



## wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 08:40 PM EST

PDB ID : 7M6A  
EMDB ID : EMD-23692  
Title : High resolution structure of the membrane embedded skeletal muscle ryanodine receptor  
Authors : Melville, Z.; Kim, K.; Clarke, O.B.; Marks, A.R.  
Deposited on : 2021-03-25  
Resolution : 3.36 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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

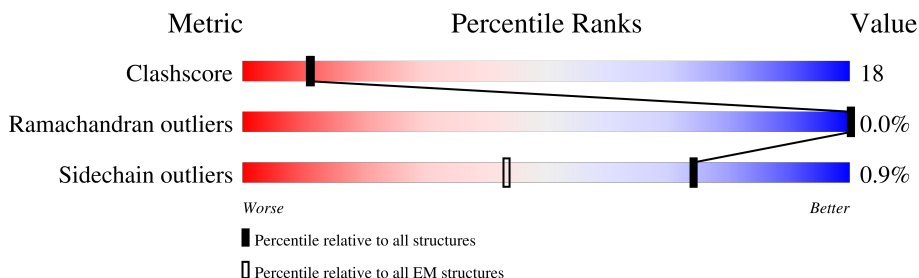
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.36 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	F	108	
1	H	108	
1	J	108	
1	O	108	
2	A	5037	
2	B	5037	
2	G	5037	
2	I	5037	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 140632 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.

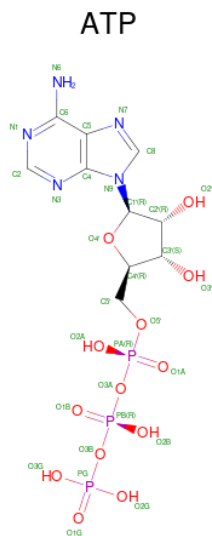
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	G	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	B	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		
2	I	4306	Total	C	N	O	S	0	0
			34293	21843	5903	6312	235		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

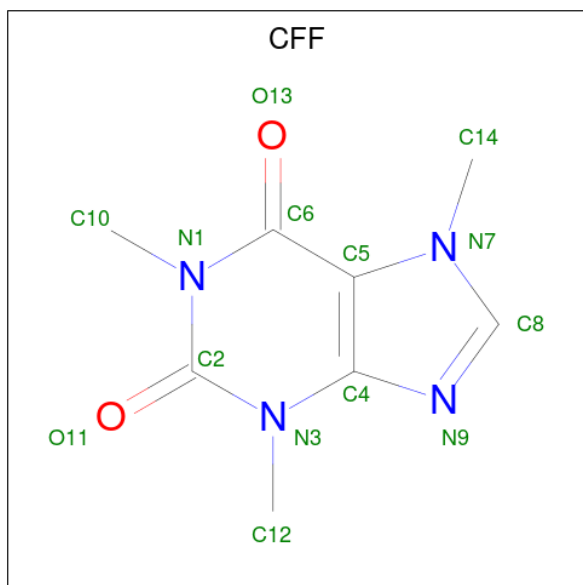
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula:  $C_8H_{10}N_4O_2$ ).

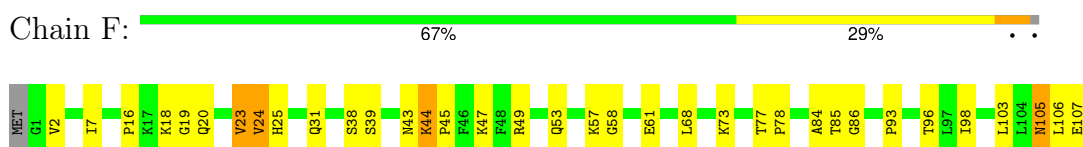


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	I	1	Total	C	N	O	0
			14	8	4	2	

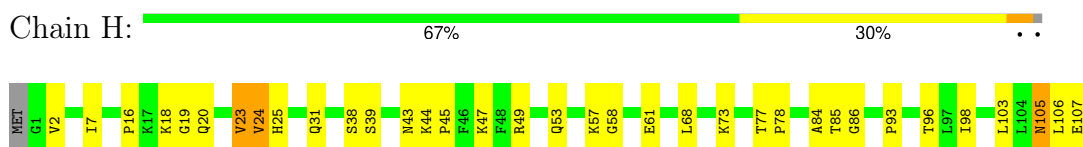
### 3 Residue-property plots

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.

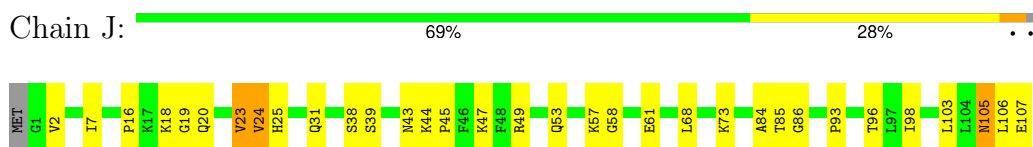
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



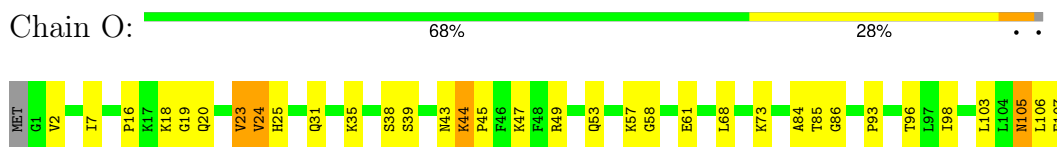
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



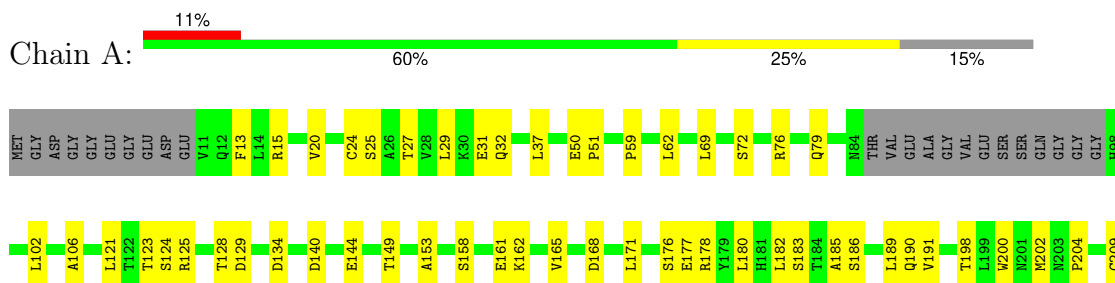
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



- Molecule 2: Ryanodine receptor 1











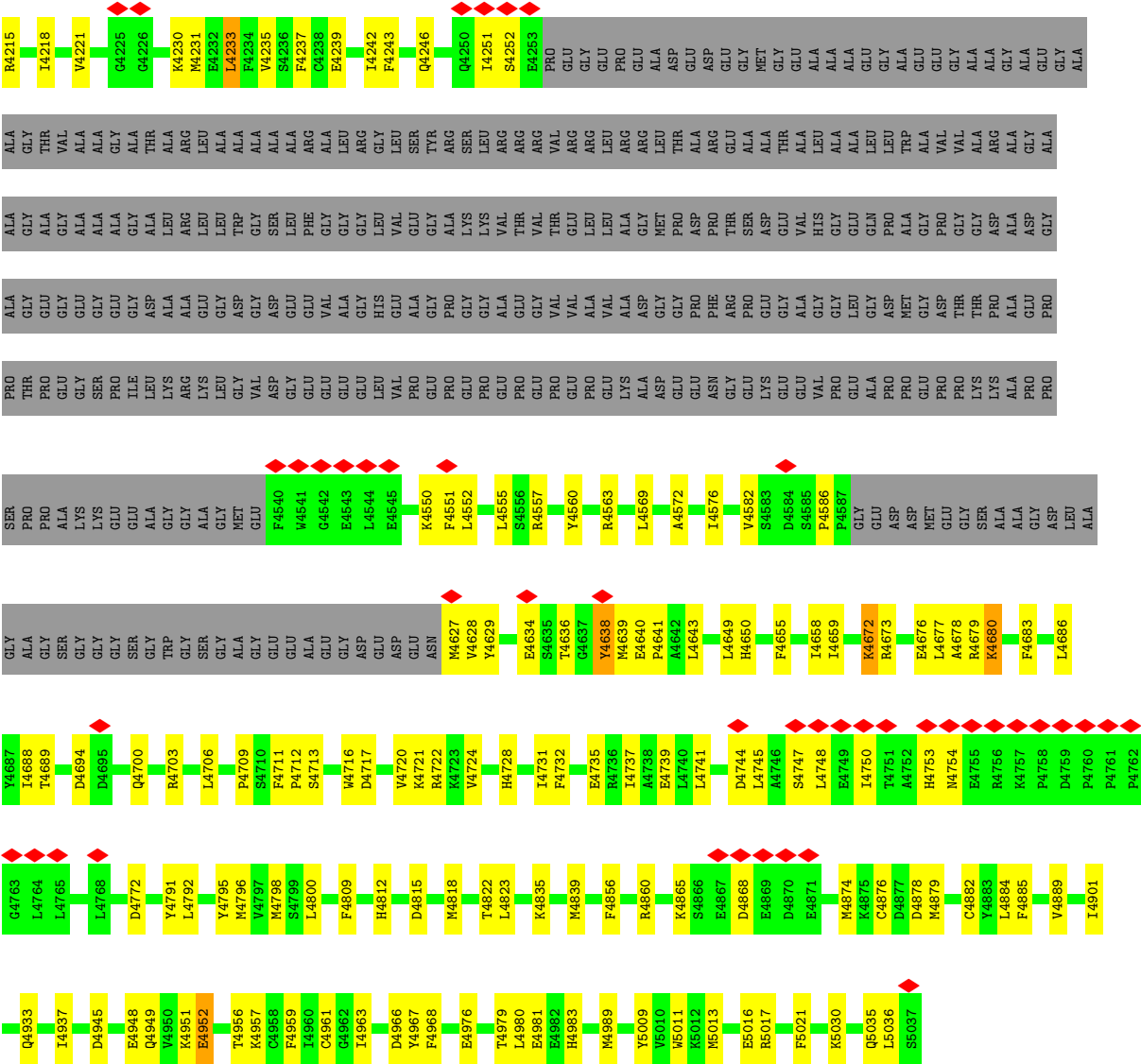
Frequency	Percentage
11%	11%
60%	60%
25%	25%
15%	15%



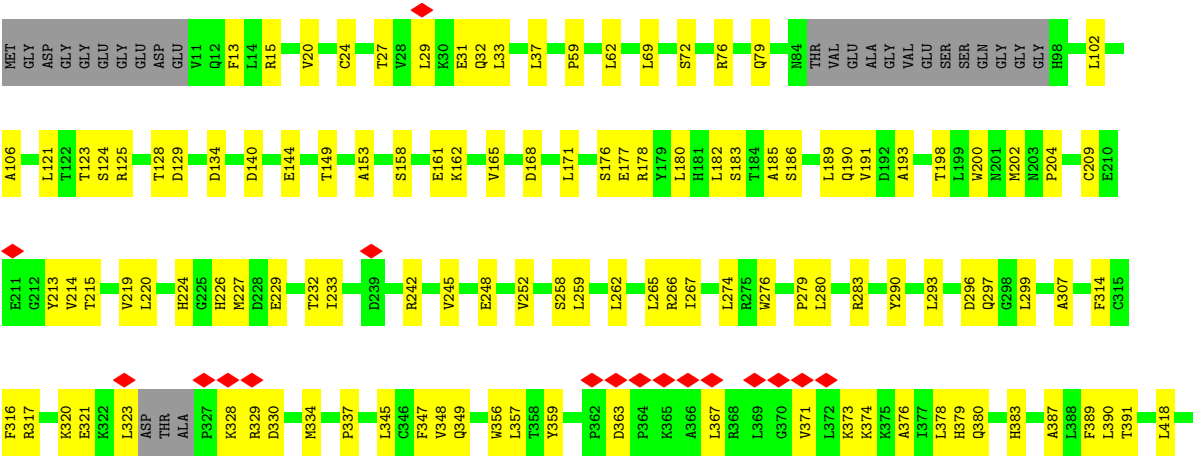


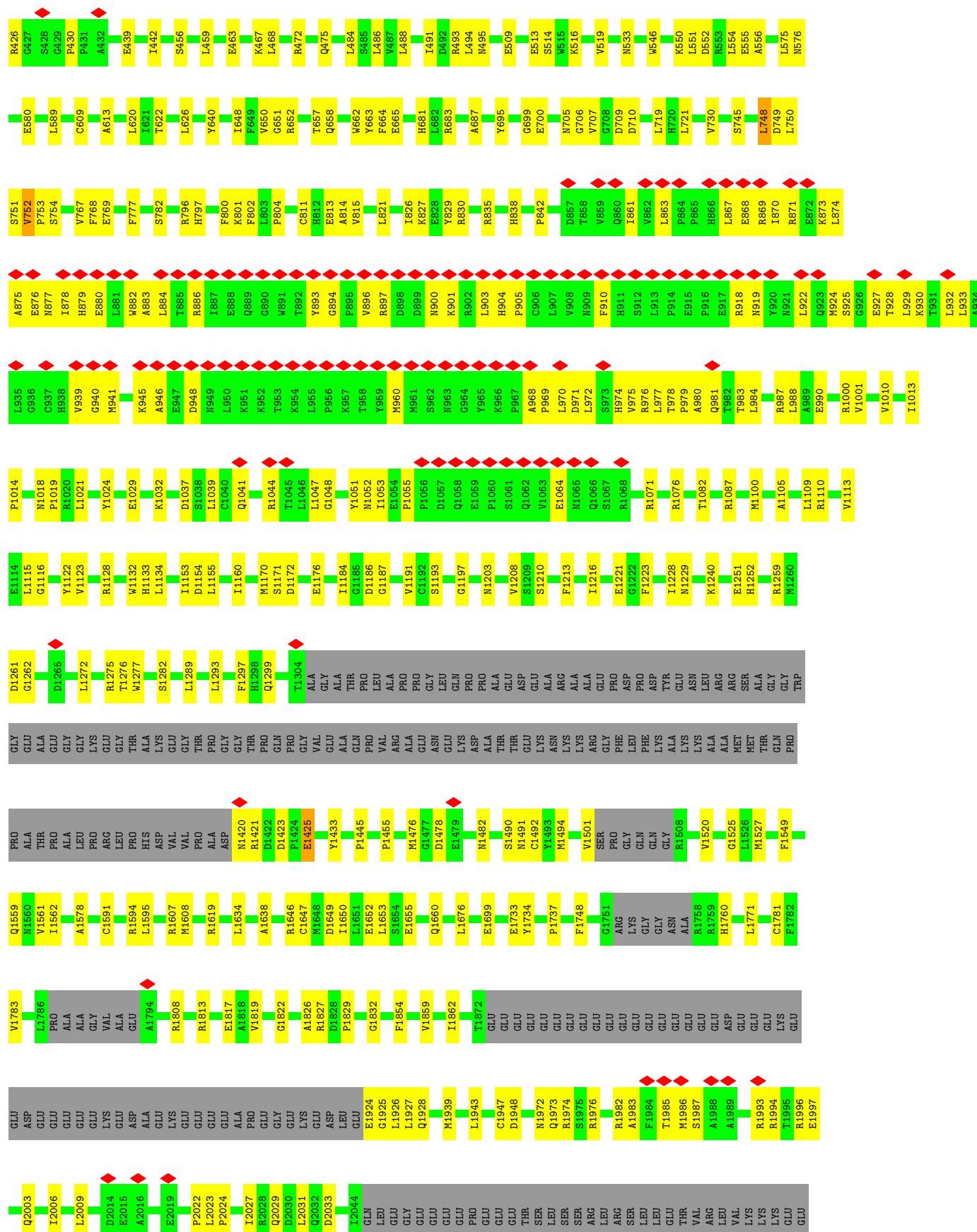


F3992	E4107	R3630	Q3554	GLY	Y3415	L3338	G3176	K3105	Y3016
F3996	T4108	A3631	N3555	GLY	V3416	I3345	T3177	M3106	A3022
M3999	C4114	Y3632	N3556	SER	D3417	V3346	Y3182	E3107	K3023
M4000	E4115	V3633	L3557	ASP	N3418	S3347	Y3182	N3109	K3024
M4001	E4116	V3634	K3560	GLN	N3419	R3348	K3185	L3110	L3025
K4002	E4117	A3634	R3560	ARG	R3420	R3348	L3186	R3111	G3026
S4007	E3712	F3636	V3563	THR	T3425	R3350	L3187	G3112	S3027
L4012	K3873	R3637	E3564	LYS	F3427	H3357	P3188	G3113	
L4016	V3751	K3638	P3567	LYS	N3428			LYS	
K4021	R3762	Y3642	R3570	ARG	E3432	T3361	C3193	VAL	N3033
M4023	Q3767	S3768	L3575	GLY	E3433	G3363	L3194	SER	K3034
M4024	S3778	R3648	Y3576	ASP	K3437	R3364	A3195	ALA	K3035
V4025	M3782	Y3682	L3579	ARG	F3442	G3370	R3196	ARG	E3037
L4031	M3782	E3682	C3581	Y3503	N3448	V3372	A3198	THR	N3038
V4036	I3802	GLN	R3582	S3504	H3449			GLN	I3039
M4044	M3809	GLU	E3583	V3505	I3450	K3367	M3201	VAL	T3040
V4045	V3812	GLU	E3584	Q3506	F3451	R3368	P3202	K3123	S3041
M4047	Q3813	GLU	F3586	T3507	K3452	A3369	V3203	G3124	L3042
L4048	Q3814	GLU	D3587	S3508	E3454	G3371	V3204	F3043	F3043
V4049	V3815	VAL	D3588	L3509	E3455	R3372	F3205	C3044	C3044
E4056	K3815	GLU	V3593	I3510	N3456	E3376	L3206	G3126	K3045
V4057	K3816	GLU	R3594	V3511	I3457	E3377	E3207	T3130	L3046
K4060	L3817	GLU	R3595	L3514	F3458	Q3378	P3208	L3136	L3049
F4061	M3836	VAL	V3596	M3517	N3459	I3379	Q3209	L3136	V3050
V4072	L3842	GLU	V3599	I3520	N3460	R3380	A3215	V3139	R3051
S4074	D3843	GLU	R3603	C3521	V3460	E3382	C3216	L3140	H3052
F4077	L3844	GLU	R3604	R3522	V3461	E3383	S3217	T3141	
Q4078	N3845	GLU	E3607	V3596	Q3462	A3383	S3218	L3143	L3056
T4082	R3947	GLU	H3611	K3597	E3463	K3384	Y3219	F3144	F3057
D4083	E3948	GLU	P3612	Q3598	I3464	R3385	T3220	Q3145	D3060
P4084	R3949	GLU	Y3613	C3525	E3465	E3386	T3221	H3146	A3061
R4085	K3850	GLU	K3614	A3526	I3466	E3387	S3223	A3148	V3064
G4086	N3851	GLU	S3615	D3529	N3467	A3387	P3224	A3149	C3067
K4090	E3854	GLU	L3615	Q3530	K3467	E3388	R3225	H3150	L3068
K4091	G3855	GLU	Y3615	L3532	E3468	E3389	E3226	Q3151	
D4092	L3856	GLU	ALA	I3533	F3469	G3390	R3227	F3152	L3071
K4095	G3857	GLU	VAL	M3534	T3471	E3391	A3228	D3155	D3076
M4097	M3729	GLU	LYS	K3537	ALA	L3392	T3229	V3156	A3077
F4103	L3735	GLU	LYS	A3541	ASP	L3393	L3230	I3157	R3078
T4104	E3718	GLU	ALA	L3542	SER	L3394	P3233	L3158	T3079
	E3718	GLU	TRP	K3543	LYS	V3394	R3234	D3159	V3080
	M3723	GLU	VAL	D3544	SER	R3395	S3235	V3161	M3081
	A3724	GLU	TRP	K3546	LYS	E3397	V3236	Q3162	P3085
	Y3725	GLU	HIS	D3547	LYS	F3398	E3237	Y3166	V3088
	M3729	GLU	LEU	T3549	LYS	V3400	E3238	R3167	K3089
	L3735	GLU	L3624	E3547	LYS	C3401	C3240	T3169	L3092
	E3718	GLU	S3625	E3548	LYS	C3402	I3243	T3172	A3099
	M3729	GLU	K3626	V3549	LYS	R3403	P3244	Y3173	S3100
	L3735	GLU	S3626	E3550	LYS	D3404	V3246	S3174	
	E3718	GLU	K3627	F3551	LYS	L3405	D3247	L3175	
	M3729	GLU	R3628	F3552	LYS	Y3409	R3248		E3104
	L3735	GLU	R3629	L3553	SER	I3412			
	E3718	GLU				I3413			
	M3729	GLU				R3414			



• Molecule 2: Ryanodine receptor 1





LYS	THR	P2319	F2494	A2570	R2650	E2724	E2784	GLN	L2904	D2968	F3043
PRO	LYS	D2320	P2495	H2574	C2651	K2725	L2785	THR	L2905	I2969	C3044
GLU	GLU	I2223	P2496	R2575	K2652	LYS	K2786	ALA	V2906	S2970	K3045
LEU	GLU	R2224	D2497	H2498	K2653	THR	T2787	GLN	P2907	Q2971	L3046
PRO	LEU	M2228	H2499	K2499	Y2654	VAL	H2788	TYR	D2908	E2972	L3049
ALA	PRO	C2237	A2500	V2579	Y2655	ASP	P2789	ASP	D2909	F2973	V3050
GLU	ALA	M2228	S2501	M2502	C2656	ALA	M2790	PRO	T2910	A2975	R3051
LYS	GLU	R2241	H2417	H2582	L2657	GLU	L2791	ARG	L2911	H2976	H3052
LYS	LYS	R2241	A2421	L2583	Q2660	GLY	R2792	GLY	L2912	L2977	L3056
P2091	P2091	Q2247	L2506	L2585	K2661	N2734	P2793	Y2855	T2913	E2978	F3057
Q2092	Q2092	R2330	D2507	T2586	F2664	D2735	Y2794	N2856	K2914	S2982	D3060
S2093	S2093	Y2331	R2508	Y2587	T2667	D2736	K2795	P2857	E2915	S2983	A3061
Q2095	L2094	Y2256	V2509	R2588	E2667	P2737	T2796	Q2858	Q2916	S2984	V3064
E2096	Q2096	F2334	L2429	L2430	E2669	R2738	F2797	P2859	A2917	Q2984	
L2097	L2097	F2337	D2431	I2512	E2670	R2739	Y2798	P2860	R2918	R2985	
V2098	V2098	A2338	R2435	E2513	E2671	V2740	S2798	D2861	D2919	V2986	
M2101	ILE	V2339	C2436	E2514	L2672	E2741	E2799	L2862		E2987	
L2123	GLY	S2345	E2439	Q2515	T2675	T2742	K2800	S2863	R2920	F2990	
R2126	GLY	V2346	M2440	L2518	R2676	L2743	D2801	G2864	E2921	H2991	
Q2127	GLY	E2347	Q2444	H2520	K2677	L2744	K2802	V2865	K2922	E2992	
G2132	GLY	E2348	E2449	V2521	F2679	V2745	E2803	T2866	Q2923	Q2993	
E2133	GLY	N2349	E2449	V2524	W2680	L2746	I2804	L2867	Q2924	E2994	
L2134	GLY	A2350	E2449	G2525	G2681	L2747	Y2805	L2867	E2925	E2995	
L2135	GLY	R2359	E2449	F2526	L2682	L2748	R2806	S2868	L2926	I2996	
R2136	GLY	E2362	E2449	L2527	L2686	E2749	V2807	R2869	L2927	F2997	
A2137	GLY	C2363	E2449	R2615	L2686	K2750	P2808	E2870	K2928	F2998	
L2155	GLY	R2369	P2462	M2618	L2686	L2751	I2809	L2871	F2929	A2999	
L2166	GLY	L2377	D2465	L2619	D2692	D2752	K2810	Q2872	L2930	K3000	
L2167	GLY	E2380	L2466	G2620	Q2693	D2753	E2811	A2873	Q2931	I3001	
V2168	GLY	E2381	V2467	H2621	E2694	S2753	S2812	M2874	N2932	L3002	
Q2169	GLY	E2382	I2469	L2622	L2695	F2754	L2813	A2875	N2933	L3003	
M2178	GLY	L2384	I2470	L2626	Y2696	K2755	K2814	E2876	G2934	P3004	
L2185	GLY	E2385	S2471	V2627	M2698	K2757	A2815	Q2877	Y2935	L3005	
M2198	GLY	K2297	L2472	A2547	M2700	F2758	M2816	L2878	A2936	I3006	
L2201	GLY	Y2301	P2473	M2551	C2702	A2759	I2817	A2879	V2937	N3007	
G2202	GLY	L2302	L2474	E2552	D2629	K2760	E2818	E2880	T2938	C3014	
M2203	GLY	C2306	Q2475	Y2553	V2630	Y2761	V2819	N2881	GLY	L3015	
T2206	GLY	G2307	I2476	L2554	V2634	T2762	E2820	Y2882	LEU	Y3016	
V2212	GLY	L2308	L2479	L2556	E2635	K2763	V2821	H2883	LYS	A3022	
G2216	GLY	ARG	VAL	L2559	F2636	E2764	T2822	N2884	ASP	K3023	
GLY	GLY	ASP	ARG	L2562	A2637	K2765	I2823	T2885	MET	V3024	
L2314	GLY	ASP	ASP	T2563	M2638	K2766	E2824	V2886	GLU	L3025	
L2315	GLY	ARG	ARG	L2566	P2640	A2767	A2826	G2887	LEU	G3026	
L2316	GLY	ARG	ARG	A2566	L2641	F2768	R2827	R2888	ASP	S3027	
GLY	GLY	ARG	ARG	P2567	L2644	D2769	E2827	K2889	THR	N3033	
P2568	GLY	GLY	GLY	L2568	T2645	K2770	R2827	K2890	LYS	S2949	
M2490	GLY	P2488	M2490	F2569	N2646	L2771	E2828	K2891	S2950	K3034	
					N2647	L2772	E2829	K2892	E2951	E3035	
					Y2719	K2773	E2830	E2893	E2952	K3036	
					S2720	N2774	GLU	E2894	K2953	E3037	
					S2721	K2775	GLU	L2894	F2959	M3038	
					K2722	N2776	THR	E2895	Q2961	I3039	
					A2723	K2777	GLU	A2896	Q2962	T3040	
						E2778	ARG	K2897	L2963	S3041	
						E2779	LYS	G2898	L2964	L3042	
						N2780	LYS	G2899	V2965		
						I2781	THR	G2900	R2966		
						D2782	ARG	G2901	M2967		
						E2783	LYS	T2901			
							ILE	H2902			
							SER	P2903			

D4157	F4158	R4159	L4160	R4161	L4164	E4166	L4166	P4176	R4180	I4181	E4182	R4189	R4192	E4199	R4202	A4203	Q4204	W4205	Q4209	E4212	S4213	K4214	R4215	I4218	W4221	Q4225	Q4226	K4230	M4231	E4232	L4233	F4234	W4235	S4236	F4237	Q4238	E4239	I4242	F4243	E4244	M4245	Q4246	Q4250	I4251									
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA								
F3933	Y3934	Y3935	Y3936	D3941	V3942	I3943	E3944	E3945	Q3946	A3954	M3955	L3965	T3966	E3967	Y3968	I3969	Q3970	Q3971	P3972	C3973	L3980	R3984	D3987	A3988	V3989	F3992	F3996	M3999	M4000	M4001	K4002	L4012	L4016	K4021	D4022	M4023	W4024	V4025	L4031	M4034	W4035	V4036	W4037	G4038									
M4044	V4045	D4046	M4047	L4048	W4049	E4056	K4060	F4061	T4071	V4072	S4073	S4074	F4077	Q4078	R4085	Q4086	K4090	K4091	D4092	K4095	A4096	M4097	F4103	T4104	E4107	T4108	C4114	D4118	E4119	T4123	M4124	F4125	E4126	F4127	F4128	A4129	M4130	R4131	F4132	Q4133	R4137	D4138	W4154	F4155	H4156								
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA								
K3123	G3124	V3125	G3126	T3130	L3136	V3139	L3140	T3141	T3142	L3143	F3144	Q3145	R3146	I3147	A3148	Q3149	H3150	Q3151	F3152	D3155	V3156	I3157	L3158	D3159	D3160	V3161	Q3162	V3166	R3167	L3168	L3169	I3172	V3173	S3174	L3175	G3176	T3177	Y3182	K3185	L3186	R3187	P3188	C3193	L3194	L3197	A3198	A3199	A3200	K3201				
P3202	V3203	A3204	F3205	L3206	E3207	A3215	C3216	S3217	Y3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	I3243	T3244	V3245	L3246	D3247	R3248	I3253	R3262	P3267	H3268	V3269	I3270	E3271	I3272	T3273	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	
P3282	R3283	W3284	R3287	E3290	L3296	P3297	A3298	Q3299	A3300	P3301	T3305	S3309	L3312	N3313	N3318	L3319	L3320	R3321	I3322	V3324	N3325	L3327	G3328	N3329	L3330	E3331	A3332	W3334	L3338	I3345	V3346	S3347	R3348	A3349	R3350	H3357	T3361	L3362	G3363	R3364	K3367	R3368	A3369	G3370									
K3371	V3372	E3375	E3376	E3377	Q3378	L3379	L3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	E3405	Y3409	L3412	T3413	R3414	Y3415	V3416	D3417	N3418	R3419	R3420	T3425	E3426	P3427	N3428	E3432	E3433	M3437	F3442	T3443	T3444	
W3445	S3448	H3449	F3451	K3452	R3453	E3454	E3455	Q3456	F3457	F3458	V3459	W3460	Q3461	K3462	E3463	I3464	N3465	N3466	K3467	F3468	F3469	L3470	T3471	ALA	ASP	SER	LYS	SER	LYS	MET	ALA	LYS	ALA	ASP	ALA	GLN	SER	GLY	GLY	GLY	ASP	GLN	GLU	THR	LYS	LYS	ARG	ARG	ASP	ARG	Y3503	S3504	V3505
Q3506	T3507	S3508	L3509	I3510	V3511	M3517	I3520	G3521	L3522	N3523	C3524	C3525	A3526	D3529	Q3530	D3531	L3532	I3533	M3534	K3537	A3541	L3542	K3543	D3544	T3545	D3546	E3547	E3548	V3549	R3550	E3551	L3553	Q3554	L3557	Q3560	V3563	E3564	P3567	R3570	L3575	Y3576	L3579	P3580	G3581	R3582								
E3583	E3584	D3585	L3586	D3587	D3588	V3593	R3594	V3595	V3596	Q3597	E3598	V3599	V3602	L3603	Y3604	E3607	H3611	P3612	Y3613	K3614	S3615	LYS	LYS	VAL	TRP	LYS	TRP	LYS	LYS	LEU	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	M3638	Y3642	R3648	Y3657	R3658	E3682	GLN	GLU	
GLU	GLU	GLU	GLU	VAL	GLU	GLU	K3693	K3694	P3695	H3699	H3700	L3701	F3705	A3709	F3715	E3718	K3723	K3724	Y3725	K3729	L3735	GLU	GLU	GLY	GLY	GLU	ASN	GLY	GLU	ALA	ALA	ASN	GLY	GLU	GLU	VAL	V3751	R3762	Q3767	S3768	H3771	T3772	A3776	E3777	K3778								
M3782	I3802	N3809	V3812	Q3813	K3815	M3816	L3817	M3836	L3842	D3843	L3844	N3845	A3846	F3847	E3848	Q3850	R3851	M3858	V3859	N3860	E3861	G3863	T3864	V3865	I3866	ASN	ARG	GLN	ASN	E3872	K3873	D3883	L3884	F3885	Q3889	C3892	E3893	F3899	W4035	V4036	W4037	G4038											
F3933	Y3934	Y3935	Y3936	D3941	V3942	I3943	E3944	E3945	Q3946	A3954	M3955	L3965	T3966	E3967	Y3968	I3969	Q3970	Q3971	P3972	C3973	L3980	R3984	D3987	A3988	V3989	F3992	F3996	M3999	M4000	M4001	K4002	L4012	L4016	K4021	D4022	M4023	W4024	V4025	L4031	M4034	W4035	V4036	W4037	G4038									
M4044	V4045	D4046	M4047	L4048	W4049	E4056	K4060	F4061	T4071	V4072	S4073	S4074	F4077	Q4078	R4085	Q4086	K4090	K4091	D4092	K4095	A4096	M4097	F4103	T4104	E4107	T4108	C4114	D4118	E4119	T4123	M4124	F4125	E4126	F4127	F4128	A4129	M4130	R4131	F4132	Q4133	R4137	D4138	W4154	F4155	H4156								





F3043	C3044	K3045	L3046	E2968	D2969	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	S2982	S2983	G2984	R2985	V2986	E2987	P2990	H2991	E2992	Q2993	E2994	K2995	F2997	F2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	N3006	K3007	Q3008	C3014	L3015	Y3016	A3022	K3023	V3024	L3025	G3026	S3027	N3033	K3034	E3035	K3036	E3037	M3038	I3039	Q3041	L3042	C3067	L3068	H3069	L3070	L3071	D3076	A3077	R3078	T3079	V3080	M3081	P3085	V3088	K3089	L3092	A3099	S3100	E3104	K3105	V3106	E3107	E3108	K3109	L3110	R3111	L3112	G3113	L3113	VAL	VAL	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125
L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	K2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	S2949	S2950	I2951	E2952	K2953	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	M2967																																						
E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	T2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	R2806	V2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	V2819	E2820	H2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	I1E	SER																																					
E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783																																					
R2850	C2851	W2852	K2853	Y2854	Y2855	L2857	G2860	W2861	F2864	T2867	S2868	E2869	E2870	N2871	L2872	T2875	K2876	K2877	L2878	F2879	W2880	G2881	L2882	L2886	D2892	Q2893	E2894	L2895	Y2896	R2897	M2898	M2900	P2901	C2902	A2905	N2906	L2910	P2911	T2912	E2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	K2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	S2949	S2950	I2951	E2952	K2953															
A2570	H2574	R2575	M2578	V2579	D2580	S2581	M2582	L2583	H2584	T2585	V2586	R2587	R2588	R2591	L2595	Q2599	E2604	D2605	C2606	R2612	Y2613	L2614	R2615	M2618	L2619	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	N2634	E2635	F2636	A2637	K2638	M2639	L2641	L2644	T2645	Y2648	E2649																																																	
F2494	V2495	P2496	D2497	H2498	K2499	A2500	S2501	M2502	L2506	P2507	R2508	V2509	I2512	E2513	N2514	Q2515	L2518	L2519	H2520	V2521	V2524	G2525	L2527	P2528	D2529	M2530	R2531	S2535	L2536	T2540	F2541	E2545	M2546	A2547	N2551	R2552	Y2553	L2554	C2555	L2559	T2562	T2563	A2566	P2567	L2568	F2569																																																	
P2319	D2320	I2321	G2322	W2323	R2415	V2416	H2417	A2421	L2422	M2423	L2429	D2430	L2432	L2433	G2434	R2435	C2436	E2439	M2440	Q2444	E2449	R2452	I2453	R2456	D2465	L2466	V2467	G2468	I2469	I2470	S2471	L2472	P2473	Q2474	Q2475	I2476	L2479	G2480	K2481	D2482	G2483	A2484	L2485	P2488	K2489	M2490																																																	
GLU	I2223	M2228	C2237	R2241	Q2247	S2255	Y2256	E2259	N2260	S2261	GLY	I1E	GLY	LEU	MET	Q2268	G2269	L2273	A2277	A2278	S2279	N2283	L2286	L2290	Q2291	D2294	L2295	E2296	K2297	Y2301	L2302	C2305	L2307	Q2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	K2316																																																					
LEU	PRO	ALA	GLU	GLU	LYS	P2091	Q2092	S2093	L2094	Q2095	E2096	L2097	V2098	W2101	L2103	R2126	Q2127	G2132	E2133	L2134	L2135	R2136	A2137	L2155	L2166	I2167	V2168	Q2169	W2178	I2185	W2186	Y2192	W2198	L2201	G2202	M2203	T2206	V2212	G2216	GLY	GLY	THR	LYS																																																				

Q4246	R4131	M4037	T3797	D3585	S3508	S448	E3375	W3284	L3206	G3126
Q4250	F4132	G4038	I3802	A3586	L3509	H3449	E3376	R3287	E3207	T3130
I4251	Q4133	M4044	N3809	D3587	V3511	N3450	E3377	E3290	Q3209	L3136
E4253	R4137	D4046	V3812	V3593	M3517	R3453	L3379	L3296	A3215	V3139
PRD	D4138	Q3927	Q3813	R3594	G3520	E3454	R3380	P3297	C3216	L3140
GLU	V4154	F3933	Q3814	R3595	G3521	E3456	L3381	P3297	S3217	T3141
GLU	D4157	F3936	R3815	V3596	L3522	Q3456	E3382	A3298	Y3219	T3142
GLU	P4158	D3941	M3816	Q3597	N3523	N3457	A3383	G3299	T3220	L3143
PRD	S4052	V3942	L3817	E3598	K3524	F3458	A3383	A3300	T3221	F3144
GLU	E4056	I3943	L3701	V3599	C3525	V3459	K3384	A3300	K3222	Q3145
ALA	K4060	F3705	F3705	V3602	A3526	V3460	A3385	P3301	S3223	H3146
ASP	F4061	A3709	A3709	L3603	D3529	Q3461	E3386	T3305	P3224	I3147
ASP	E4165	E3715	E3715	L3604	Q3530	N3462	A3387	G3149	R3225	A3148
GLU	L4164	K3718	E3718	E3607	D3532	I3464	E3388	S3309	E3226	H3150
GLY	L4166	M3723	M3723	H3611	L3533	N3466	E3389	N3312	R3227	F3151
MET	R4180	F3847	F3847	P3612	K3537	M3467	G3390	L3313	A3228	F3152
GLU	E4182	A3846	A3846	Y3613	A3541	F3468	E3391	N3318	L3229	D3155
ALA	E4182	E3848	E3848	K3614	L3542	F3469	E3392	T3319	G3231	V3156
ALA	R4188	Q3850	Q3850	S3615	K3543	L3470	L3393	L3320	L3232	T3157
ALA	R4189	L3735	L3735	LVS	D3544	T3471	R3395	R3321	P3233	L3158
GLU	Q4077	GLU	GLU	ALA	D3546	ALA	D3396	I3322	N3234	D3159
GLY	Q4078	GLY	GLY	VAL	D3547	ASP	E3397	I3323	S3235	D3160
GLY	Q4079	GLY	GLY	TRP	D3548	SER	F3398	V3324	E3236	V3161
ALA	Q4085	GLY	GLY	ALA	E3549	LVS	S3399	N3325	V3237	Q3162
GLU	G4086	GLY	GLY	L3624	E3551	ALA	V3400	N3326	E3238	V3166
GLU	R4086	GLY	GLY	S3625	F3552	GLY	L3401	L3327	E3239	V3166
GLU	G4086	GLY	GLY	K3626	Q3554	ASP	C3402	G3328	C3240	R3167
GLY	K4090	GLY	GLY	R3628	Q3555	ALA	R3403	I3329	T3243	T3172
ALA	K4091	GLY	GLY	R3629	N3556	GLY	D3404	D3330	P3244	V3173
ALA	D4092	GLY	GLY	R3630	Q3557	GLY	L3405	E3331	V3245	S3174
GLY	Q4209	GLY	GLY	A3631	L3557	ASP	Y3409	T3333	D3247	L3175
ALA	E4212	GLY	GLY	V3632	Q3560	ALA	L3412	W3334	R3248	Q3176
GLY	S4213	GLY	GLY	V3633	V3563	GLY	L3413	L3338	I3253	T3177
ALA	R4215	GLY	GLY	A3634	E3564	GLY	Y3415	I3345	R3262	V3182
THR	I4218	GLY	GLY	C3635	P3567	SER	V3416	V3346	P3267	K3185
VAL	V4221	GLY	GLY	R3636	R3570	ASP	D3417	R3347	H3268	L3186
ALA	G4225	GLY	GLY	M3638	L3575	GLN	N3418	A3349	V3269	R3187
ALA	K4230	GLY	GLY	Y3642	Y3576	ARG	R3420	R3350	I3270	P3188
ARG	M4231	GLY	GLY	R3648	P3567	THR	T3425	H3357	E3271	C3193
LEU	E4232	GLY	GLY	R3658	R3579	LVS	E3426	L3272	I3272	L3194
ALA	L4233	GLY	GLY	Y3658	F3580	LVS	P3427	T3361	T3273	L3197
ALA	R4234	GLY	GLY	R3658	G3581	ARG	N3428	I3362	L3274	L3197
ALA	S4236	GLY	GLY	E3582	E3584	GLY	ARG	G3363	M3276	A3198
ALA	P4237	GLY	GLY	E3582	E3584	GLY	GLY	R3364	L3277	L3277
ARG	C4238	GLY	GLY	E3582	E3584	ASP	E3432	K3367	C3278	K3201
ARG	E4239	GLY	GLY	GLN	E3584	ARG	E3433	R3368	S3279	F3202
ALA	I4242	GLY	GLY	GLU	E3584	ARG	M3437	A3369	Y3280	V3203
ALA	F4243	GLY	GLY	GLU	E3584	ARG	F3442	G3370	L3281	A3204
LEU		GLY	GLY	GLU	E3584	ARG	T3443	K3371	P3282	F3205
		GLY	GLY	GLU	E3584	ARG	Y3444	V3372	R3283	
		GLY	GLY	GLU	E3584	ARG	W3445			

F4968	D4815	K4721	V4628	L4552	GLU	PRO	ALA	GLU	SER
E4976	K4722	R4723	Y4629	L4555	PRO	PRO	PRO	GLY	TYR
T4979	M4818	V4724	E4634	S4556	GLU	PRO	GLY	LVS	ARG
L4980	T4822	H4728	S4635	R4557	PRO	PRO	GLY	LVS	LEU
E4981	L4823		T4636	Y4560	GLU	GLU	ALA	VAL	ARG
E4982	M4839	T4731	G4637		PRO	PRO	GLU	THR	ARG
H4983		F4732	Y4638	R4563	GLU	GLU	VAL	THR	ARG
M4989	F4856	E4735	M4639	L4569	GLU	GLU	VAL	GLU	ARG
Y5009	R4860	R4736	E4640		PRO	PRO	ALA	LEU	ARG
W5011	A4738	L4737	P4641	A4572	GLU	LVS	VAL	LEU	ARG
K5012	K4865	E4739	A4642		ALA	ALA	ASP	GLY	ARG
M5013	S4866	L4740	L4643	L4576	ASP	ASP	GLY	MET	LEU
E4987	E4868	L4741	L4646		GLU	GLU	GLY	PRO	THR
D4868	D4744		L4649	D4584	GLU	GLU	PRO	ASP	ALA
E4869	L4745	L4746	H4650	S4585	ASN	ASN	PHE	PRO	ARG
D4870	E4746		F4655	P4586	GLU	GLU	ARG	THR	ALA
E4871	S4747	A4746		P4587	LVS	LVS	GLU	ASP	ALA
M4874	L4748	L4748	I4658	GLY	GLU	GLU	GLY	GLU	THR
K4875	E4749	E4749	I4659	ASP	VAL	VAL	ALA	VAL	ALA
C4876	L4750	L4750	K4672	ASP	PRO	PRO	GLY	HIS	LEU
D4877	T4751	T4751	R4673	GLU	VAL	VAL	GLY	GLY	ALA
D4878	A4752	A4752		GLY	GLU	GLU	GLY	GLN	LEU
M4879	H4753	H4753	E4676	SER	PRO	PRO	ASP	PRO	LEU
C4882	L4754	L4754	A4677	ALA	GLU	GLU	MET	ALA	TRP
F4885	E4755	E4755	R4679	ASP	PRO	PRO	GLY	GLY	ALA
V4889	R4756	R4756	K4680	LEU	LVS	LVS	THR	GLY	ARG
I4901	K4757	K4757	F4683	ALA	ALA	ALA	PRO	ASP	ARG
Q4933	P4758	P4758	L4686	GLY	PRO	PRO	GLU	ASP	GLY
T4937	D4759	D4759	Y4687	GLY	PRO	PRO	GLY	GLY	ALA
D4945	P4760	P4760	I4688	SER	SER	SER	THR	GLY	GLY
E4948	P4761	P4761	T4689	GLY	PRO	PRO	PRO	GLU	ALA
Q4949	P4762	P4762		GLY	ALA	ALA	GLU	GLY	GLY
V4950	C4763	C4763	G4693	SER	LVS	LVS	GLY	GLU	ALA
K4951	L4764	L4764	D4694	SER	LVS	LVS	SER	GLY	ALA
E4952	L4766	L4766	D4695	TRP	GLU	GLU	ILE	GLY	GLY
T4956			Q4700	GLY	ALA	ALA	LEU	ASP	LEU
K4957	W4767	W4767		SER	GLY	GLY	LVS	ALA	LEU
C4958	L4768	L4768	R4703	GLY	GLY	GLY	ARG	ALA	ARG
I4960	W4769	W4769		ALA	ALA	ALA	LEU	GLU	ARG
C4961	L4796	L4796	L4706	GLY	GLY	GLY	LEU	GLY	LEU
G4962	V4797	V4797		GLU	MET	MET	GLY	ASP	TRP
I4963	W4798	W4798	L4706	GLU	GLU	GLU	VAL	GLY	SER
D4966	D4772	D4772	P4709	ALA	ASP	ASP	ASP	ASP	SER
Y4967	Y4791	Y4791	S4710	GLU	F4640	F4640	GLY	GLU	LEU
F4959	L4792	L4792	F4711	GLY	W4541	W4541	GLY	GLU	PHE
I4960			P4712	ASP	G4642	G4642	GLU	VAL	GLY
C4961	Y4795	Y4795	S4713	GLU	G4643	G4643	GLU	ALA	GLY
G4962	M4796	M4796		ASP	L4644	L4644	GLU	GLY	GLY
I4963	V4797	V4797	W4716	ASP	L4644	L4644	GLU	GLY	GLY
D4966	W4798	W4798	D4717	ASN			LEU	HIS	LEU
Y4967	S4799	S4799	Y4720	M4627	K4650	K4650	VAL	GLU	VAL
S5037				F4551					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	53882	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.119	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.121	Depositor
Map size (Å)	425.472, 425.472, 425.472	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	F	0.78	0/834	0.70	1/1123 (0.1%)
1	H	0.78	0/834	0.71	1/1123 (0.1%)
1	J	0.78	0/834	0.70	1/1123 (0.1%)
1	O	0.78	0/834	0.70	1/1123 (0.1%)
2	A	0.46	1/35070 (0.0%)	0.55	31/47504 (0.1%)
2	B	0.46	1/35070 (0.0%)	0.55	31/47504 (0.1%)
2	G	0.46	1/35070 (0.0%)	0.55	32/47504 (0.1%)
2	I	0.46	1/35070 (0.0%)	0.55	31/47504 (0.1%)
All	All	0.47	4/143616 (0.0%)	0.56	129/194508 (0.1%)

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	A	0	1
2	B	0	1
2	G	0	1
2	I	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3188	PRO	N-CD	-8.43	1.36	1.47
2	B	3188	PRO	N-CD	-8.43	1.36	1.47
2	I	3188	PRO	N-CD	-8.43	1.36	1.47
2	G	3188	PRO	N-CD	-8.37	1.36	1.47

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3850	GLN	CA-CB-CG	8.89	132.95	113.40
2	A	3850	GLN	CA-CB-CG	8.88	132.94	113.40
2	I	3850	GLN	CA-CB-CG	8.87	132.92	113.40
2	G	3850	GLN	CA-CB-CG	8.86	132.90	113.40
2	B	2676	ARG	CB-CG-CD	-8.82	88.66	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4638	TYR	Peptide
2	B	4638	TYR	Peptide
2	G	4638	TYR	Peptide
2	I	4638	TYR	Peptide

## 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	F	818	0	824	36	0
1	H	818	0	824	35	0
1	J	818	0	824	34	0
1	O	818	0	824	36	0
2	A	34293	0	33897	1228	0
2	B	34293	0	33897	1219	0
2	G	34293	0	33897	1242	0
2	I	34293	0	33897	1219	0
3	A	31	0	12	2	0
3	B	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1	0	0	0	0
6	A	14	0	10	1	0
6	B	14	0	10	1	0
6	G	14	0	10	1	0
6	I	14	0	10	1	0
All	All	140632	0	138972	4997	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 18.

The worst 5 of 4997 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:3989:VAL:HG23	2:I:4023:MET:CE	1.38	1.52
2:B:3989:VAL:HG23	2:B:4023:MET:CE	1.38	1.51
2:A:3989:VAL:HG23	2:A:4023:MET:CE	1.38	1.49
2:G:3989:VAL:HG23	2:G:4023:MET:CE	1.38	1.49
2:G:2615:ARG:NH2	2:G:2618:MET:HE1	1.16	1.48

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	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	J	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	O	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	A	4260/5037 (85%)	4079 (96%)	179 (4%)	2 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	4260/5037 (85%)	4078 (96%)	180 (4%)	2 (0%)	100	100
2	G	4260/5037 (85%)	4080 (96%)	178 (4%)	2 (0%)	100	100
2	I	4260/5037 (85%)	4079 (96%)	179 (4%)	2 (0%)	100	100
All	All	17460/20580 (85%)	16720 (96%)	732 (4%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	801	LYS
2	G	801	LYS
2	B	801	LYS
2	I	801	LYS
2	A	3267	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	88/89 (99%)	78 (89%)	10 (11%)	4	17
1	H	88/89 (99%)	78 (89%)	10 (11%)	4	17
1	J	88/89 (99%)	78 (89%)	10 (11%)	4	17
1	O	88/89 (99%)	78 (89%)	10 (11%)	4	17
2	A	3738/4276 (87%)	3713 (99%)	25 (1%)	81	89
2	B	3738/4276 (87%)	3713 (99%)	25 (1%)	81	89
2	G	3738/4276 (87%)	3713 (99%)	25 (1%)	81	89
2	I	3738/4276 (87%)	3713 (99%)	25 (1%)	81	89
All	All	15304/17460 (88%)	15164 (99%)	140 (1%)	74	87

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	751	SER

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Mol	Chain	Res	Type
2	I	1128	ARG
2	I	4031	LEU
1	J	25	HIS
1	J	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	2127	GLN
2	I	2324	ASN
2	I	3052	HIS
2	G	2127	GLN
2	G	877	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	ATP	I	5301	-	28,33,33	0.84	0	34,52,52	1.25	4 (11%)
6	CFF	I	5304	-	8,15,15	2.10	2 (25%)	8,23,23	1.20	1 (12%)
6	CFF	G	5304	-	8,15,15	2.11	2 (25%)	8,23,23	1.20	1 (12%)
6	CFF	B	5304	-	8,15,15	2.11	2 (25%)	8,23,23	1.21	1 (12%)
3	ATP	A	5301	-	28,33,33	0.84	0	34,52,52	1.25	4 (11%)
3	ATP	G	5301	-	28,33,33	0.84	0	34,52,52	1.25	4 (11%)
3	ATP	B	5301	-	28,33,33	0.84	0	34,52,52	1.25	4 (11%)
6	CFF	A	5304	-	8,15,15	2.11	2 (25%)	8,23,23	1.20	1 (12%)

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	ATP	I	5301	-	-	2/18/38/38	0/3/3/3
6	CFF	I	5304	-	-	-	0/2/2/2
6	CFF	G	5304	-	-	-	0/2/2/2
6	CFF	B	5304	-	-	-	0/2/2/2
3	ATP	A	5301	-	-	2/18/38/38	0/3/3/3
3	ATP	G	5301	-	-	2/18/38/38	0/3/3/3
3	ATP	B	5301	-	-	2/18/38/38	0/3/3/3
6	CFF	A	5304	-	-	-	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5304	CFF	C5-C6	4.19	1.48	1.41
6	A	5304	CFF	C5-C6	4.19	1.48	1.41
6	B	5304	CFF	C5-C6	4.19	1.48	1.41
6	I	5304	CFF	C5-C6	4.14	1.48	1.41
6	A	5304	CFF	C5-C4	3.74	1.45	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5301	ATP	N3-C2-N1	-3.74	123.59	128.67
3	B	5301	ATP	N3-C2-N1	-3.74	123.59	128.67
3	A	5301	ATP	N3-C2-N1	-3.74	123.59	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5301	ATP	N3-C2-N1	-3.72	123.63	128.67
3	B	5301	ATP	C4-C5-N7	-2.35	106.85	109.34

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

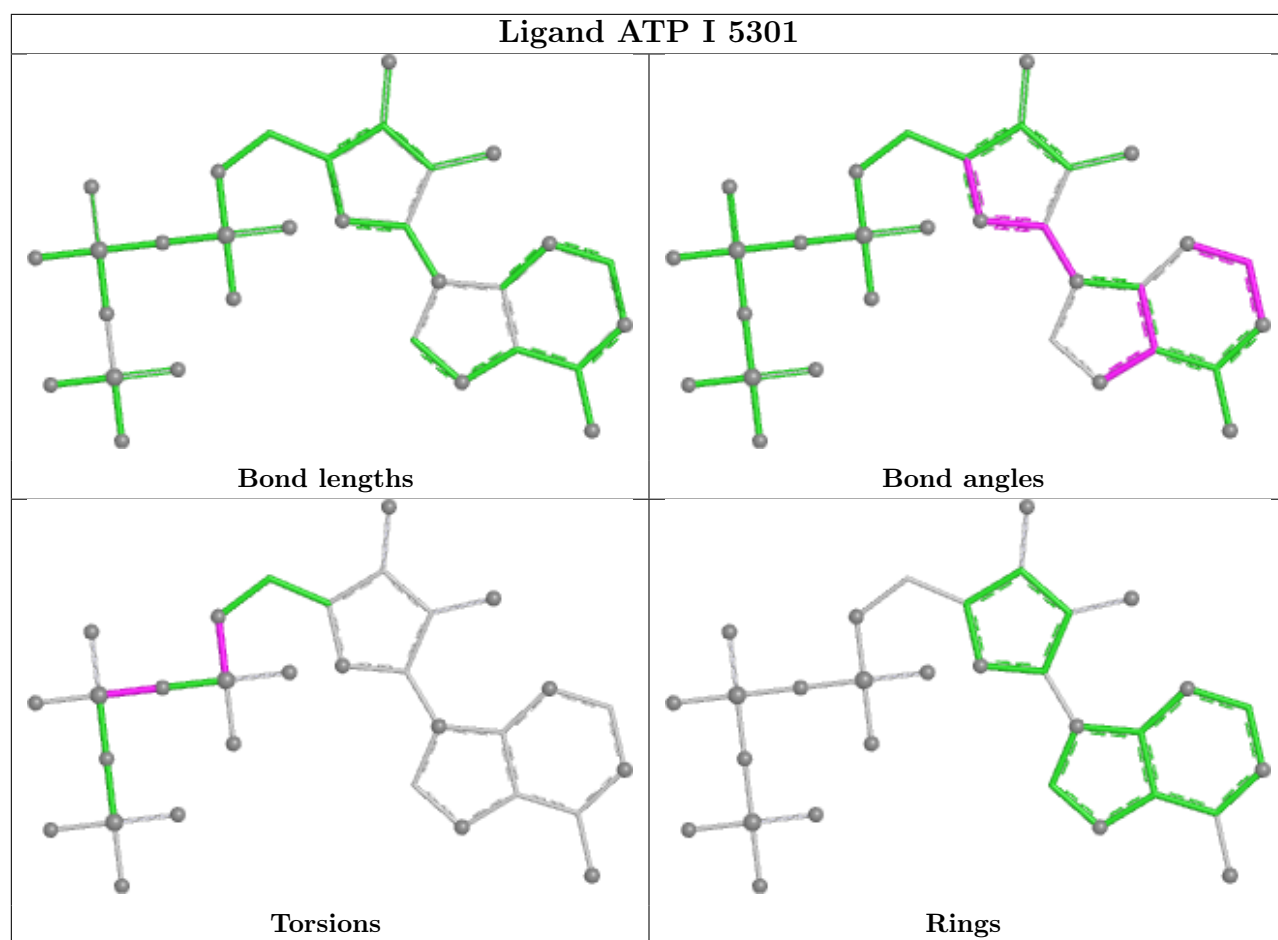
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O3A
3	G	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	I	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	PA-O3A-PB-O1B

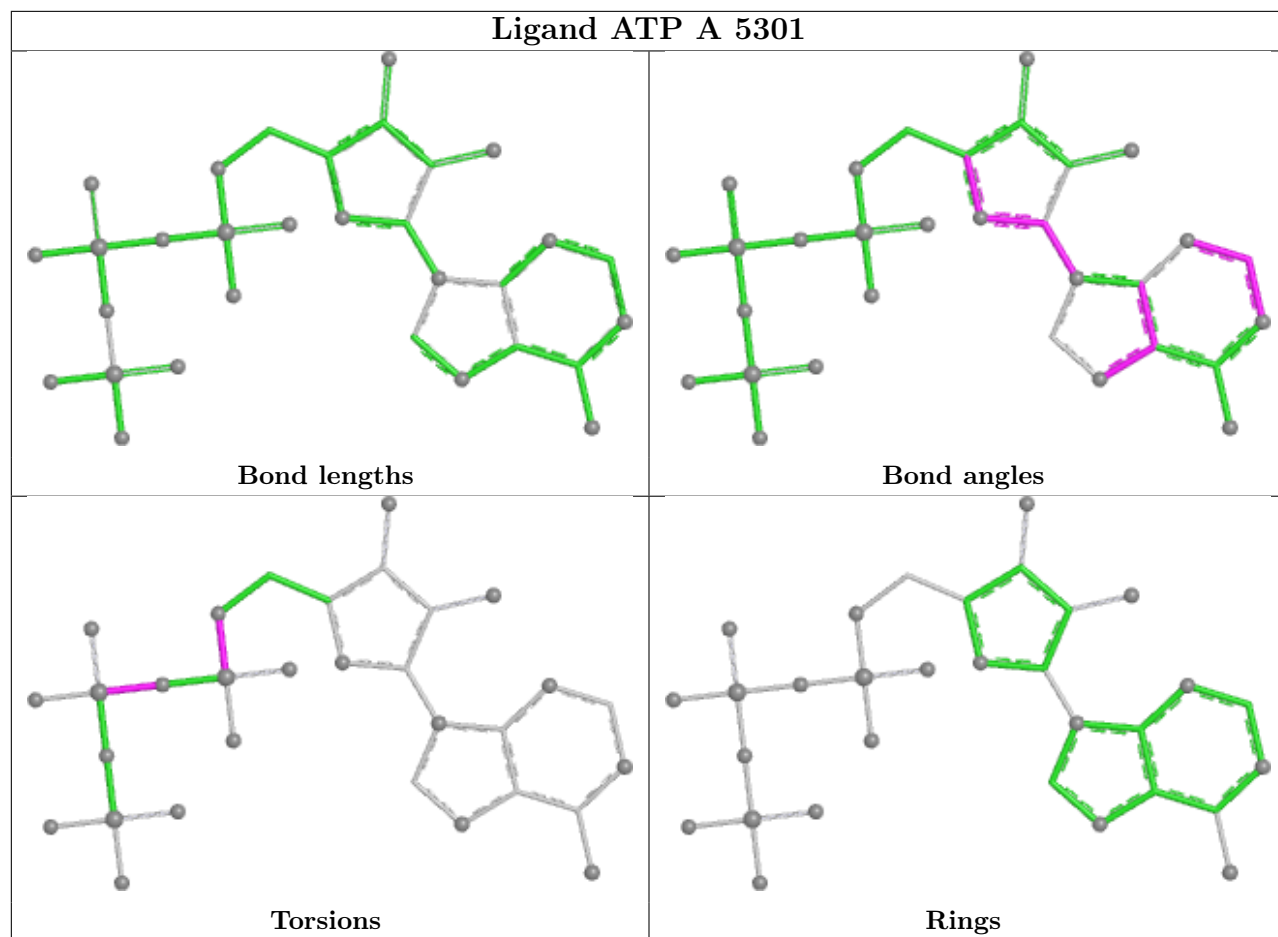
There are no ring outliers.

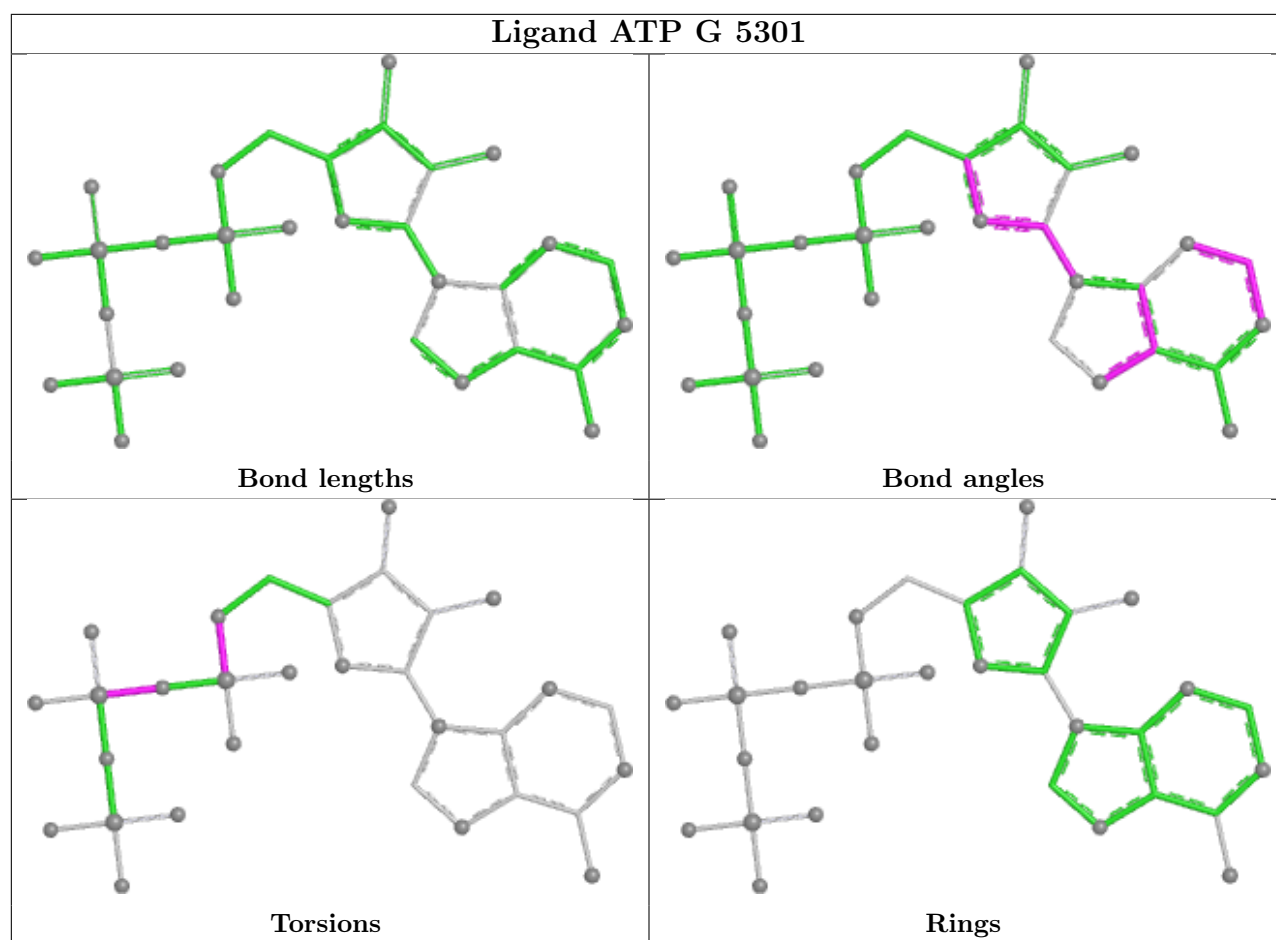
8 monomers are involved in 12 short contacts:

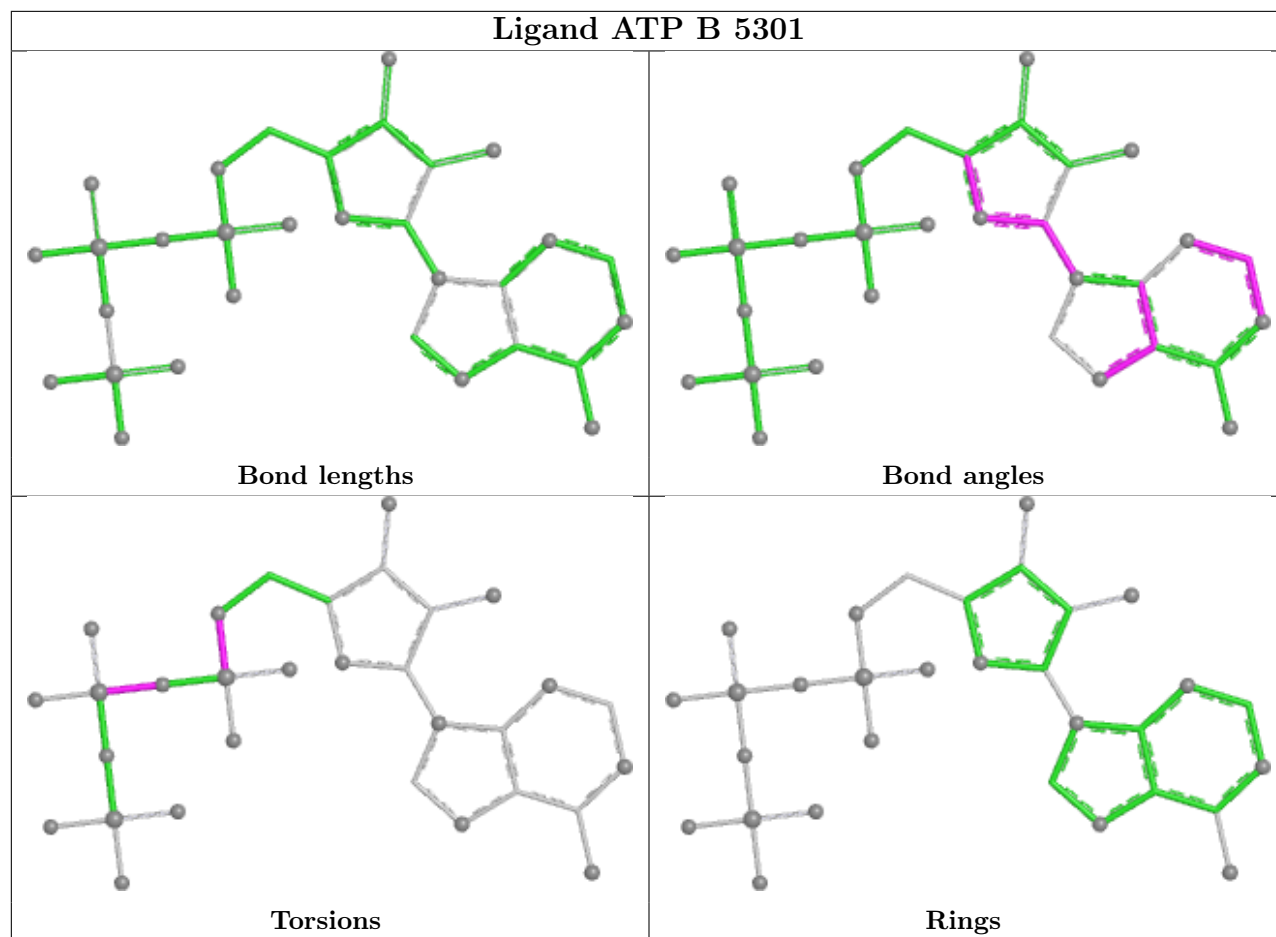
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	5301	ATP	2	0
6	I	5304	CFF	1	0
6	G	5304	CFF	1	0
6	B	5304	CFF	1	0
3	A	5301	ATP	2	0
3	G	5301	ATP	2	0
3	B	5301	ATP	2	0
6	A	5304	CFF	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

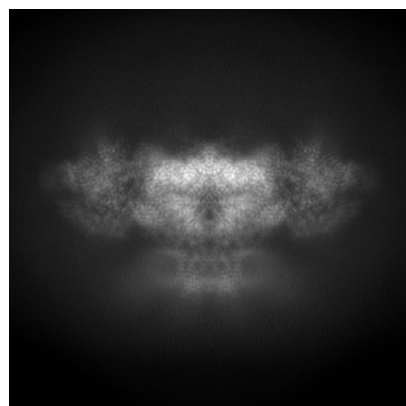
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23692. These allow visual inspection of the internal detail of the map and identification of artifacts.

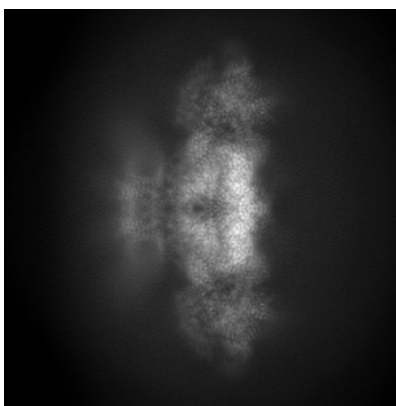
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

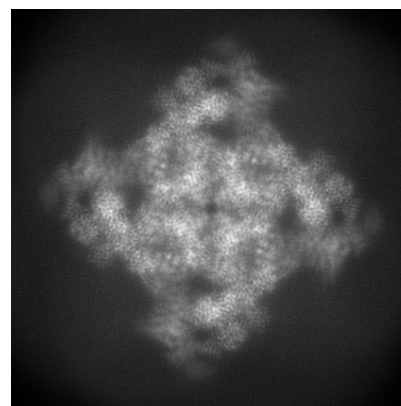
#### 6.1.1 Primary map



X

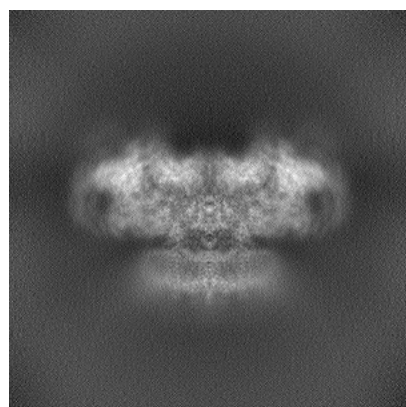


Y

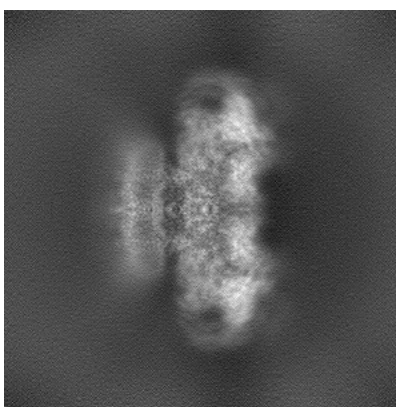


Z

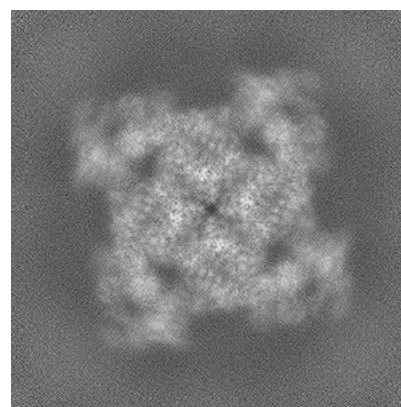
#### 6.1.2 Raw map



X



Y

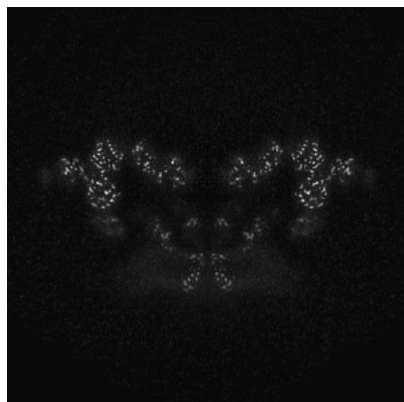


Z

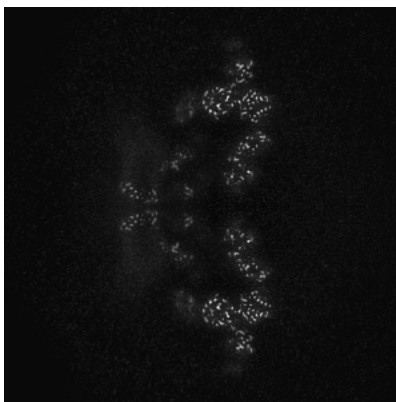
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

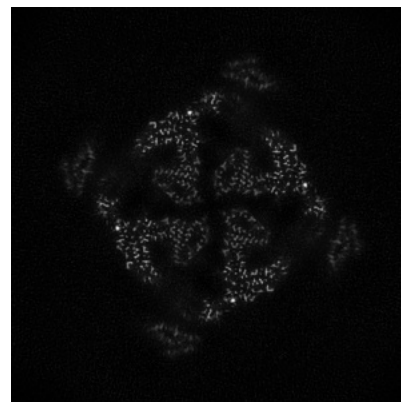
### 6.2.1 Primary map



X Index: 256

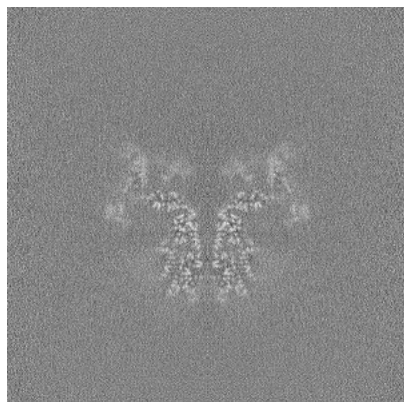


Y Index: 256

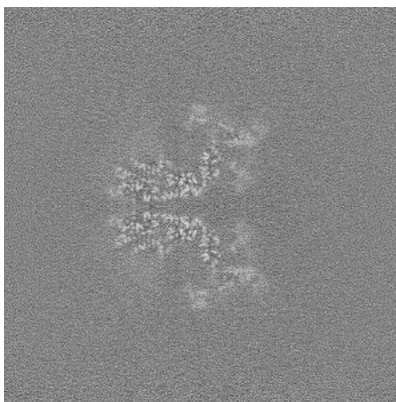


Z Index: 256

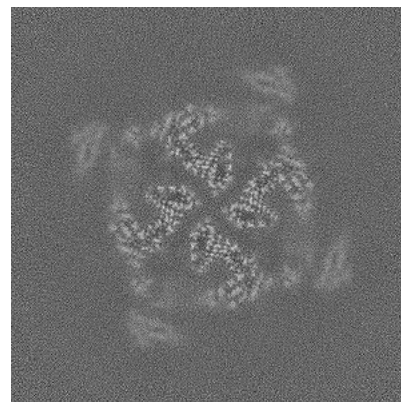
### 6.2.2 Raw map



X Index: 256



Y Index: 256

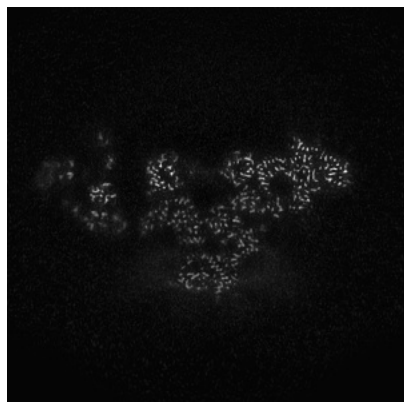


Z Index: 256

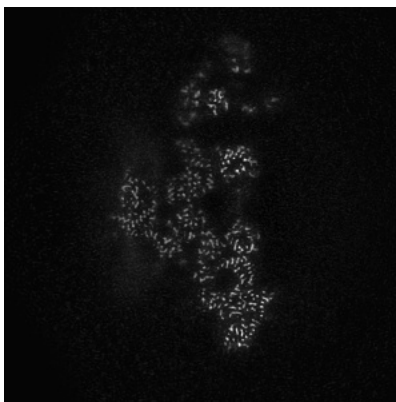
The images above show central slices of the map in three orthogonal directions.

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

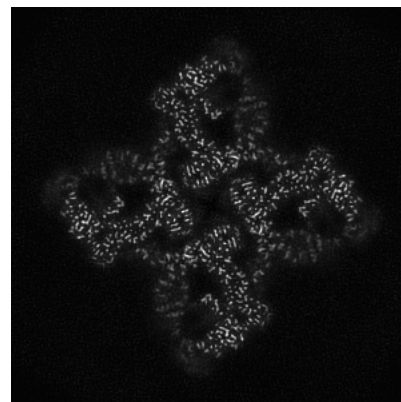
### 6.3.1 Primary map



X Index: 236

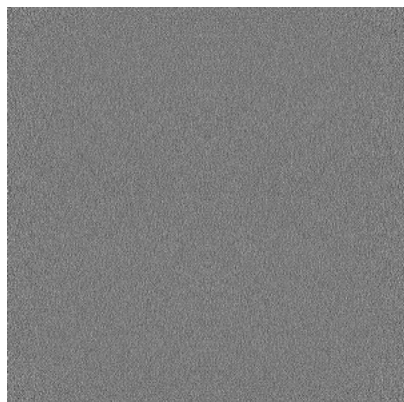


Y Index: 236

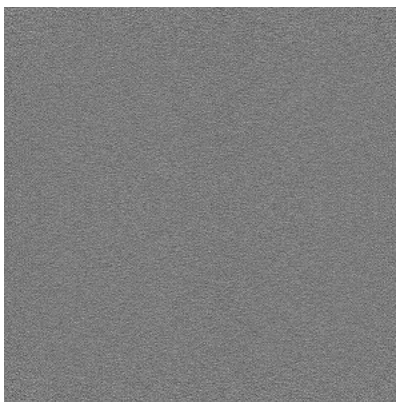


Z Index: 304

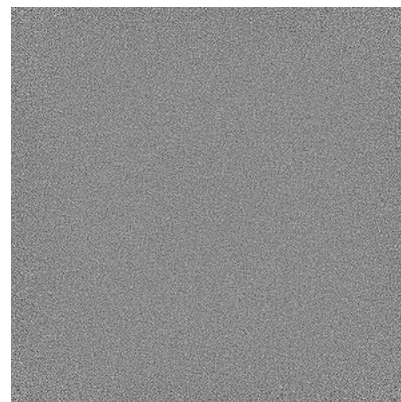
### 6.3.2 Raw map



X Index: 0



Y Index: 0

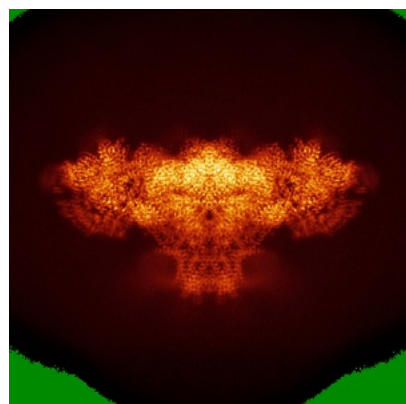


Z Index: 0

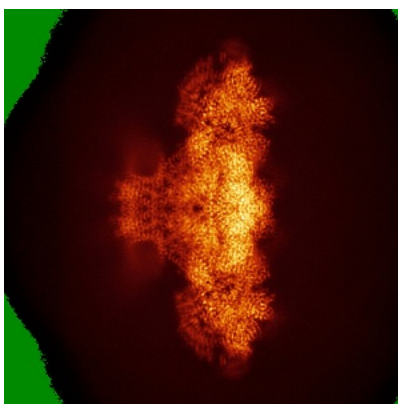
The images above show the largest variance slices of the map in three orthogonal directions.

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

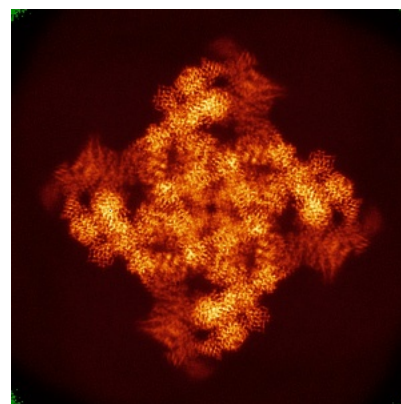
### 6.4.1 Primary map



X

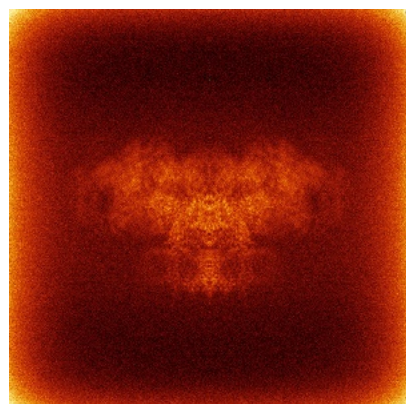


Y

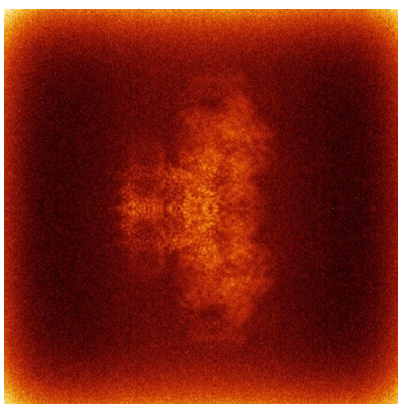


Z

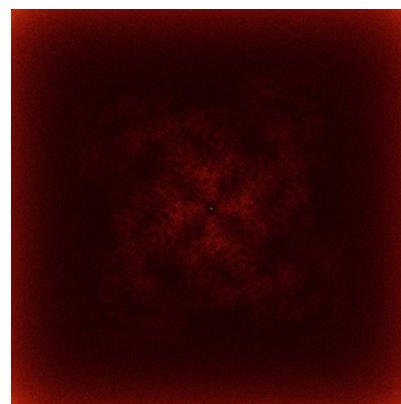
### 6.4.2 Raw map



X



Y

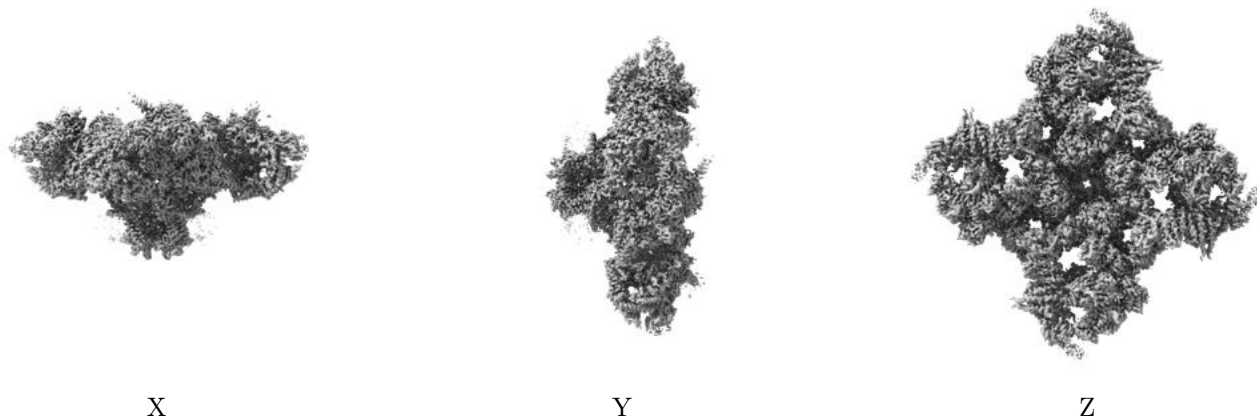


Z

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.

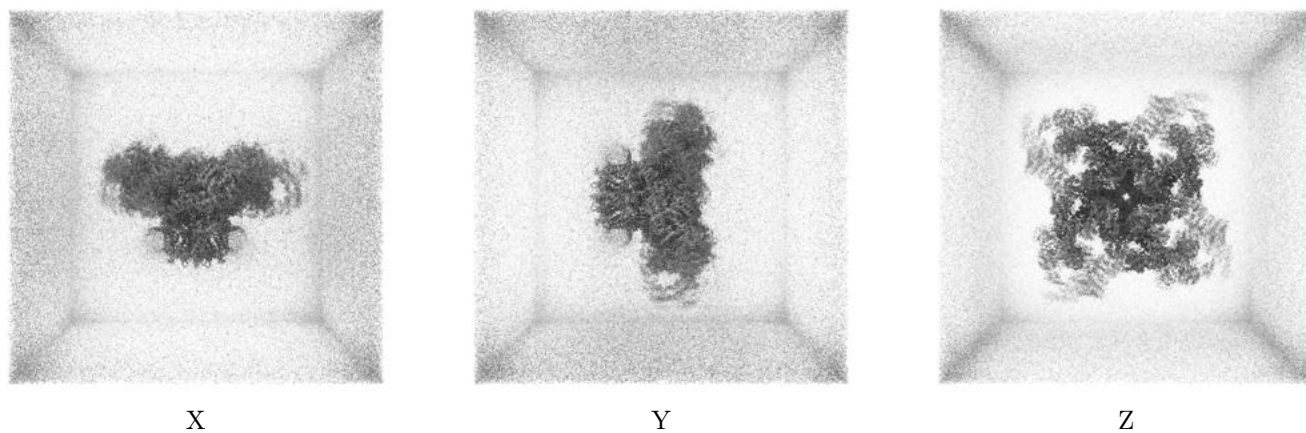
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.121. 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.

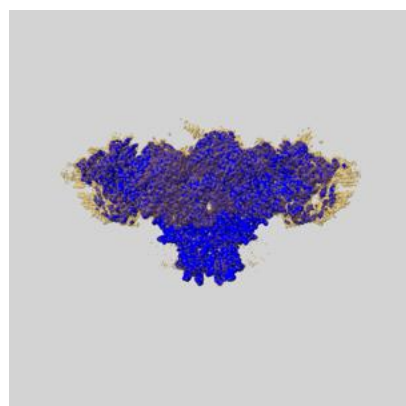
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

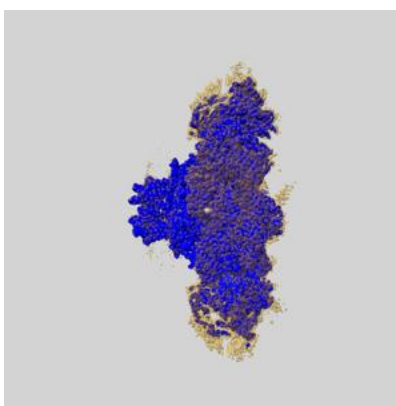
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

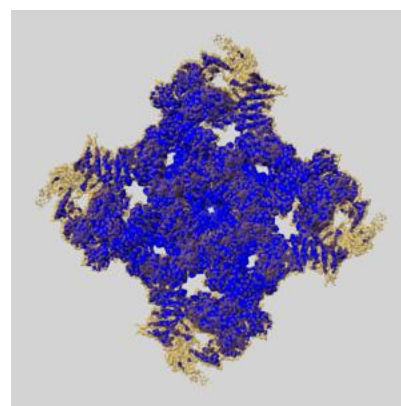
### 6.6.1 emd\_23692\_msk\_1.map [i](#)



X



Y

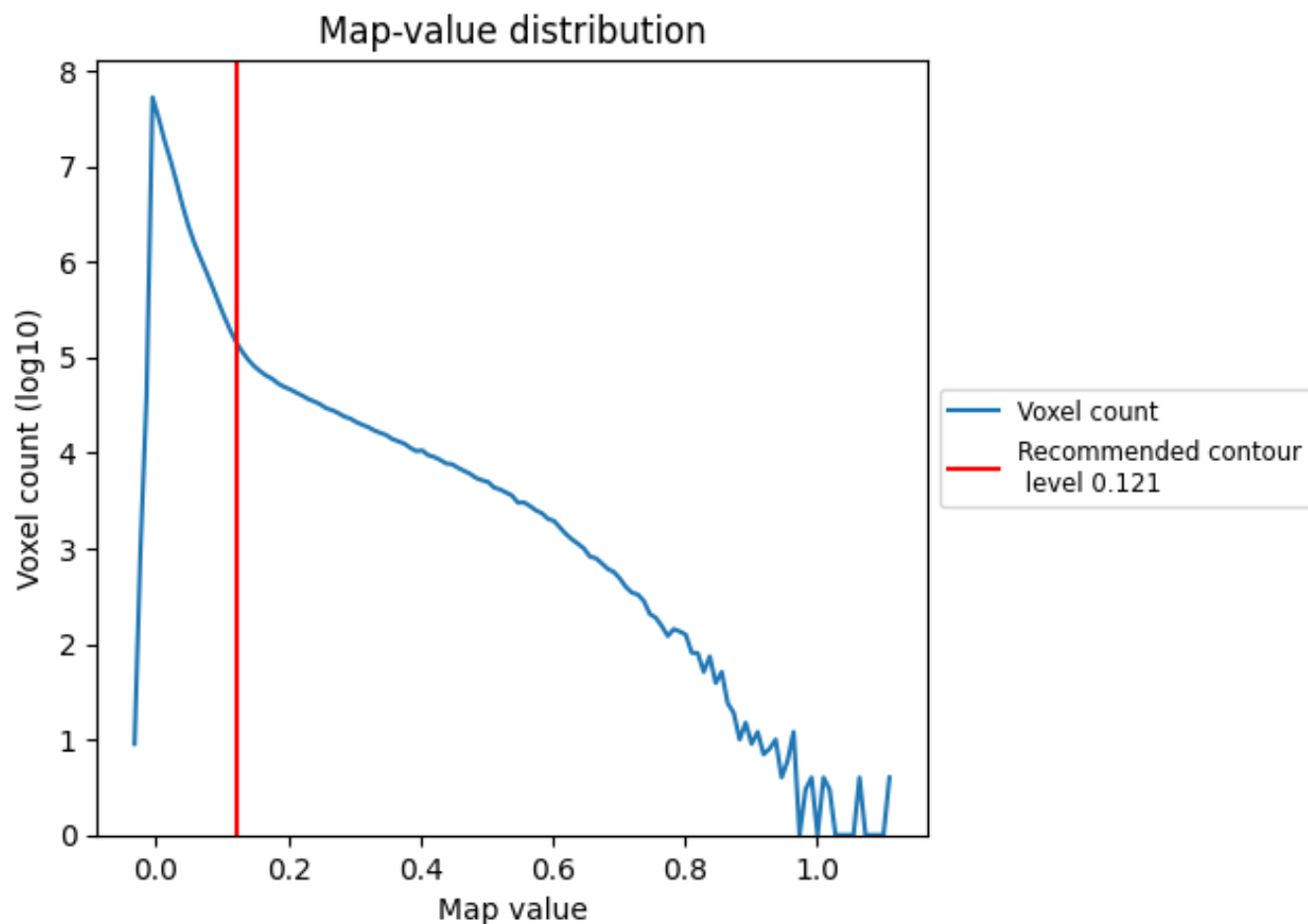


Z

## 7 Map analysis [i](#)

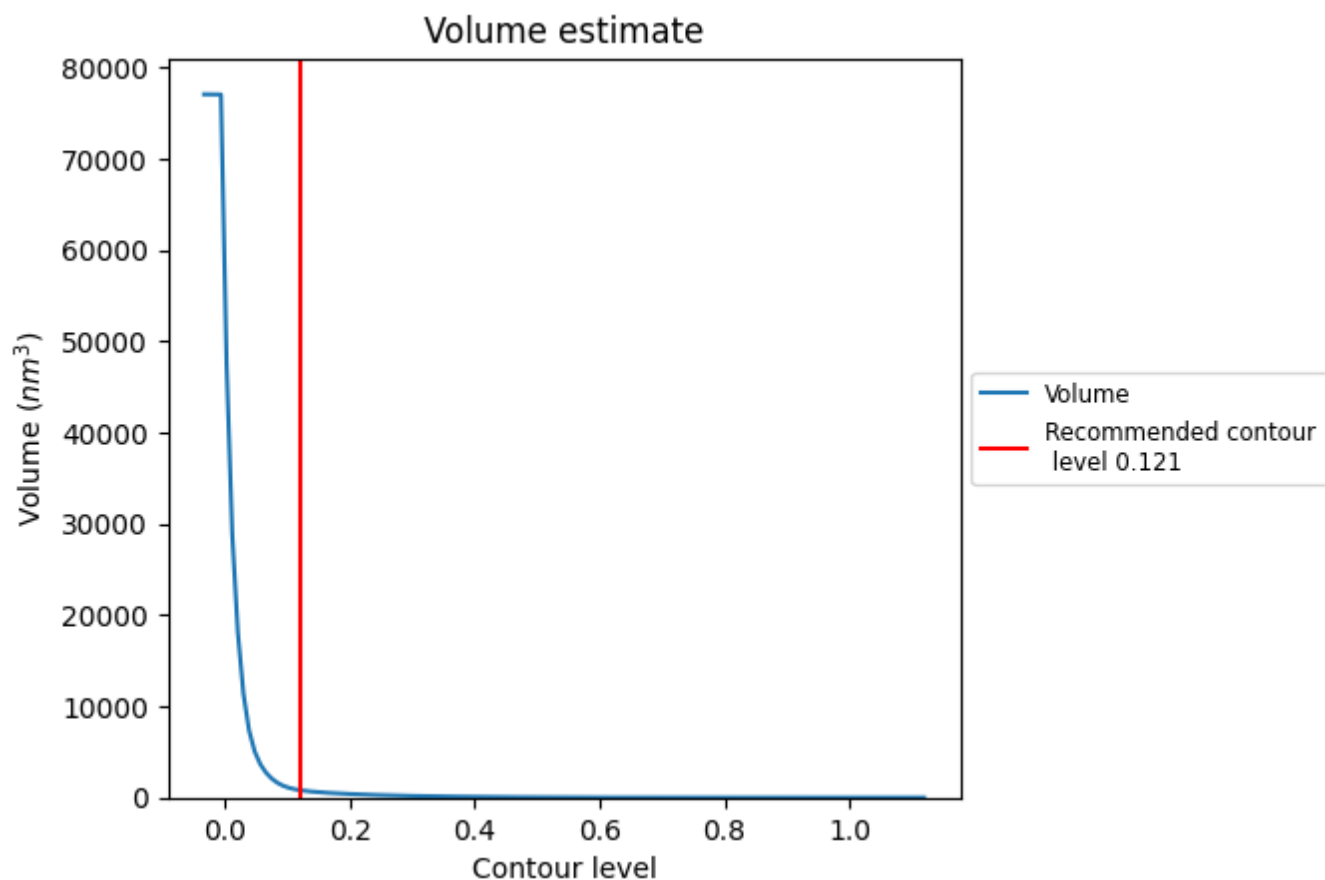
This section contains the results of statistical analysis of the map.

### 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.

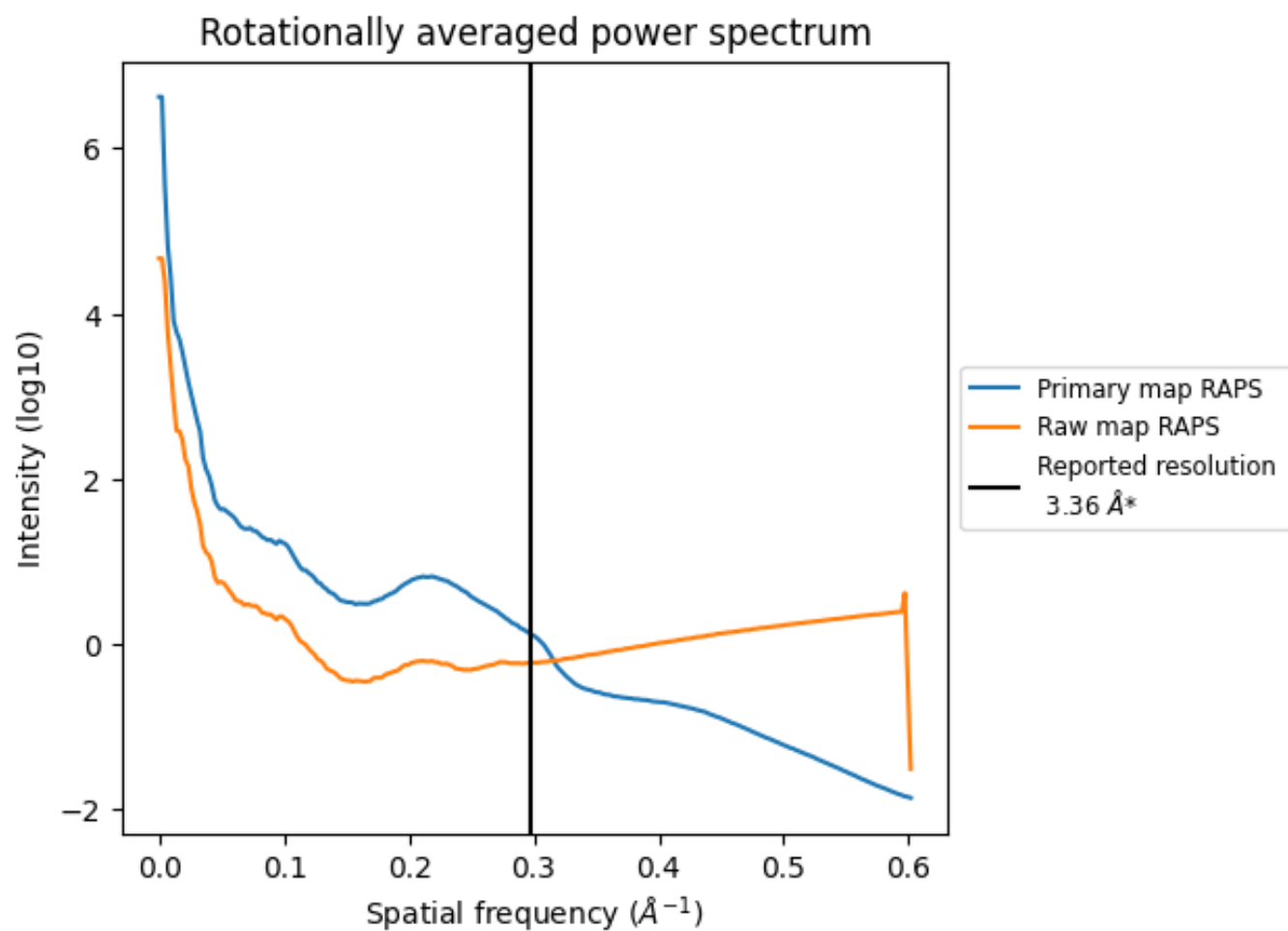
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 808 nm<sup>3</sup>; this corresponds to an approximate mass of 730 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

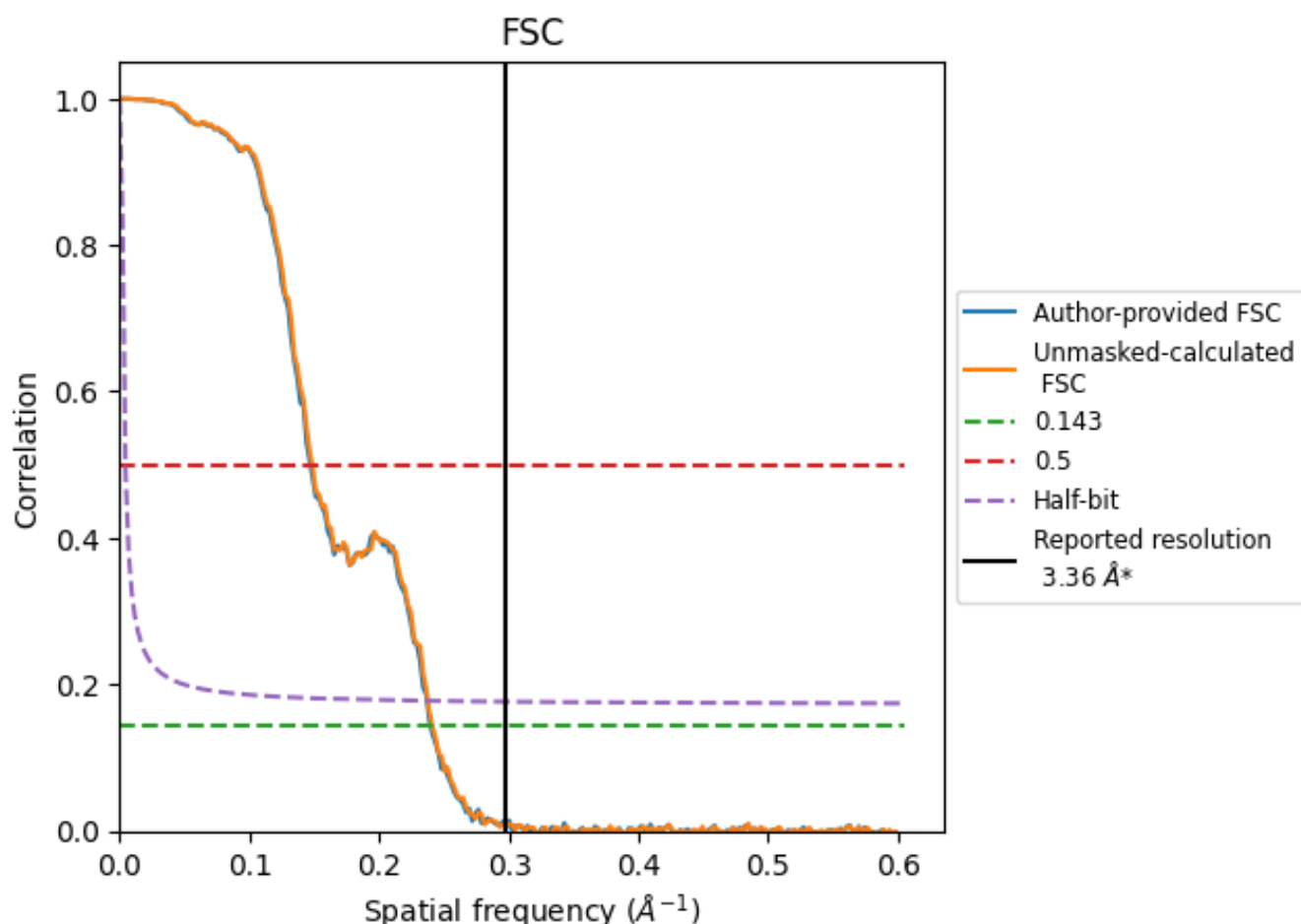


\*Reported resolution corresponds to spatial frequency of 0.298 Å<sup>-1</sup>

## 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 0.298 Å<sup>-1</sup>

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	4.17	6.79	4.22
Unmasked-calculated*	4.15	6.73	4.21

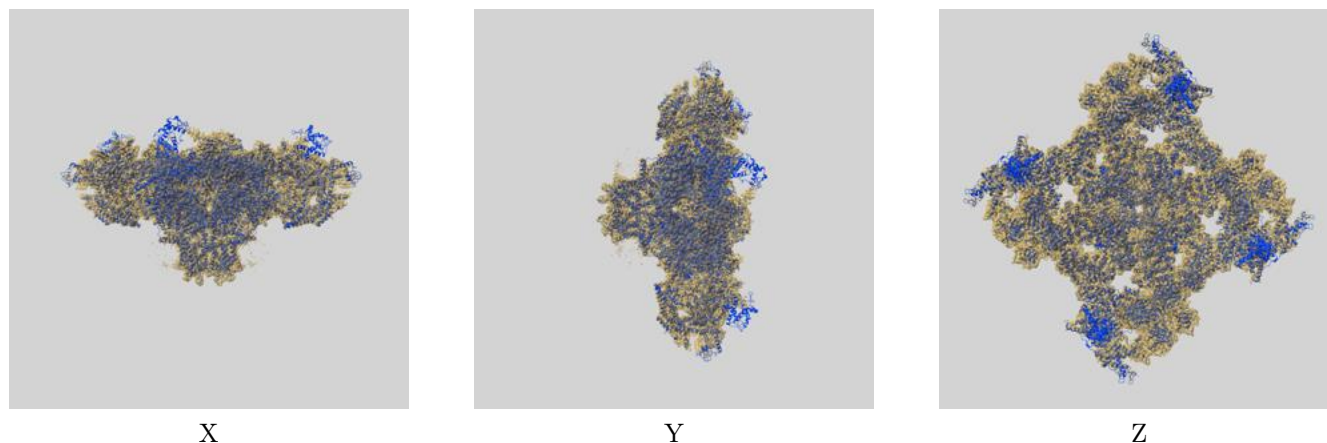
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.36 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.36 by more than 10 %

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

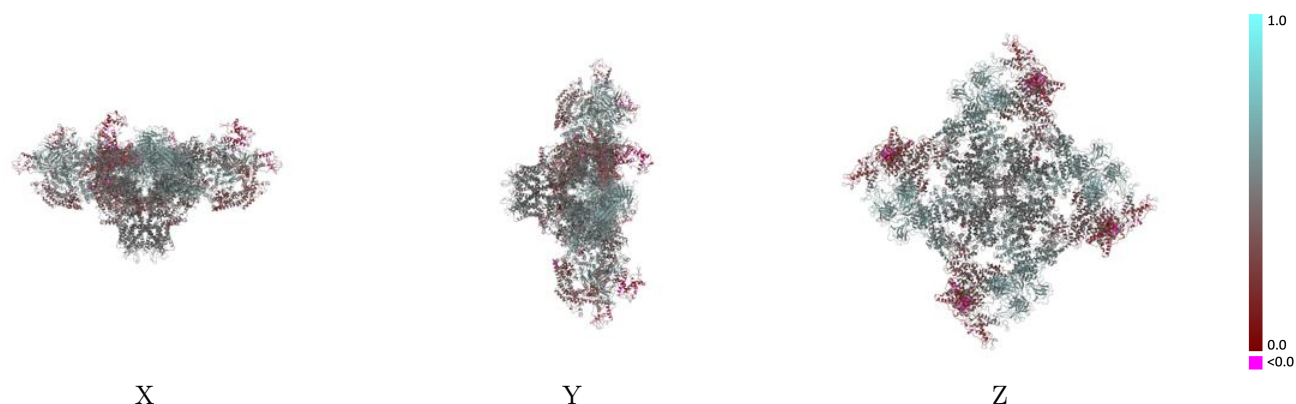
This section contains information regarding the fit between EMDB map EMD-23692 and PDB model 7M6A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



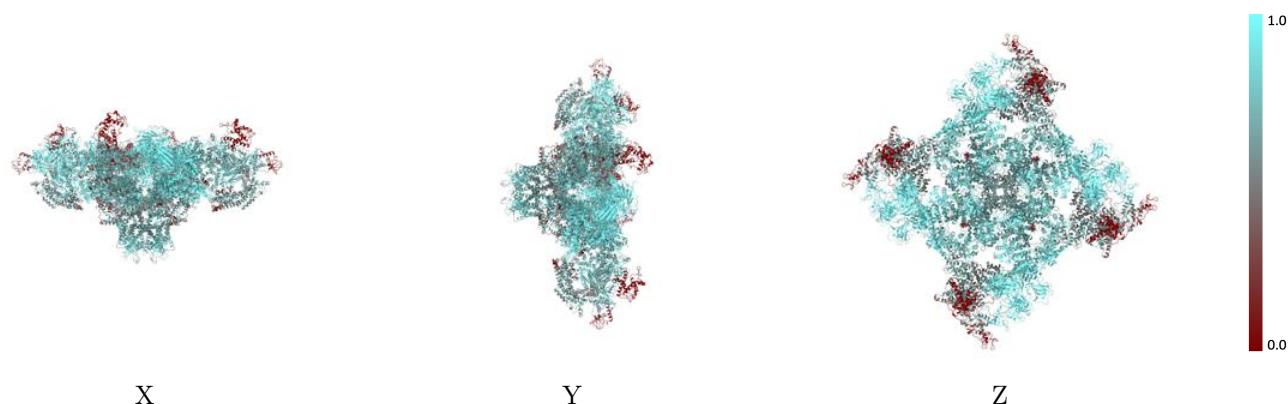
The images above show the 3D surface view of the map at the recommended contour level 0.121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



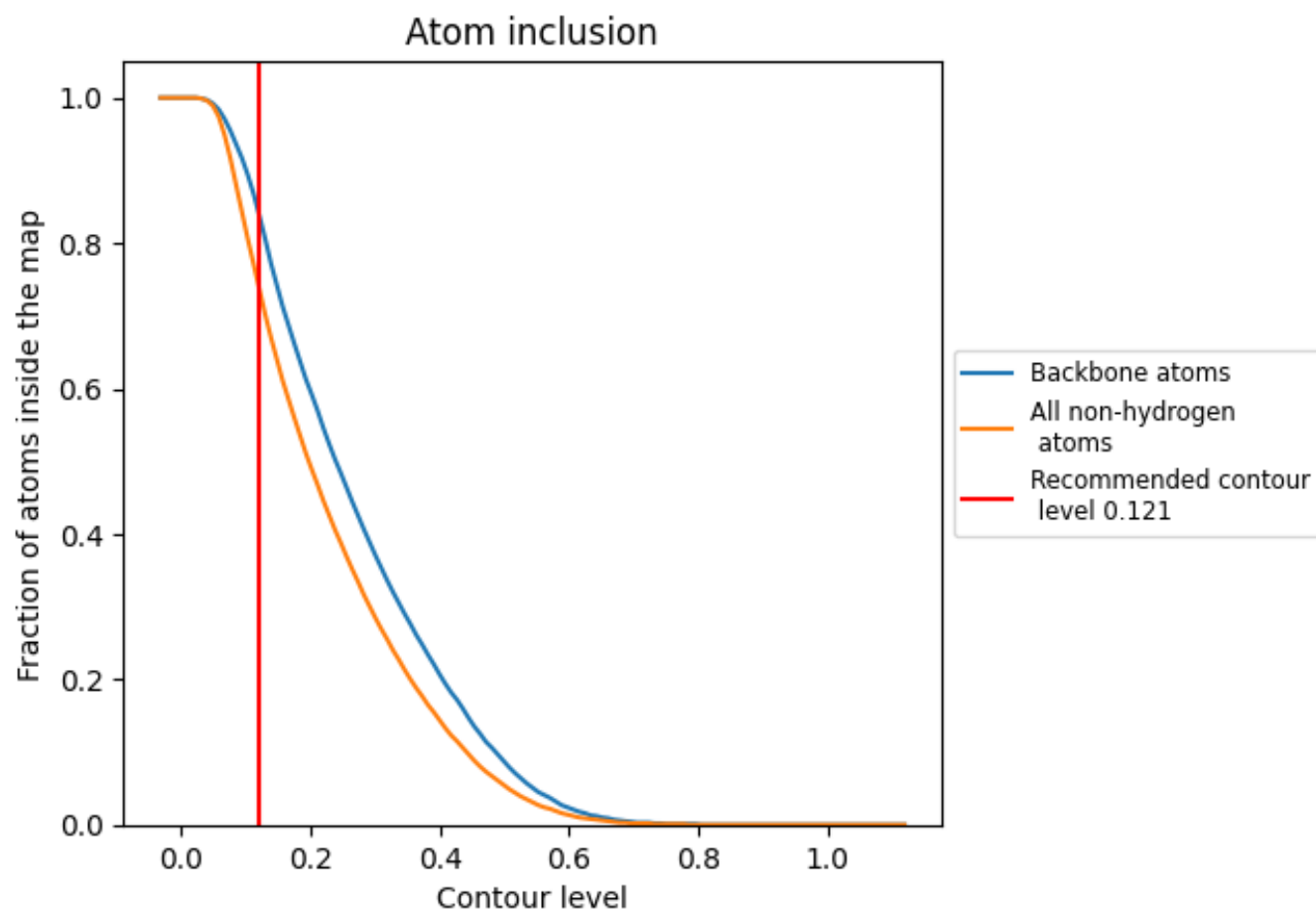
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.121).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.4570
A	<div></div> 0.7320	<div></div> 0.4580
B	<div></div> 0.7300	<div></div> 0.4530
F	<div></div> 0.8820	<div></div> 0.5530
G	<div></div> 0.7320	<div></div> 0.4540
H	<div></div> 0.8670	<div></div> 0.5530
I	<div></div> 0.7310	<div></div> 0.4530
J	<div></div> 0.8780	<div></div> 0.5500
O	<div></div> 0.8820	<div></div> 0.5520

1.0

0.0

<0.0