



## wwPDB EM Validation Summary Report ⓘ

Jul 10, 2023 – 12:36 PM EDT

PDB ID : 8SET  
EMDB ID : EMD-40428  
Title : Cryo-EM Structure of RyR1 + cAMP  
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 : 3.42 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.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

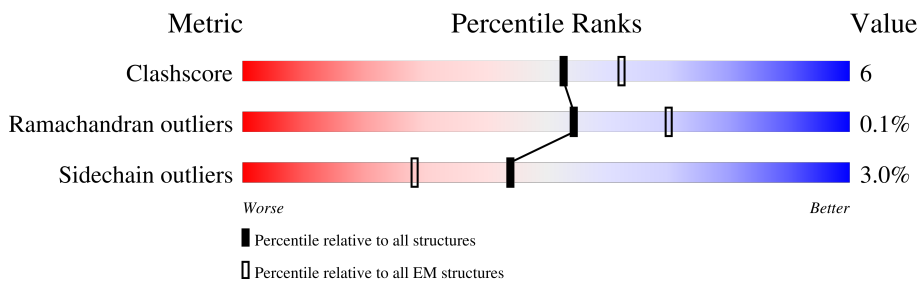
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	350	
2	F	350	
2	G	350	
2	H	350	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 143048 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	34921	22219	6024	6442	236	9	0
1	B	4378	34921	22219	6024	6442	236	9	0
1	C	4378	34921	22219	6024	6442	236	9	0
1	D	4378	34921	22219	6024	6442	236	9	0

- 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	818	516	144	154	4	0	0
2	F	107	818	516	144	154	4	0	0
2	G	107	818	516	144	154	4	0	0
2	H	107	818	516	144	154	4	0	0

There are 100 discrepancies between the modelled and reference sequences:

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

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

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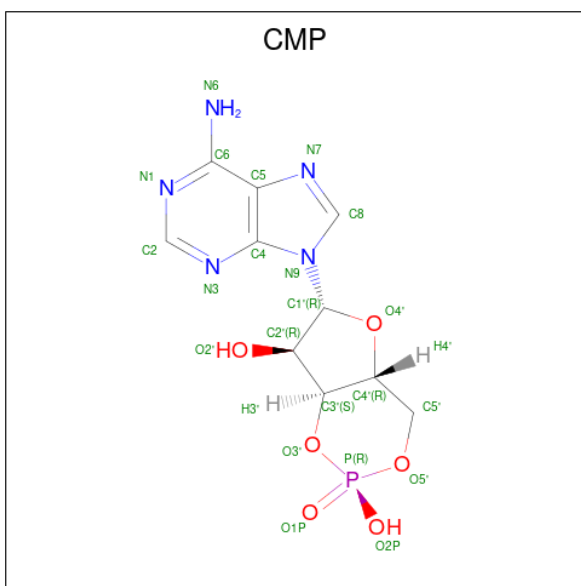
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression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

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

- Molecule 3 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	B	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	D	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

### 3 Residue-property plots

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

#### • Molecule 1: Ryanodine receptor 1

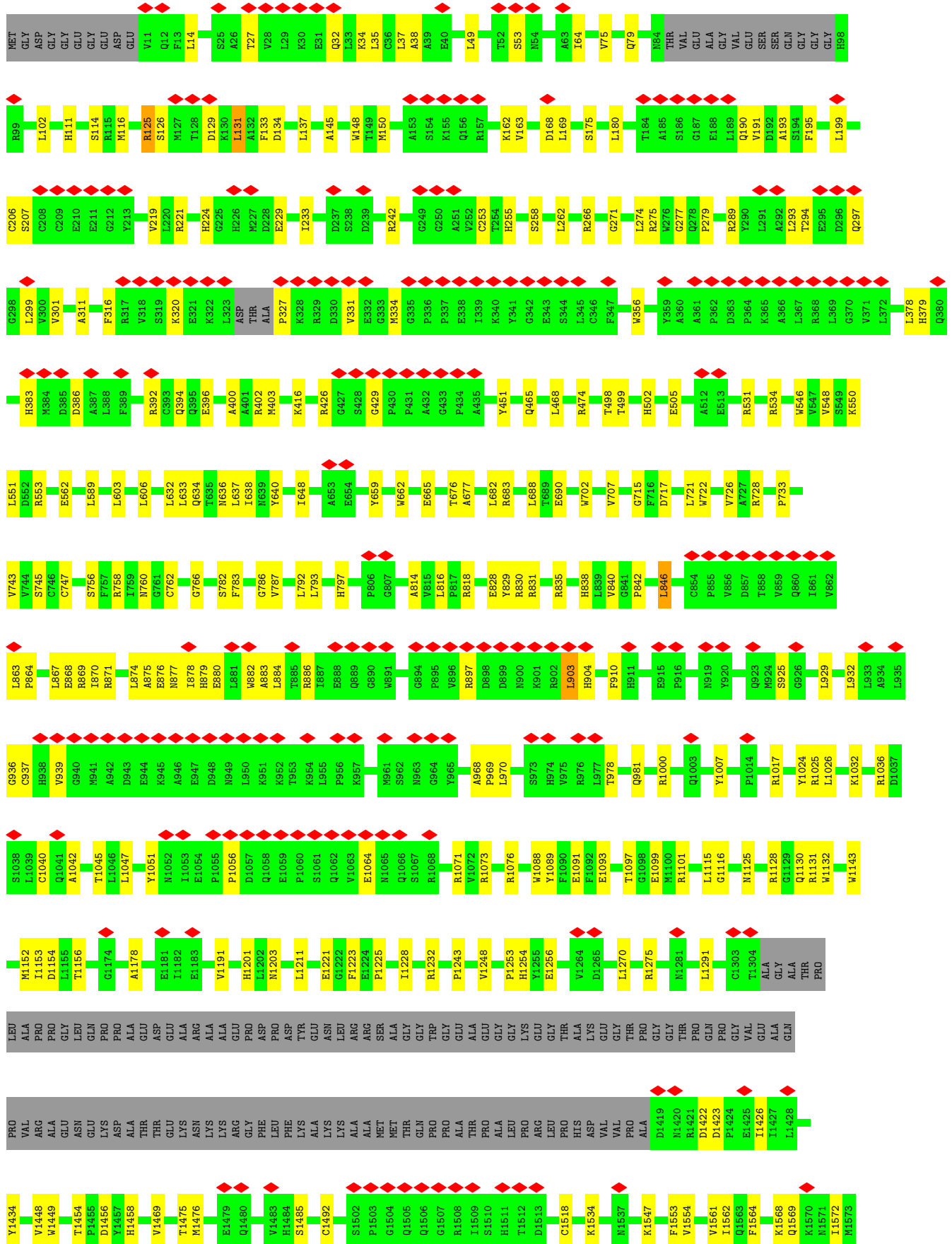


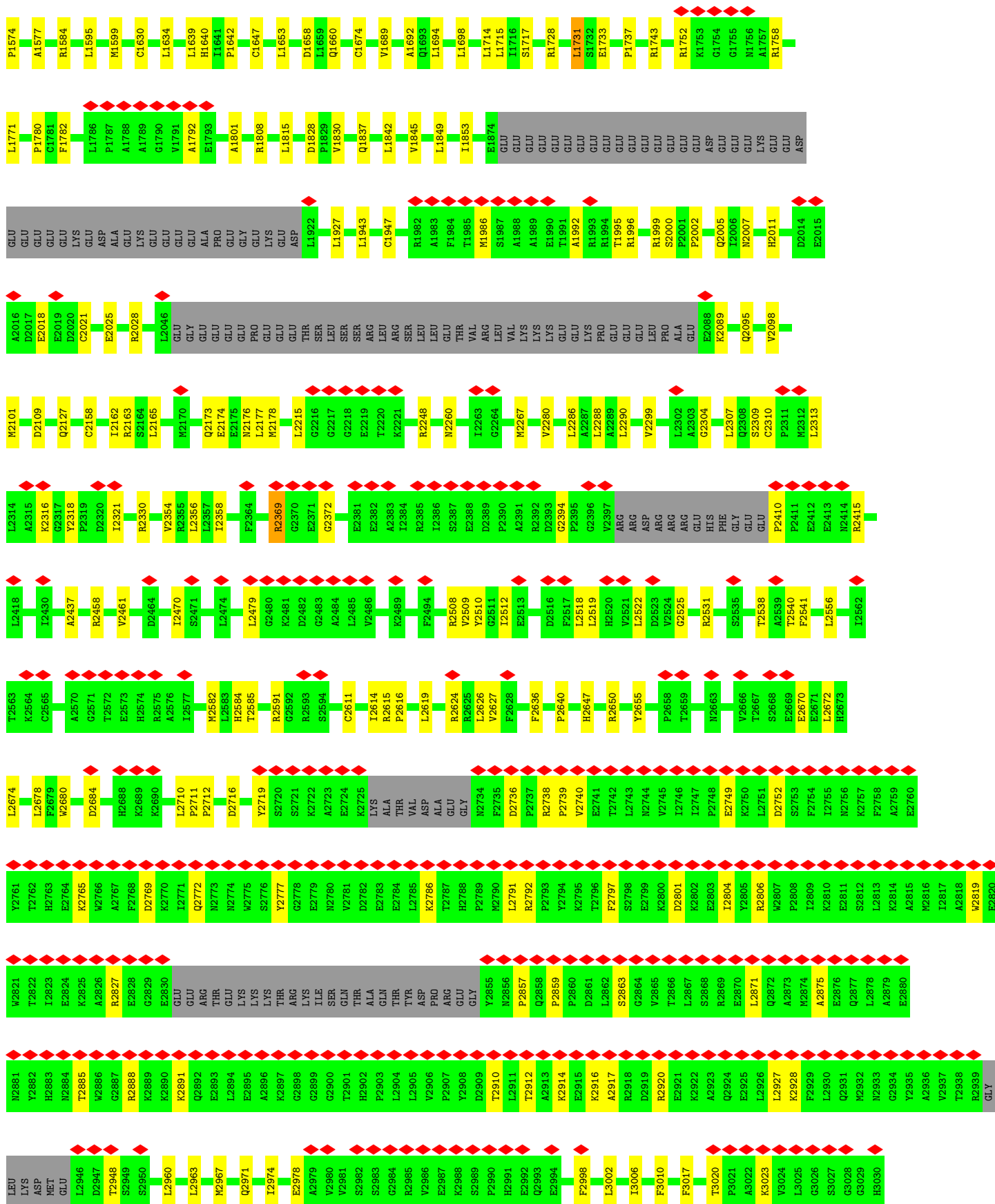




Q3683	Q3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3690	K3691	K3692	K3693	D3719	Y3722	E3736	GLU	GLY	GLY	E3610	H3611	P3612	Y3613	Y3614	K3614	S3615	K3616	K3617	A3618	V3619	V3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	K3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	L3641	L3644	E3655	K3658	A3680									
L3322	N3326	L3327	G3328	L3329	A3332	K3335	K3336	R3337	V3340	L3345	V3346	S3347	R3348	E3352	L3353	L3354	H3355	S3356	H3357	F3358	L3359	L3362	R3366	K3371	E3377	Q3378	L3379	R3380	L3381	A3382	A3383	A3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	N3392	P3393	P3394	A3395	L3396	N3211	E3212	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	S3309	D3310	L3315	L3316			
F3144	Q3146	V3065	I3147	A2979	V2980	V2981	S2982	G3153	A2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	F2998	L3002	I3006	F3010	F3017	T3020	P3021	A3022	K3023	V3024	L3025	M2932	M2933	G2934	Y2935	A2936	V2937	T2938	E2939	GLY	LEU	LYS	ASP	MET	L2946	R2947	K2989	T2948	A2926	R2827	E2828	Q2892	E2893	L2894	E2895	A2896	K2897	G2898					
P3224	R3225	E3226	R3227	A3228	L3229	L3230	G3231	L3232	K3335	K3336	R3337	V3340	L3345	V3346	S3347	R3348	E3352	L3353	L3354	H3355	S3356	H3357	F3358	L3359	L3362	R3366	K3371	E3377	Q3378	L3379	R3380	L3381	A3382	A3383	A3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	N3392	P3393	P3394	A3395	L3396	N3211	E3212	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	S3309	D3310	L3315	L3316
V3416	D3417	H3418	H3419	R3420	A3421	H3422	H3423	L3424	T3425	F3435	F3436	K3437	V3438	G3439	E3440	I3441	F3442	I3443	Y3444	M3445	S3446	K3447	S3448	M3457	Q3461	M3465	M3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	K3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR							
LYS	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	Q3506	V3511	K3515	K3516	M3517	L3520	N3523	M3524	D3531	M3534	L3535	A3536	K3537	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	T3545	D3546	E3547	E3548	E3551	F3552	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	Y3576	L3579													
P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	R3588	P3589	E3590	K3591	L3592	V3593	R3594	H3605	L3606	E3607	E3610	H3611	P3612	Y3613	Y3614	K3614	S3615	K3616	K3617	A3618	V3619	V3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	K3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	L3641	L3644	E3655	K3658	A3680										
Q2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	P2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	T2821	H2822	E2823	L2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	LYS	LYS	Q2778				
THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ALA	THR	ASP	PRO	R2985	ARG	GLU	GLY	Y2855	M2856	P2857	Q2858	P2859	D2860	I2862	S2863	V2865	G2864	T2866	L2867	R2868	S2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	M2884	T2885	W2886	G2887	R2888	K2889	A2890	K2891	Q2892	E2893	E2894	L2894	E2895	A2896	K2897	G2898
G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	R2985	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	A3022	K3023	V3024	L3025	M2932	M2933	G2934	Y2935	A2936	V2937	T2938	E2939	GLY	LEU	LYS	ASP	MET	L2946	R2947	K2989	T2948	A2926	R2827	E2828	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	
I2974	E2978	A2979	V2980	V2981	S2982	G3153	A2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	F2998	L3002	I3006	F3010	F3017	T3020	P3021	A3022	K3023	V3024	L3025	M2932	M2933	G2934	Y2935	A2936	V2937	T2938	E2939	GLY	LEU	LYS	ASP	MET	L2946	R2947	K2989	T2948	A2926	R2827	E2828	Q2892	E2893	L2894	E2895	A2896	K2897	G2898							
P3062	V3065	I3068	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	L3157	S3083	G3084	F3085	E3086	I3087	V3088	K3089	L3092	R3093	L3172	S3094	F3095	S3098	I3103	E3104	K3105	K3106	R3111	L3112	E3183	N3180	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	N3128	Y3131	T3132	T3133	U3134	A3135	L3136	V3139										

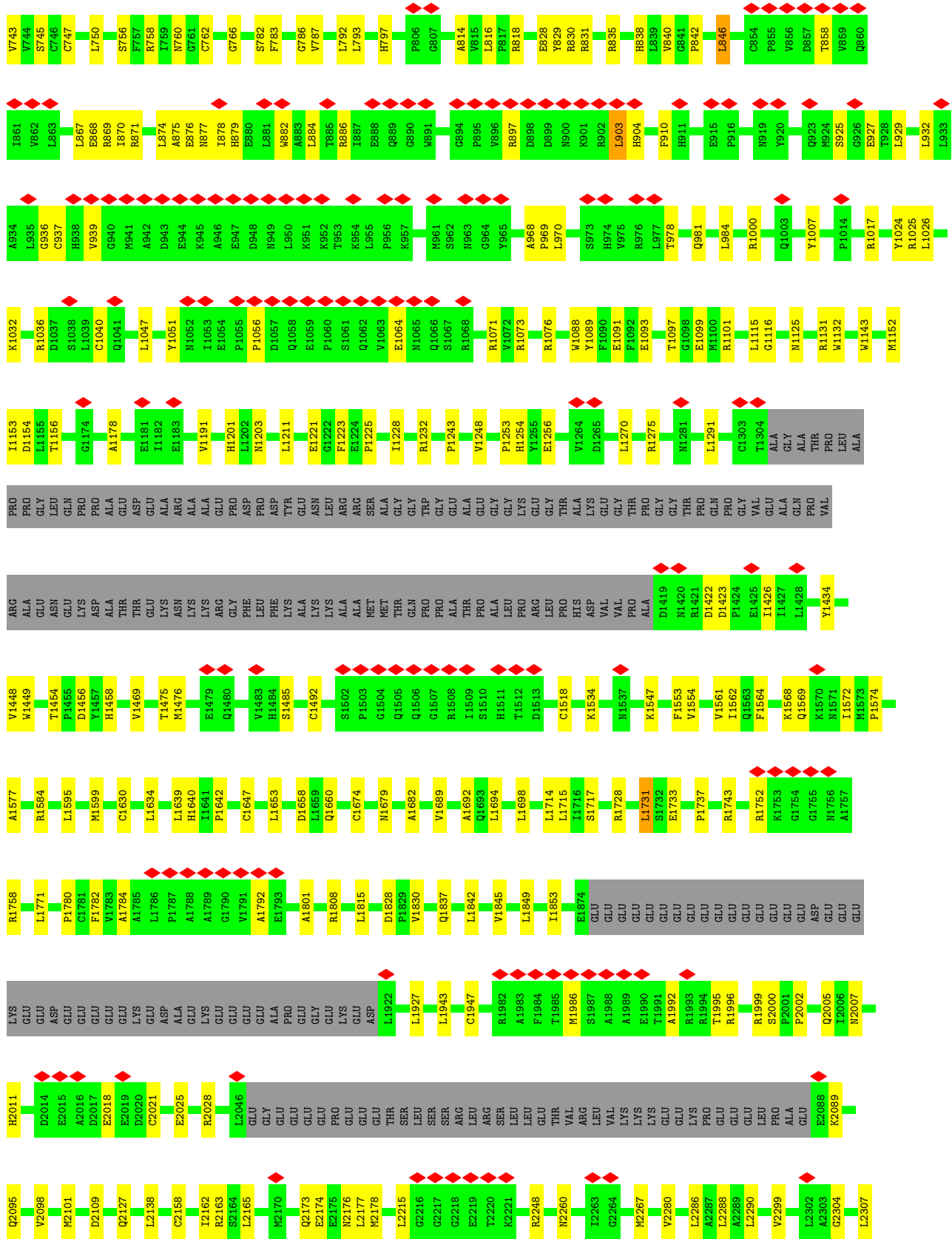




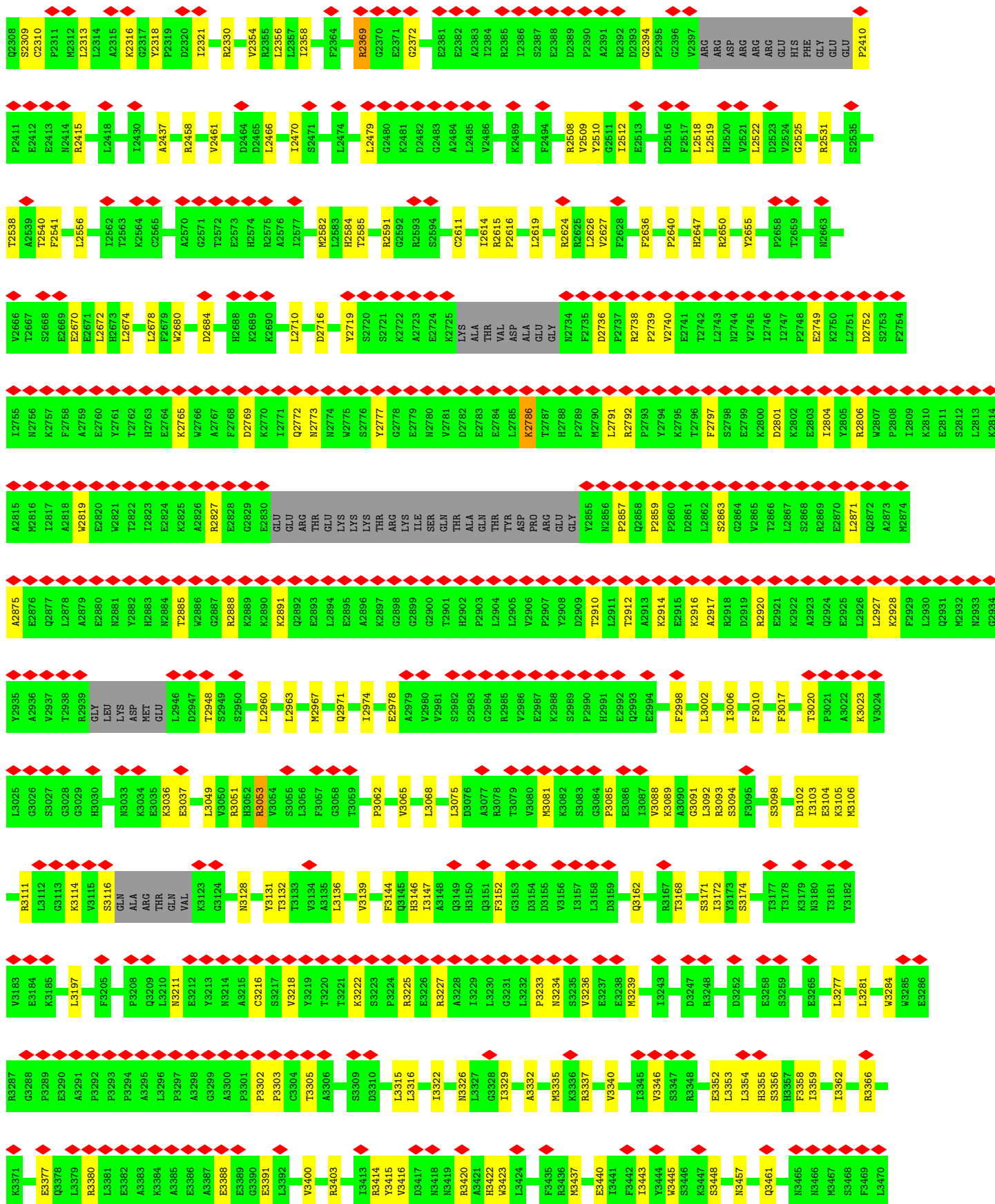




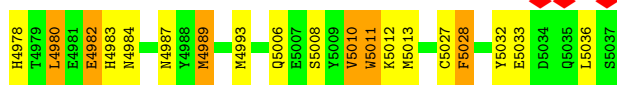




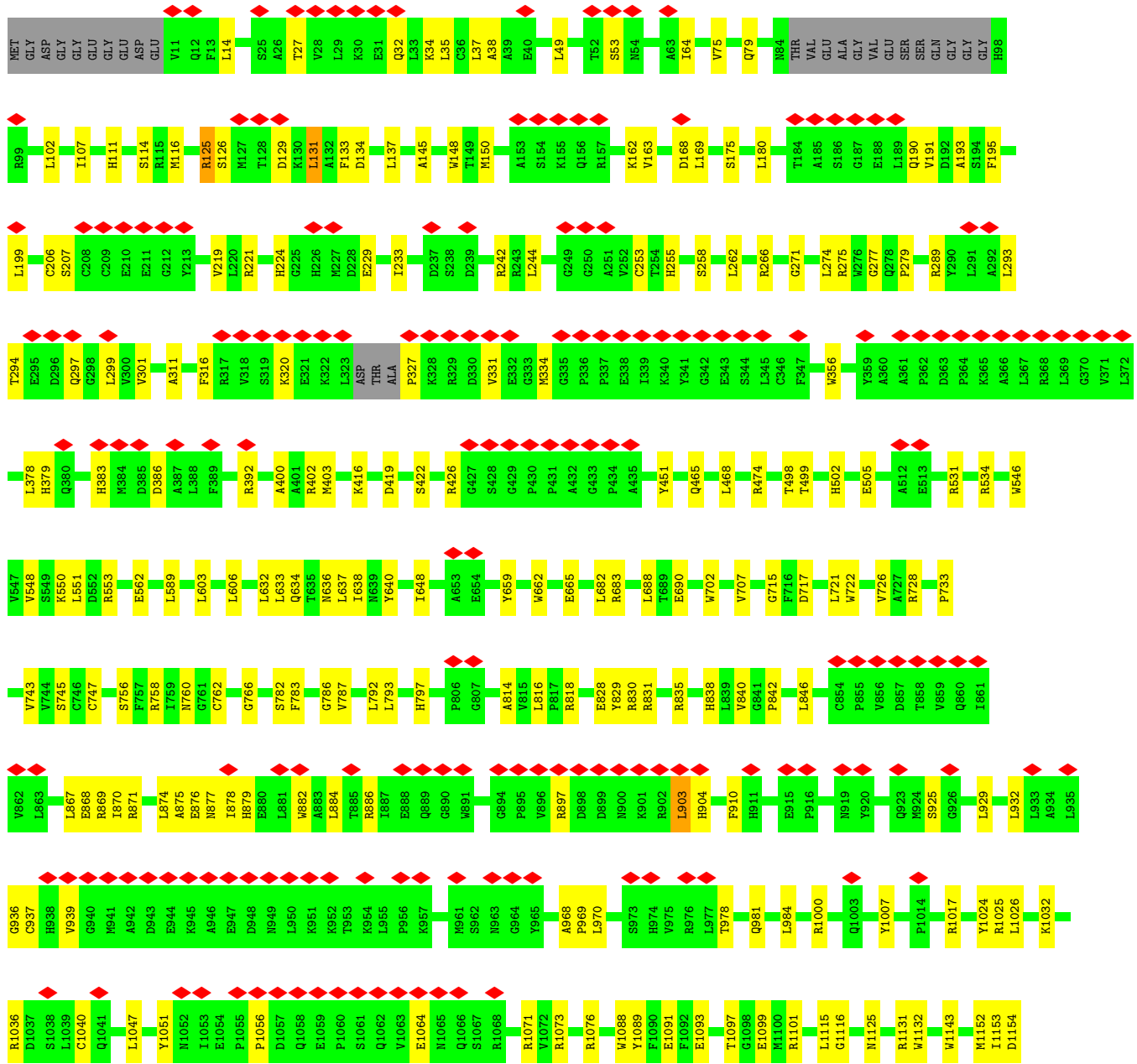








• Molecule 1: Ryanodine receptor 1





Y2771	Q2772	R2773	H2774	S2775	S2776	Y2777	G2778	E2779	H2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	F2789	H2790	L2791	R2792	F2793	Y2794	L2795	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	Q2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	H2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	K2825	A2826	R2827	E2828	G2829	E2830	
GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	E2877	Q2878	L2879	S2880	A2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	L2890
K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	L2931	Q2932	N2933	Q2934	A2935	Y2936	N2937	V2938	R2939	GLY	LEU	LYS	ASP	MET	L2946	D2947	T2948	S2949	S2950
L2960	L2963	H2967	Q2971	L2974	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	F2998	L3002	L3006	N3007	F3010	T3011	F3017	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	N3033	K3034	E3035	K3036	E3037	L3049													
V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	T3058	P3062	V3065	L3068	L3075	D3076	A3077	R3078	V3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	L3087	V3088	K3089	L3092	R3093	S3094	F3095	S3098	I3103	E3104	M3106	R3111	L3112	L3113	G3114	V3115	S3116	ALA	ARG	THR	GLN	VAL	K3123	G3124											
R3128	Y3131	V3134	Y3139	F3144	H3145	L3146	L3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	L3157	L3158	D3159	Q3162	R3167	T3168	S3171	L3172	V3173	S3174	T3177	T3178	K3179	N3180	T3181	V3182	V3183	E3184	K3185	L3194	L3197	F3205	P3208	Q3209	L3210	N3211	E3212	ASP	N3214	A3215	C3216											
S3217	V3218	Y3219	T3220	K3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3236	E3237	E3238	M3239	I3243	D3247	R3248	D3252	E3258	S3259	E3265	L3277	L3281	V3284	W3285	E3286	R3287	G3288	P3289	E3290	A3291	P3292	L3293	P3294	A3295	R3296	P3297	A3298	G3299	P3300	P3301	P3302	P3303								
G3304	T3305	A3306	S3309	D3310	L3315	L3316	I3322	N3326	L3327	G3328	I3329	I3329	A3332	M3335	K3336	R3337	V3340	I3345	V3346	S3347	R3348	E3352	L3353	L3354	H3355	S3356	R3357	F3358	I3359	I3362	R3366	K3371	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391											
L3392	V3400	R3403	I3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	A3421	H3422	W3423	L3424	F3435	R3436	M3437	E3440	I3441	F3442	I3443	Y3444	W3445	S3446	K3447	N3457	Q3461	N3465	N3466	H3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	A3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY								
GLY	SER	ASP	GLN	GLU	ARC	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Y3503	P3509	E3590	K3591	L3592	V3593	R3594	Y3604	H3605	L3606	E3607	Q3608	T3609	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	N3638	L3641	L3644	
L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	D3719	Y3722	E3736	GLU	GLY	GLU	ASN	GLY	GLU	ALA	V3874	N3875	L3876	D3877	D3878	Q3882	L3888	L3924	E3928	S3929	F3933	Y3936	E3944	E3945	Q3946	R3949	V3957	A3981	L3805	N3809															
Y3819	K3823	S3840	V3841	L3842	L3843	L3844	R3849	G3857	H3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	I3866	N3867	R3868	R3869	N3870	E3871	E3872	K3873	V3874	N3875	L3876	D3877	D3878	Q3882	L3888	L3924	E3928	S3929	F3933	Y3936	E3944	E3945	Q3946	R3949	V3957	A3981	L3805	N3809														





SER	ASN	ALA	G1	I4	I7	S8	P9	K18	G19	Q20	T21	G22	V23	V24	H25	Y26	T27	K35	R40	D41	R42	K47	F48	R49	E54	Q70	K73	L74	T77	F78	D79	V80	A81	Y82	L104	M105	L106	E107														
MET	LYS	SER	LEU	ALA	PHE	PRO	LYS	VAL	CYS	PHE	LYS	LYS	ARG	PHE	ILE	GLU	SER	LYS	ALA	ILE	GLN	GLU	TYR	MET	PHE	GLU	LYS	TRP	TRP	THR	LEU	GLN	ALA	PHE	GLY	GLY	ASP	GLY	ASP	HIS	PRO	PRO	LYS	GLY	ILE	GLU	GLU	ASN	LEU	TYR	PHE	GLN
ARG	ILE	ALA	TYR	SER	LYS	ASP	PHE	THR	THR	CYS	LEU	VAL	ASP	PHE	ILE	LEU	PRO	LEU	ALA	ILE	GLN	GLU	TYR	MET	PHE	GLU	LYS	TRP	TRP	THR	LEU	GLN	ALA	PHE	GLY	GLY	ASP	HIS	PRO	PRO	LYS	GLY	ILE	GLU	GLU	ASN	LEU	TYR	PHE	GLN		
LEU	GLY	LEU	GLU	PRO	PHE	ASN	LEU	PRO	TYR	TYR	ILE	ASP	GLY	ASP	ASP	VAL	PRO	LEU	ILE	LEU	VAL	THR	GLN	TYR	TRP	TRP	TRP	TRP	THR	LEU	LEU	LEU	GLY	CYS	PRO	GLU	LYS	GLU	ARG	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
MET	LYS	SER	LEU	ALA	PHE	PRO	LYS	VAL	CYS	PHE	LYS	LYS	ARG	PHE	ILE	GLU	SER	LYS	ALA	ILE	GLN	GLU	TYR	MET	PHE	GLU	LYS	TRP	TRP	THR	LEU	GLN	ALA	PHE	GLY	GLY	ASP	HIS	PRO	PRO	LYS	GLY	ILE	GLU	GLU	ASN	LEU	TYR	PHE	GLN		



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	206618	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	0.725	Depositor
Minimum map value	-0.299	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.126	Depositor
Map size ( $\text{\AA}$ )	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.288, 1.288, 1.288	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.33	0/35738	0.64	8/48398 (0.0%)
1	B	0.33	0/35738	0.64	8/48398 (0.0%)
1	C	0.33	0/35738	0.64	8/48398 (0.0%)
1	D	0.33	0/35738	0.64	8/48398 (0.0%)
2	E	0.33	0/834	0.65	0/1123
2	F	0.33	0/834	0.65	0/1123
2	G	0.33	0/834	0.65	0/1123
2	H	0.33	0/834	0.64	0/1123
All	All	0.33	0/146288	0.64	32/198084 (0.0%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5028	PHE	CB-CG-CD1	7.53	126.07	120.80
1	C	5028	PHE	CB-CG-CD1	7.43	126.00	120.80
1	B	5028	PHE	CB-CG-CD1	7.42	126.00	120.80
1	D	5028	PHE	CB-CG-CD1	7.42	126.00	120.80
1	A	903	LEU	CA-CB-CG	6.29	129.76	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34921	0	34546	387	0
1	B	34921	0	34546	399	0
1	C	34921	0	34546	392	0
1	D	34921	0	34546	391	0
2	E	818	0	824	12	0
2	F	818	0	824	12	0
2	G	818	0	824	13	0
2	H	818	0	824	13	0
3	A	22	0	11	2	0
3	B	22	0	11	2	0
3	C	22	0	11	2	0
3	D	22	0	11	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	143048	0	141524	1601	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 6.

The worst 5 of 1601 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)
3:B:5101:CMP:H2	3:B:5101:CMP:C2	0.97	1.49
3:A:5101:CMP:C2	3:A:5101:CMP:H2	0.97	1.49
3:C:5101:CMP:H2	3:C:5101:CMP:C2	0.97	1.48
3:D:5101:CMP:H2	3:D:5101:CMP:C2	0.97	1.47
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.61	0.74

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%)	4218 (97%)	133 (3%)	4 (0%)	51	83
1	B	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	51	83
1	C	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	51	83
1	D	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	51	83
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%)	17287 (97%)	537 (3%)	16 (0%)	54	83

5 of 16 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	4691	GLN

### 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%)	3687 (97%)	120 (3%)	39	69
1	B	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
1	C	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
1	D	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
2	E	88/304 (29%)	87 (99%)	1 (1%)	73	87
2	F	88/304 (29%)	87 (99%)	1 (1%)	73	87
2	G	88/304 (29%)	87 (99%)	1 (1%)	73	87
2	H	88/304 (29%)	87 (99%)	1 (1%)	73	87

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15580/18320 (85%)	15096 (97%)	484 (3%)	44 70

5 of 484 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5010	VAL
1	D	4821	LYS
1	C	4550	LYS
1	D	4750	ILE
1	D	5012	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4707	ASN
1	D	4984	ASN
2	H	87	HIS
1	B	4043	GLN
1	B	3605	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

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

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

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CMP	C	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)
3	CMP	D	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)
3	CMP	A	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)
3	CMP	B	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CMP	C	5101	-	-	0/0/31/31	0/4/4/4
3	CMP	D	5101	-	-	0/0/31/31	0/4/4/4
3	CMP	A	5101	-	-	0/0/31/31	0/4/4/4
3	CMP	B	5101	-	-	0/0/31/31	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	CMP	P-O3'	3.21	1.63	1.57
3	D	5101	CMP	P-O3'	3.21	1.63	1.57
3	C	5101	CMP	P-O3'	3.21	1.63	1.57
3	A	5101	CMP	P-O3'	3.21	1.63	1.57
3	D	5101	CMP	O5'-C5'	-2.57	1.42	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5101	CMP	N3-C2-N1	-3.35	123.44	128.68
3	A	5101	CMP	N3-C2-N1	-3.35	123.44	128.68
3	D	5101	CMP	N3-C2-N1	-3.35	123.44	128.68
3	B	5101	CMP	N3-C2-N1	-3.35	123.45	128.68
3	B	5101	CMP	O2P-P-O1P	3.23	118.86	108.73

There are no chirality outliers.

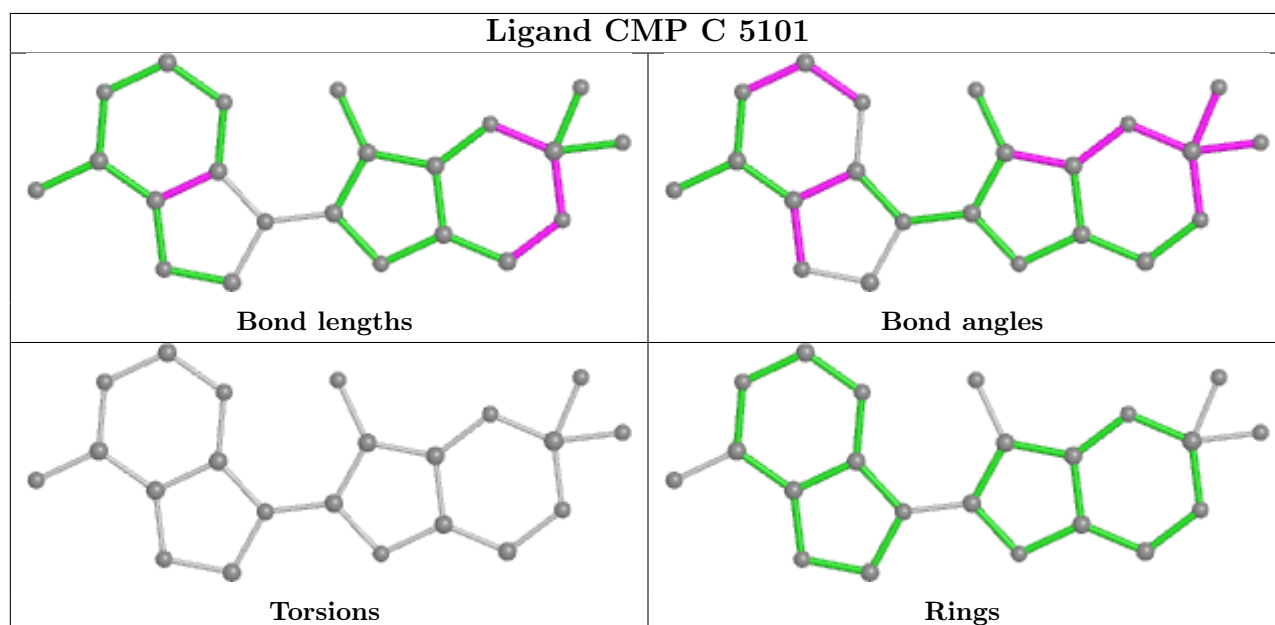
There are no torsion outliers.

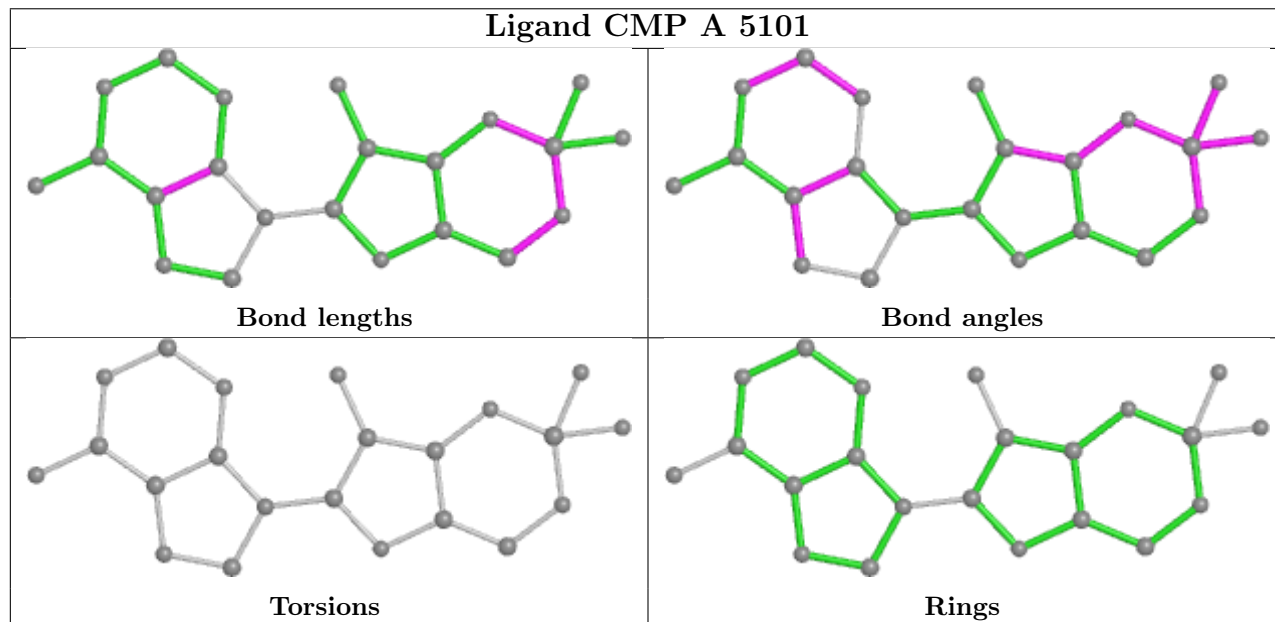
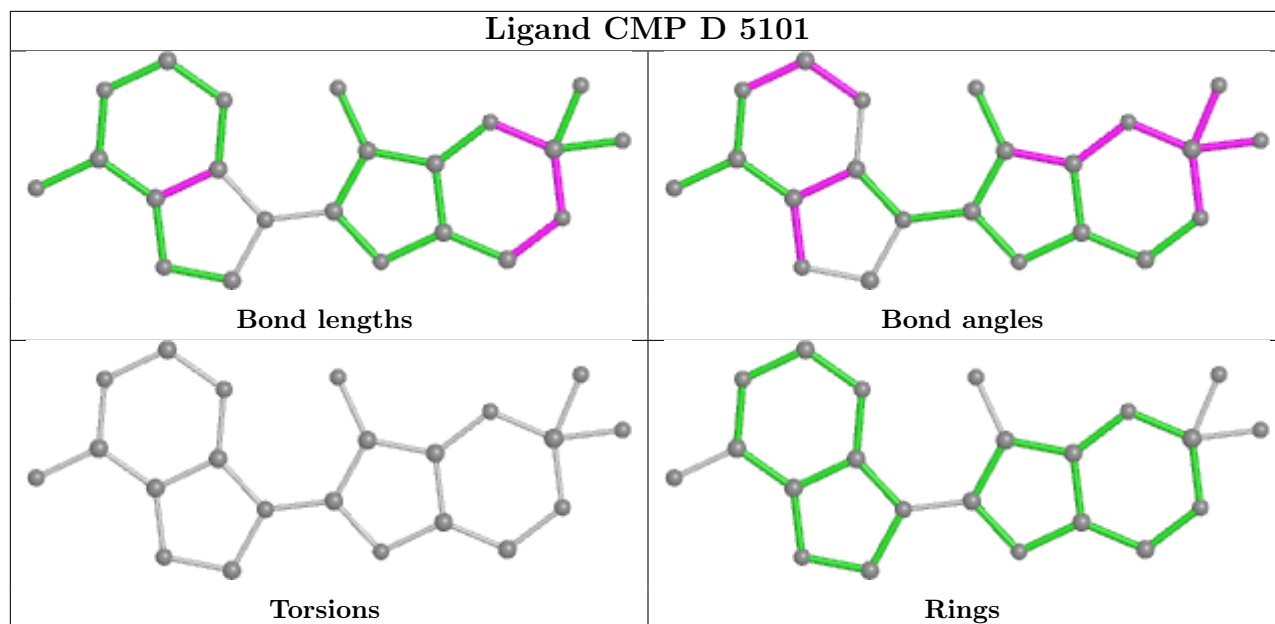
There are no ring outliers.

4 monomers are involved in 8 short contacts:

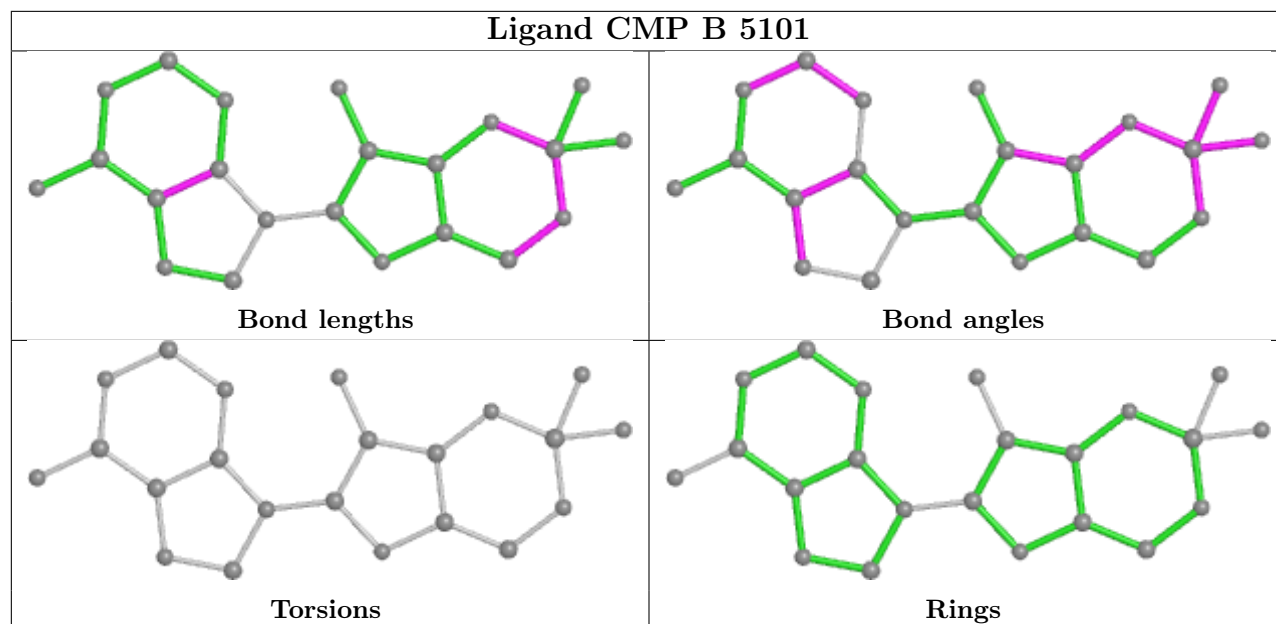
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5101	CMP	2	0
3	D	5101	CMP	2	0
3	A	5101	CMP	2	0
3	B	5101	CMP	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

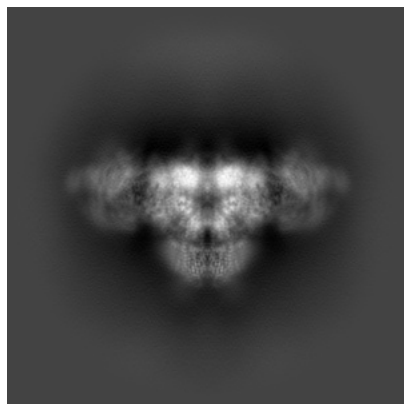
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40428. These allow visual inspection of the internal detail of the map and identification of artifacts.

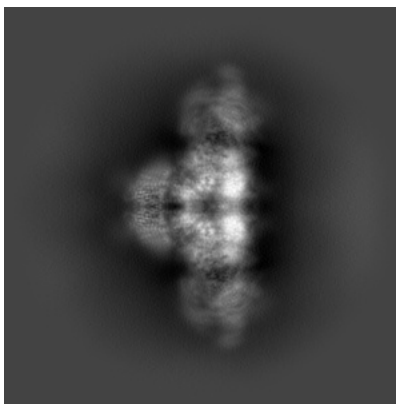
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

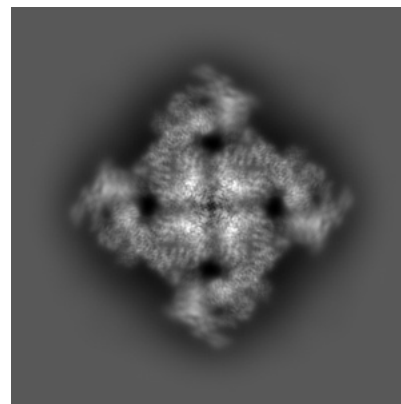
#### 6.1.1 Primary map



X

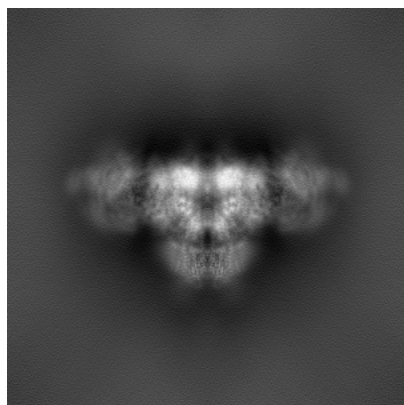


Y

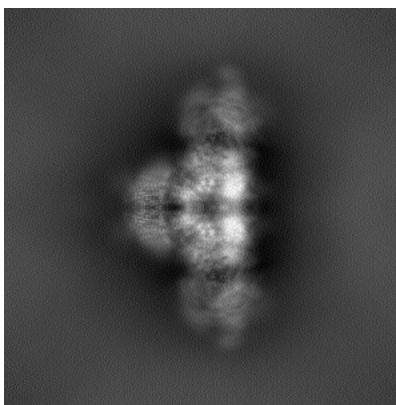


Z

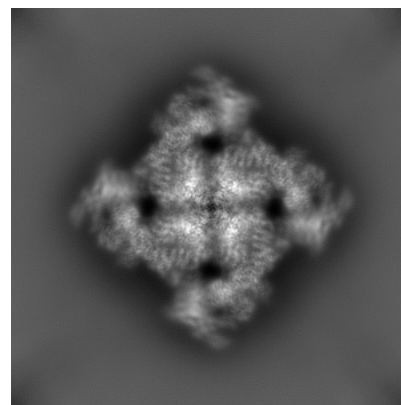
#### 6.1.2 Raw map



X



Y

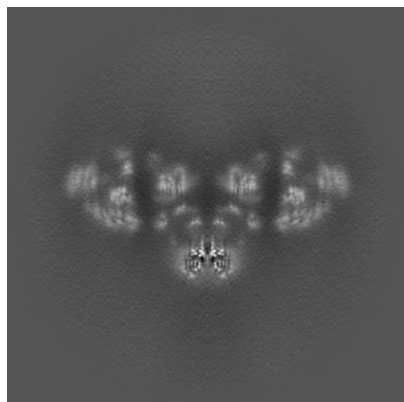


Z

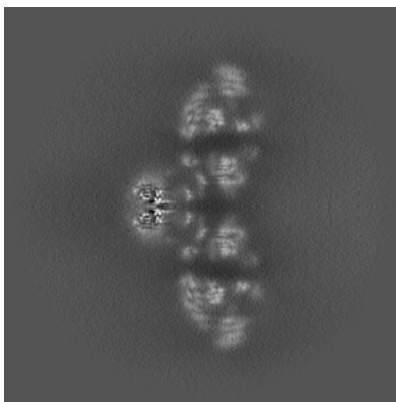
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

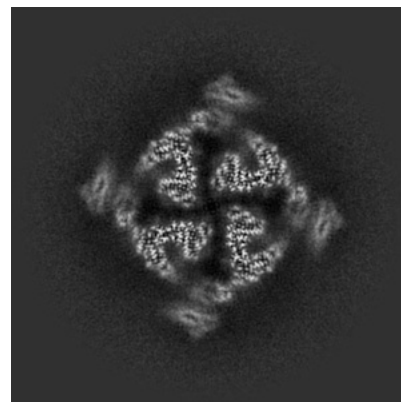
### 6.2.1 Primary map



X Index: 200

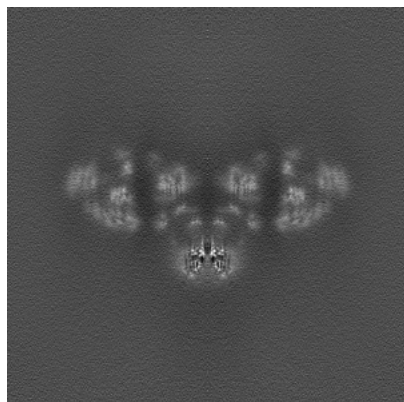


Y Index: 200

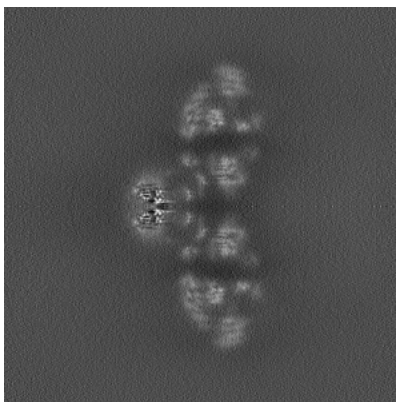


Z Index: 200

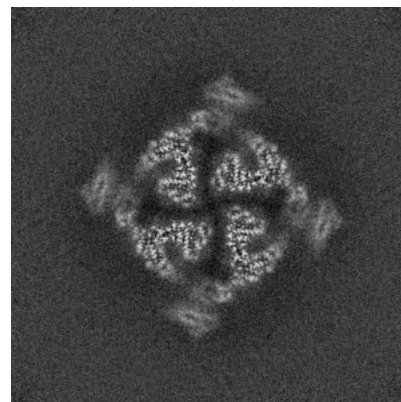
### 6.2.2 Raw map



X Index: 200



Y Index: 200

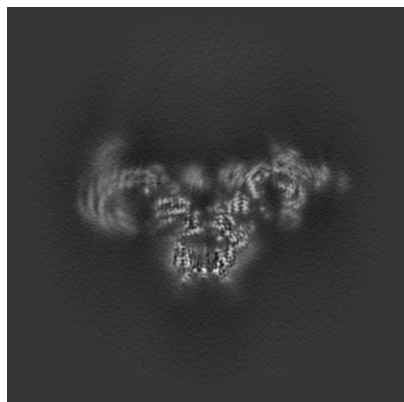


Z Index: 200

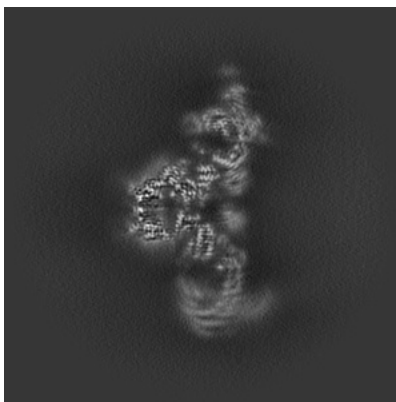
The images above show central slices of the map in three orthogonal directions.

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

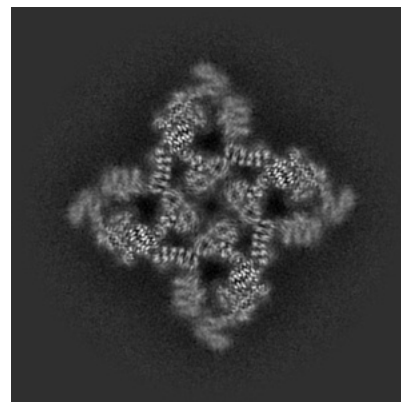
### 6.3.1 Primary map



X Index: 182

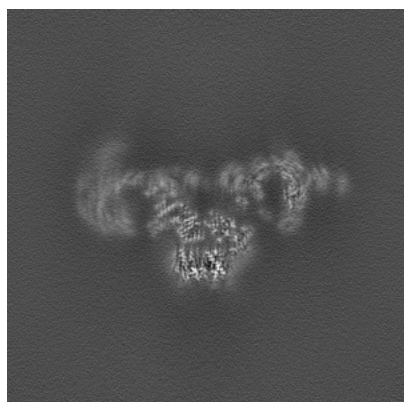


Y Index: 218

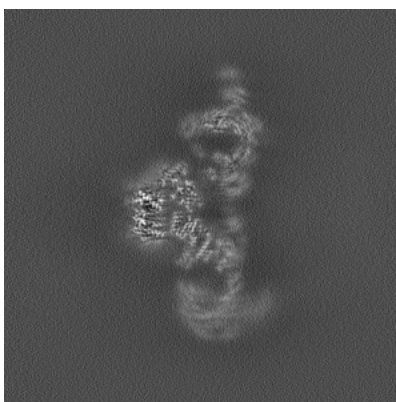


Z Index: 224

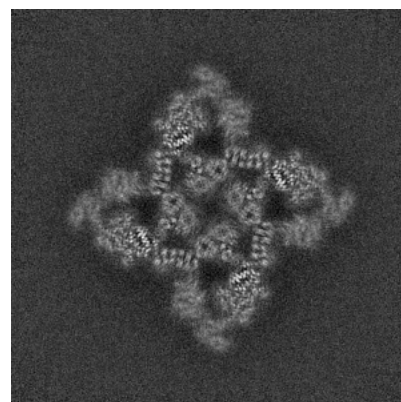
### 6.3.2 Raw map



X Index: 186



Y Index: 214

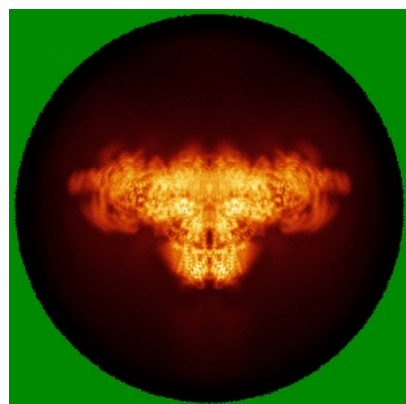


Z Index: 223

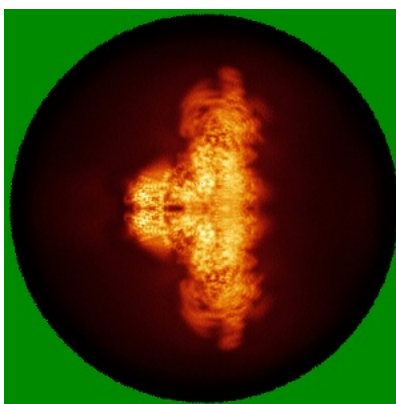
The images above show the largest variance slices of the map in three orthogonal directions.

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

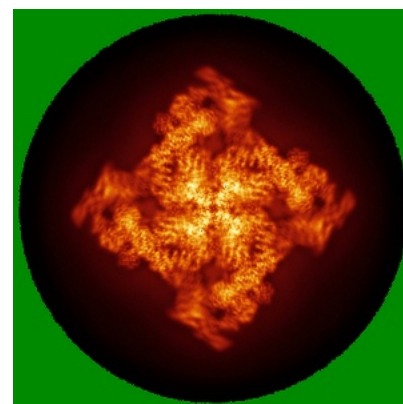
### 6.4.1 Primary map



X

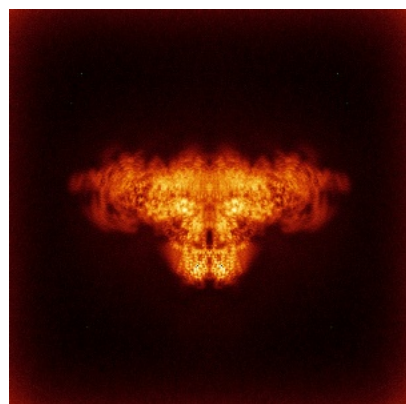


Y

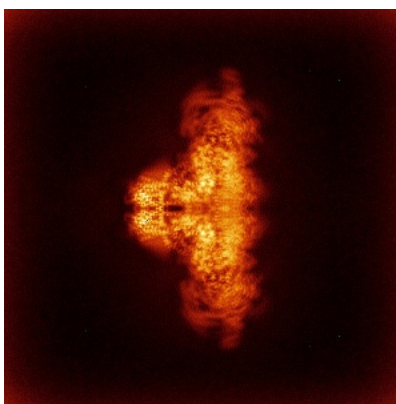


Z

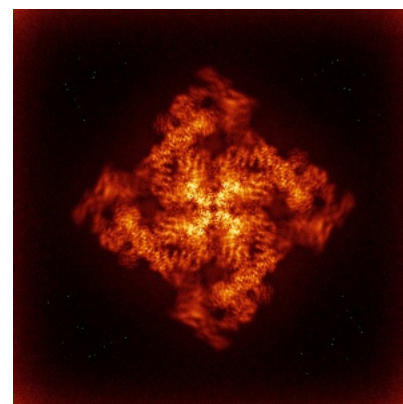
### 6.4.2 Raw map



X



Y



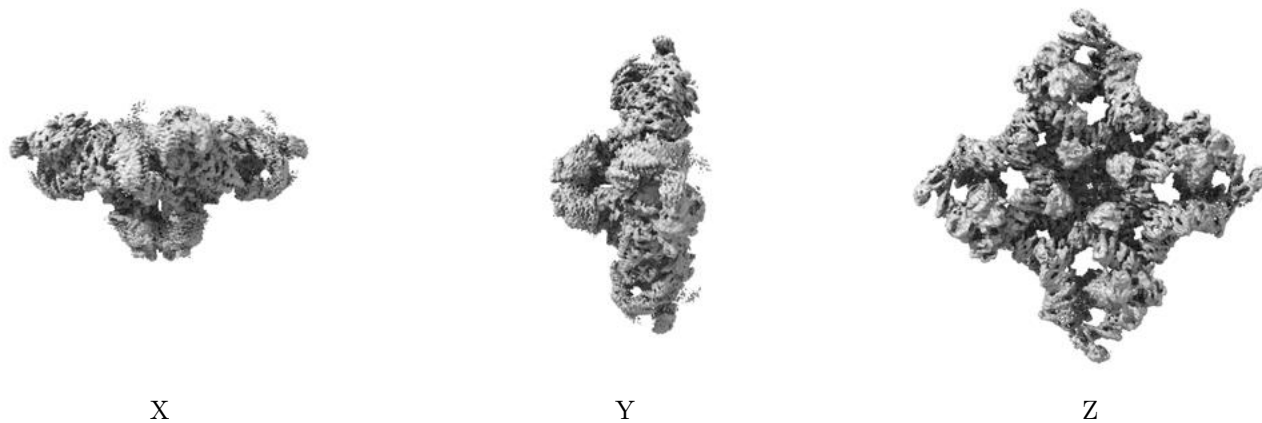
Z

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



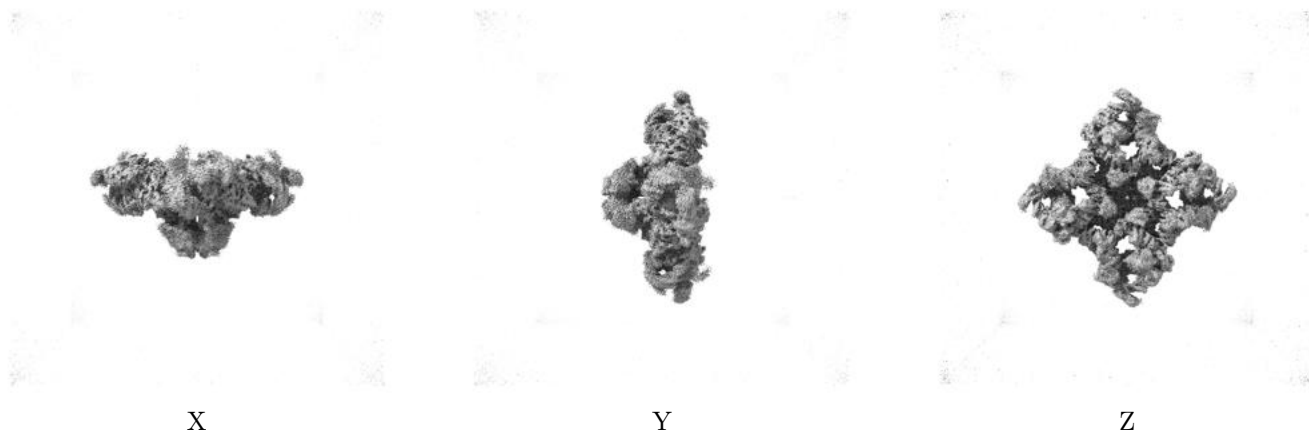
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.126. 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.

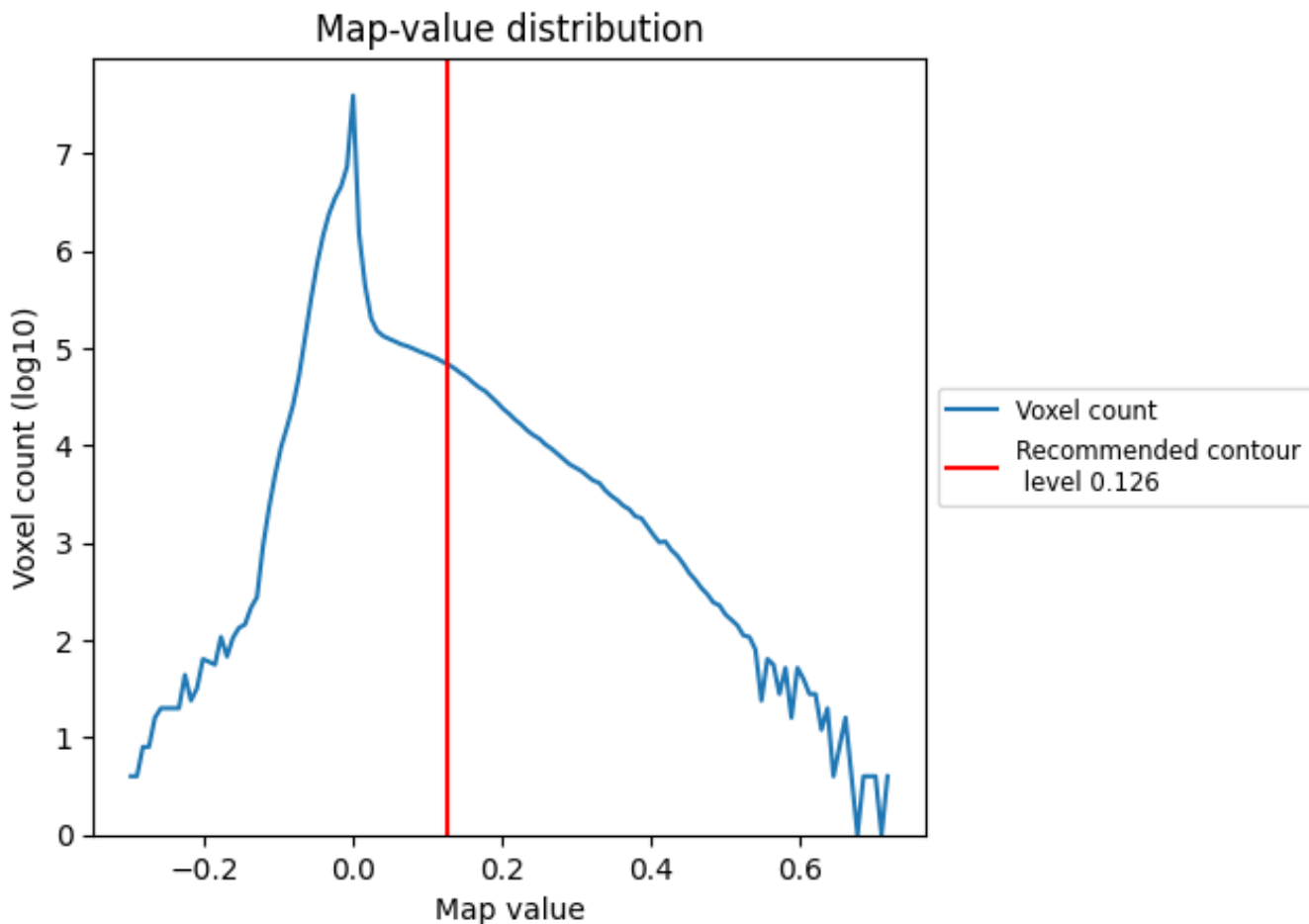
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

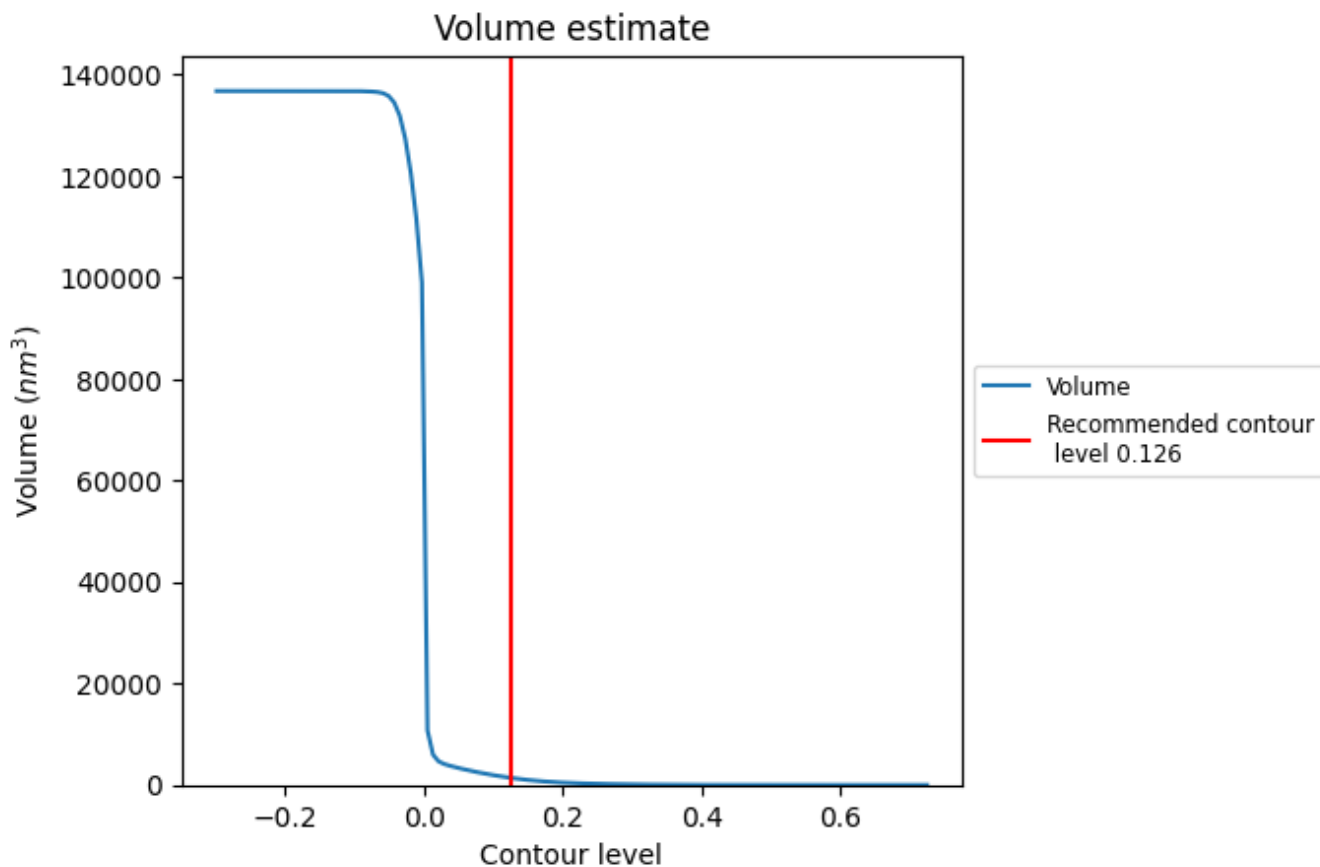
This section contains the results of statistical analysis of the map.

### 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](#)

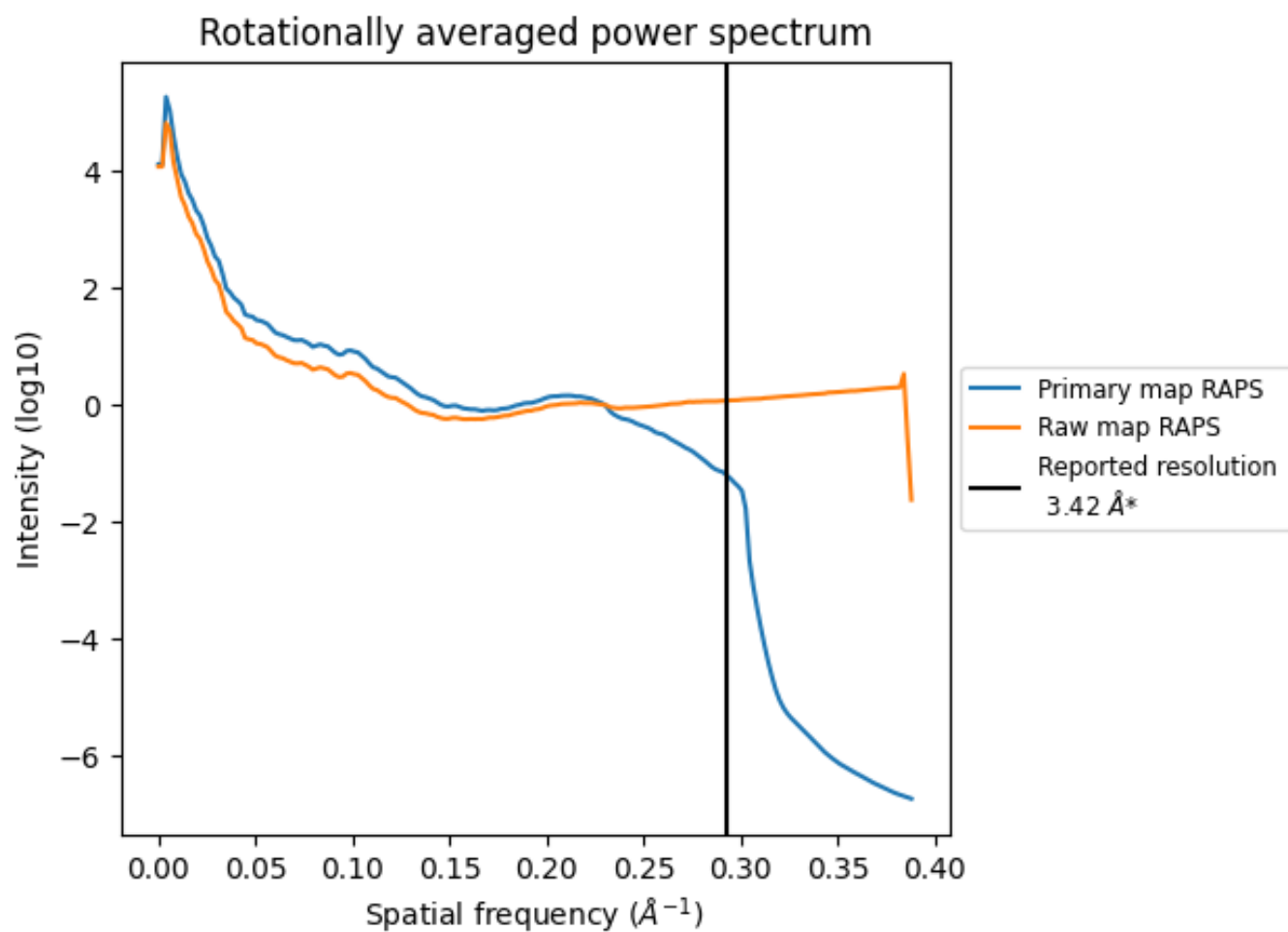


The volume at the recommended contour level is 1379  $\text{nm}^3$ ; this corresponds to an approximate mass of 1246 kDa.

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

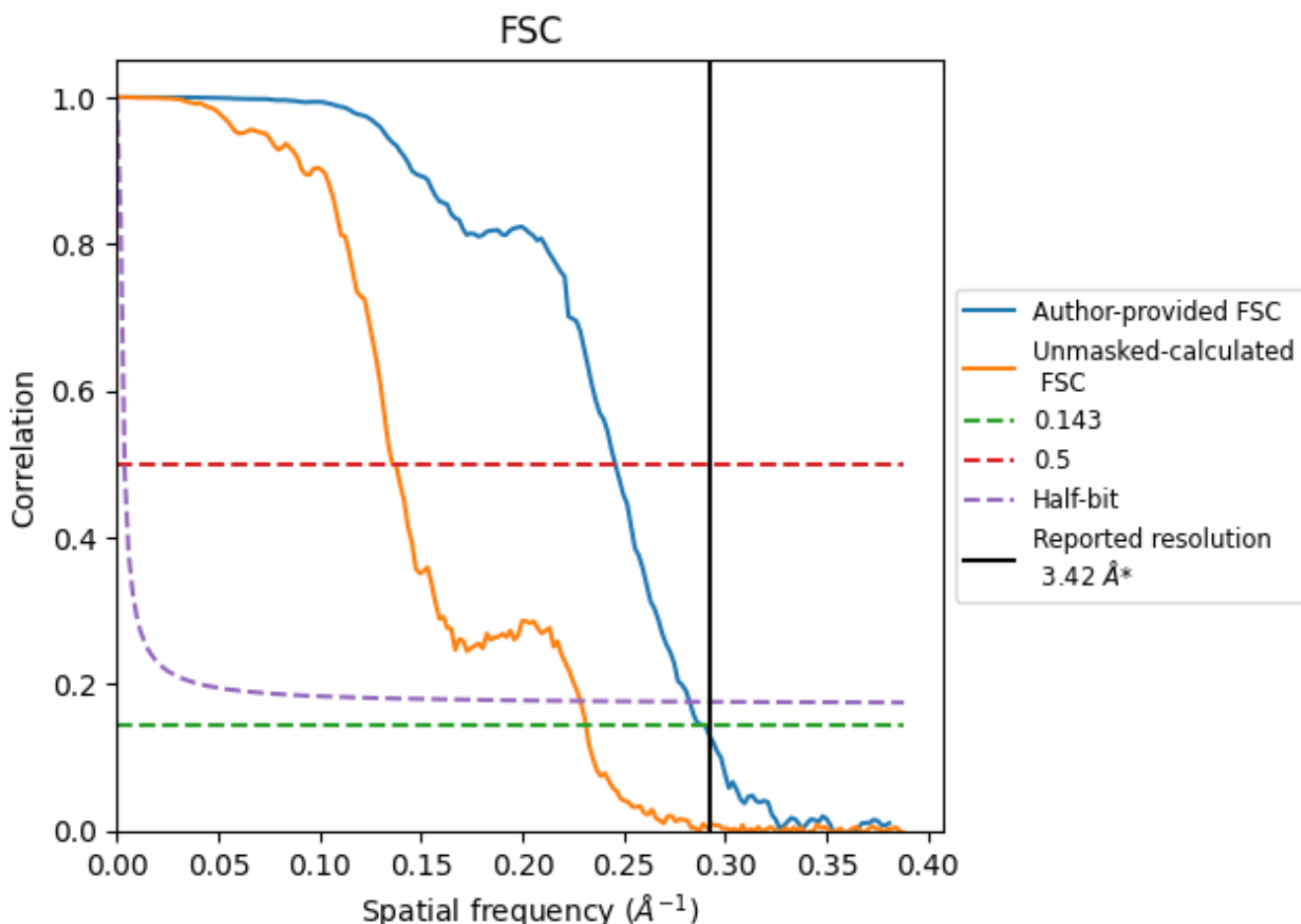


\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.292 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

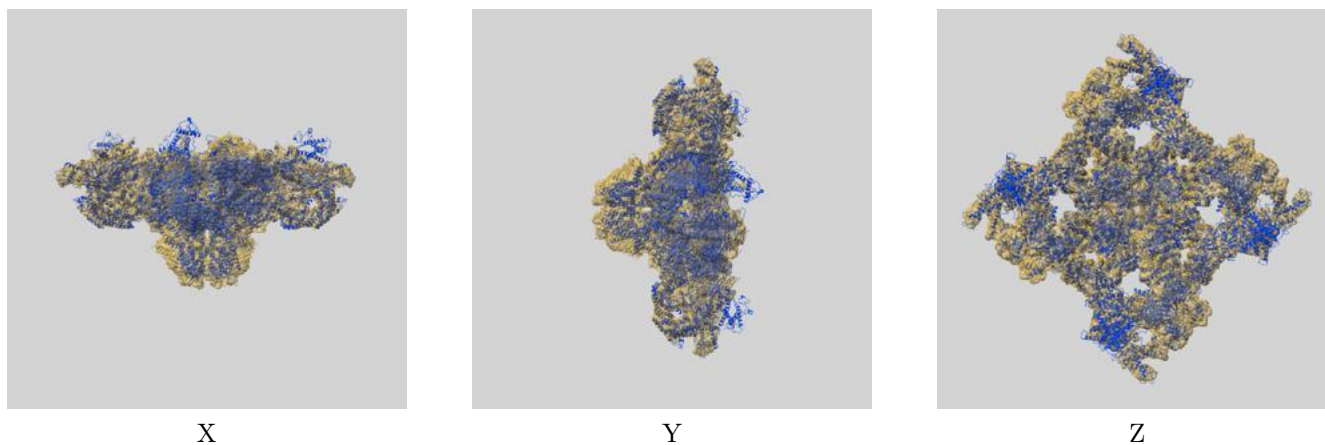
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.45	4.07	3.54
Unmasked-calculated*	4.32	7.36	4.37

\*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 4.32 differs from the reported value 3.42 by more than 10 %

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

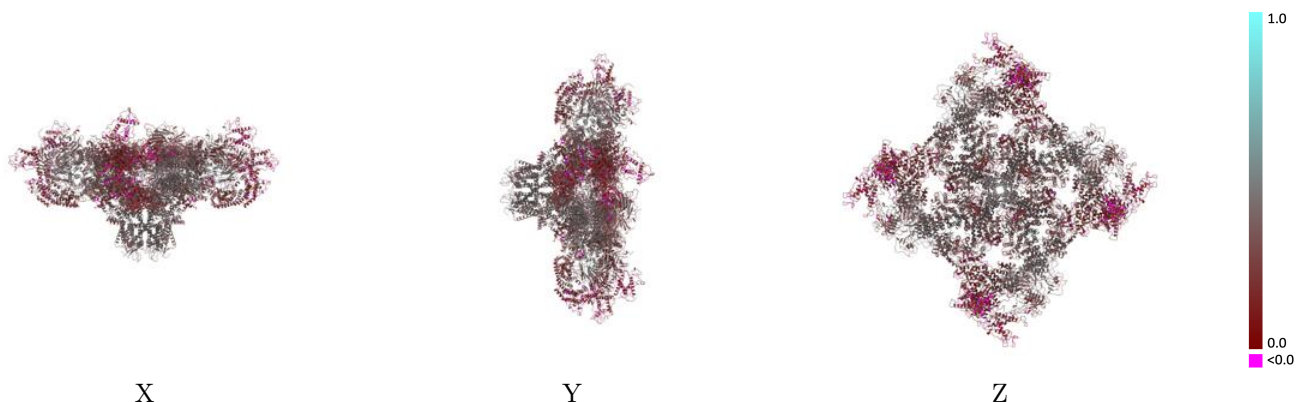
This section contains information regarding the fit between EMDB map EMD-40428 and PDB model 8SET. Per-residue inclusion information can be found in section 3 on page 8.

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



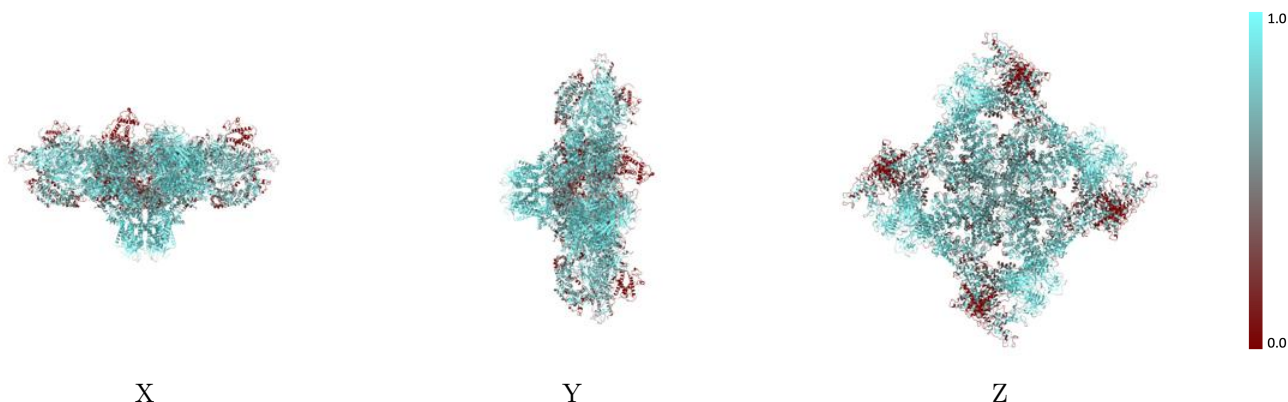
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



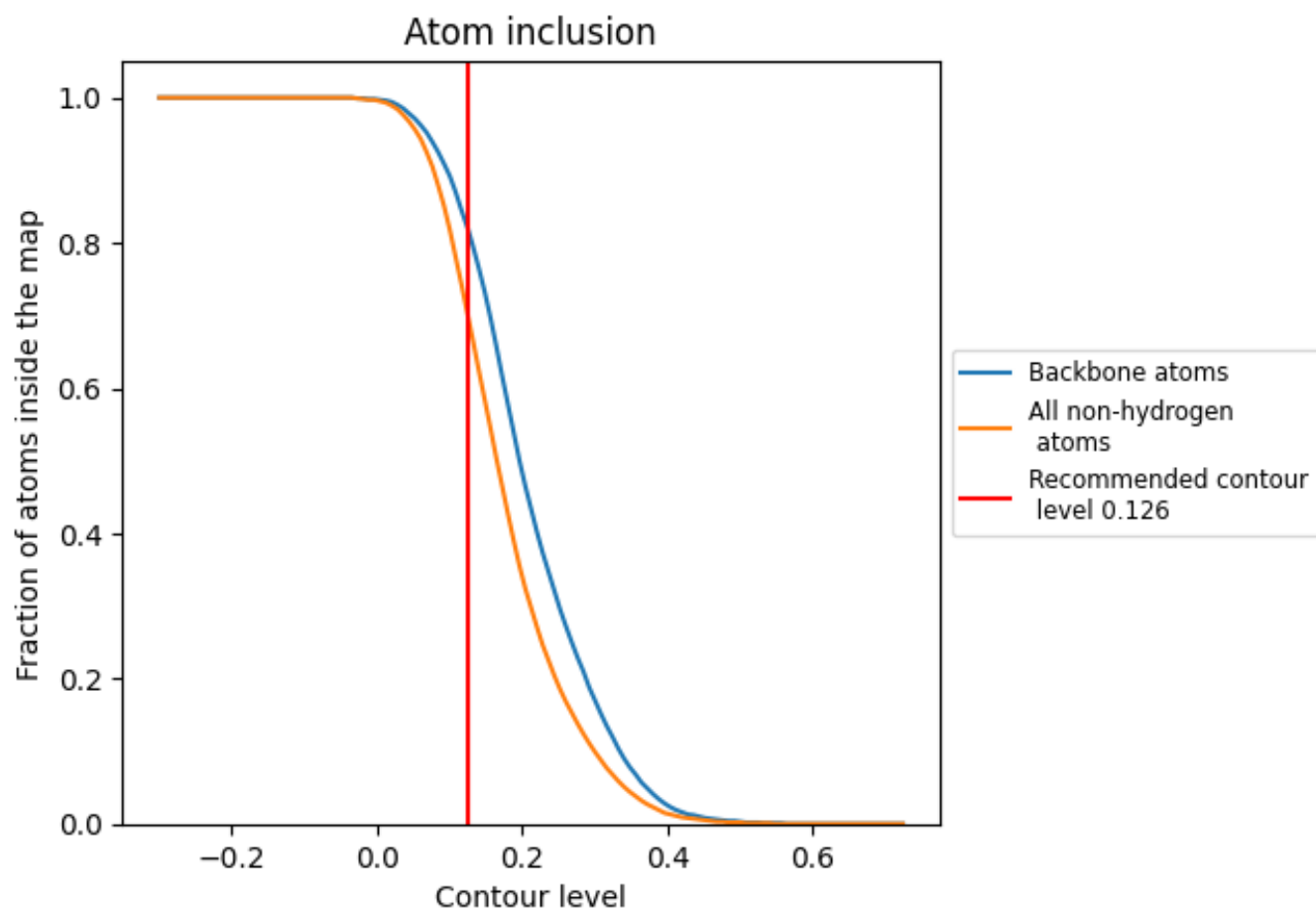
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.126).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.3090
A	 0.6960	 0.3070
B	 0.6960	 0.3070
C	 0.6960	 0.3070
D	 0.6960	 0.3070
E	 0.8410	 0.3850
F	 0.8410	 0.3870
G	 0.8410	 0.3850
H	 0.8410	 0.3860

