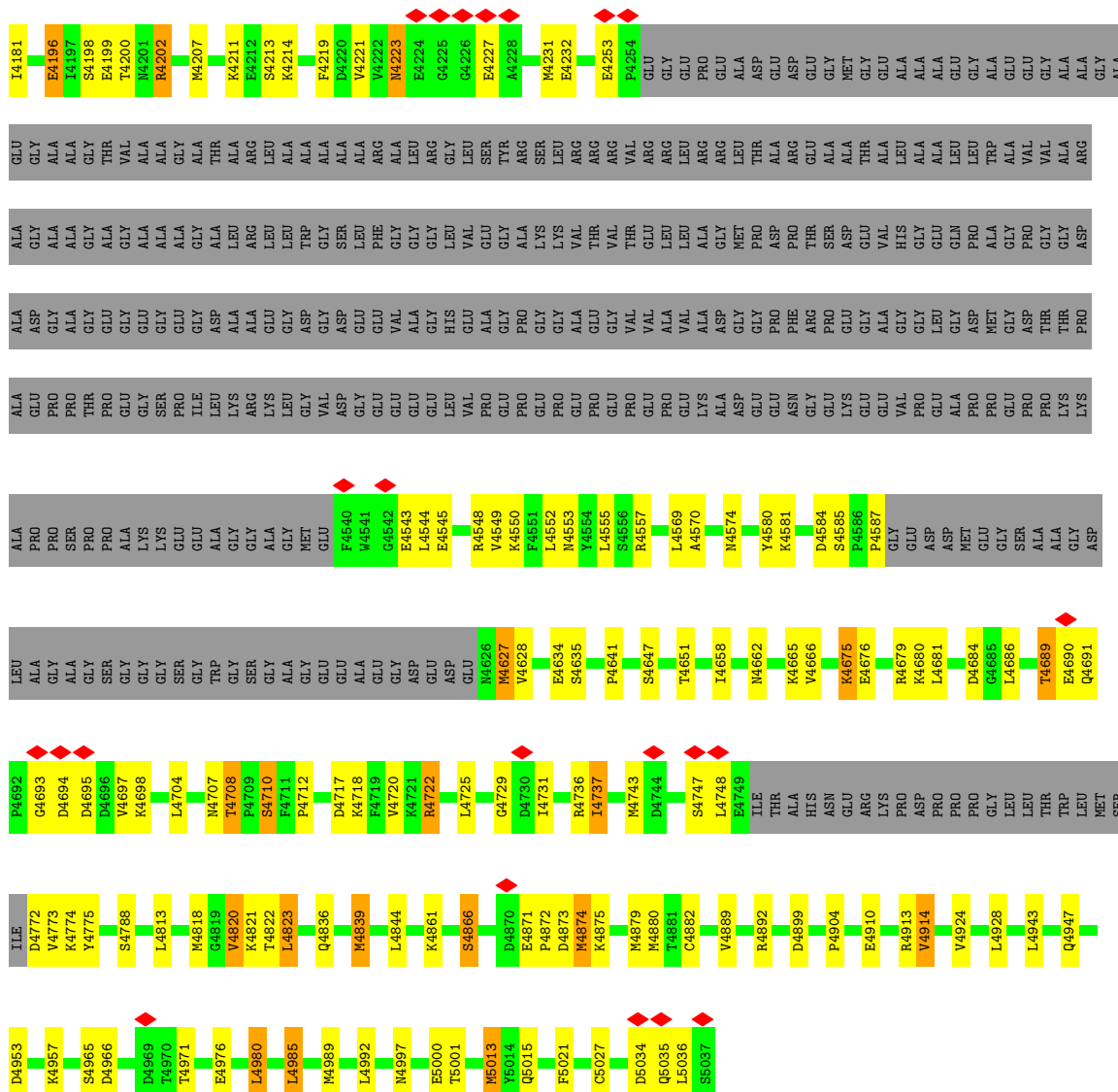


• Molecule 1: Ryanodine receptor 1

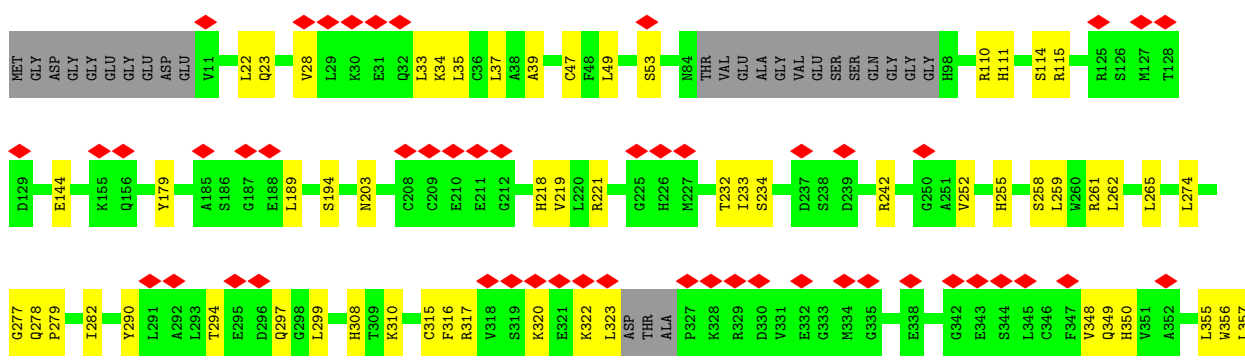
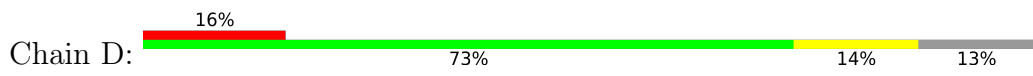




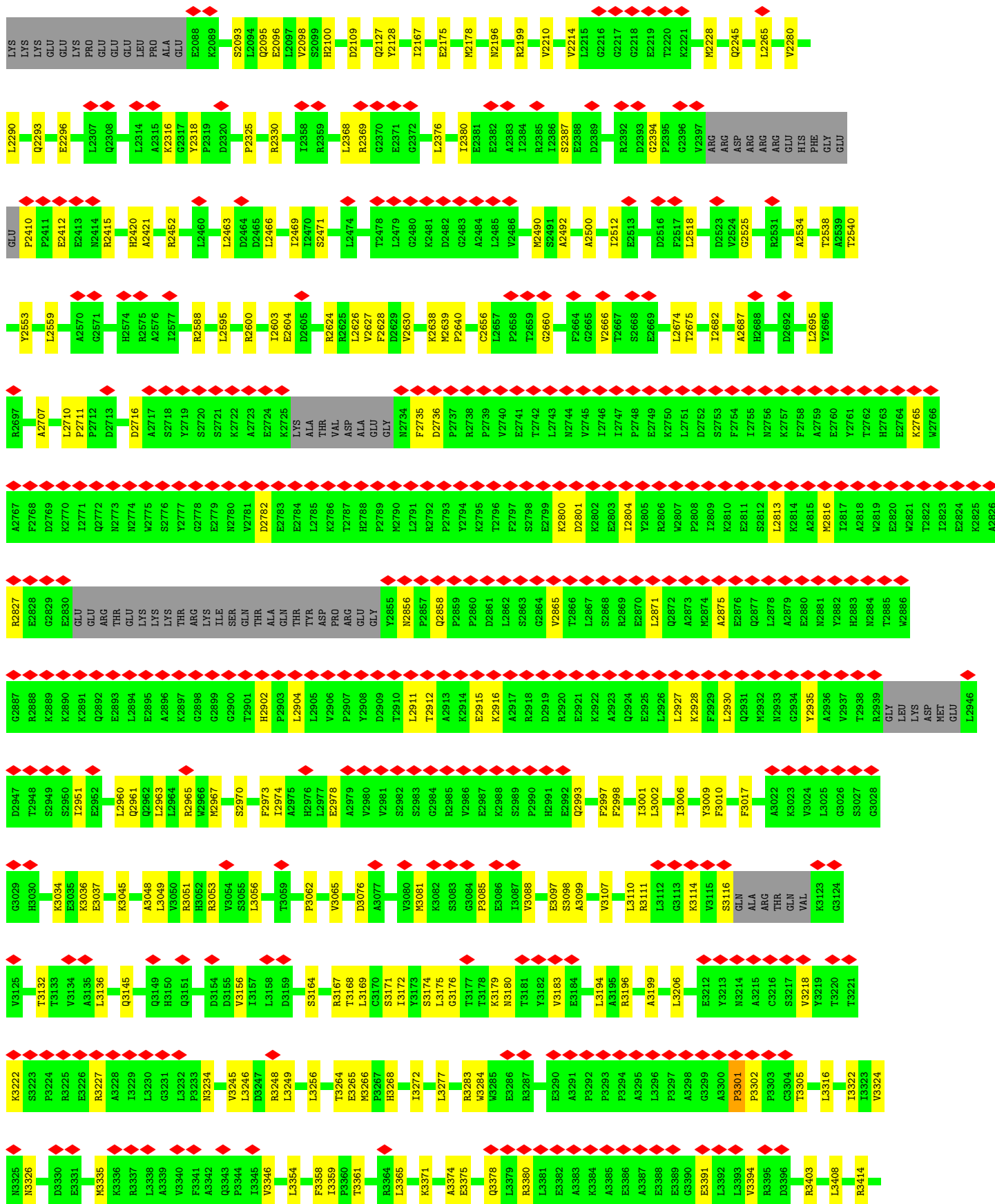
R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	ALA	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	F2857	Q2858	F2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	R2868	R2869	E2870	L2871	Q2872	A2873	N2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	
G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	T2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	R2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946
D2947	T2948	S2949	S2950	T2951	E2952	L2953	L2954	R2955	W2956	M2957	S2970	F2973	T2974	A2975	H2976	L2977	E2978	A2979	V2980	Y2981	S2982	S2983	G2984	P2985	V2986	E2987	K2988	S2989	P2990	D2991	F2992	Q2993	F2998	L3002	I3006	Y3009	F3010	F3017	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030												
K3034	E3035	K3036	E3037	K3045	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	T3059	P3062	V3065	D3076	A3077	V3080	M3081	K3082	S3083	G3084	P3085	E3086	L3087	V3088	E3089	S3098	A3099	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	K3123	G3124	G3026	V3125	T3132											
T3133	V3134	A3135	L3136	Q3145	Q3149	H3150	R3151	D3154	D3155	V3156	I3157	L3158	D3159	S3164	R3167	T3168	L3169	G3170	S3171	I3172	V3173	S3174	L3175	G3176	T3177	N3180	T3181	Y3182	V3183	E3184	L3194	A3195	R3196	L3206	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	V3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227									
A3228	T3229	L3230	G3231	L3232	P3233	N3234	V3245	L3246	R3248	L3256	T3264	E3265	K3266	P3267	H3268	I3272	K3284	K3285	E3286	I3287	R3287	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	L3316	T3322	L3323	V3324	N3325	N3326	D3330	E3331	K3335	K3336	R3337	L3338										
A3339	V3340	F3341	A3342	Q3343	P3344	I3345	L3354	F3356	I3359	T3361	R3364	L3365	K3371	A3374	E3375	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	R3403	L3408	R3414	R3417	R3420	L3424	N3430	E3433	L3434																
F3435	R3436	N3437	F3442	H3449	N3450	R3453	V3459	V3460	Q3461	N3462	E3463	I3464	N3465	N3466	H3467	S3468	F3469	T3471	A3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	ALA	GLY	ASP	ALA	GLN	SER	GLY	SER	GLY	ASP	GLN	GLU	THR	LYS	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	Q3506	T3507					
V3511	I3520	M3524	T3528	I3533	K3534	A3541	L3542	K3543	D3544	T3545	E3548	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	M3573	L3579	P3580	G3581	E3582	E3583	E3584	D3585	A3586	D3587	I3592	V3593	R3594	R3595	V3596	H3605	L3606	T3609	E3610	H3611	F3612	Y3613	K3614	S3615													
K3616	K3617	A3618	V3619	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3630	A3631	V3632	A3634	C3635	F3636	R3637	M3638	Y3642	R3648	M3652	E3655	A3659	L3663	D3676	G3681	E3682	Q3683	E3684	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	K3694	P3695	H3699	F3705	T3708																
E3736	GLU	GLY	GLU	ASN	GLY	GLU	ALA	GLU	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	S3768	R3769	L3770	H3771	I3772	R3773	G3801	R3802	L3805	L3817	K3821	D3822	K3823	L3835	S3840	V3841	L3842	K3852	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	I3866	N3867	R3868										
Q3869	N3870	G3871	E3872	K3873	V3874	M3875	A3876	D3877	F3880	L3888	L3891	F3899	Q3900	N3901	R3904	S3929	Y3937	D3941	E3945	K3948	R3949	Y3968	N3976	M4001	K4002	D4006	L4017	F4061	L4068	K4069	D4070	V4072	G4073	S4074	E4075	A4076	D4079	Y4080	V4081	T4082																			
D4083	F4084	R4085	I4088	S4089	K4090	K4091	A3876	D4092	F4093	Q4094	R4095	A4096	H4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	E4107	L4108	Q4109	F4110	L4111	L4112	S4115	E4116	A4117	D4118	E4119	M4120	M4121	M4122	L4123	F4125	A4129	P4135	D4138	F4141	M4142	P4155	R4161	Y4080	E4165	P4176	R4180										



● Molecule 1: Ryanodine receptor 1













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.402	Depositor
Minimum map value	-0.437	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.428	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

## 5 Model quality [i](#)

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

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

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	0.27	0/35738	0.59	9/48398 (0.0%)
1	B	0.27	0/35738	0.59	9/48398 (0.0%)
1	C	0.27	0/35738	0.59	9/48398 (0.0%)
1	D	0.27	0/35738	0.59	9/48398 (0.0%)
2	E	0.21	0/834	0.52	0/1123
2	F	0.21	0/834	0.52	0/1123
2	G	0.21	0/834	0.52	0/1123
2	H	0.21	0/834	0.52	0/1123
All	All	0.27	0/146288	0.59	36/198084 (0.0%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3301	PRO	N-CD-CG	-7.38	92.12	103.20
1	B	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	C	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	D	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	A	3301	PRO	CA-N-CD	-7.25	101.85	112.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34921	0	34541	370	0
1	B	34921	0	34541	371	0
1	C	34921	0	34541	363	0
1	D	34921	0	34541	371	0
2	E	818	0	824	12	0
2	F	818	0	824	14	0
2	G	818	0	824	13	0
2	H	818	0	824	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	142960	0	141460	1508	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 1508 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1561:VAL:HG12	1:A:1562:ILE:HG12	1.73	0.71
1:C:1561:VAL:HG12	1:C:1562:ILE:HG12	1.73	0.71
1:B:1561:VAL:HG12	1:B:1562:ILE:HG12	1.73	0.71
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.56	0.70
1:D:1561:VAL:HG12	1:D:1562:ILE:HG12	1.73	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	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48 79

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
1	C	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
1	D	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	48	79
2	E	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	F	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	G	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	H	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
All	All	17840/21548 (83%)	17332 (97%)	488 (3%)	20 (0%)	49	79

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	B	3615	SER
1	C	3615	SER
1	D	3615	SER
1	A	3616	LYS

### 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	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
1	B	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
1	C	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
1	D	3807/4276 (89%)	3697 (97%)	110 (3%)	37	60
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15580/18320 (85%)	15140 (97%)	440 (3%)	38	61

5 of 440 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4199	GLU
1	C	4736	ARG
1	D	5034	ASP
1	D	4747	SER
1	C	4223	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2877	GLN
1	D	1511	HIS
1	C	3313	ASN
1	D	23	GLN
1	D	2127	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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](#)

There are no chain breaks in this entry.

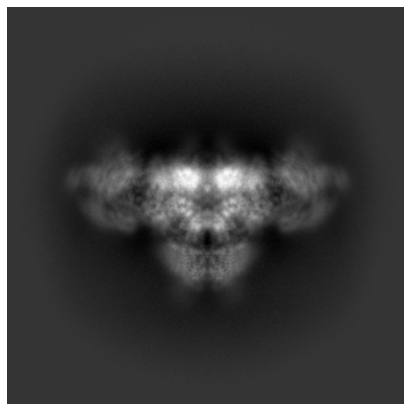
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40422. These allow visual inspection of the internal detail of the map and identification of artifacts.

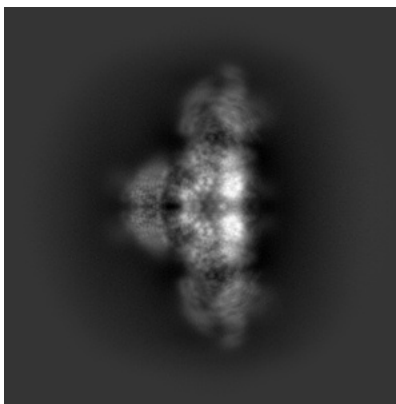
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

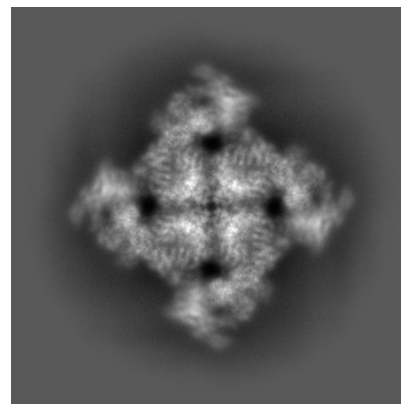
#### 6.1.1 Primary map



X

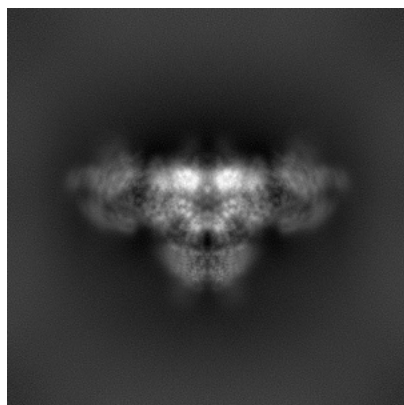


Y

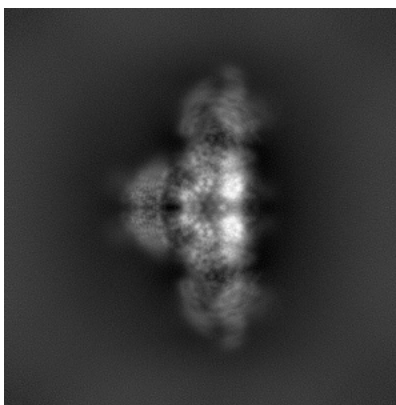


Z

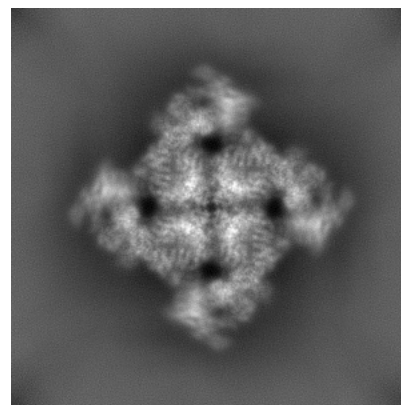
#### 6.1.2 Raw map



X



Y

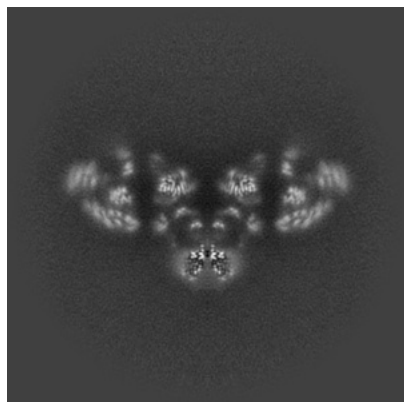


Z

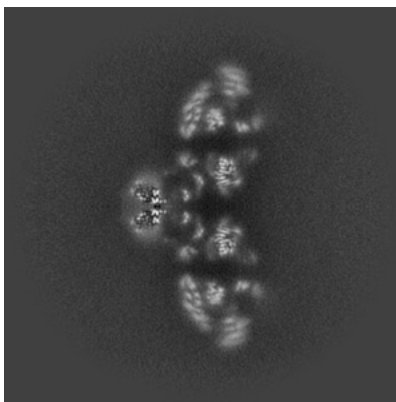
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

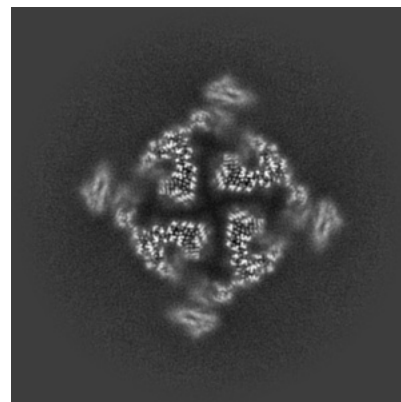
### 6.2.1 Primary map



X Index: 200

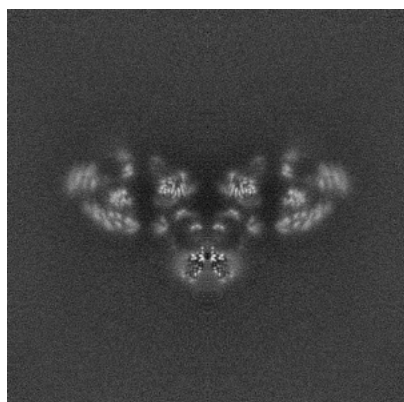


Y Index: 200

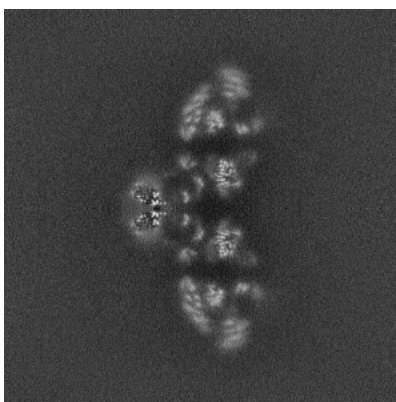


Z Index: 200

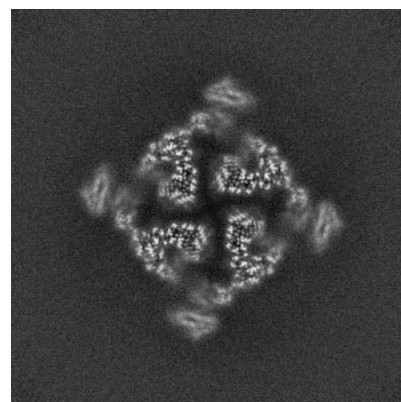
### 6.2.2 Raw map



X Index: 200



Y Index: 200

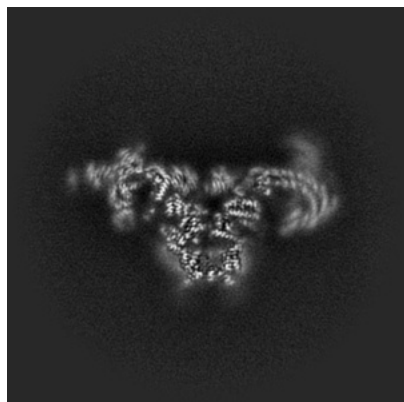


Z Index: 200

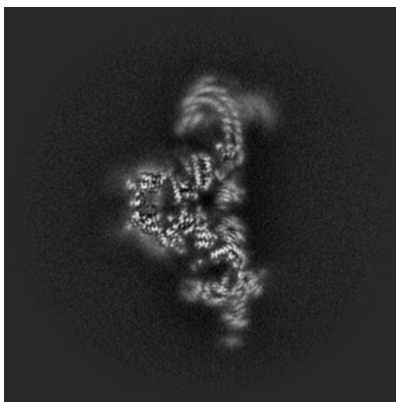
The images above show central slices of the map in three orthogonal directions.

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

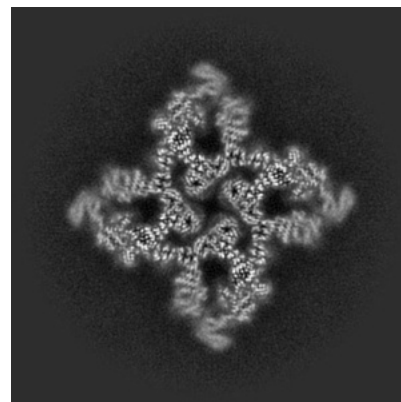
### 6.3.1 Primary map



X Index: 218

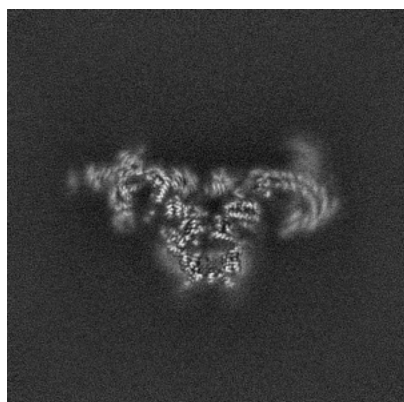


Y Index: 182

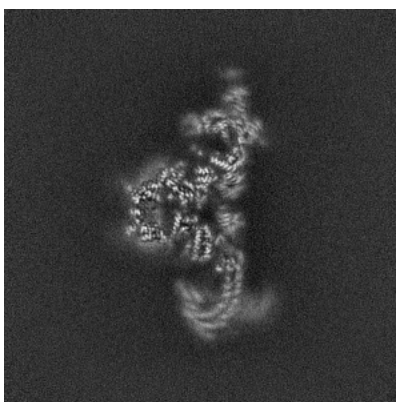


Z Index: 225

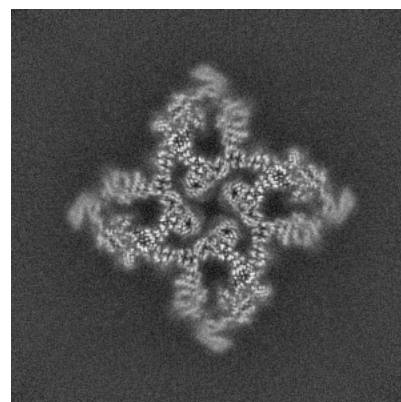
### 6.3.2 Raw map



X Index: 218



Y Index: 218

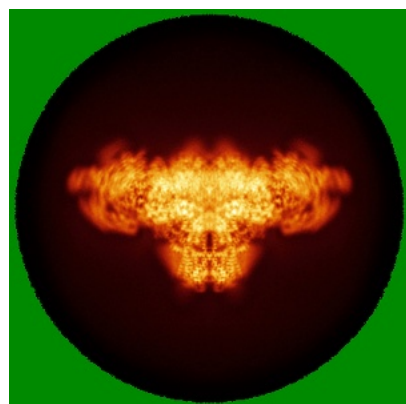


Z Index: 225

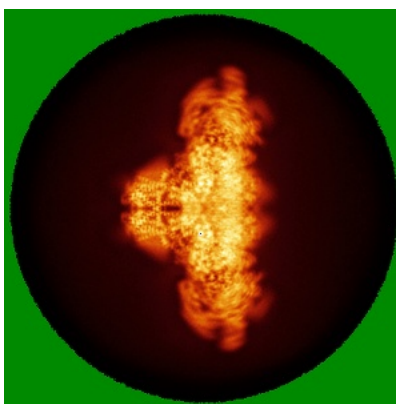
The images above show the largest variance slices of the map in three orthogonal directions.

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

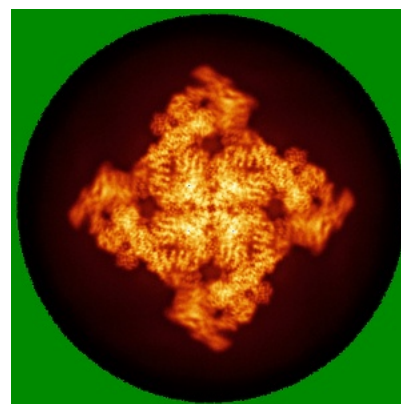
### 6.4.1 Primary map



X

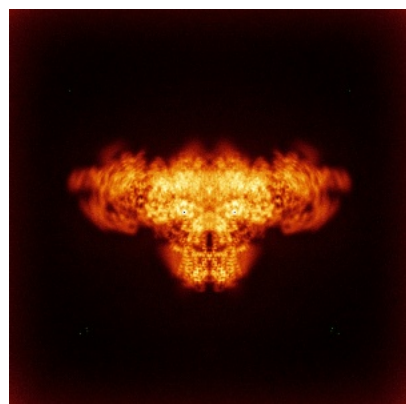


Y

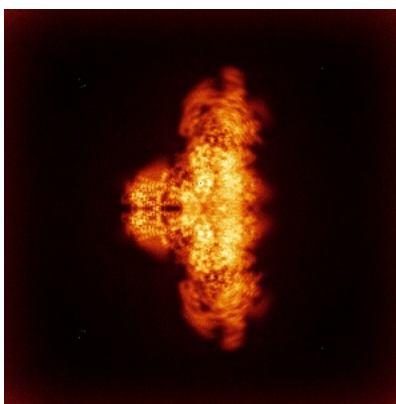


Z

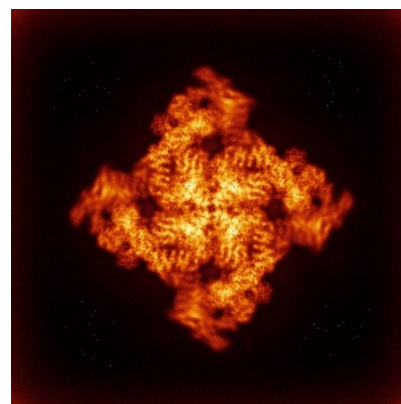
### 6.4.2 Raw map



X



Y

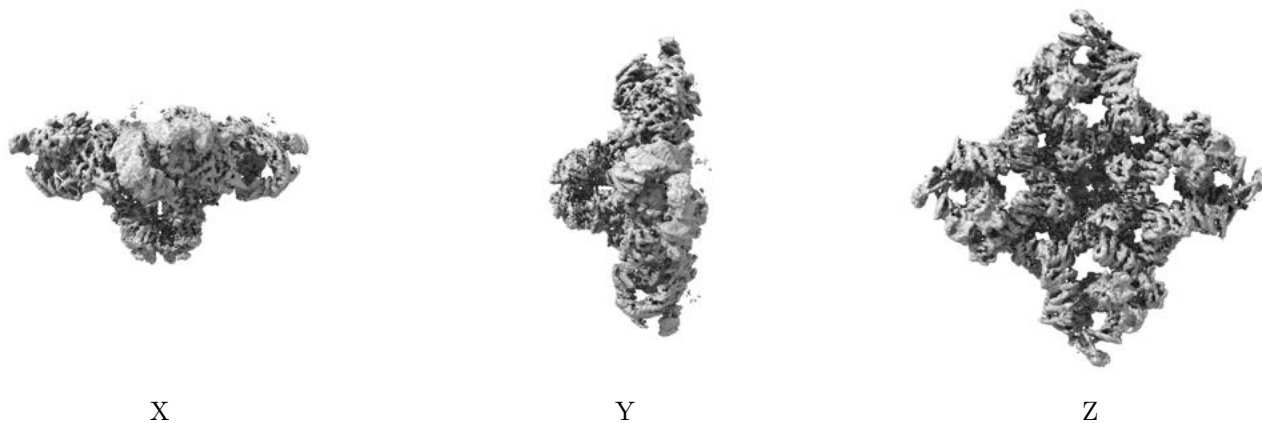


Z

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.

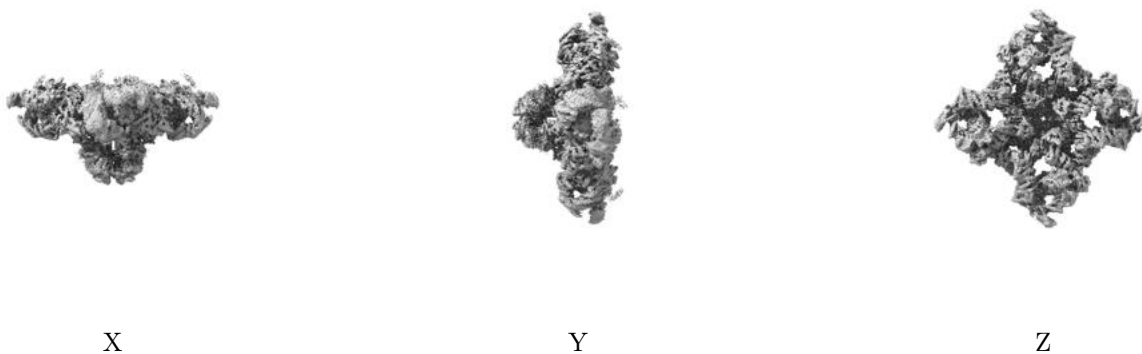
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.428. 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.

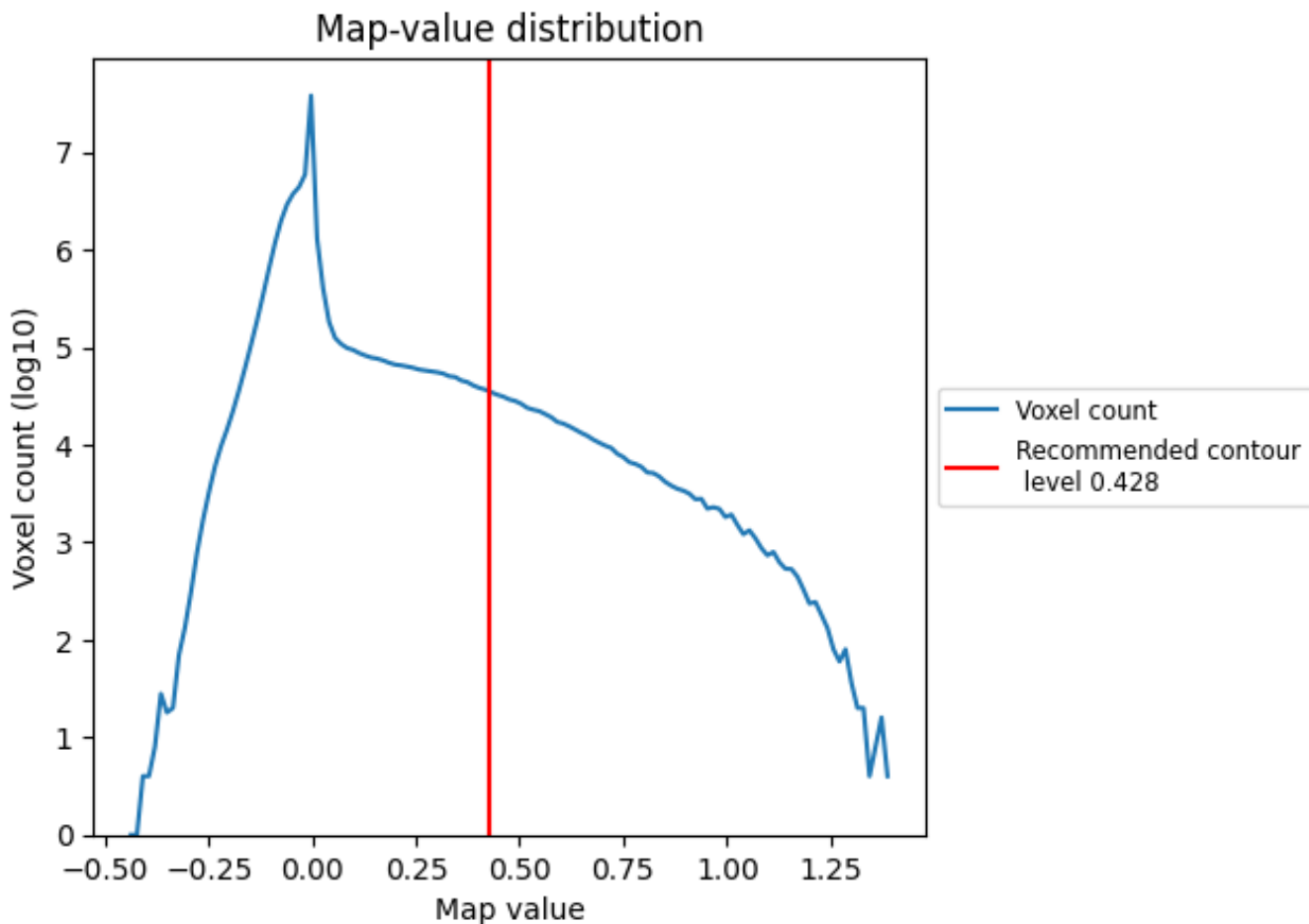
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

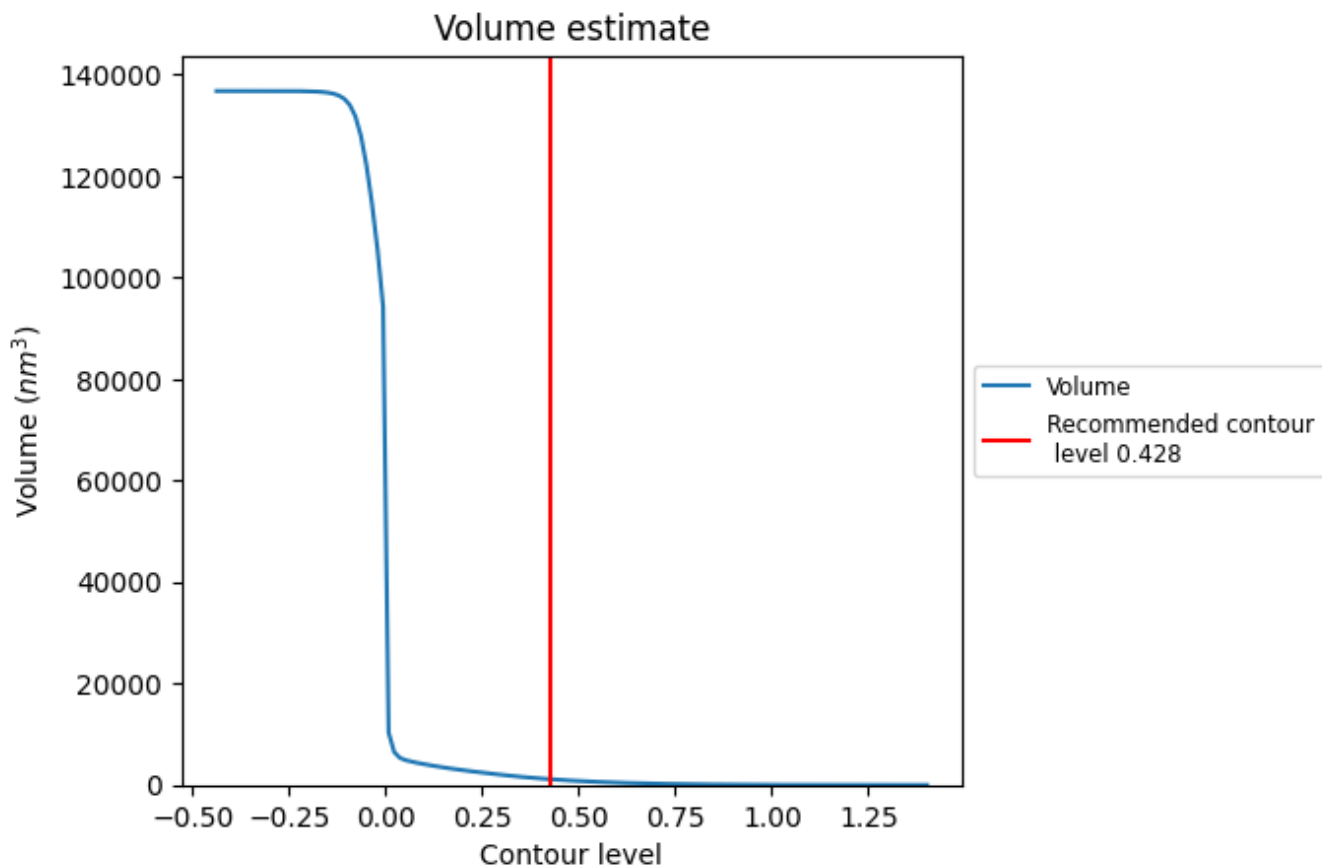
This section contains the results of statistical analysis of the map.

### 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.

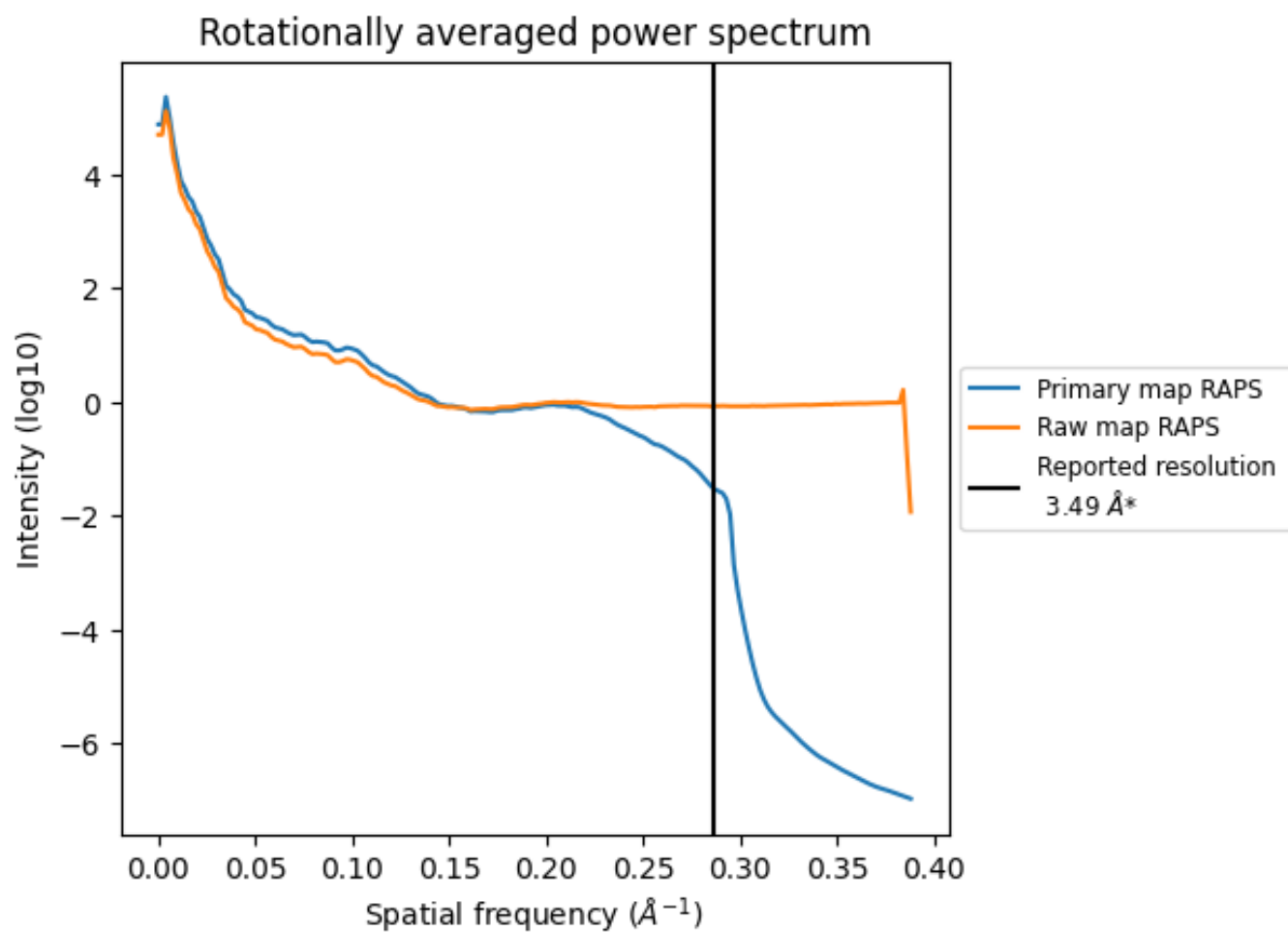
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1121 nm<sup>3</sup>; this corresponds to an approximate mass of 1013 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

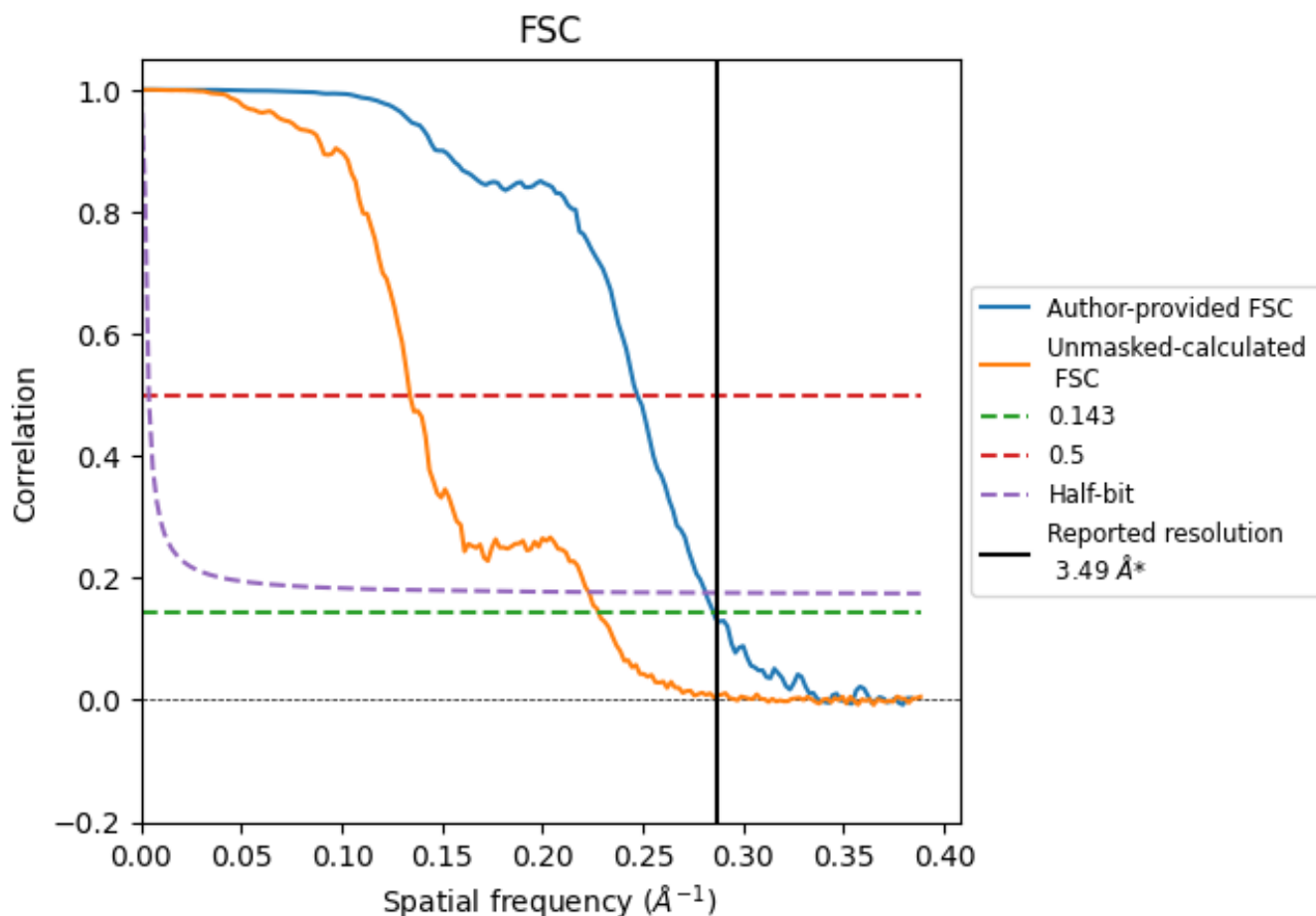


\*Reported resolution corresponds to spatial frequency of  $0.287 \text{ \AA}^{-1}$

## 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 0.287 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

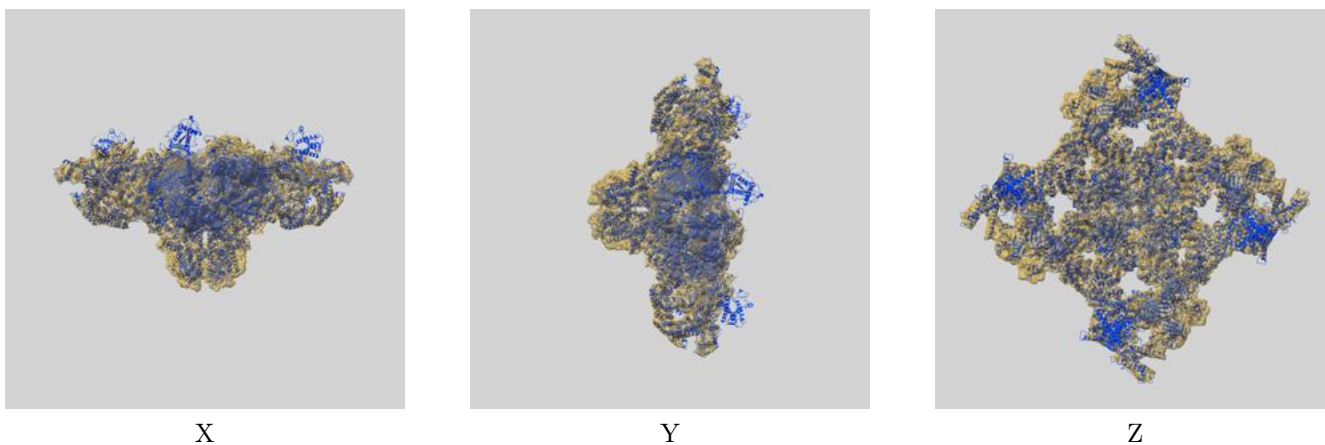
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.51	4.05	3.56
Unmasked-calculated*	4.39	7.47	4.48

\*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 4.39 differs from the reported value 3.49 by more than 10 %

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

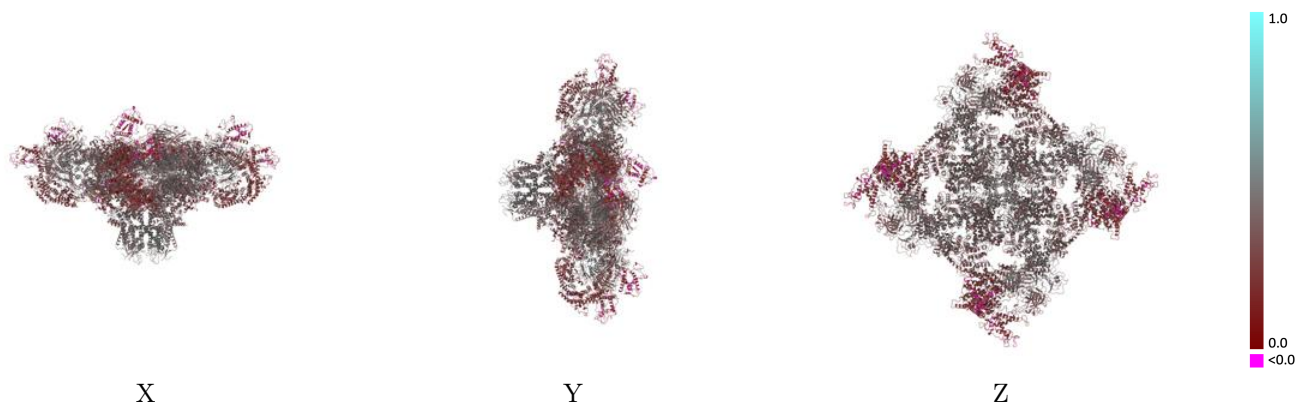
This section contains information regarding the fit between EMDB map EMD-40422 and PDB model 8SEN. Per-residue inclusion information can be found in section 3 on page 8.

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



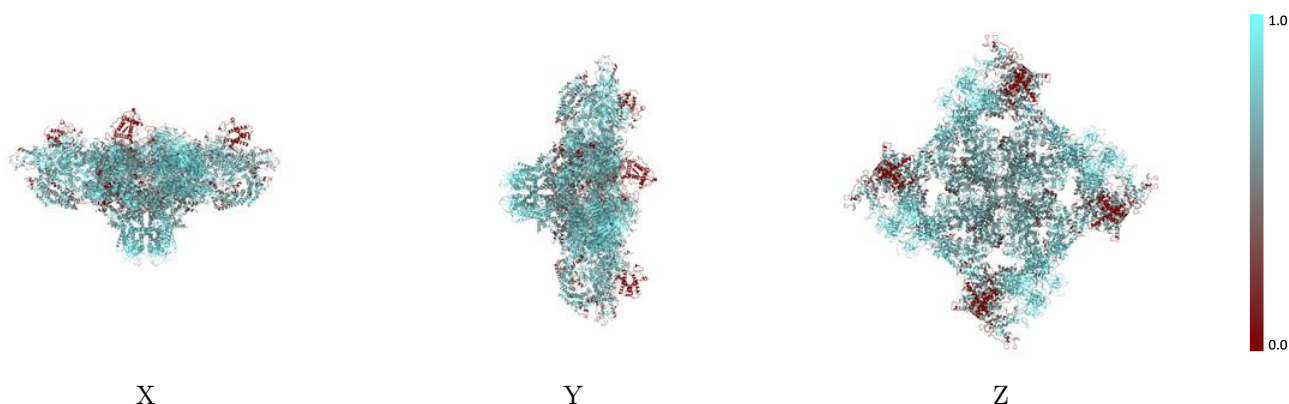
The images above show the 3D surface view of the map at the recommended contour level 0.428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



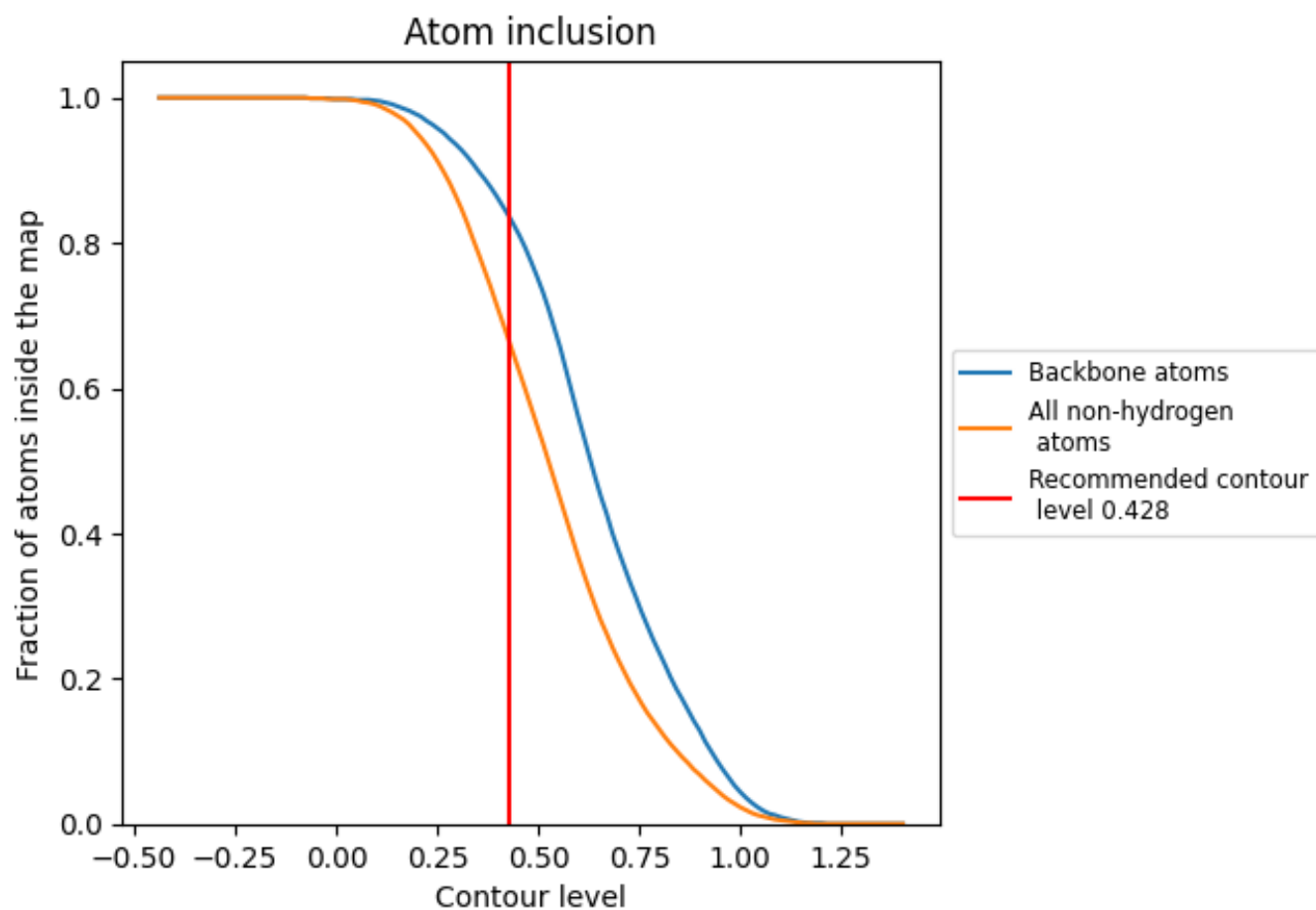
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.428).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3380
A	 0.6600	 0.3370
B	 0.6600	 0.3360
C	 0.6600	 0.3360
D	 0.6600	 0.3370
E	 0.8210	 0.4140
F	 0.8210	 0.4130
G	 0.8210	 0.4130
H	 0.8210	 0.4160

