



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 03:02 AM UTC

PDB ID : 9E1C / pdb_00009e1c
EMDB ID : EMD-47389
Title : Structure of RyR1 in the primed state in the presence of IBMX
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 2.63 Å (reported)
Based on initial model : 7TZC

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

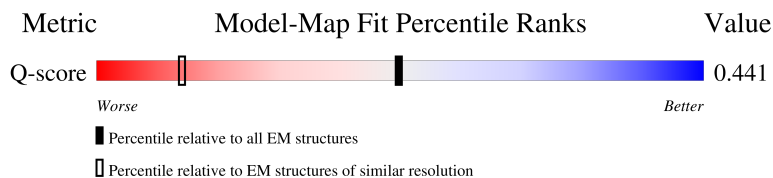
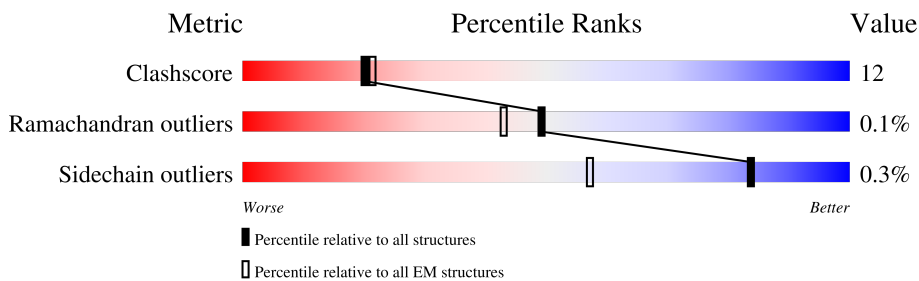
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.63 Å.

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



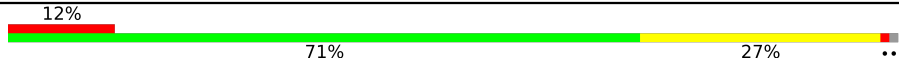

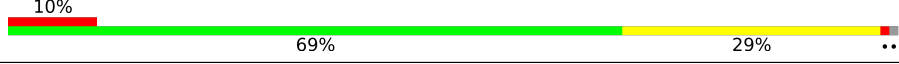
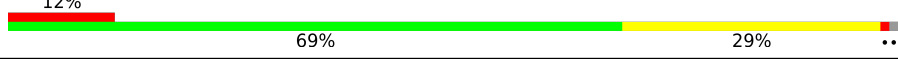
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	108	 12% 71% 27% ..
2	F	108	 11% 71% 27% ..
2	G	108	 10% 69% 29% ..
2	H	108	 12% 69% 29% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 144120 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	4404	35150	22365	6063	6485	237	9	0
1	B	4404	35150	22365	6063	6485	237	9	0
1	D	4404	35150	22365	6063	6485	237	9	0
1	C	4404	35150	22365	6063	6485	237	9	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	831	527	146	154	4	0	0
2	H	107	831	527	146	154	4	0	0
2	G	107	831	527	146	154	4	0	0
2	F	107	831	527	146	154	4	0	0

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



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

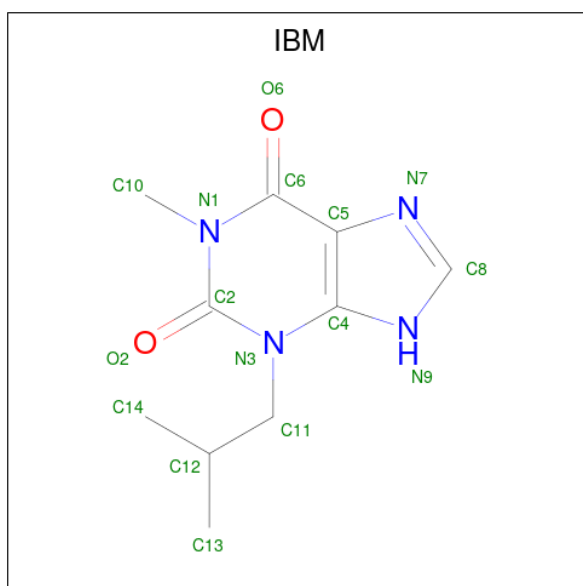
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	Total	Zn	0
			1	1	

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

- Molecule 6 is 3-ISOBUTYL-1-METHYLNANTHINE (CCD ID: IBM) (formula: C₁₀H₁₄N₄O₂) (labeled as "Ligand of Interest" by depositor).

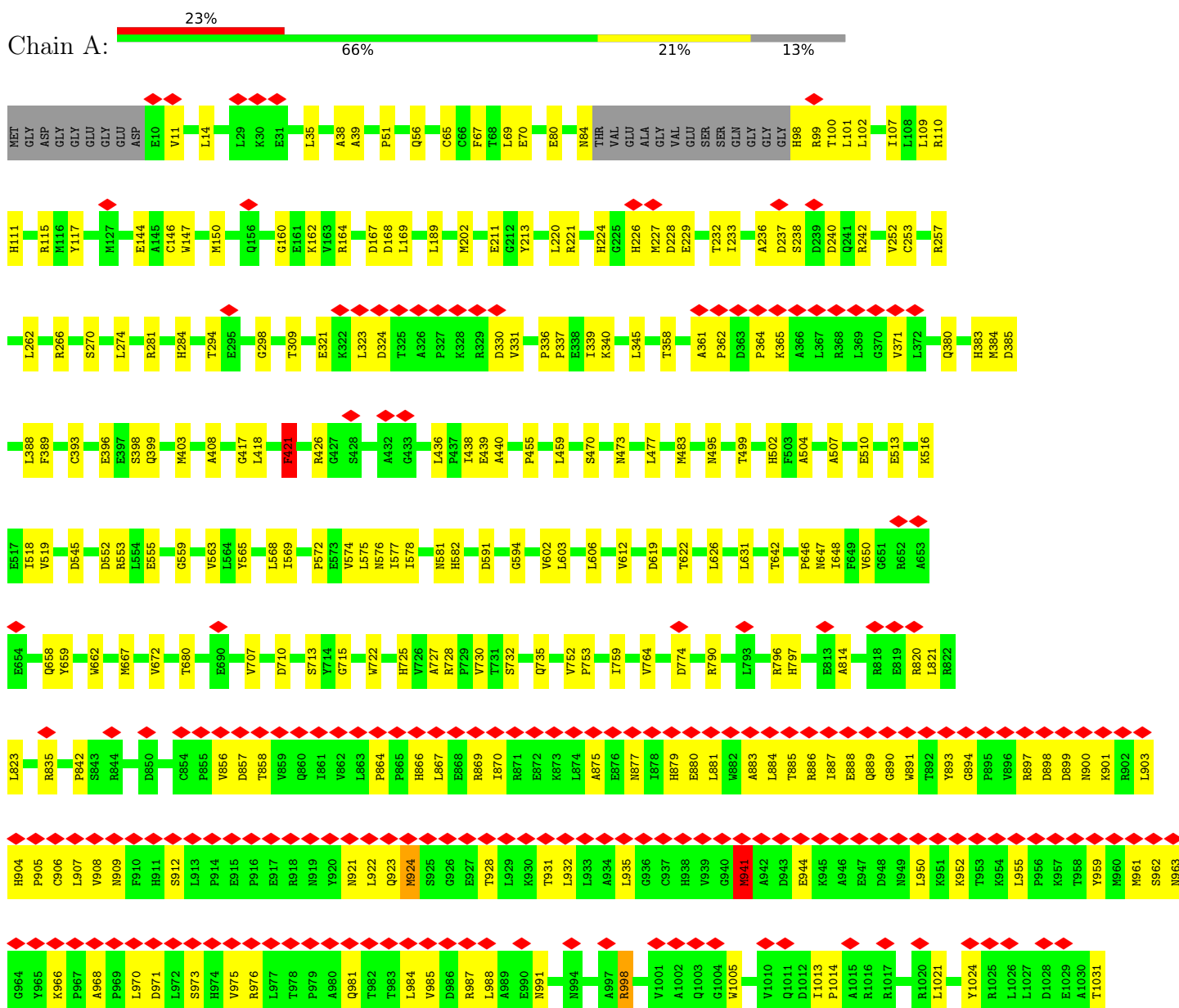


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			16	10	4	2	
6	B	1	Total	C	N	O	0
			16	10	4	2	
6	D	1	Total	C	N	O	0
			16	10	4	2	
6	C	1	Total	C	N	O	0
			16	10	4	2	

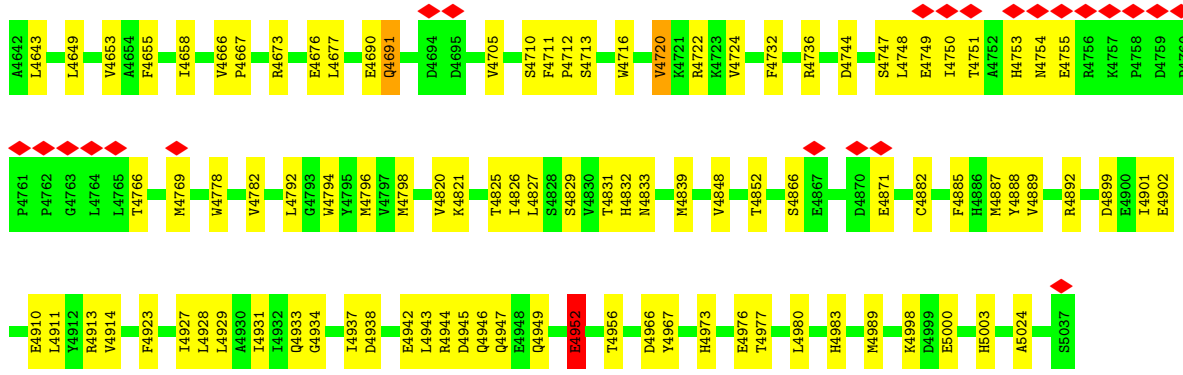
3 Residue-property plots [i](#)

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

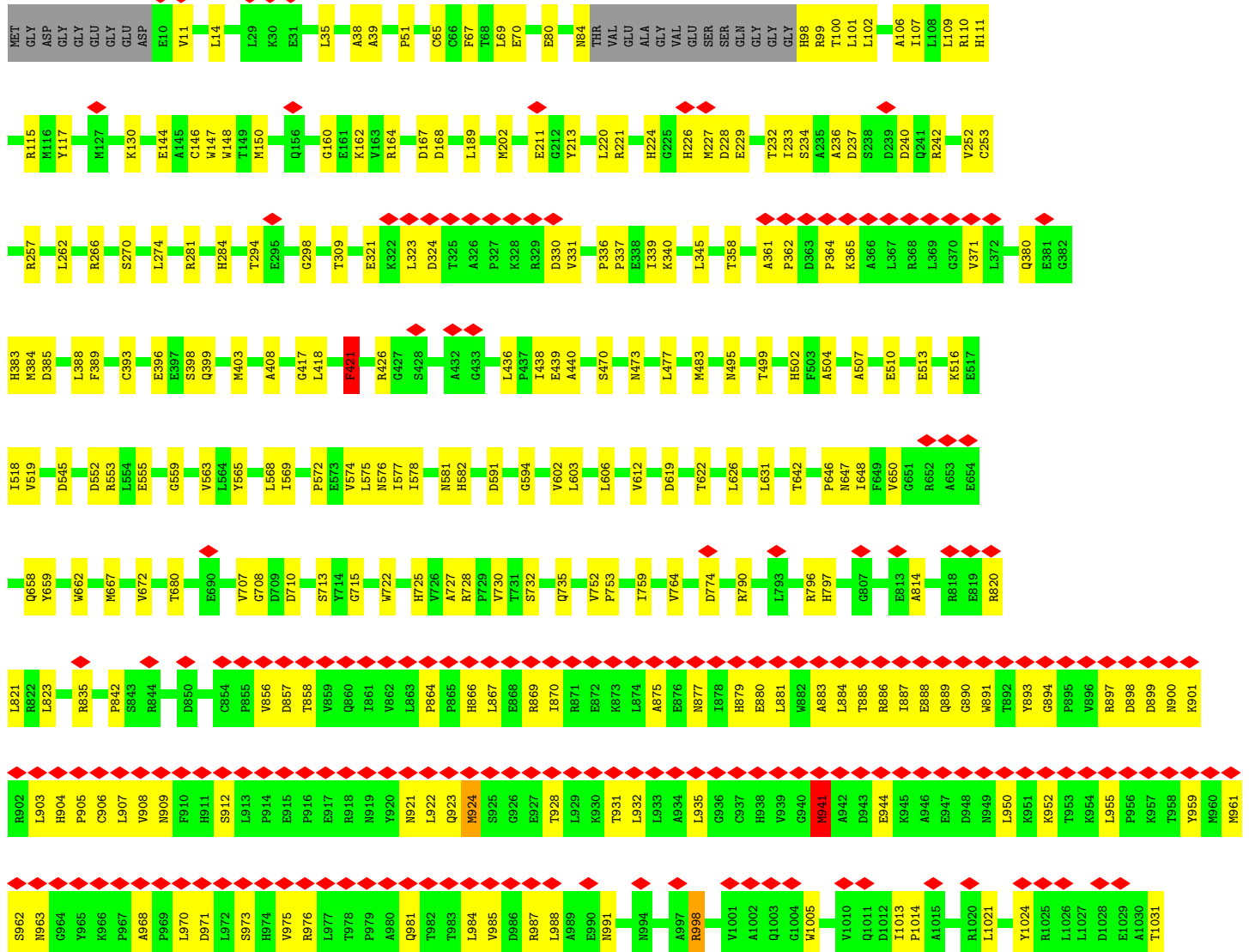
- Molecule 1: Ryanodine receptor 1

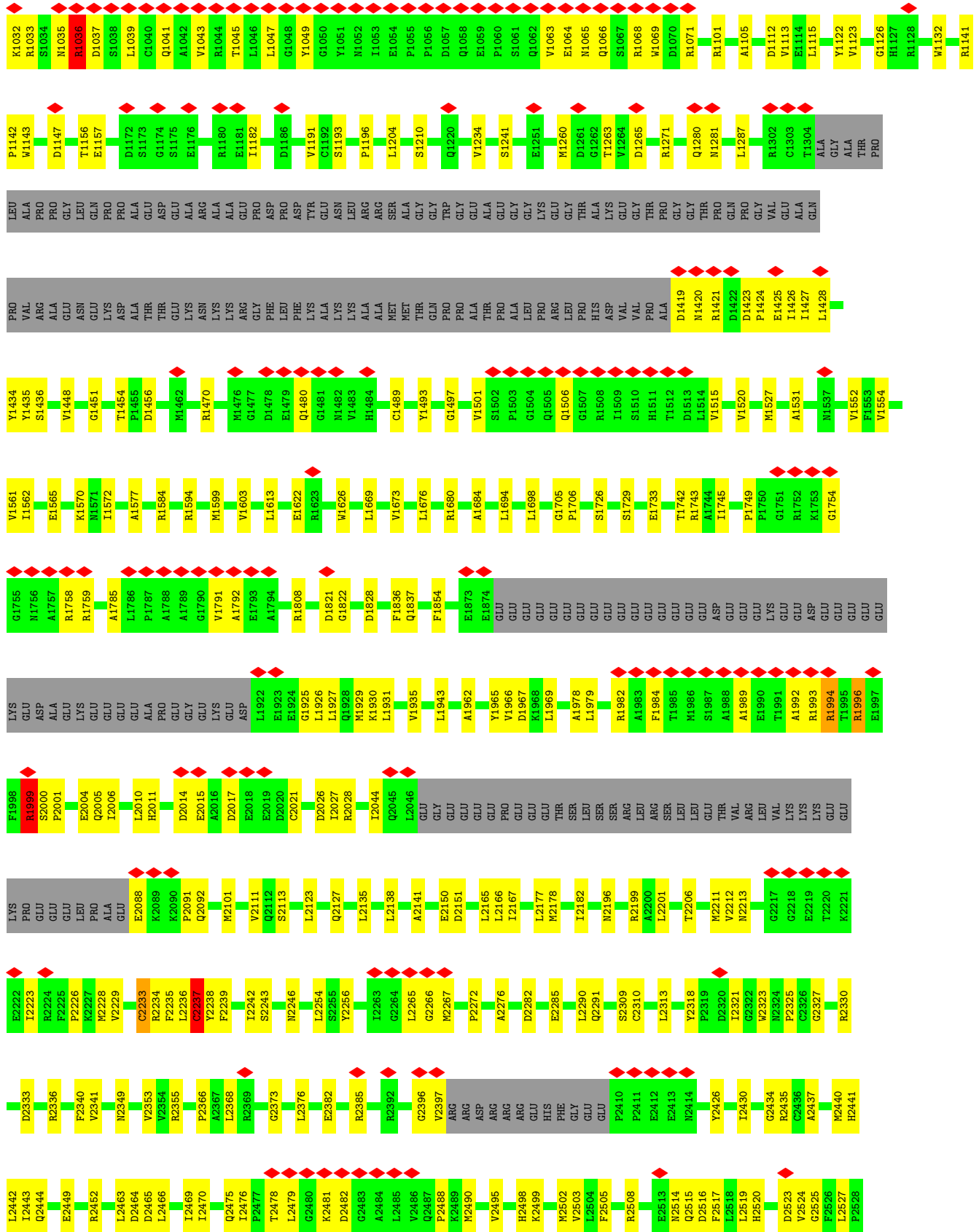


L2562	K2642	P2712	Q2772	E2952	H3013	L3075	A3135	A3200	R3262	I3323
L2568	L2643	D2713	N2773	K2963	C3014	D3076	L3136	M3201	Y3263	V3324
F2569	L2644	Y2714	M2774	R2954	L3015	A3077	L3137	P3202	T3264	N3325
A2570	T2645	Z2715	N2775	F2955	Y3016	R3078	P3138	V3203	E3265	N3326
E2573	H2647	D2716	S2776	F3017	L3018	T3079	V3139	A3204	M3266	L3327
H2574	Y2648	A2717	G2778	R2896	S3019	V3080	L3140	F3205	P3267	G3328
R2575	E2649	S2718	E2779	G2898	T3020	K3081	L3141	L3206	H3268	I3329
A2576	R2650	S2719	E2779	G2899	P3021	K3082	F3144	E3207	V3269	D3330
I2577	C2651	S2720	I2780	F2959	P3022	S3083	F3144	A3208	I3270	E3331
H2578	Y2655	S2721	N2781	L2960	A3022	G3084	Q3145	Q3208	E3271	A3332
S2581	C2656	K2722	D2782	H2902	L2963	F3085	Q3149	Q3209	I3272	T3333
N2582	L2657	A2723	E2783	P2903	L2964	E3086	H3150	L3210	T3273	N3334
L2583	P2658	K2724	E2784	L2904	R2965	I3087	Q3151	E3212	L3274	H3335
H2584	T2659	E2725	L2785	L2905	V2966	V3088	G3026	Y3213	P3275	K3336
T2585	G2660	K2725	L2786	V2906	M2967	K3089	S3027	G3028	M3276	R3337
A2586	Y2666	LYS	K2787	P2907	I2969	G3090	G3029	G3091	H3269	H3338
V2587	S2668	THR	H2788	Y2908	S2970	G3091	G3029	G3091	I3270	I3339
Y2588	E2669	VAL	P2789	D2909	Q2971	L3092	H3030	L3092	I3270	C3340
R2591	H2673	ALA	M2790	T2910	E2972	S3094	A3031	R3093	Y3280	Y3340
O2592	L2674	ALA	L2791	T2911	F2973	F3095	S3032	F3095	L3281	F3341
R2593	L2675	THR	R2792	L2912	Q2974	F3096	N3033	F3096	P3282	A3342
S2594	T2675	GLY	P2793	A2913	L2974	E3097	K3034	F3096	R3283	O3343
L2595	R2676	ASP	Y2794	K2914	H2976	S3098	E3035	D3159	M3284	P3344
R2600	K2677	GLU	K2795	E2915	L2977	A3099	F3036	D3160	W3285	I3345
E2604	L2678	GLY	D2861	K2916	E2978	S3100	F3037	V3161	S3279	Y3346
M2608	I2682	M2734	F2797	A2917	Q2978	E3101	M3038	C3165	L3280	R3347
A2609	F2683	N2735	S2798	R2918	V2980	D3102	L3039	R3167	L3281	R3348
L2610	D2684	Q2858	E2799	D2919	V2981	I3103	L3042	L3168	P3289	G3349
T2614	S2685	Q2859	K2800	E2920	S2982	E3104	F3043	L3169	E3290	A3350
R2615	A2687	D2736	D2801	E2921	G2984	K3105	C3044	C3170	E3226	L3353
H2618	H2688	L2743	K2802	K2922	Q2984	M3106	K3045	S3171	R3227	L3354
L2623	R2689	M2744	E2803	A2923	R2985	V3107	L3046	I3172	A3228	H3357
R2624	K2690	Y2745	E2804	Q2924	Y2986	E3108	A3047	Y3173	G3231	F3358
L2626	Y2691	I2746	L2805	Q2925	K2988	N3109	A3048	S3174	I3232	I3359
V2627	Q2693	L2747	L2806	E2926	K2988	L3110	L3049	L3175	P3233	T3361
F2628	E2694	P2748	R2806	L2926	P2989	R3111	H3052	T3177	M3234	A3298
D2629	E2694	E2749	Q2807	K2927	S2989	G3112	R3053	T3178	S3235	G3299
V2630	L2695	K2750	P2808	L2927	H2991	G3113	V3054	K3179	E3236	A3300
F2631	Y2696	L2751	L2809	F2929	E2992	K3114	V3055	N3180	E3237	P3301
L2632	R2697	D2752	K2810	E2993	E2994	S3115	L3056	T3181	E3238	P3302
P2631	A2698	F2753	E2811	Q2993	E2994	G3116	F3057	Y3182	M3239	P3303
L2633	M2700	S2754	S2812	Q2993	E2995	S3116	L3057	V3183	P3241	C3304
E2635	P2701	L2755	S2812	I2995	K2996	ALA	G3058	V3184	D3242	T3305
L2636	P2702	K2756	E2816	K2996	F2997	ARG	T3059	E3184	L3243	A3306
F2636	L2703	M2756	M2816	Y2935	F2998	THR	D3060	K3185	P3244	V3307
A2637	A2705	L2762	E2818	V2937	A2999	GLN	P3062	L3186	V3245	T3308
K2638	I2706	I2762	E2818	K3000	K3000	VAL	A3061	R3187	L3246	S3309
M2639	E2707	K2762	E2818	I3001	I3001	ALA	A3063	P3188	G3124	D3310
P2640	G2708	H2763	E2818	L3002	L3002	ARG	V3064	P3188	V3125	H3311
L2641	A2709	E2764	E2818	L3003	L3003	THR	V3065	R3189	V3126	L3312
		W2766	E2818	P3004	R3066	ALA	R3066	R3189	G3127	L3313
		K2768	E2818	S3004	C3067	ARG	C3067	R3189	Q3127	H3314
		D2769	E2818	I3006	L3068	THR	L3068	R3190	N3128	I3315
		K2770	E2818	I3007	H3069	VAL	H3069	L3190	L3129	H3316
		E2828	E2818	L3007	T3070	ALA	T3070	L3191	L3129	L3317
		E2829	E2818	L3008	L3071	ARG	L3071	L3191	L3129	L3318
		E2830	E2818	L3009	A3072	THR	A3072	L3191	L3129	L3319
			E2818	L3010	R3073	VAL	R3073	L3191	L3129	L3320
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			E2818	L3012		ARG		L3191	L3129	L3322

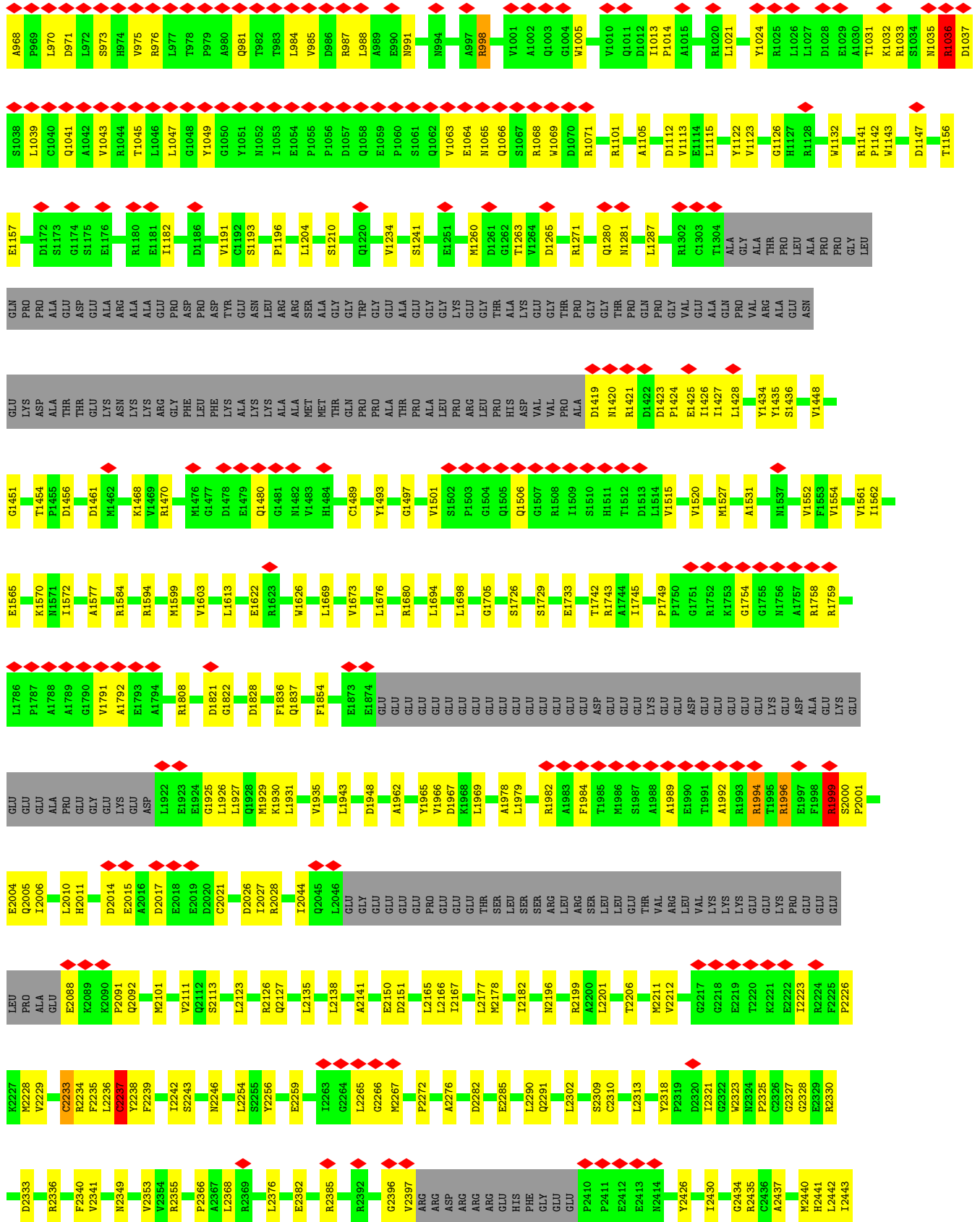


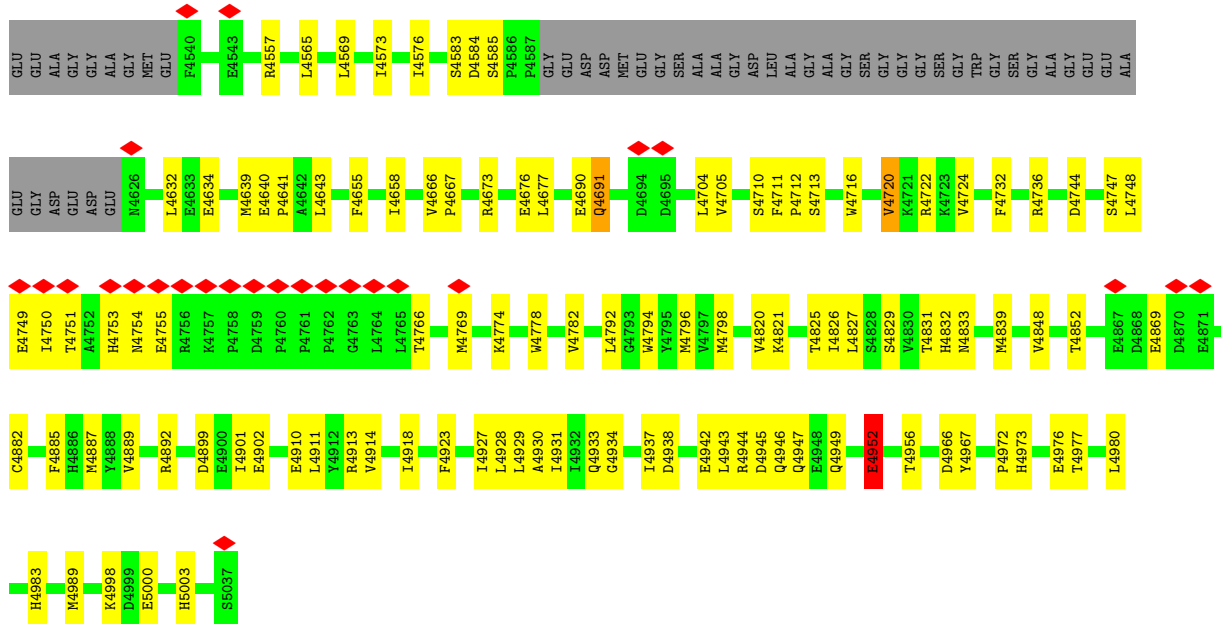
• Molecule 1: Ryanodine receptor 1



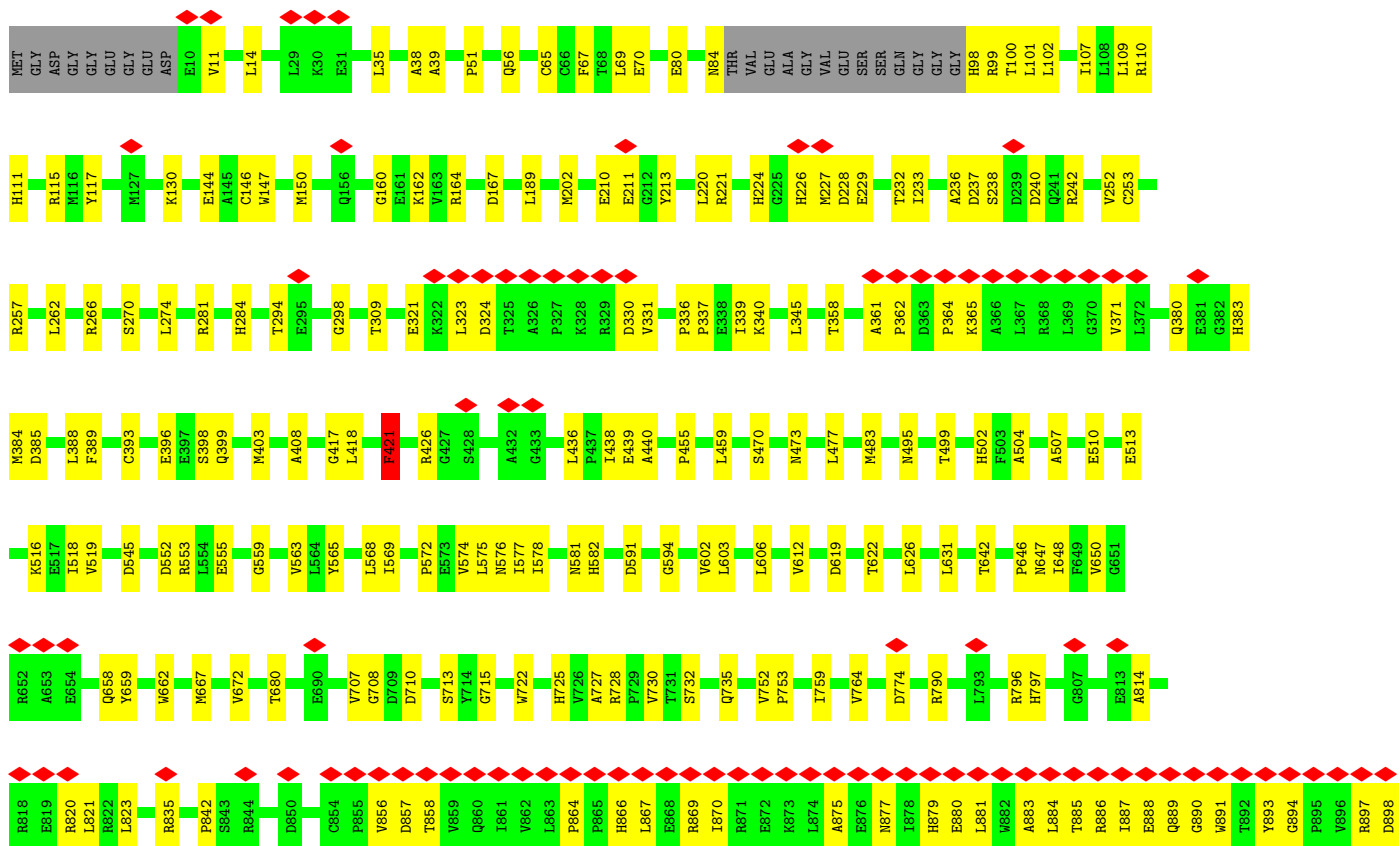


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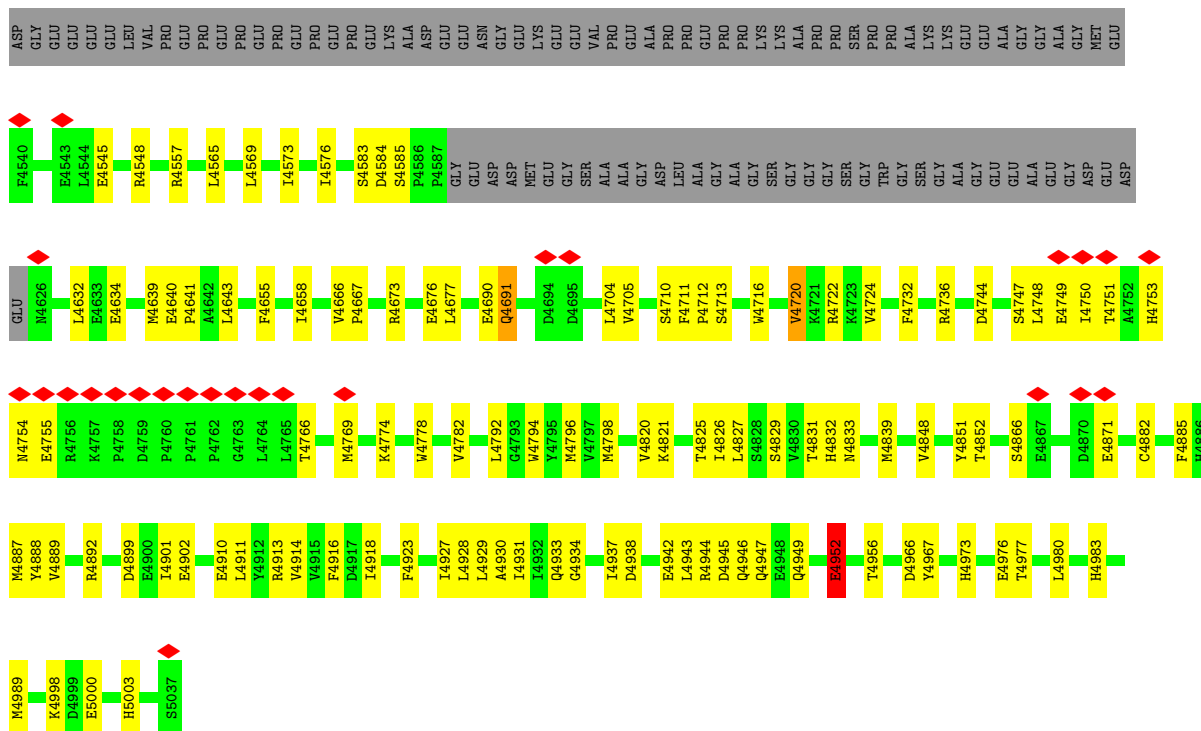




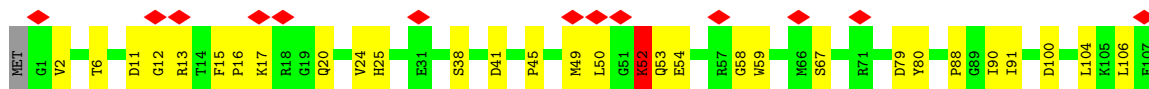
• Molecule 1: Ryanodine receptor 1



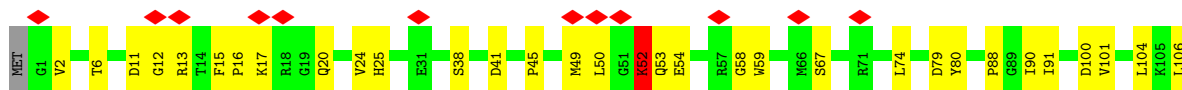
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VAL	GLY	GLY	ALA	ALA	G4225	K4060	F3899	M3758	K6668	G3579	V3611	N3450	E3375	L3312	L3249
GLY	GLY	GLY	LEU	LEU	F4062	F4061	T3905	R3762	D3666	P3580	L3614	F3451	E3376	N3313	M3250
HIS	LEU	VAL	GLY	ARG	G4227	M4064	T3912	R3765	D3671	G3581	K3515	K3452	E3377	L3316	M3251
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ALA	GLY	TYR	GLY	TYR	T4241	K4069	L3924	R3769	R3673	R3583	L3379	R3454	Q3378	G3317	I3253
ALA	GLY	ARG	GLY	ARG	I4242	D4070	Q3927	R3773	R3674	E3585	L3380	R3455	Q3379	N3318	A3267
PRO	PRO	ARG	LYS	SER	M4245	I4071	Q3927	R3773	E3684	D3586	L3320	E3456	Q3380	I3319	E3258
VAL	VAL	ARG	VAL	ARG	M4253	G4086	D3941	M3782	E3685	D3587	L3381	E3455	E3382	L3321	G3269
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GLY	GLY	THR	ARG	ARG	GLY	K4091	Q3946	C3786	E3687	P3527	L3383	E3456	E3384	I3323	A3261
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GLU	GLU	ARG	ARG	ARG	GLY	K4095	R3949	G3791	E3688	T3528	L3385	E3456	E3386	N3325	Y3263
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LEU	LEU	ARG	ARG	ARG	GLY	S4099	S3952	V3794	V3690	Q3531	L3388	E3456	E3389	G3328	E3265
LEU	LEU	ARG	ARG	ARG	ASP	S4099	S3952	V3794	E3691	D3532	L3389	E3456	E3390	G3329	M3266
LEU	LEU	ARG	ARG	ARG	GLY	F4110	K3953	Q3813	E3692	L3533	L3390	E3456	E3391	I3329	F3267
LEU	LEU	ARG	ARG	ARG	GLY	F4110	V3957	L3817	E3693	L3534	L3391	E3456	E3392	D3330	H3268
LEU	LEU	ARG	ARG	ARG	GLY	E4121	V3961	D3822	E3694	L3535	L3392	E3456	E3393	D3331	H3269
LEU	LEU	ARG	ARG	ARG	GLY	M4122	V3961	D3823	K3694	L3536	L3393	E3456	E3394	A3332	I3270
LEU	LEU	ARG	ARG	ARG	GLY	F4125	V3967	K3824	E3695	L3537	L3394	E3456	E3395	A3333	I3271
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LEU	LEU	ARG	ARG	ARG	GLY	E3969	I3969	E3827	E3699	Y3540	L3398	E3456	E3399	M3337	L3275
LEU	LEU	ARG	ARG	ARG	GLY	E3970	Q3970	S3831	E3709	Y3541	L3399	E3456	E3400	M3338	L3276
LEU	LEU	ARG	ARG	ARG	GLY	E3971	V3957	S3832	A3709	Y3542	L3400	E3456	E3401	M3339	C3278
LEU	LEU	ARG	ARG	ARG	GLY	E3972	V3961	S3833	A3710	Y3543	L3401	E3456	E3402	M3340	S3279
LEU	LEU	ARG	ARG	ARG	GLY	E3973	V3967	S3834	A3711	Y3544	L3402	E3456	E3403	M3341	Y3280
LEU	LEU	ARG	ARG	ARG	GLY	E3974	V3967	S3835	A3712	Y3545	L3403	E3456	E3404	M3342	R3283
LEU	LEU	ARG	ARG	ARG	GLY	E3975	V3967	S3836	A3713	Y3546	L3404	E3456	E3405	M3343	K3284
LEU	LEU	ARG	ARG	ARG	GLY	E3976	V3967	S3837	A3714	Y3547	L3405	E3456	E3406	M3344	M3285
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LEU	LEU	ARG	ARG	ARG	GLY	E3982	V3967	S3843	A3720	Y3553	L3411	E3456	E3412	M3350	A3291
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LEU	LEU	ARG	ARG	ARG	GLY	E3985	V3967	S3846	A3723	Y3556	L3414	E3456	E3415	M3353	P3294
LEU	LEU	ARG	ARG	ARG	GLY	E3986	V3967	S3847	A3724	Y3557	L3415	E3456	E3416	M3354	A3295
LEU	LEU	ARG	ARG	ARG	GLY	E3987	V3967	S3848	A3725	Y3558	L3416	E3456	E3417	M3355	L3296
LEU	LEU	ARG	ARG	ARG	GLY	E3988	V3967	S3849	A3726	Y3559	L3417	E3456	E3418	M3356	P3297
LEU	LEU	ARG	ARG	ARG	GLY	E3989	V3967	S3850	A3727	Y3560	L3418	E3456	E3419	M3357	G3298
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LEU	LEU	ARG	ARG	ARG	GLY	E3992	V3967	S3853	A3730	Y3563	L3421	E3456	E3422	M3360	P3301
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LEU	LEU	ARG	ARG	ARG	GLY	E3999	V3967	S3860	A3737	Y3570	L3428	E3456	E3429	M3367	P3308
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LEU	LEU	ARG	ARG	ARG	GLY	E4001	V3967	S3862	A3739	Y3572	L3430	E3456	E3431	M3369	C3304
LEU	LEU	ARG	ARG	ARG	GLY	E4002	V3967	S3863	A3740	Y3573	L3431	E3456	E3432	M3370	T3305
LEU	LEU	ARG	ARG	ARG	GLY	E4003	V3967	S3864	A3741	Y3574	L3432	E3456	E3433	M3371	A3306
LEU	LEU	ARG	ARG	ARG	GLY	E4004	V3967	S3865	A3742	Y3575	L3433	E3456	E3434	M3372	P3307
LEU	LEU	ARG	ARG	ARG	GLY	E4005	V3967	S3866	A3743	Y3576	L3434	E3456	E3435	M3373	I3307
LEU	LEU	ARG	ARG	ARG	GLY	E4006	V3967	S3867	A3744	Y3577	L3435	E3456	E3436	M3374	P3308
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LEU	LEU	ARG	ARG	ARG	GLY	E4008	V3967	S3869	A3746	Y3579	L3437	E3456	E3438	M3376	T3305
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LEU	LEU	ARG	ARG	ARG	GLY	E4011	V3967	S3872	A3749	Y3582	L3440	E3456	E3441	M3379	P3302
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LEU	LEU	ARG	ARG	ARG	GLY	E4013	V3967	S3874	A3751	Y3584	L3442	E3456	E3443	M3381	C3304
LEU	LEU	ARG	ARG	ARG	GLY	E4014	V3967	S3875	A3752	Y3585	L3443	E3456	E3444	M3382	T3305
LEU	LEU	ARG	ARG	ARG	GLY	E4015	V3967	S3876	A3753	Y3586	L3444	E3456	E3445	M3383	A3306
LEU	LEU	ARG	ARG	ARG	GLY	E4016	V3967	S3877	A3754	Y3587	L3445	E3456	E3446	M3384	P3301
LEU	LEU	ARG	ARG	ARG	GLY	E4017	V3967	S3878	A3755	Y3588	L3446	E3456	E3447	M3385	P3302
LEU	LEU	ARG	ARG	ARG	GLY	E4018	V3967	S3879	A3756	Y3589	L3447	E3456	E3448	M3386	P3303
LEU	LEU	ARG	ARG	ARG	GLY	E4019	V3967	S3880	A3757	Y3590	L3448	E3456	E3449	M3387	C3304
LEU	LEU	ARG	ARG	ARG	GLY	E4020	V3967	S3881	A3758	Y3591	L3449	E3456	E3450	M3388	T3305
LEU	LEU	ARG	ARG	ARG	GLY	E4021	V3967	S3882	A3759	Y3592	L3450	E3456	E3451	M3389	A3306
LEU	LEU	ARG	ARG	ARG	GLY	E4022	V3967	S3883	A3760	Y3593	L3451	E3456	E3452		



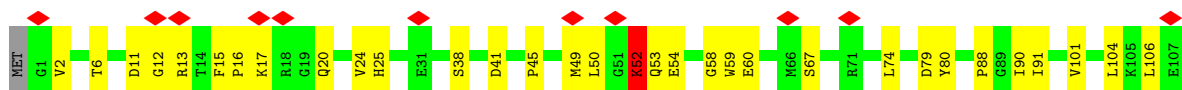
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



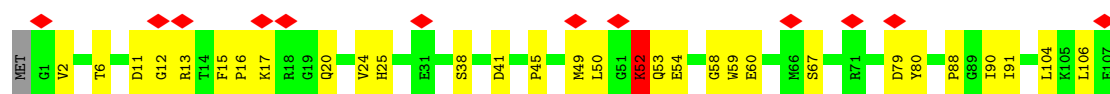
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128983	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.485	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.835, 0.835, 0.835	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	1/35977 (0.0%)	0.46	26/48726 (0.1%)
1	B	0.21	1/35977 (0.0%)	0.46	28/48726 (0.1%)
1	C	0.21	1/35977 (0.0%)	0.46	26/48726 (0.1%)
1	D	0.21	1/35977 (0.0%)	0.46	24/48726 (0.0%)
2	E	0.37	0/850	0.70	2/1146 (0.2%)
2	F	0.37	0/850	0.70	2/1146 (0.2%)
2	G	0.37	0/850	0.70	2/1146 (0.2%)
2	H	0.37	0/850	0.70	2/1146 (0.2%)
All	All	0.22	4/147308 (0.0%)	0.47	112/199488 (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
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1999	ARG	CB-CG	5.45	1.68	1.52
1	A	1999	ARG	CB-CG	5.42	1.68	1.52
1	C	1999	ARG	CB-CG	5.42	1.68	1.52
1	B	1999	ARG	CB-CG	5.40	1.68	1.52

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	998	ARG	CG-CD-NE	12.45	139.38	112.00
1	A	998	ARG	CG-CD-NE	12.44	139.36	112.00
1	B	998	ARG	CG-CD-NE	12.43	139.35	112.00
1	C	998	ARG	CG-CD-NE	12.42	139.32	112.00
1	B	998	ARG	CB-CG-CD	11.95	138.77	111.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1994	ARG	Sidechain
1	A	1996	ARG	Sidechain
1	A	1999	ARG	Sidechain
1	A	2237	CYS	Peptide
1	A	421	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35150	0	34793	876	0
1	B	35150	0	34793	884	0
1	C	35150	0	34793	871	0
1	D	35150	0	34793	870	0
2	E	831	0	831	19	0
2	F	831	0	831	22	0
2	G	831	0	831	21	0
2	H	831	0	831	20	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	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
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	16	0	14	2	0
6	B	16	0	14	2	0
6	C	16	0	14	2	0
6	D	16	0	14	2	0
All	All	144120	0	142600	3527	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 12.

The worst 5 of 3527 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1032:LYS:HB3	1:D:1036:ARG:HH12	1.14	1.13
1:A:935:LEU:HD13	1:A:987:ARG:HE	1.16	1.10
1:C:1032:LYS:HB3	1:C:1036:ARG:HH12	1.14	1.09
1:B:935:LEU:HD13	1:B:987:ARG:HE	1.16	1.08
1:A:1032:LYS:HB3	1:A:1036:ARG:HH12	1.14	1.08

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	4385/5037 (87%)	4245 (97%)	136 (3%)	4 (0%)	48	64
1	B	4385/5037 (87%)	4245 (97%)	136 (3%)	4 (0%)	48	64
1	C	4385/5037 (87%)	4245 (97%)	136 (3%)	4 (0%)	48	64
1	D	4385/5037 (87%)	4245 (97%)	136 (3%)	4 (0%)	48	64
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	G	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
All	All	17960/20580 (87%)	17376 (97%)	568 (3%)	16 (0%)	49	64

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3300	ALA
1	B	3300	ALA
1	D	3300	ALA
1	C	3300	ALA
1	A	2669	GLU

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	3836/4276 (90%)	3824 (100%)	12 (0%)	86	93
1	B	3836/4276 (90%)	3824 (100%)	12 (0%)	86	93
1	C	3836/4276 (90%)	3824 (100%)	12 (0%)	86	93
1	D	3836/4276 (90%)	3824 (100%)	12 (0%)	86	93
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	66
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	66
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	66
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	66
All	All	15700/17464 (90%)	15644 (100%)	56 (0%)	84	91

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3951	PHE

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Mol	Chain	Res	Type
1	C	4952	GLU
1	D	998	ARG
1	C	4720	VAL
1	C	2870[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3683	GLN
1	C	1691	GLN
1	D	4100	GLN
1	C	461	HIS
1	C	3109	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	C	5301	-	32,33,33	0.28	0	48,52,52	0.76	1 (2%)
3	ATP	B	5301	-	32,33,33	0.28	0	48,52,52	0.76	1 (2%)
3	ATP	D	5301	-	32,33,33	0.28	0	48,52,52	0.76	1 (2%)
6	IBM	B	5304	-	17,17,17	0.66	0	19,25,25	0.93	1 (5%)
6	IBM	C	5304	-	17,17,17	0.66	0	19,25,25	0.92	1 (5%)
6	IBM	D	5304	-	17,17,17	0.66	0	19,25,25	0.93	1 (5%)
3	ATP	A	5301	-	32,33,33	0.28	0	48,52,52	0.76	1 (2%)
6	IBM	A	5304	-	17,17,17	0.67	0	19,25,25	0.92	1 (5%)

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	C	5301	-	-	8/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	8/22/38/38	0/3/3/3
3	ATP	D	5301	-	-	8/22/38/38	0/3/3/3
6	IBM	B	5304	-	-	2/4/4/4	0/2/2/2
6	IBM	C	5304	-	-	2/4/4/4	0/2/2/2
6	IBM	D	5304	-	-	2/4/4/4	0/2/2/2
3	ATP	A	5301	-	-	8/22/38/38	0/3/3/3
6	IBM	A	5304	-	-	2/4/4/4	0/2/2/2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5304	IBM	N9-C4-N3	3.14	132.37	127.81
6	D	5304	IBM	N9-C4-N3	3.14	132.37	127.81
6	C	5304	IBM	N9-C4-N3	3.14	132.37	127.81
6	A	5304	IBM	N9-C4-N3	3.14	132.37	127.81
3	D	5301	ATP	O2'-C2'-C3'	-2.26	104.57	111.82

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

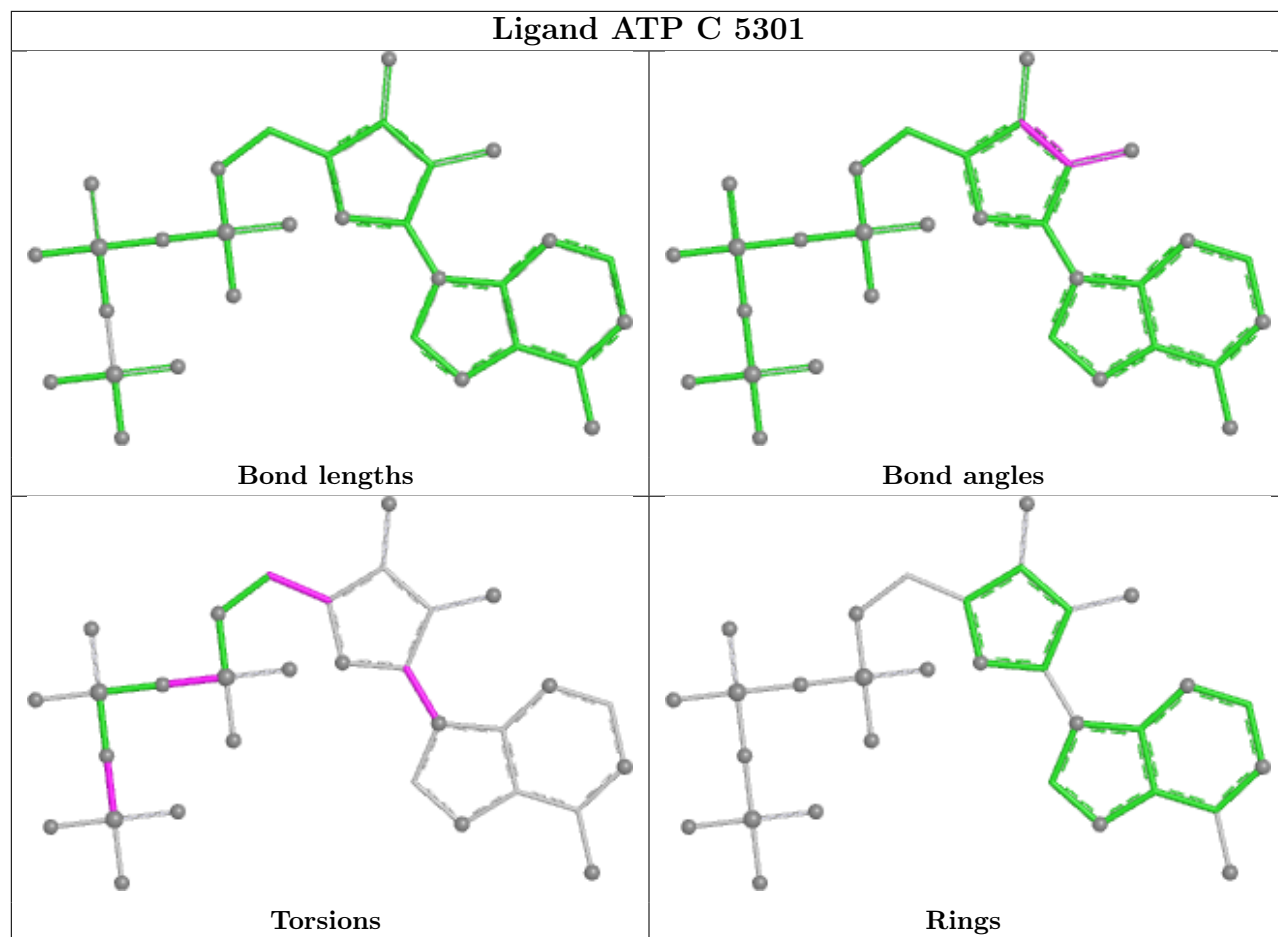
Mol	Chain	Res	Type	Atoms
6	A	5304	IBM	N3-C11-C12-C14
6	B	5304	IBM	N3-C11-C12-C14
6	D	5304	IBM	N3-C11-C12-C14
6	C	5304	IBM	N3-C11-C12-C14
6	A	5304	IBM	N3-C11-C12-C13

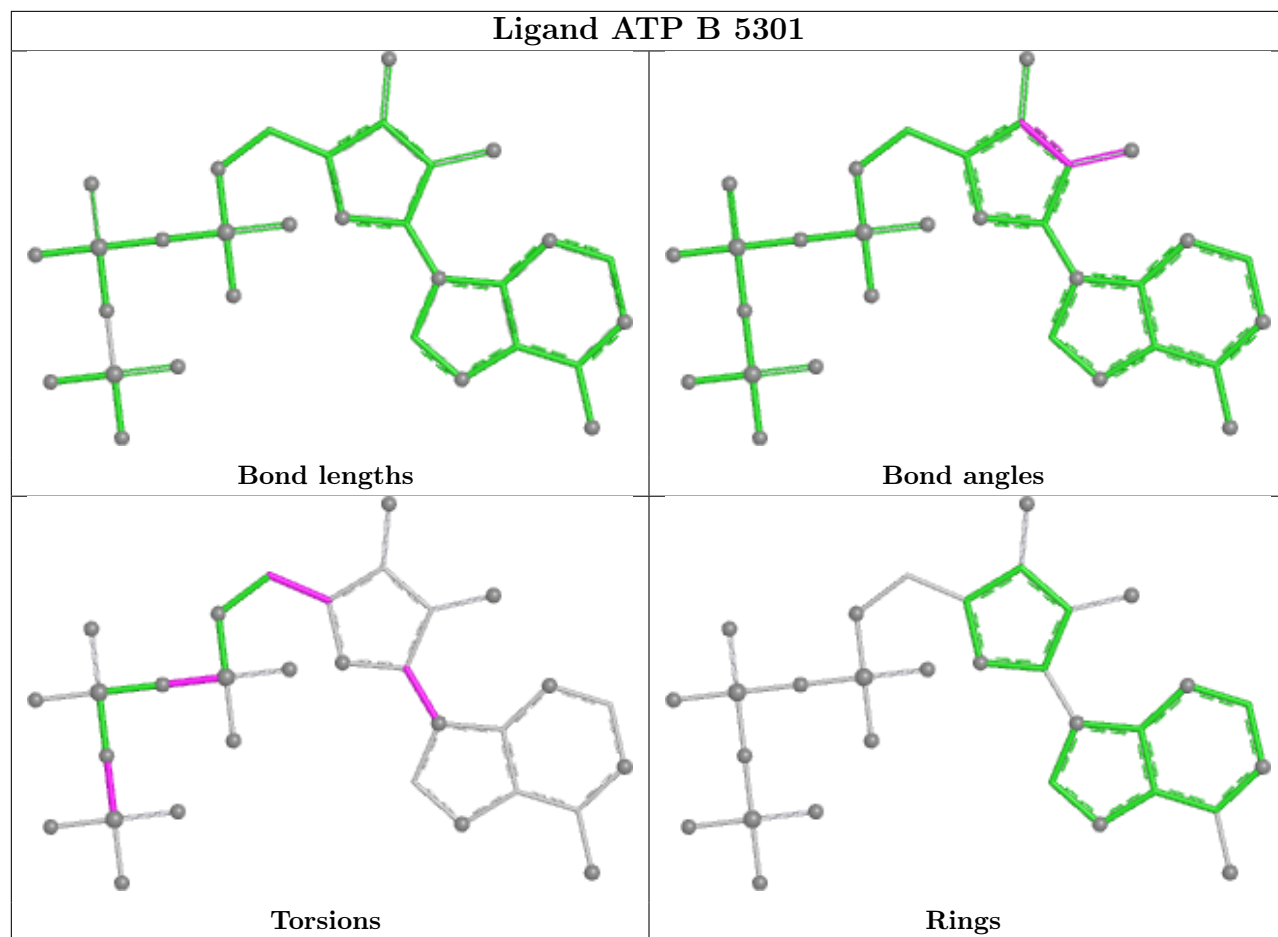
There are no ring outliers.

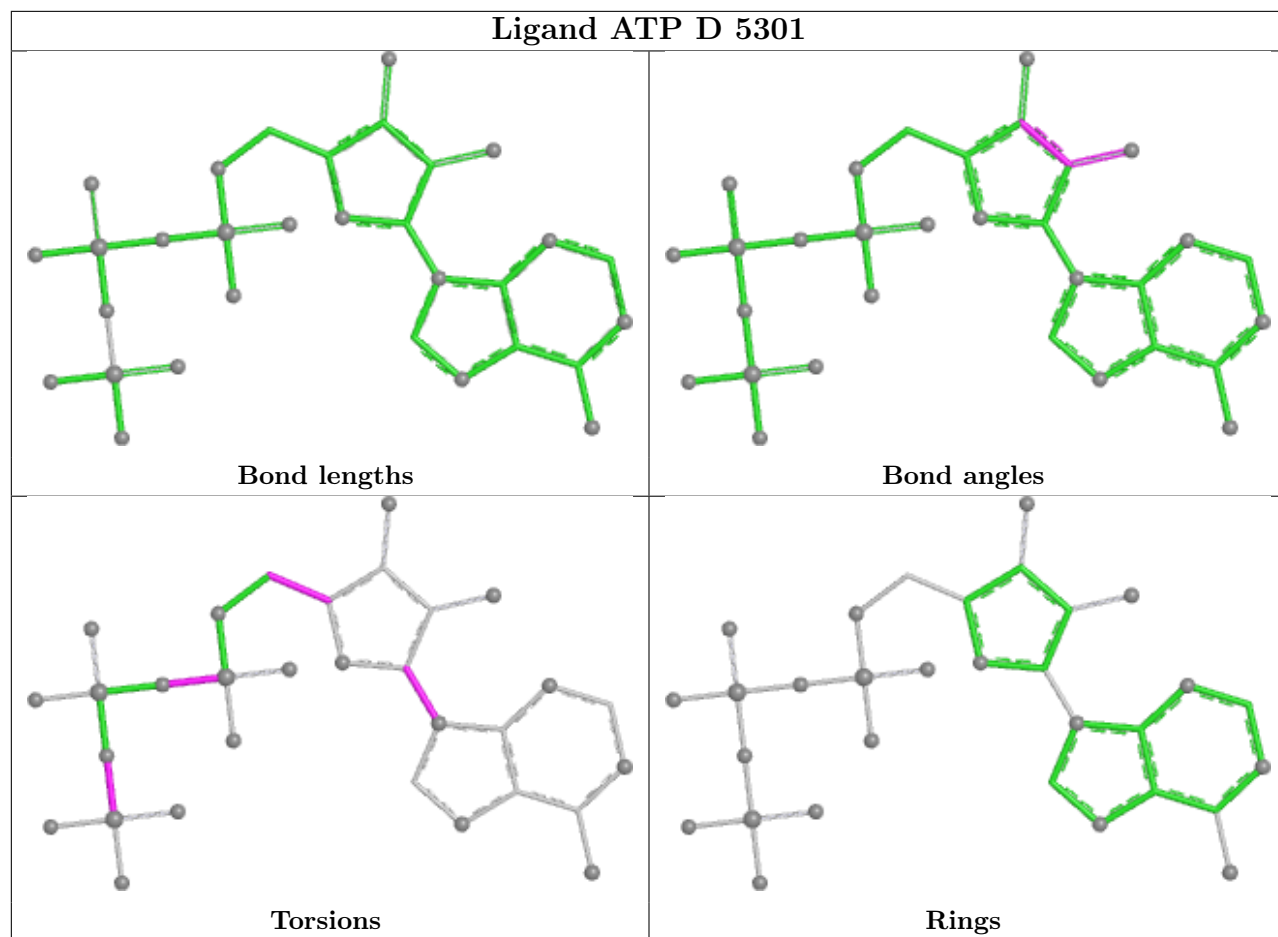
8 monomers are involved in 12 short contacts:

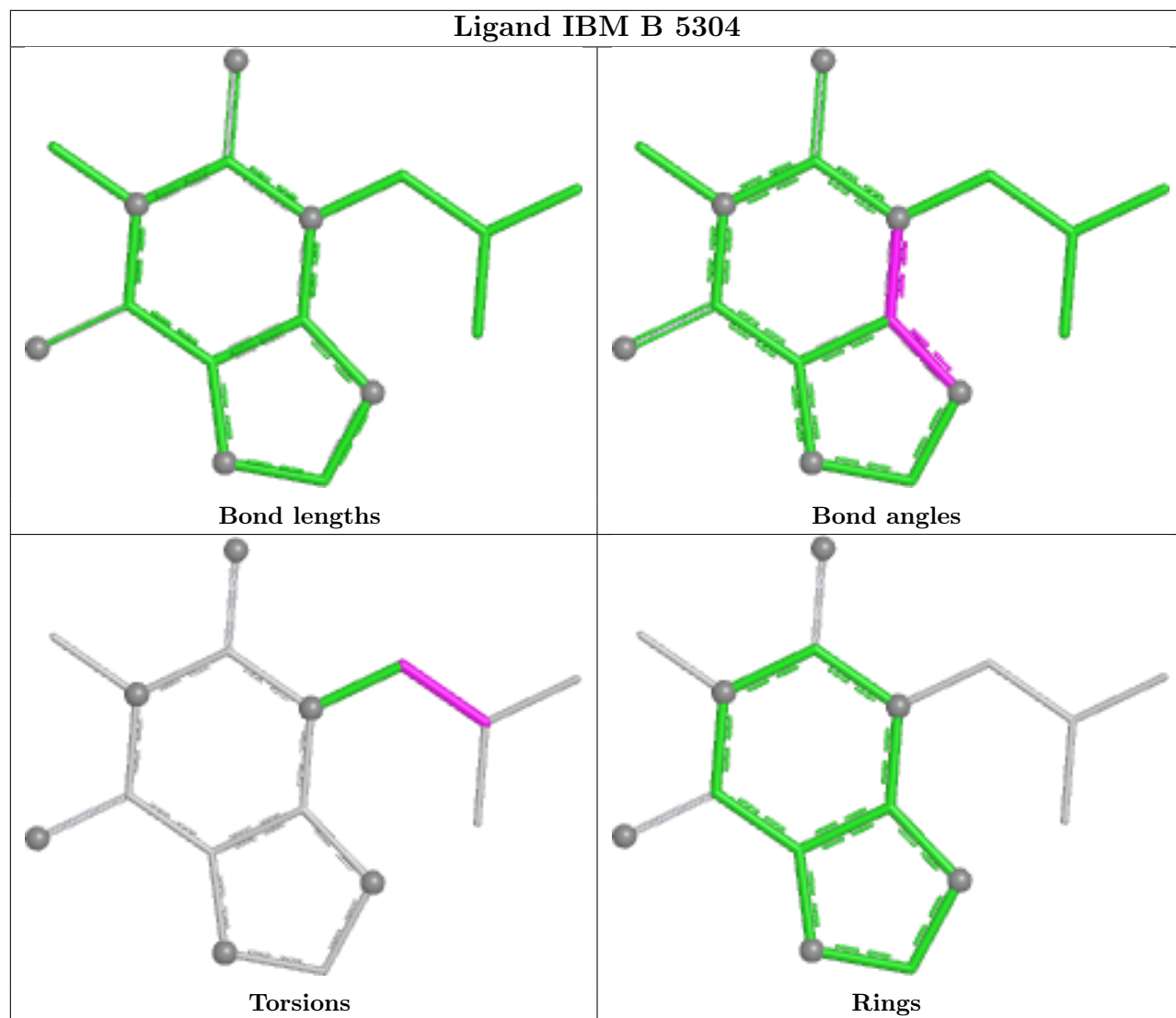
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5301	ATP	1	0
3	B	5301	ATP	1	0
3	D	5301	ATP	1	0
6	B	5304	IBM	2	0
6	C	5304	IBM	2	0
6	D	5304	IBM	2	0
3	A	5301	ATP	1	0
6	A	5304	IBM	2	0

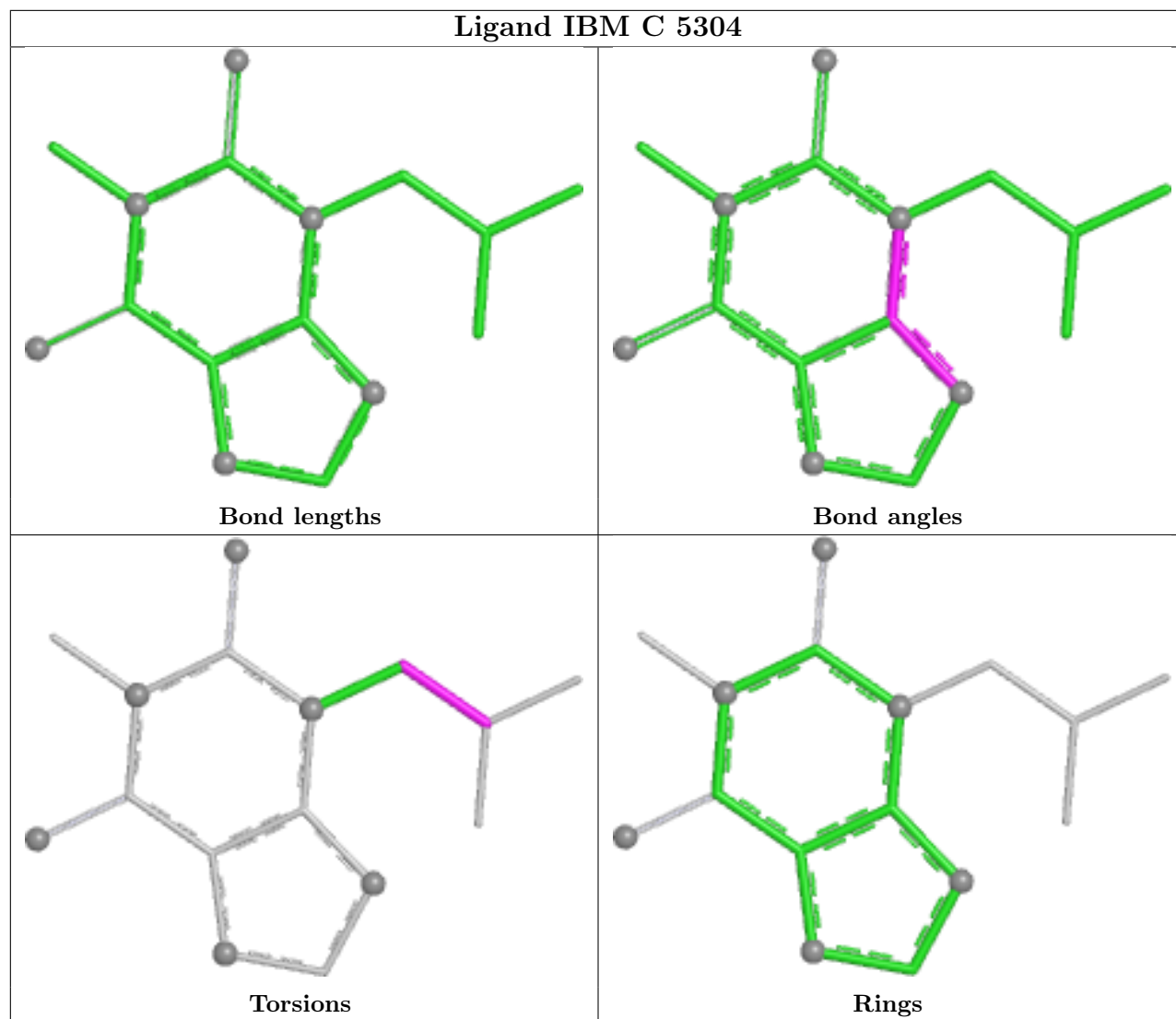
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

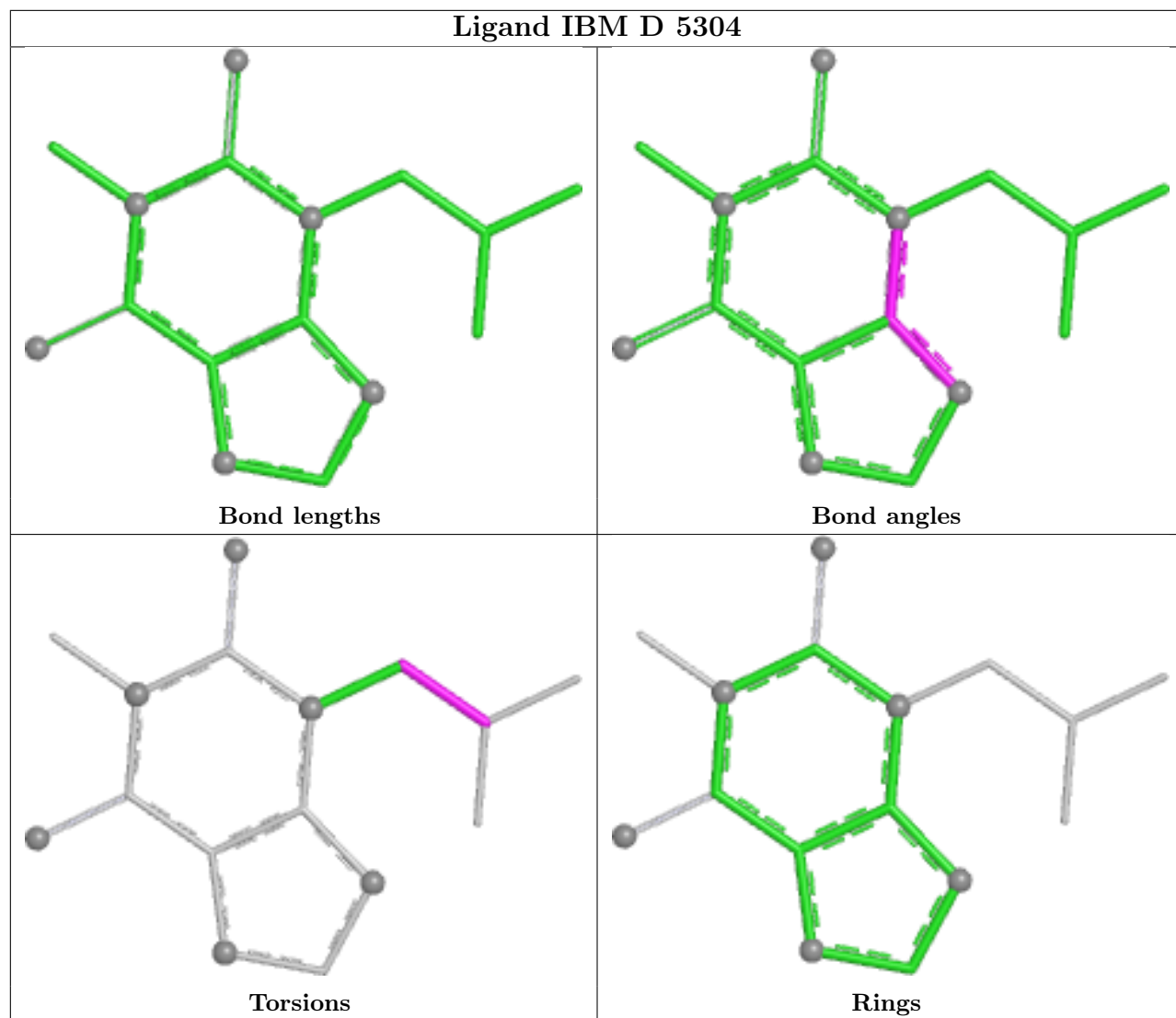


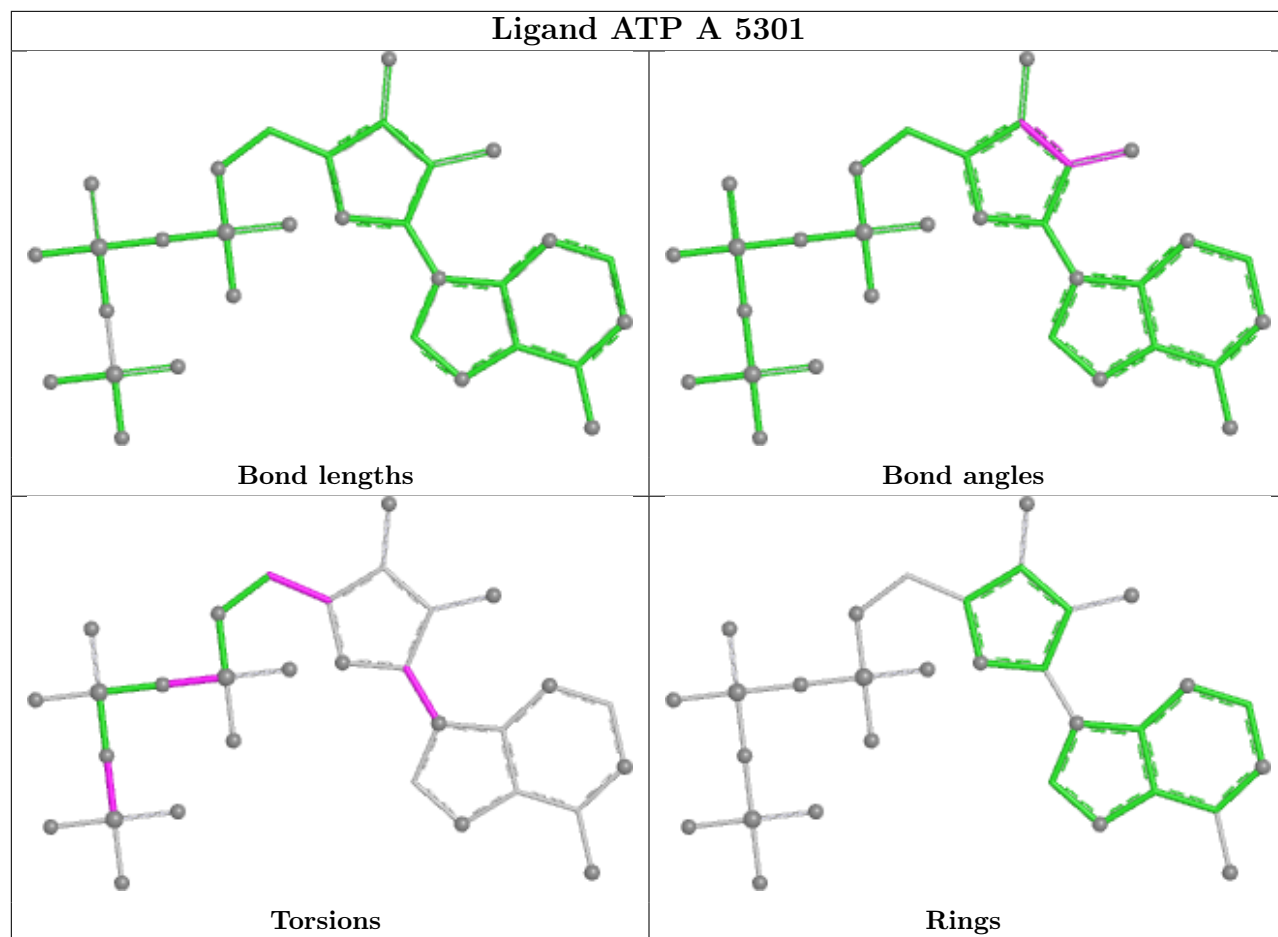


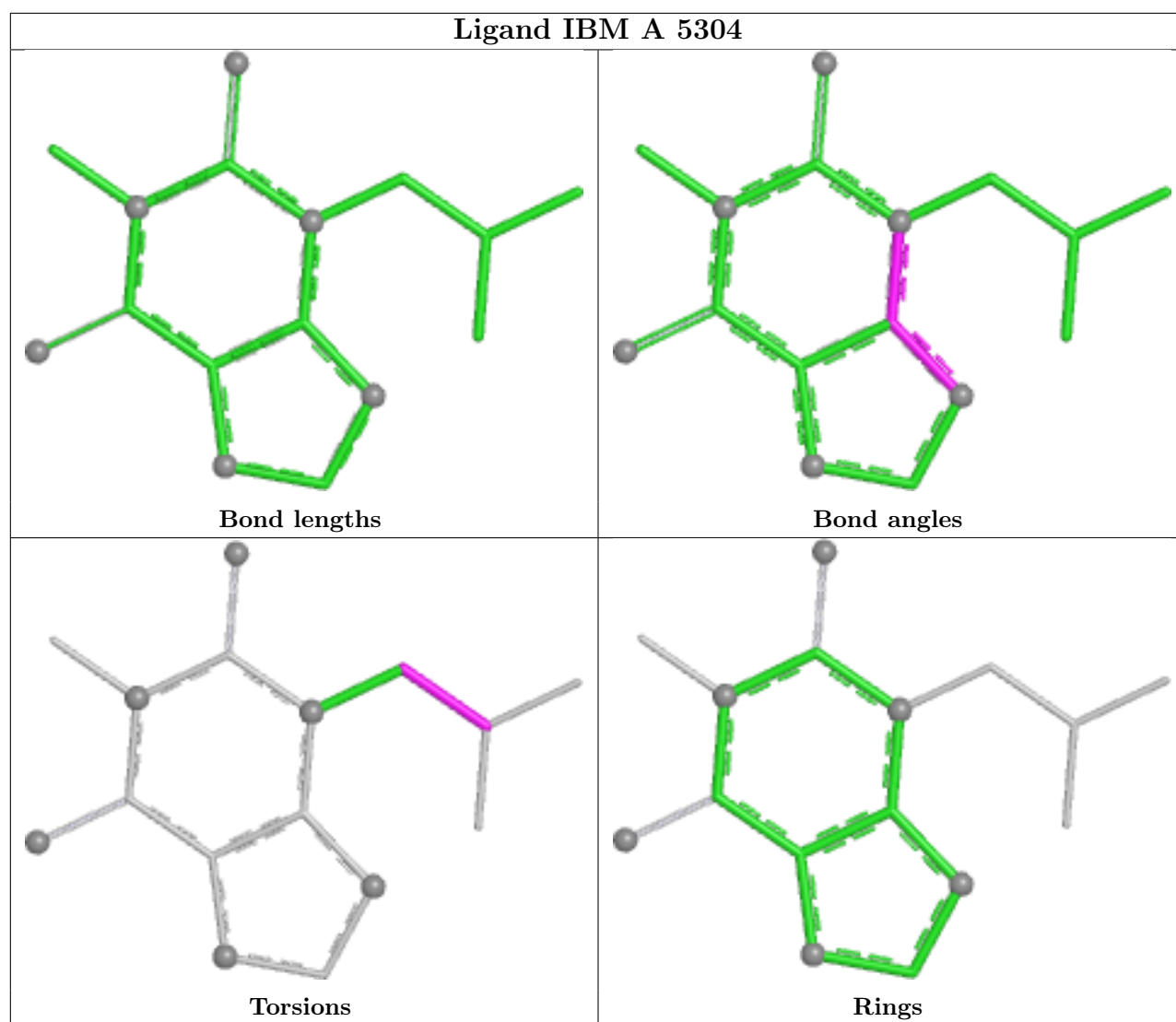












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

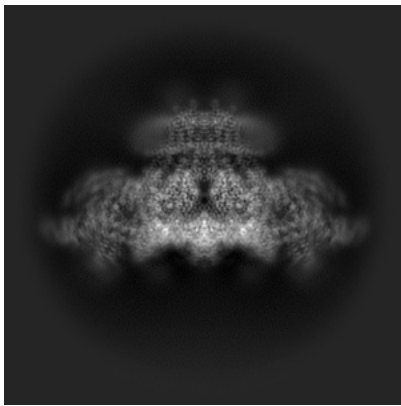
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47389. These allow visual inspection of the internal detail of the map and identification of artifacts.

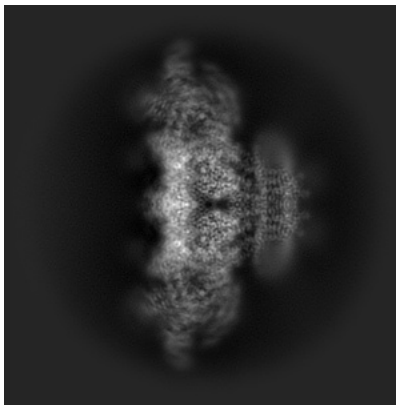
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

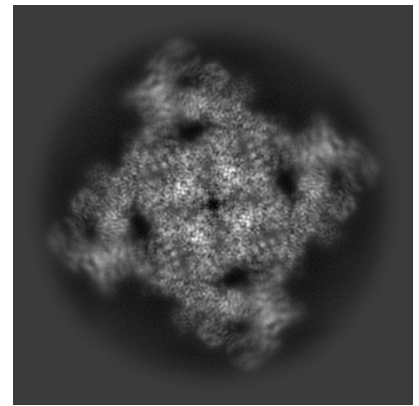
6.1.1 Primary map



X

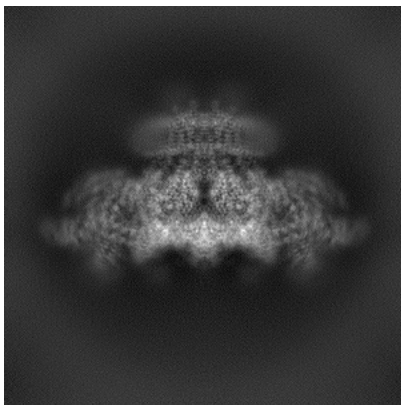


Y

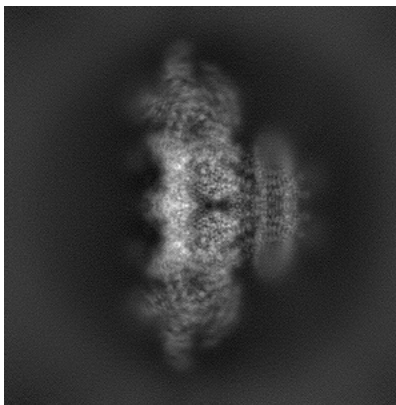


Z

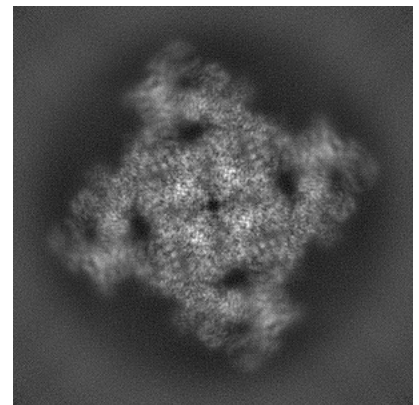
6.1.2 Raw map



X



Y

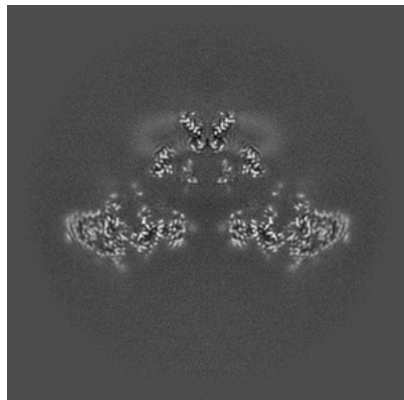


Z

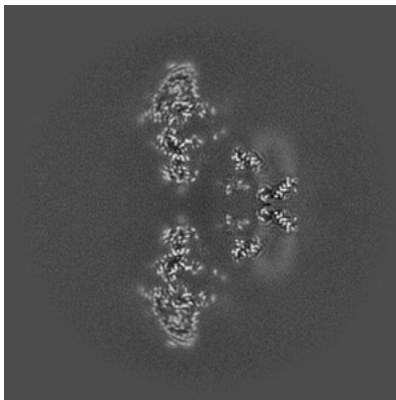
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

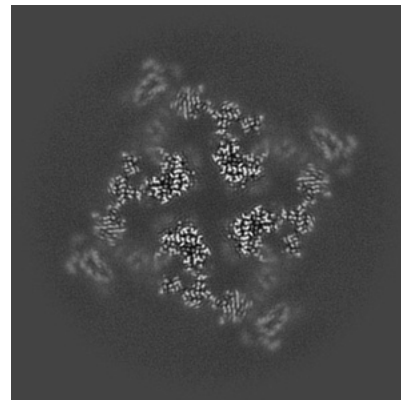
6.2.1 Primary map



X Index: 256

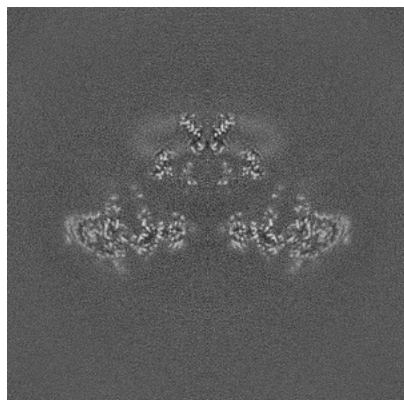


Y Index: 256

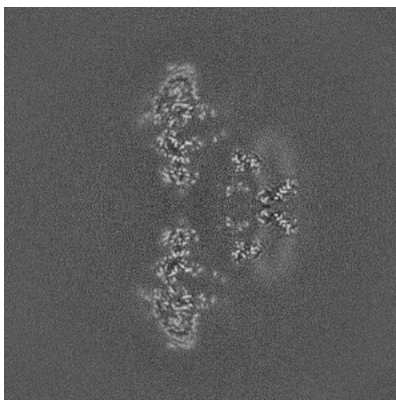


Z Index: 256

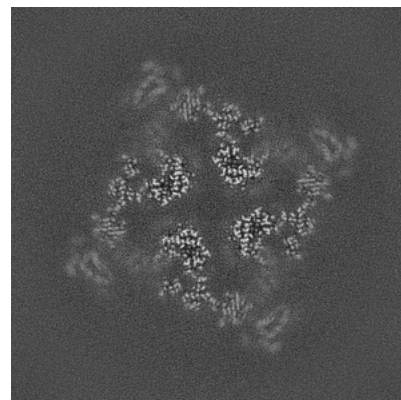
6.2.2 Raw map



X Index: 256



Y Index: 256

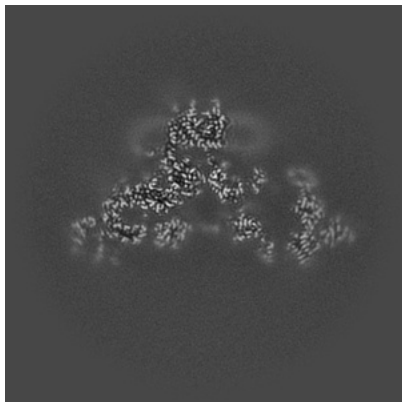


Z Index: 256

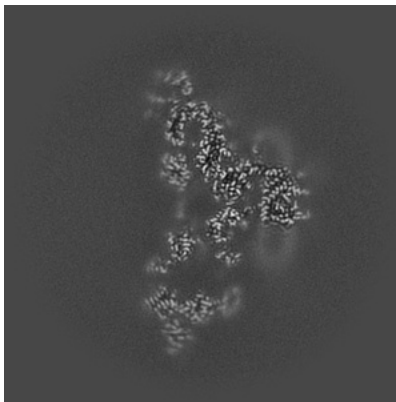
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

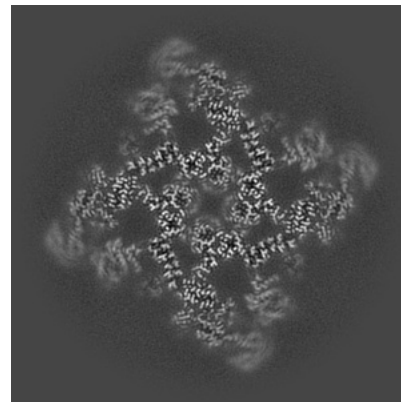
6.3.1 Primary map



X Index: 239

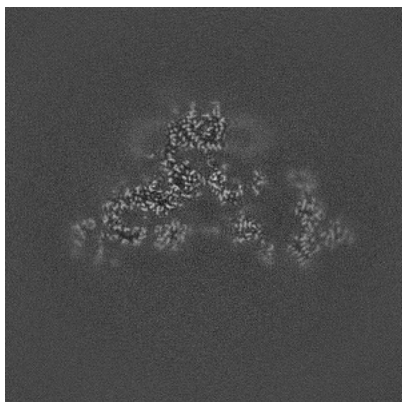


Y Index: 239

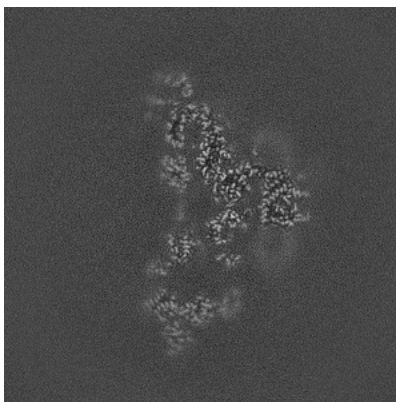


Z Index: 229

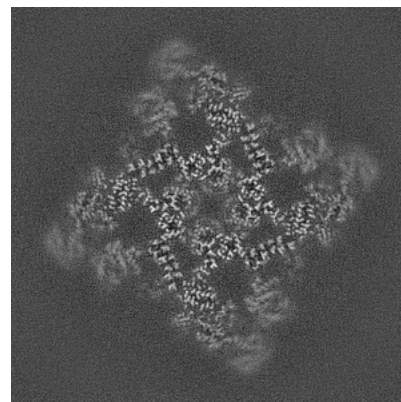
6.3.2 Raw map



X Index: 239



Y Index: 239

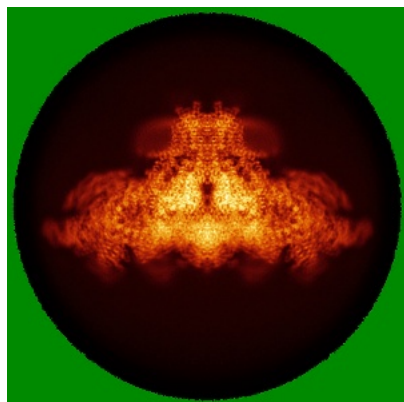


Z Index: 229

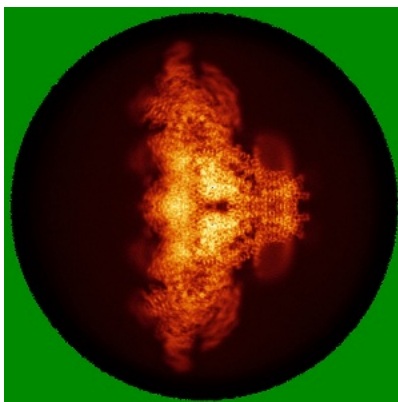
The images above show the largest variance slices of the map in three orthogonal directions.

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

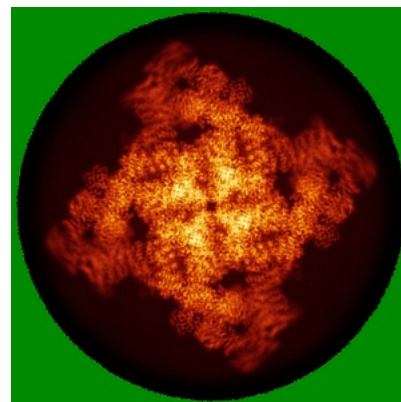
6.4.1 Primary map



X

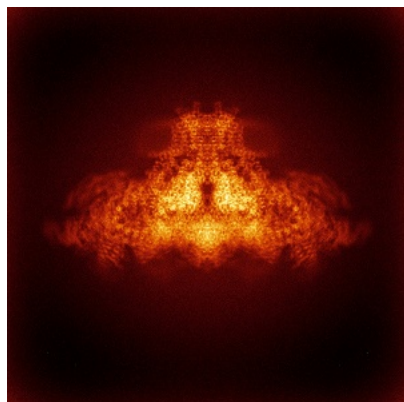


Y

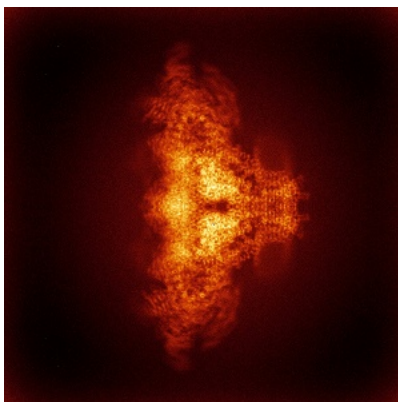


Z

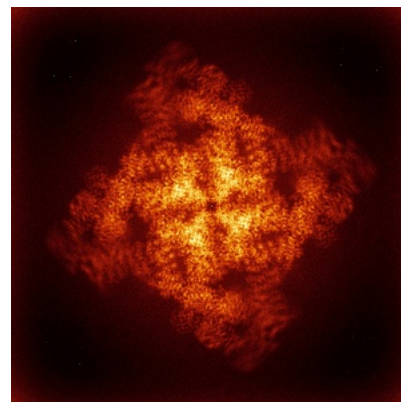
6.4.2 Raw map



X



Y

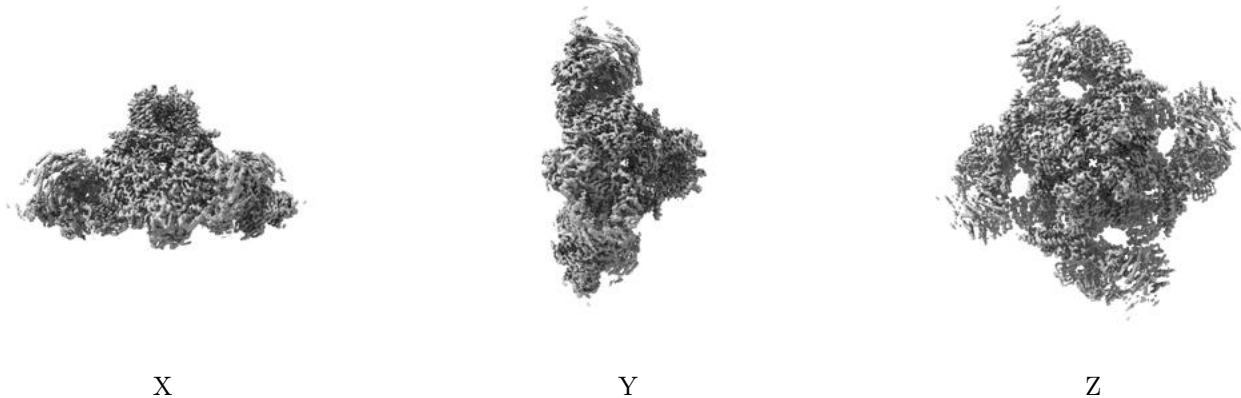


Z

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.

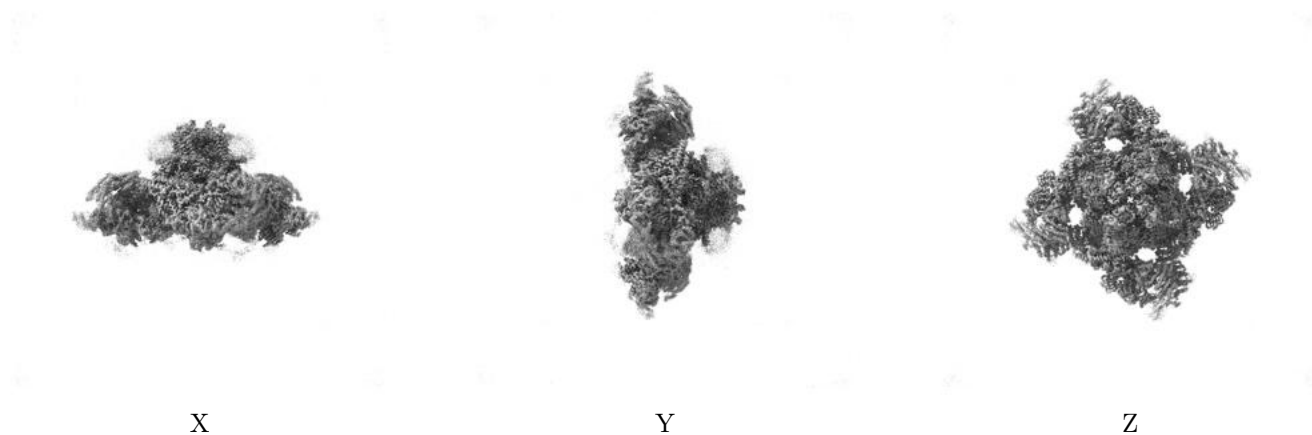
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

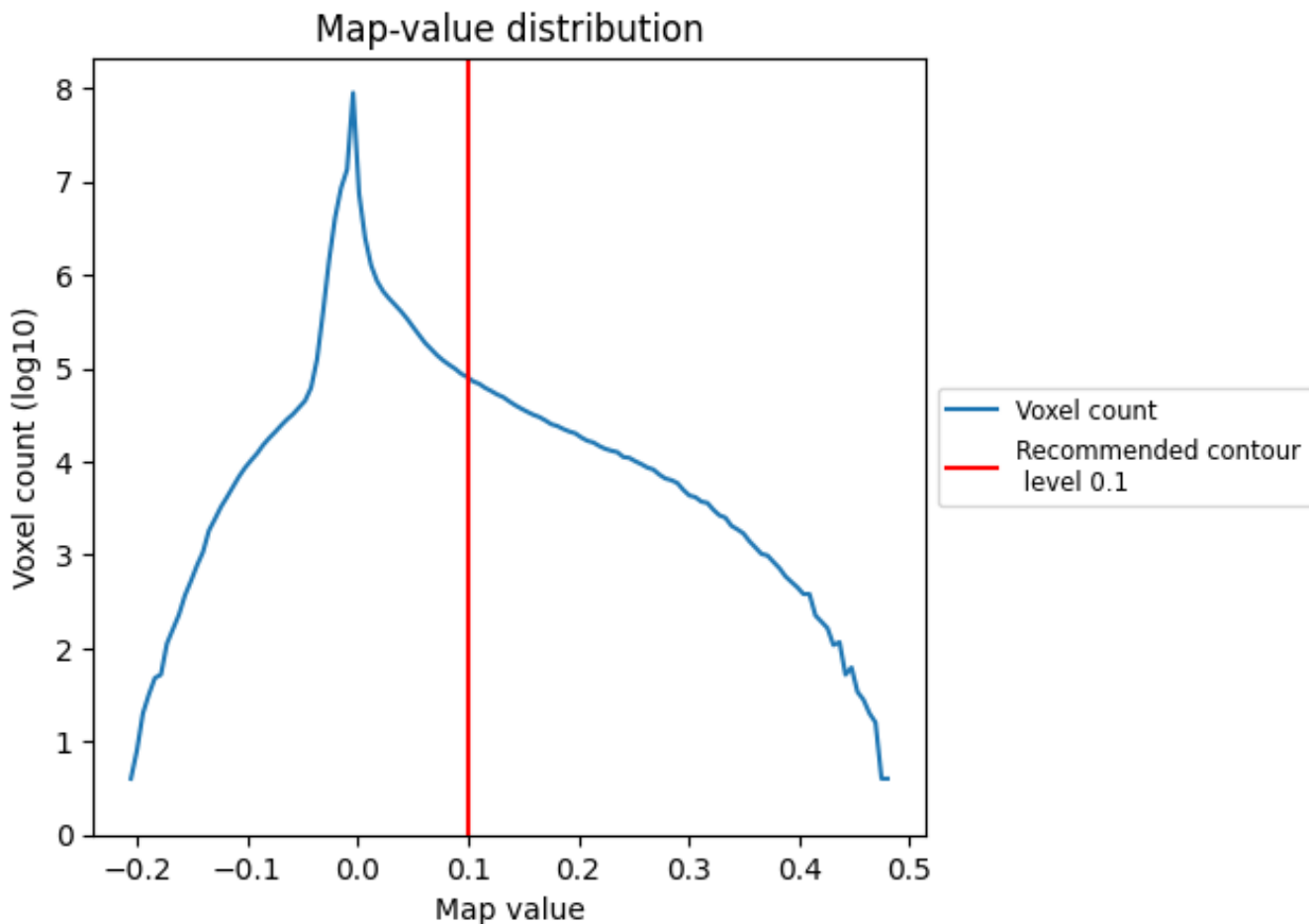
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

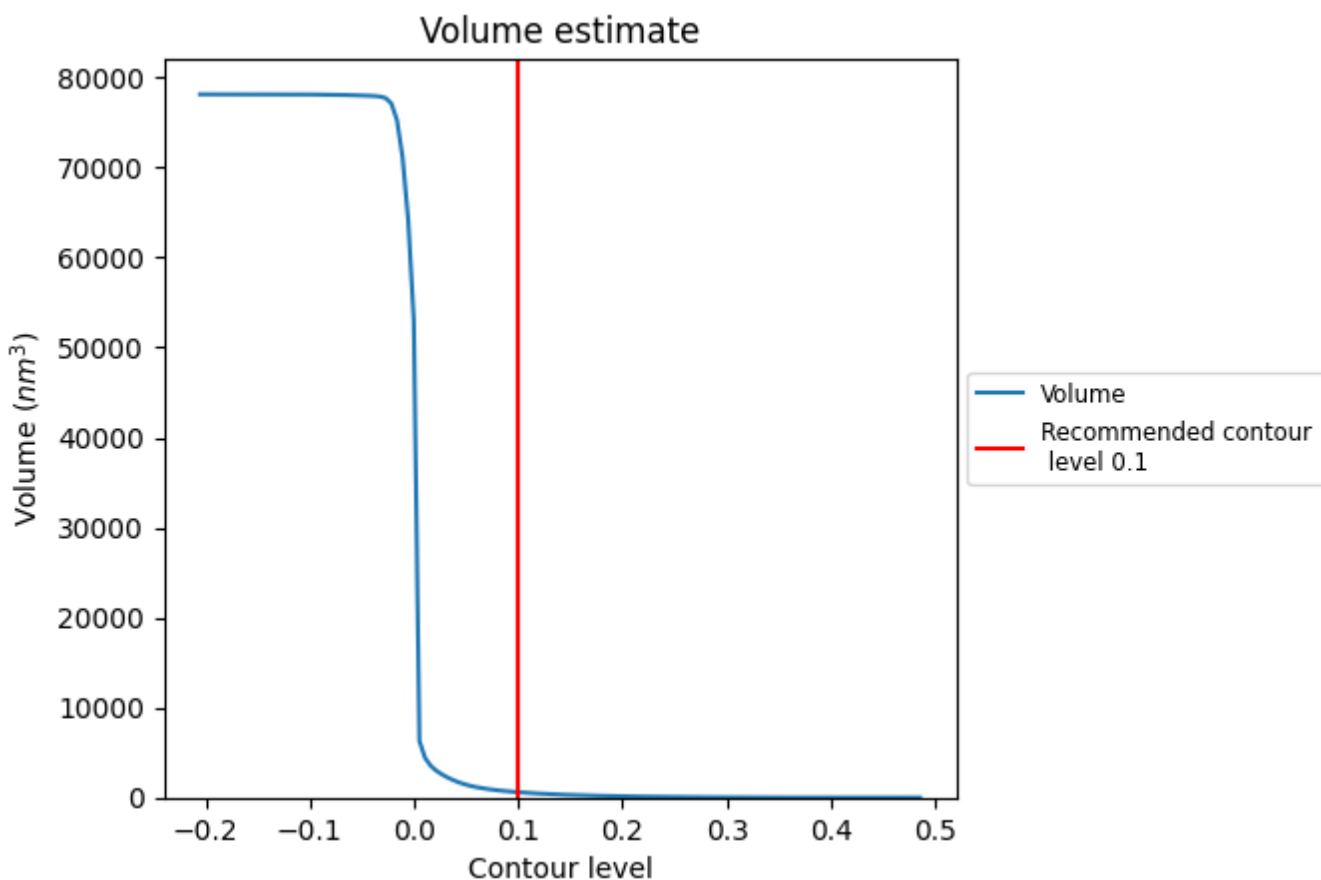
This section contains the results of statistical analysis of the map.

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.

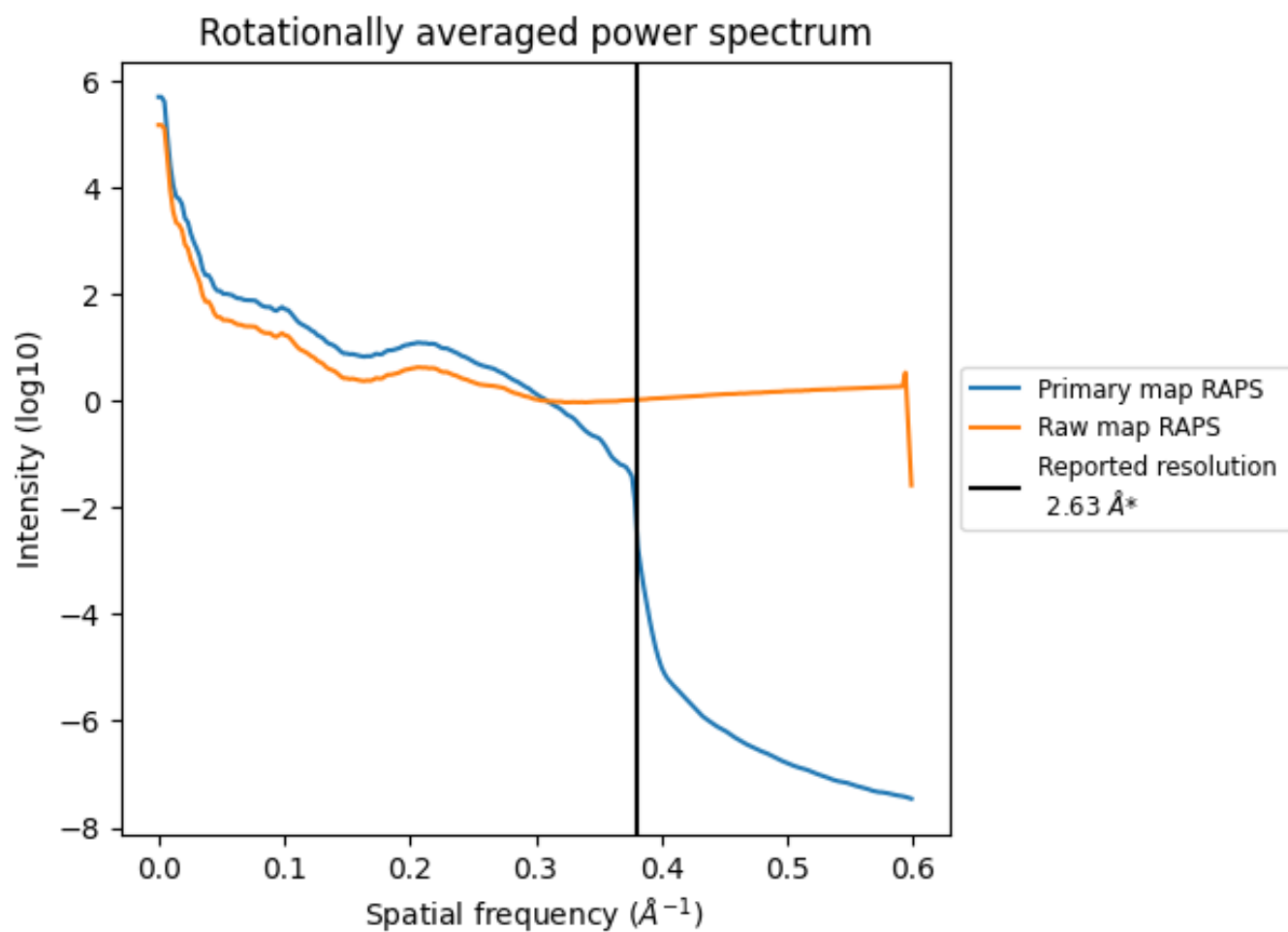
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 594 nm³; this corresponds to an approximate mass of 536 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

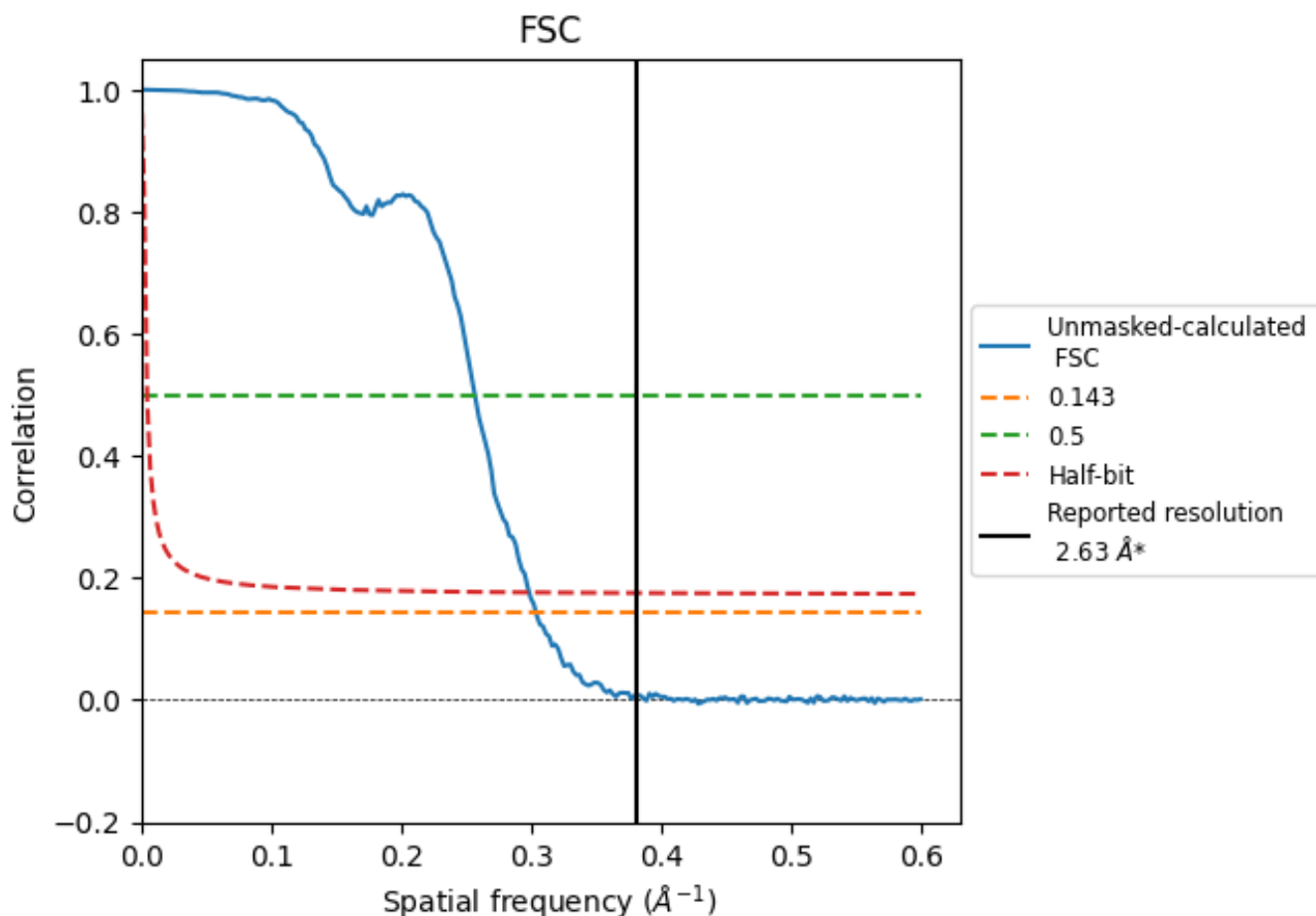


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.380 \AA^{-1}

8.2 Resolution estimates [i](#)

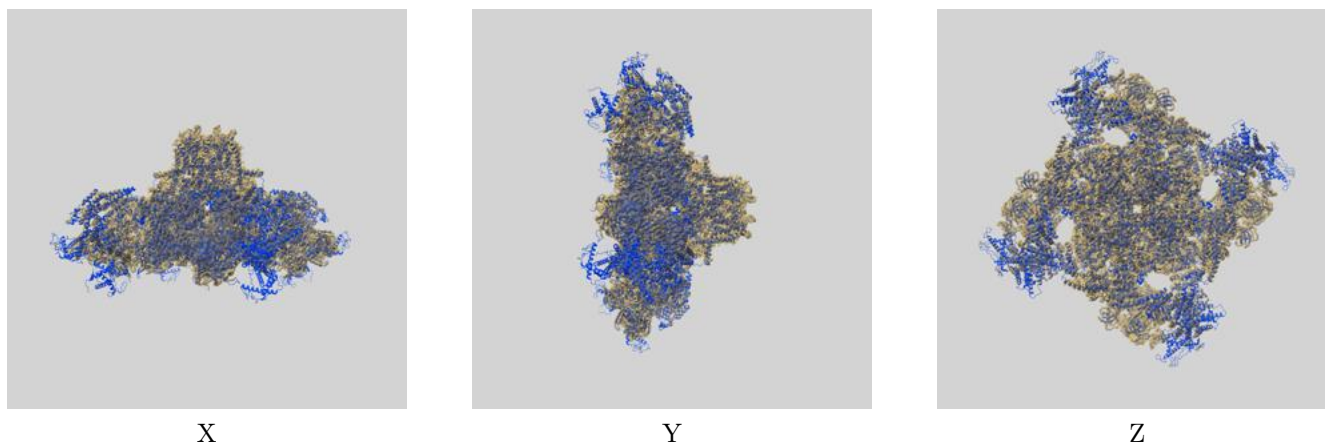
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.30	3.90	3.35

*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 3.30 differs from the reported value 2.63 by more than 10 %

9 Map-model fit [i](#)

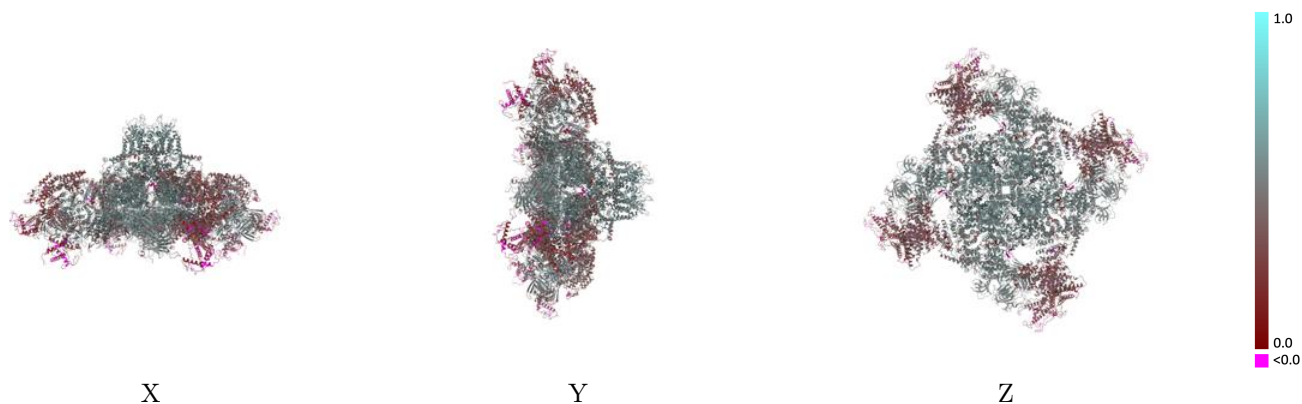
This section contains information regarding the fit between EMDB map EMD-47389 and PDB model 9E1C. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



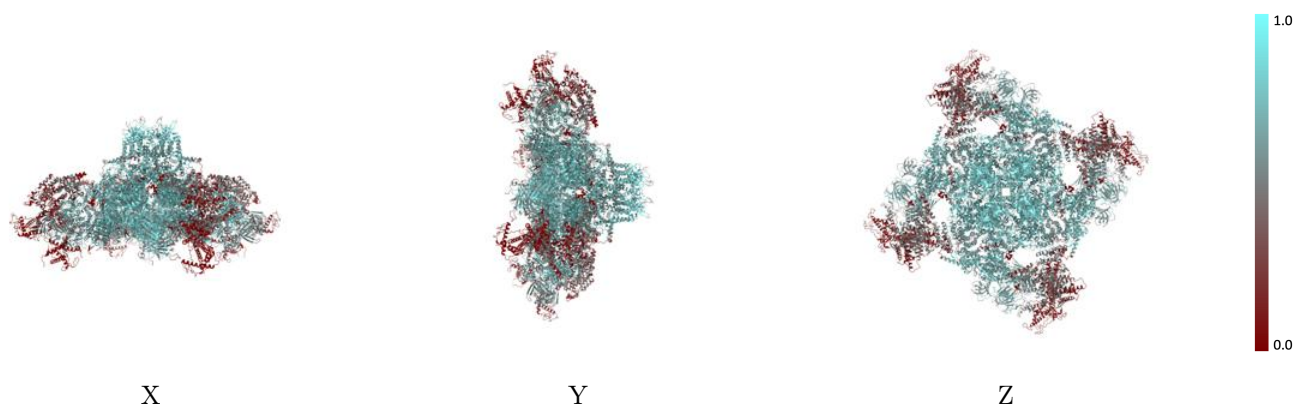
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



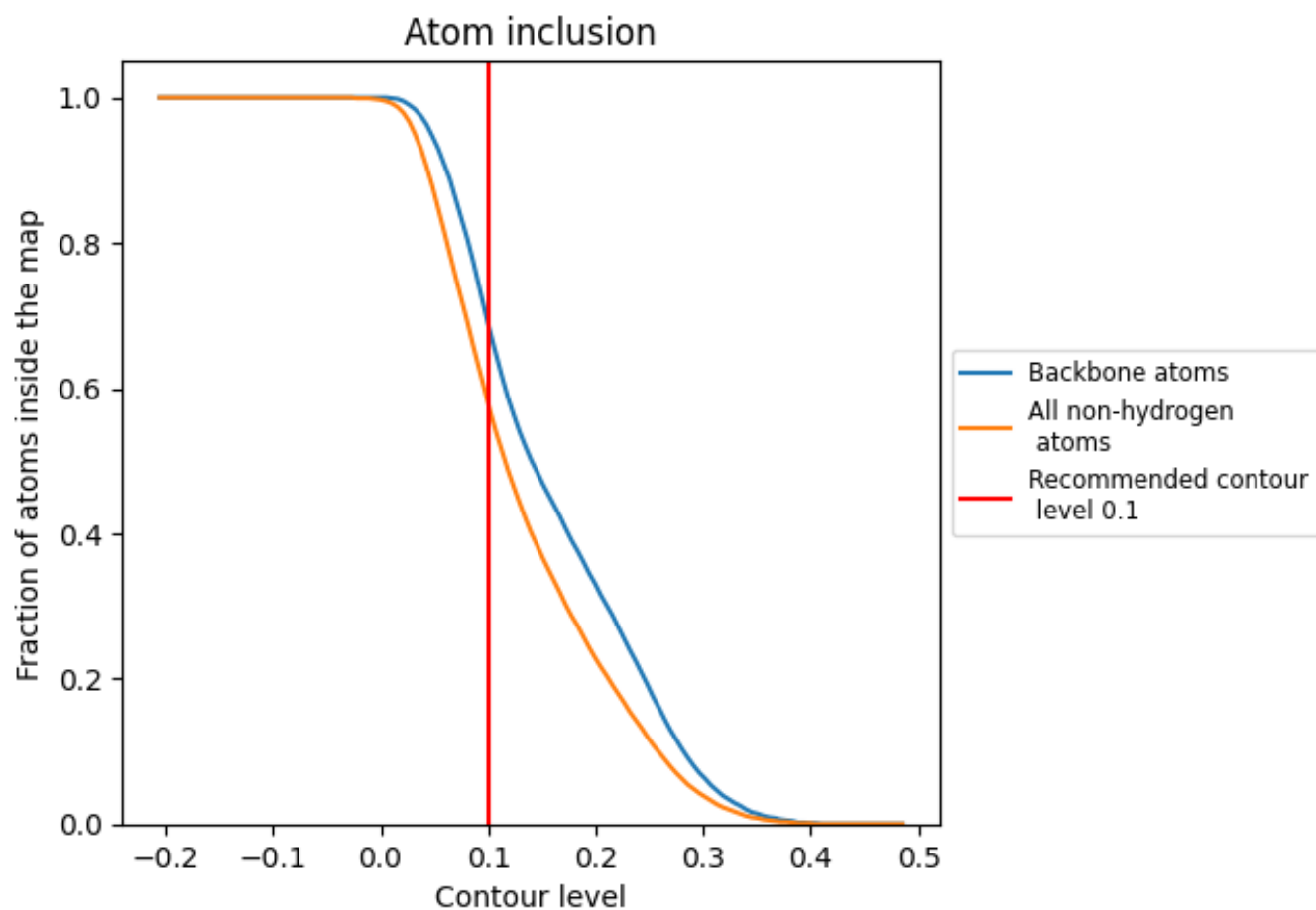
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.4410
A	 0.5780	 0.4390
B	 0.5780	 0.4400
C	 0.5780	 0.4390
D	 0.5780	 0.4390
E	 0.5880	 0.5100
F	 0.5930	 0.5090
G	 0.5930	 0.5050
H	 0.5890	 0.5050

