



wwPDB EM Validation Summary Report ⓘ

Jun 16, 2025 – 04:12 PM EDT

PDB ID : 9E1G / pdb_00009e1g
EMDB ID : EMD-47393
Title : Structure of RyR1 in the primed state in the presence of oxypurinol
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.17 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

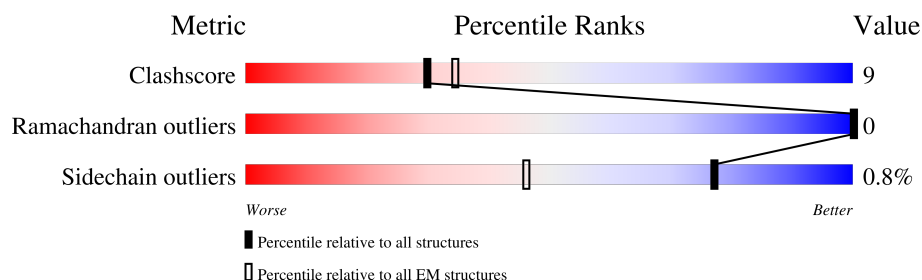
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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 ≥ 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	<div> <div>40%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div>
1	B	5037	<div> <div>40%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div>
1	C	5037	<div> <div>40%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>
1	D	5037	<div> <div>40%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>
2	E	108	<div> <div>66%</div> <div>69%</div> <div>29%</div> <div>..</div> </div>
2	F	108	<div> <div>66%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	G	108	<div> <div>65%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>
2	H	108	<div> <div>65%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144104 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
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

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

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

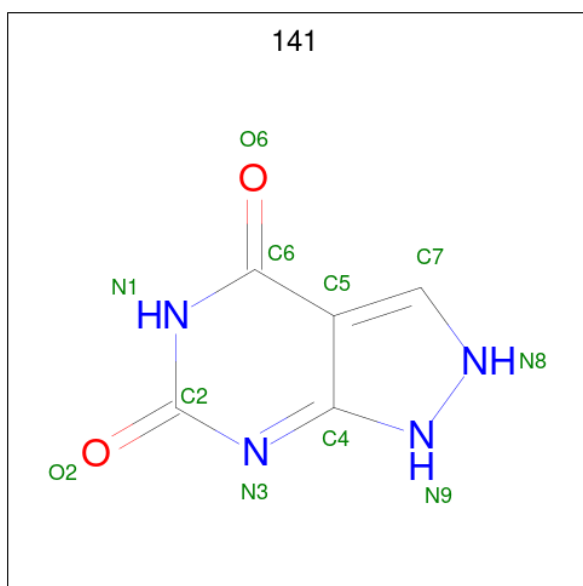
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
5	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 Oxypurinol (CCD ID: 141) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			11	5	4	2	
6	B	1	Total	C	N	O	0
			11	5	4	2	
6	D	1	Total	C	N	O	0
			11	5	4	2	
6	C	1	Total	C	N	O	0
			11	5	4	2	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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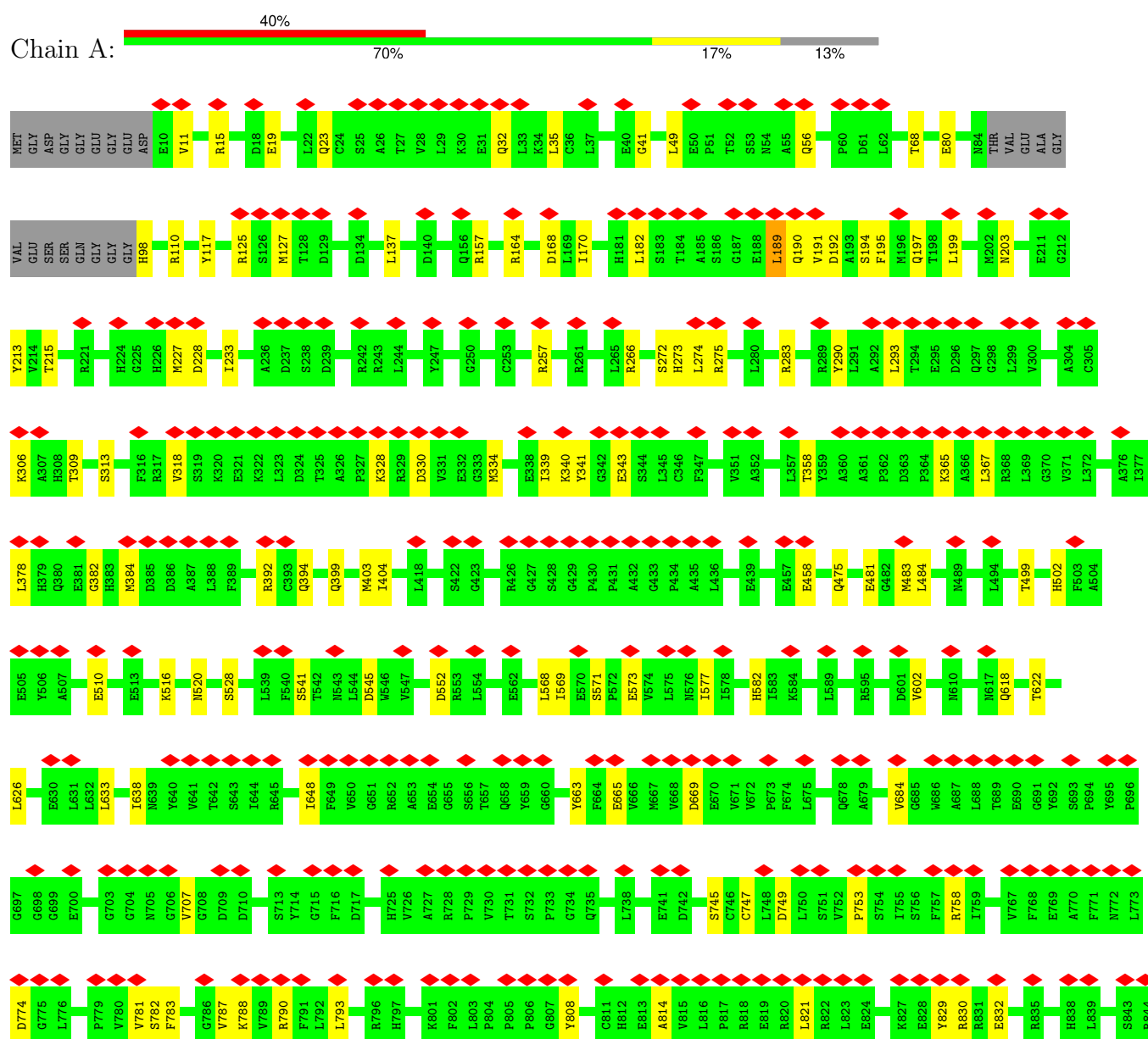
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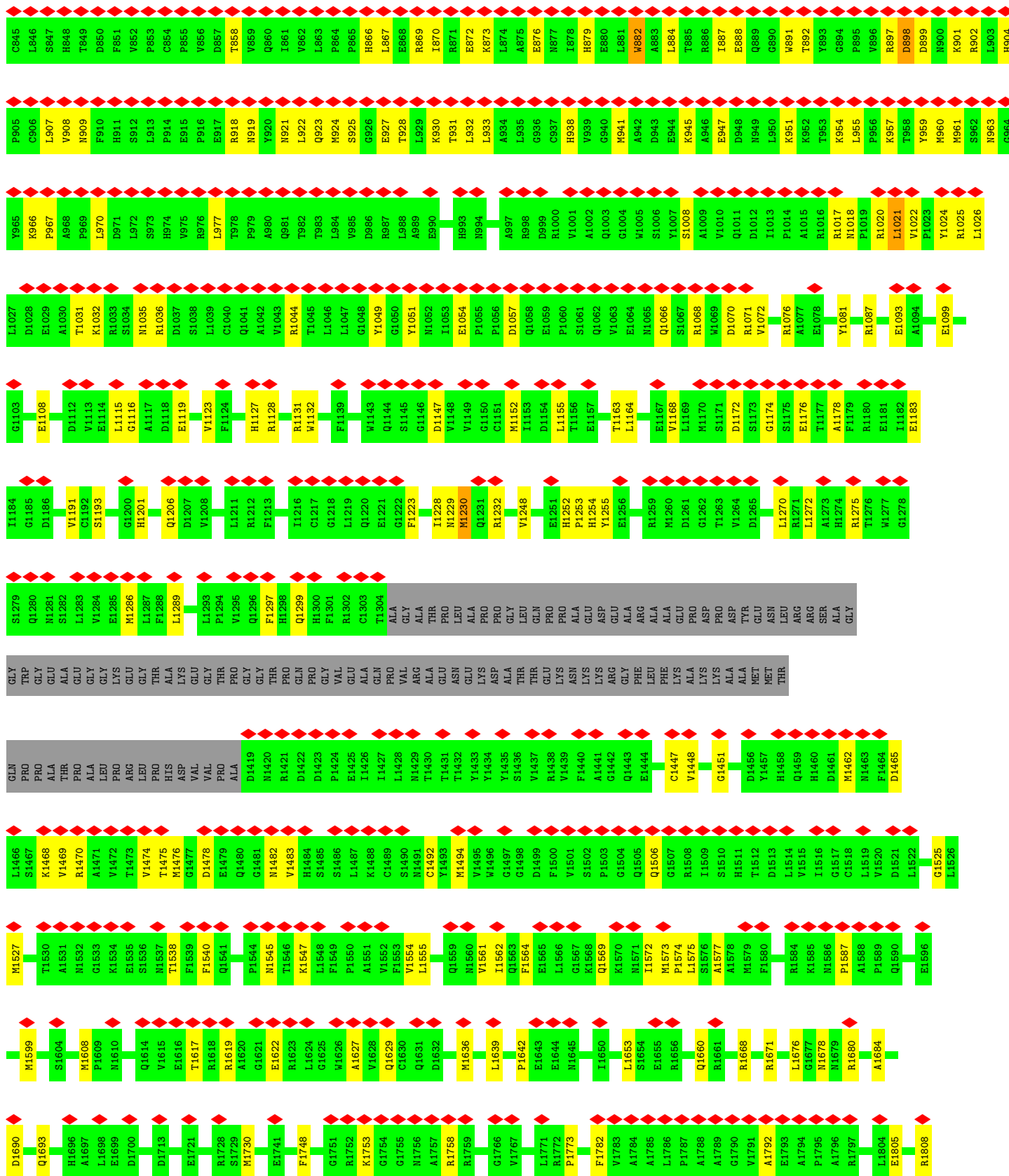
Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	O 1	0
7	C	1	Total 1	O 1	0

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











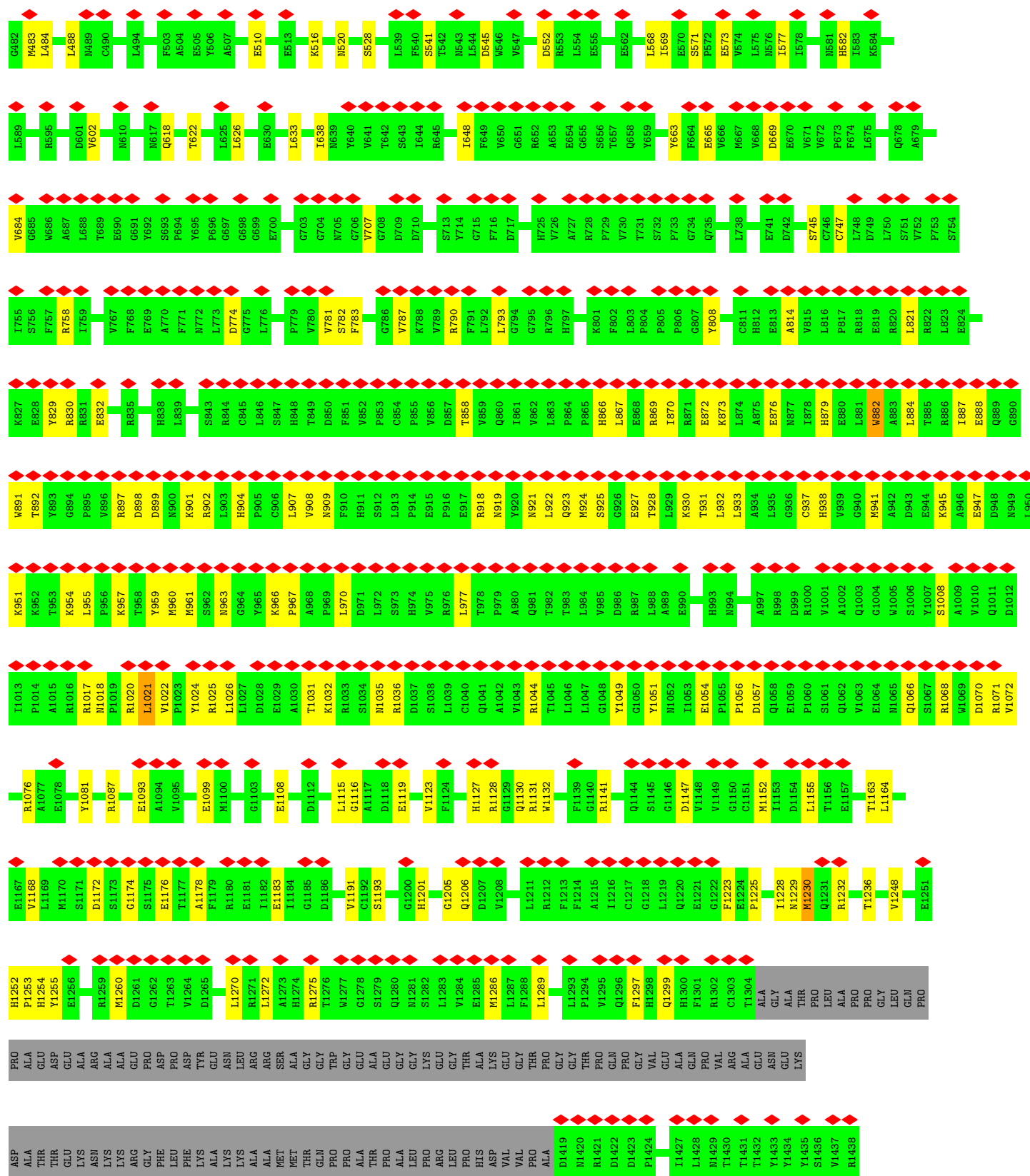
Chain B:







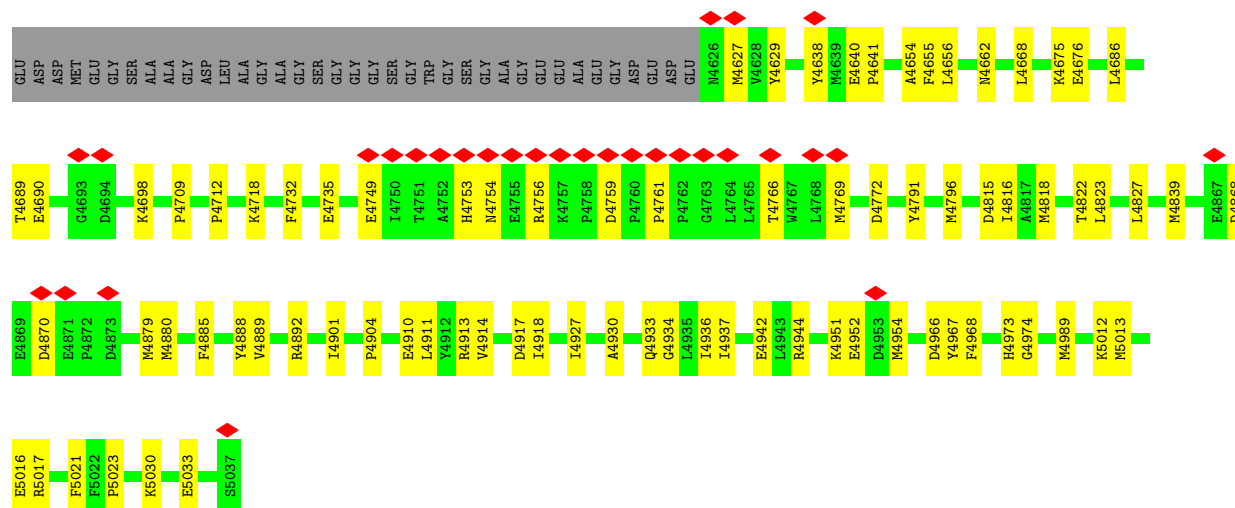
D4018	L3866	L3735	E3630	L3569	L3509	H3449	E3389	I3329	V3289	Q3209	Q3149	K3089
L4019	N3867	E3736	A3631	R3570	I3510	N3450	G3390	D3330	I3270	L3210	H3150	A3090
K4020	R3868	GLU	V3632	K3571	V3511	F3451	E3391	E3331	E3271	N3211	Q3151	G3091
D4022	Q3869	GLY	V3633	M3573	A3512	K3453	L3392	A3332	I3272	E3212	F3152	L3092
M4039	N3870	GLU	A3634	A3574	T3513	R3453	L3393	I3333	T3273	N3213	G3153	R3093
I4040	K3871	ASN	C3635	L3575	L3514	E3454	V3394	M3334	L3274	N3214	D3154	S3094
M4044	E3872	GLY	F3636	T3576	K3515	Q3455	R3395	M3335	F3275	A3215	D3155	F3095
M4047	K3873	GLU	R3637	R3577	K3516	N3457	D3396	K3336	M3276	C3216	V3156	F3096
M4047	M3638	GLU	M3638	R3577	M3517	F3458	E3397	R3337	L3277	C3217	L3157	E3097
E4056	T3639	GLU	T3639	Q3578	L3518	V3459	F3398	L3338	C3278	V3217	L3158	S3098
F3880	F3640	GLU	F3640	L3579	P3519	V3460	S3399	A3339	S3279	F3219	D3159	A3099
D4063	L3641	GLU	L3641	F3580	I3520	Q3461	V3400	V3340	V3280	T3220	D3160	S3100
M4064	F3642	GLU	F3642	G3581	G3521	N3462	L3401	F3341	L3281	K3221	F3161	E3101
F4065	N3643	GLU	N3643	R3582	L3522	E3463	C3402	A3342	P3282	K3222	Q3162	D3102
L4066	P3645	GLU	P3645	E3583	N3523	I3464	R3403	Q3343	R3283	S3223	V3163	I3103
K4067	R3648	GLU	R3648	E3584	M3524	N3465	D3404	Q3344	W3284	P3224	S3164	E3104
K4068	M3652	GLU	M3652	C3525	C3525	N3466	L3405	I3345	W3285	R3225	C3165	K3105
C3918	E3753	GLU	E3753	A3586	A3526	M3467	V3406	V3346	E3286	E3226	Y3166	M3106
S3929	E3755	GLU	E3755	D3587	P3527	S3468	A3407	S3347	R3287	R3227	R3167	V3107
F3933	K3765	GLU	K3765	D3588	T3528	F3469	L3408	R3348	G3288	A3228	T3168	E3108
W3935	Q3766	GLU	Q3766	P3589	D3529	N3470	Y3409	A3349	P3289	I3229	L3169	N3109
K3940	S3768	GLU	S3768	E3590	Q3530	T3471	P3410	R3350	E3290	L3230	C3170	L3110
D3941	R3769	GLU	R3769	D3591	D3531	A3472	L3411	P3351	A3291	G3231	S3171	R3111
Q4102	L3770	GLU	L3770	I3592	L3532	D3473	L3412	E3352	P3292	L3232	I3172	L3112
Q3946	T3772	GLU	T3772	V3593	L3533	Q3474	L3413	L3353	P3293	P3233	Y3173	G3113
R3949	R3773	GLU	R3773	R3594	M3534	K3475	R3414	L3354	P3294	M3234	S3174	K3114
N3950	E3881	GLU	E3881	R3595	L3535	S3476	Y3415	H3355	A3295	S3235	L3175	V3115
F3951	Q3882	GLU	Q3882	V3596	A3536	K3477	V3416	S3356	L3296	V3236	G3176	S3116
K3959	E3883	GLU	E3883	E3598	K3537	M3478	D3417	H3357	P3297	E3237	T3177	GLN
L3980	E3885	GLU	E3885	V3599	T3538	A3479	N3418	F3358	A3298	I3359	K3178	ALA
L3985	E3886	GLU	E3886	Y3602	Y3540	LYS	N3419	P3360	G3299	M3239	THR	THR
W3986	E3887	GLU	E3887	L3603	A3541	ALA	K3420	T3361	A3300	C3240	N3180	GLN
D3987	E3888	GLU	E3888	L3604	L3542	ASP	A3421	I3362	P3241	P3241	T3181	VAL
A3988	E3889	GLU	E3889	H3605	K3543	GLN	H3422	G3363	Y3182	Y3182	K3123	K3123
V3989	L3844	GLU	L3844	L3606	D3544	SER	L3424	R3364	V3183	G3124	V3183	G3124
V3995	Q3850	GLU	Q3850	E3607	T3545	GLY	L3425	L3365	I3243	P3244	E3184	V3125
F3996	E3892	GLU	E3892	Q3608	D3546	SER	E3426	R3367	V3245	V3245	K3185	G3126
M3999	K3693	GLU	K3693	T3609	E3547	ASP	P3427	K3367	L3246	R3187	L3186	Q3127
M4000	L3856	GLU	L3856	E3610	E3548	GLN	N3428	R3368	V3307	D3247	P3188	R3128
M4001	D3695	GLU	D3695	H3611	V3549	GLU	A3429	A3369	T3308	P3188	P3188	L3129
K4002	D3696	GLU	D3696	F3612	R3550	ARG	N3430	A3369	T3309	A3189	A3189	T3130
D4006	H3699	GLU	H3699	Y3613	E3551	THR	N3431	G3370	L3249	L3190	G3191	Y3131
Q4009	K3715	GLU	K3715	S3615	L3553	LYS	A3432	K3371	H3311	M3250	T3132	T3132
E4015	L3716	GLU	L3716	K3616	Q3554	R3498	E3433	V3372	L3312	A3251	E3192	T3133
E3861	D3717	GLU	D3717	K3617	N3555	R3499	F3435	V3373	L3313	D3252	E3192	T3133
Q3863	E3718	GLU	E3718	V3618	L3557	D3501	R3437	A3374	G3317	I3253	C3193	V3134
T3864	Y3725	GLU	Y3725	W3620	H3558	Y3503	V3438	E3377	L3315	G3254	A3195	A3135
V3865	M3729	GLU	M3729	H3621	L3559	S3504	E3439	Q3378	L3316	G3255	R3196	L3136
	C3733	GLU	C3733	K3622	Q3560	V3505	G3440	R3380	G3317	L3256	L3197	L3137
	H3734	GLU	H3734	L3624	V3563	T3507	T3441	E3382	G3319	A3257	L3197	P3138
				S3625	E3564	Q3508	F3443	A3383	A3199	S3259	A3198	V3139
				K3626	G3565		W3445	E3385	A3200	G3260	A3200	L3140
				Q3627	S3566		S3446	A3387	M3201	A3261	M3201	T3141
				R3628	P3567		V3447	E3387	P3202	R3262	P3202	L3143
				R3629	S3568		S3448	E3388	V3263	F3144	F3144	F3144
									A3204	A3204	A3204	Q3145
									F3205	F3205	F3205	H3146
									L3206	L3206	L3206	T3147
									E3207	E3207	E3207	A3148



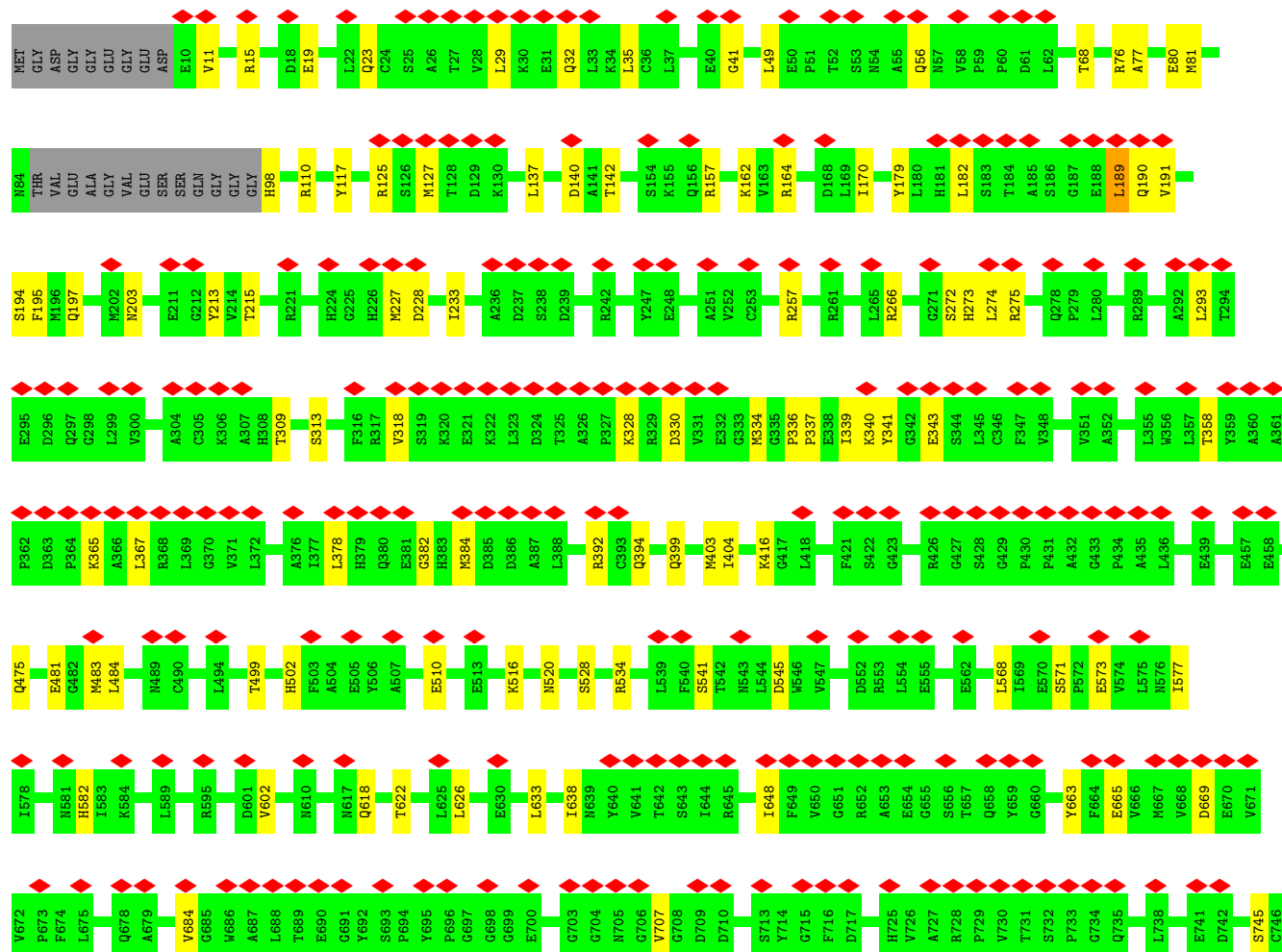
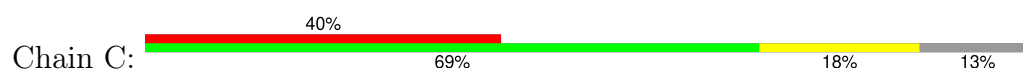


S3309	L3249	A3189	L3129	H3069	Y3009	S2949	K2889	G2829	D2769	A2709	H2647	V2586
D3310	M3250	L3190	T3130	I3070	F3010	S2950	K2890	E2830	K2770	L2710	Y2648	Y2587
H3311	A3251	G3191	Y3131	L3071	T3011	I2951	K2891	GLU	I2771	P2711	E2649	R2588
N3312	I3252	E3192	T3132	A3072	N3012	E2952	Q2892	ARG	Q2772	P2712	R2650	L2589
N3313	I3253	C3193	T3133	R3073	H3013	K2953	E2893	THR	N2773	D2713	C2651	S2590
S3314	G3254	G3254	V3134	S3074	H3014	R2954	L2894	GLU	N2774	Y2714	Y2655	R2591
L3315	G3255	L3194	A3135	L3075	L3015	F2955	E2895	LYS	W2775	V2715	C2656	Q2592
L3316	L3256	A3195	L3136	D3076	Y3016	A2956	K2896	LYS	S2776	D2716	L2657	R2593
G3317	A3257	R3196	L3137	A3077	F3017	F2957	K2897	THR	G2777	A2717	P2658	S2594
N3318	E3258	L3197	P3138	R3078	L3018	G2958	G2898	ARG	Y2778	S2718	T2659	L2595
I3319	S3259	A3198	V3139	T3079	S3019	F2959	G2899	LYS	E2779	A2719	G2660	A2598
L3320	G3260	A3200	L3140	V3080	T3020	Q2961	G2900	SER	N2780	S2720	W2661	Q2599
A3261	M3201	M3081	T3141	M3081	F3021	Q2962	H2901	GLN	W2781	S2721	A2662	R2600
R3262	P3202	P3202	T3142	K3082	A3022	L2963	H2902	THR	D2782	K2722	N2663	D2601
Y3263	V3203	S3083	L3143	S3083	K3023	L2964	P2903	ALA	E2783	A2723	F2664	V2602
T3264	F3204	G3084	F3144	G3084	V3024	R2965	L2904	THR	E2784	E2724	G2665	I2603
E3265	A3205	F3085	L3145	F3085	L3025	W2966	L2905	TYR	L2785	E2725	V2666	E2604
M3266	L3206	E3086	H3146	E3086	G3026	M2967	V2906	ASP	K2786	L2725	T2667	D2605
P3267	E3207	I3087	I3147	V3088	S3027	M2968	P2907	PRO	T2787	ALA	S2668	C2606
H3268	P3208	K3089	A3148	K3089	G3028	I2969	Y2908	ARG	H2788	THR	E2669	L2607
V3269	G3209	A3090	K3149	A3090	G3029	I2970	D2909	GLY	P2789	ASP	E2670	H2608
I3270	L3210	K3211	H3150	K3211	H3030	S2970	T2910	GLY	M2790	ALA	A2609	L2610
E3271	N3211	G3091	Q3151	G3091	A3031	Q2971	L2911	N2856	L2791	GLU	E2671	C2611
I3272	E3212	L3092	F3152	L3092	S3032	E2972	T2912	P2857	R2792	N2734	L2672	G2611
T3273	G3153	R3093	G3153	R3093	N3033	F2973	A2913	Q2858	Y2793	H2673	H2673	R2612
L3274	L3214	S3094	K3154	S3094	K3034	L2974	K2914	P2859	F2794	L2674	T2675	V2613
P3275	A3215	F3095	E3155	F3095	E3035	A2975	E2915	P2860	K2795	D2736	R2676	I2614
M3276	C3216	F3096	V3156	F3096	K3036	H2976	K2916	D2861	T2796	P2737	K2677	R2615
L3277	S3217	E3097	I3157	E3097	E3037	L2977	A2917	L2862	F2797	R2738	L2678	P2616
C3278	V3218	S3098	L3158	S3098	M3038	E2978	R2918	S2863	S2798	P2739	F2679	S2617
S3279	Y3219	A3099	D3159	A3099	T3039	A2979	D2919	G2864	E2799	V2740	W2680	M2618
L3281	T3220	S3100	D3160	S3100	T3040	V2980	R2920	V2865	K2800	G2681	G2681	L2619
A3282	T3221	E3101	V3161	E3101	S3041	V2981	E2921	T2866	L2742	T2682	Q2620	Q2620
S3283	S3223	D3102	Q3162	D3102	L3042	S2982	K2922	L2867	D2801	L2743	F2683	H2621
W3284	S3164	I3103	V3163	I3103	F3043	S2983	A2923	R2868	K2802	N2744	L2623	L2623
M3285	P3224	S3104	C3164	S3104	C3044	Q2984	Q2924	R2869	E2803	V2745	S2685	R2624
E3286	R3225	K3105	C3165	K3105	K3045	Q2985	E2925	E2870	I2804	I2746	L2686	R2625
R3287	E3226	M3106	Y3166	M3106	L3046	V2986	E2926	L2871	R2805	I2747	A2687	L2626
G3288	R3227	V3107	R3167	V3107	A3047	E2987	L2926	Q2872	R2806	P2748	H2688	V2627
P3289	A3228	E3108	L3169	E3108	A3048	K2988	L2927	A2873	W2807	E2749	K2689	F2628
E3290	T3229	N3109	C3170	N3109	L3049	S2989	K2928	R2874	P2808	K2750	K2690	D2629
A3291	G3231	L3110	S3171	L3110	V3050	P2990	F2929	A2875	I2809	L2751	Y2691	V2630
P3292	L3232	R3111	I3172	R3111	R3051	H2991	L2930	E2876	K2810	D2752	P2631	P2631
P3293	P3233	G3112	F3173	G3112	H3052	E2992	Q2931	Q2877	E2811	S2753	Q2693	L2632
P3294	N3234	K3114	S3174	K3114	R3053	E2993	W2932	L2878	S2812	F2754	E2694	L2633
A3295	S3235	V3115	L3175	V3115	V3054	E2994	G2934	A2879	L2813	I2755	L2695	N2634
L3296	V3236	GLN	G3176	GLN	S3055	I2995	Y2935	N2881	A2815	K2756	Y2696	E2635
P3297	E3237	ALA	T3177	ALA	L3056	K2996	A2936	N2882	M2816	K2757	R2697	F2636
A3298	E3238	ARG	T3178	ARG	F3057	F2997	T2937	H2883	I2817	F2758	M2698	A2637
G3299	M3239	THR	K3179	THR	T3059	A2999	T2938	H2884	A2818	A2759	K2638	K2638
A3300	C3240	GLN	D3181	GLN	D3060	K3000	R2939	T2885	W2819	E2760	M2700	M2639
P3301	P3241	VAL	T3182	VAL	A3061	I3001	GLY	W2886	E2820	T2762	C2702	L2641
L3302	D3242	K3123	Y3183	K3123	P3062	L3002	LYS	G2887	W2821	H2763	L2703	K2642
C3303	I3243	G3124	V3184	G3124	A3063	L3003	ASP	R2888	T2822	E2764	C2704	L2643
C3304	P3244	V3125	K3185	V3125	V3064	P3004	WET		I2823	K2765	A2705	L2644
L3305	V3245	G3126	L3186	G3126	V3065	L3005	GLU		E2824	W2766	L2706	T2645
A3306	L3246	Q3127	F3187	Q3127	N3066	I3006			K2825	A2767	A2707	H2646
L3307	D3247	N3128	P3188	N3128	C3067	N3007			A2826	F2768	G2708	
R3308	R3248				L3068	Q3008			E2827			





• Molecule 1: Ryanodine receptor 1

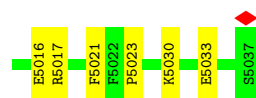




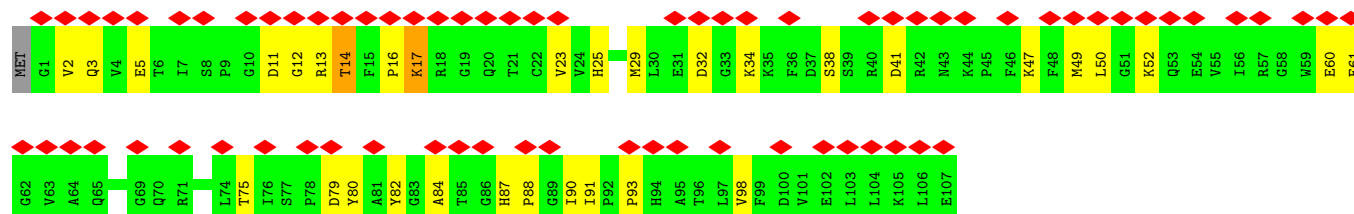




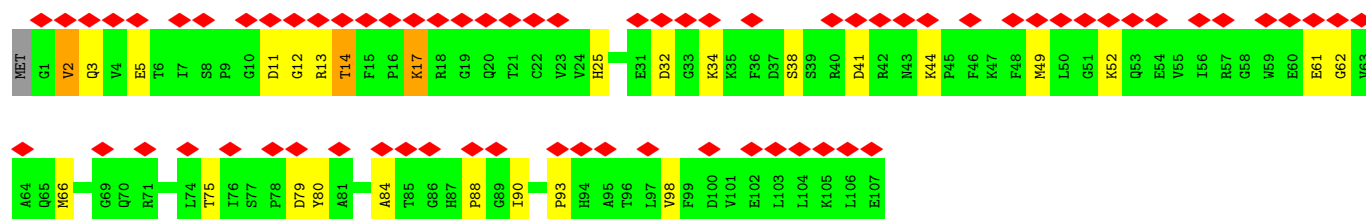




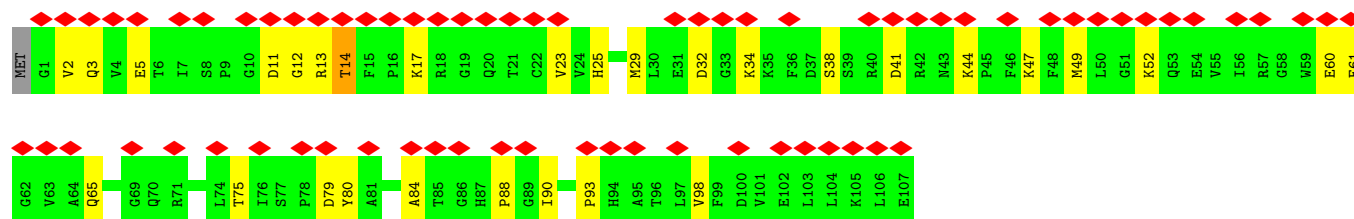
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



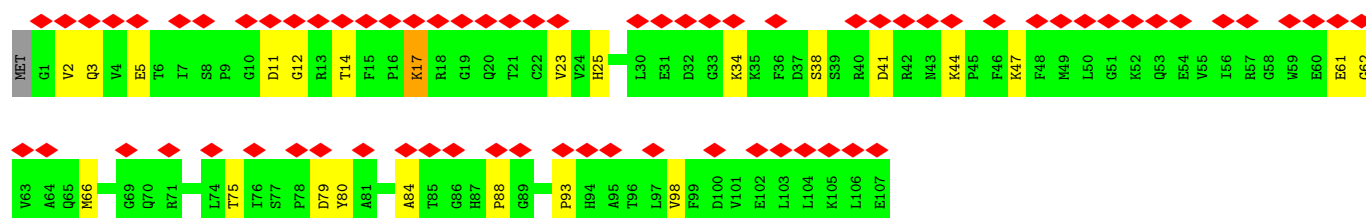
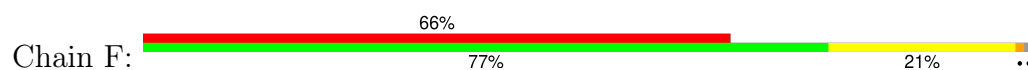
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• 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	17393	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	0.436	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.288, 428.288, 428.288	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8365, 0.8365, 0.8365	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, 141, 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	0.29	0/35977	0.38	1/48726 (0.0%)
1	B	0.29	0/35977	0.38	1/48726 (0.0%)
1	C	0.29	0/35977	0.38	1/48726 (0.0%)
1	D	0.29	0/35977	0.38	1/48726 (0.0%)
2	E	0.30	0/850	0.43	0/1146
2	F	0.27	0/850	0.40	0/1146
2	G	0.28	0/850	0.40	0/1146
2	H	0.29	0/850	0.41	0/1146
All	All	0.29	0/147308	0.38	4/199488 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3239	MET	CB-CG-SD	7.01	133.72	112.70
1	A	3239	MET	CB-CG-SD	7.00	133.71	112.70
1	C	3239	MET	CB-CG-SD	7.00	133.69	112.70
1	B	3239	MET	CB-CG-SD	6.99	133.67	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35150	0	34797	630	0
1	B	35150	0	34797	622	0
1	C	35150	0	34797	648	0
1	D	35150	0	34797	650	0
2	E	831	0	831	25	0
2	F	831	0	831	18	0
2	G	831	0	831	23	0
2	H	831	0	831	21	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	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
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	11	0	4	0	0
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144104	0	142576	2538	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 9.

The worst 5 of 2538 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:C:1573:MET:HE3	1:C:1574:PRO:HD2	1.37	1.05
1:A:1573:MET:HE3	1:A:1574:PRO:HD2	1.37	1.03
1:D:1573:MET:HE3	1:D:1574:PRO:HD2	1.37	1.02
1:B:1573:MET:HE3	1:B:1574:PRO:HD2	1.37	1.02
1:B:3467:MET:HE1	1:C:1174:GLY:CA	1.99	0.93

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%)	4246 (97%)	139 (3%)	0	100	100
1	B	4385/5037 (87%)	4245 (97%)	140 (3%)	0	100	100
1	C	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	D	4385/5037 (87%)	4246 (97%)	139 (3%)	0	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17960/20580 (87%)	17392 (97%)	568 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	3808 (99%)	28 (1%)	81	91
1	B	3836/4276 (90%)	3808 (99%)	28 (1%)	81	91
1	C	3836/4276 (90%)	3808 (99%)	28 (1%)	81	91
1	D	3836/4276 (90%)	3807 (99%)	29 (1%)	79	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	89/90 (99%)	83 (93%)	6 (7%)	13	41
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	61
2	G	89/90 (99%)	84 (94%)	5 (6%)	17	47
2	H	89/90 (99%)	85 (96%)	4 (4%)	23	53
All	All	15700/17464 (90%)	15569 (99%)	131 (1%)	77	89

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1979	LEU
1	C	2577	ILE
1	C	4973	HIS
1	B	318	VAL
1	B	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	255	HIS
1	D	2342	ASN
1	C	3211	ASN
1	D	581	ASN
1	D	1640	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A	5301	-	28,33,33	0.74	0	34,52,52	0.92	2 (5%)
6	141	D	5304	-	11,12,12	1.77	3 (27%)	11,17,17	0.97	0
3	ATP	B	5301	-	28,33,33	0.74	0	34,52,52	0.92	2 (5%)
6	141	B	5304	-	11,12,12	1.76	3 (27%)	11,17,17	0.97	0
6	141	C	5304	-	11,12,12	1.76	3 (27%)	11,17,17	0.98	0
3	ATP	D	5301	-	28,33,33	0.75	0	34,52,52	0.92	2 (5%)
3	ATP	C	5301	-	28,33,33	0.74	0	34,52,52	0.93	2 (5%)
6	141	A	5304	-	11,12,12	1.76	3 (27%)	11,17,17	0.97	0

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	A	5301	-	-	6/18/38/38	0/3/3/3
6	141	D	5304	-	-	-	0/2/2/2
3	ATP	B	5301	-	-	6/18/38/38	0/3/3/3
6	141	B	5304	-	-	-	0/2/2/2
6	141	C	5304	-	-	-	0/2/2/2
3	ATP	D	5301	-	-	6/18/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/18/38/38	0/3/3/3
6	141	A	5304	-	-	-	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5304	141	C5-C4	-4.04	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5304	141	C5-C4	-4.01	1.38	1.45
6	B	5304	141	C5-C4	-3.99	1.38	1.45
6	D	5304	141	C5-C4	-3.99	1.38	1.45
6	B	5304	141	C7-N8	2.49	1.35	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5301	ATP	C4'-O4'-C1'	-4.10	106.17	109.92
3	A	5301	ATP	C4'-O4'-C1'	-4.09	106.18	109.92
3	B	5301	ATP	C4'-O4'-C1'	-4.08	106.19	109.92
3	C	5301	ATP	C4'-O4'-C1'	-4.08	106.19	109.92
3	C	5301	ATP	C5-C6-N6	2.35	123.89	120.31

There are no chirality outliers.

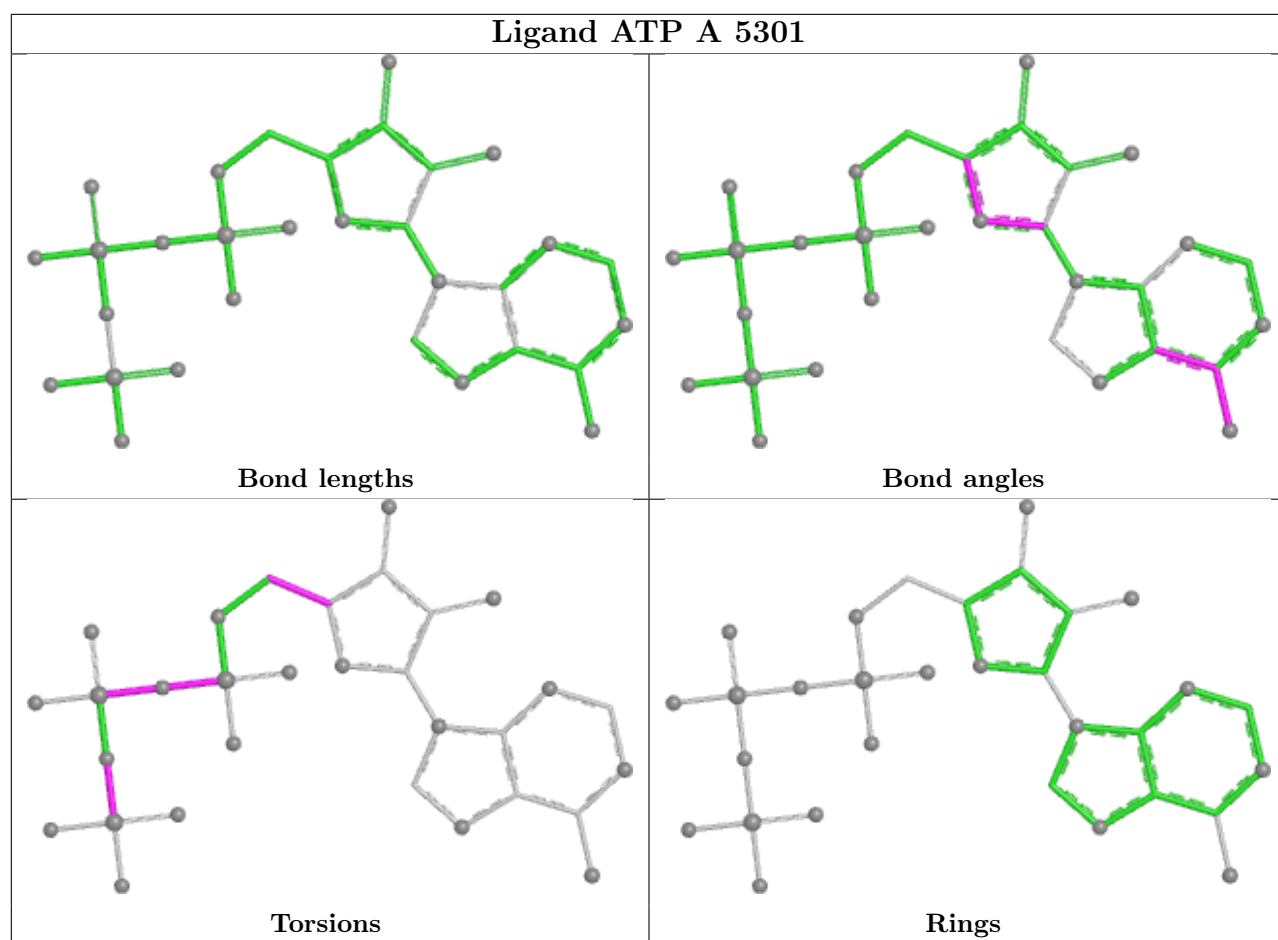
5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O2G
3	B	5301	ATP	PB-O3B-PG-O2G
3	D	5301	ATP	PB-O3B-PG-O2G
3	C	5301	ATP	PB-O3B-PG-O2G
3	A	5301	ATP	O4'-C4'-C5'-O5'

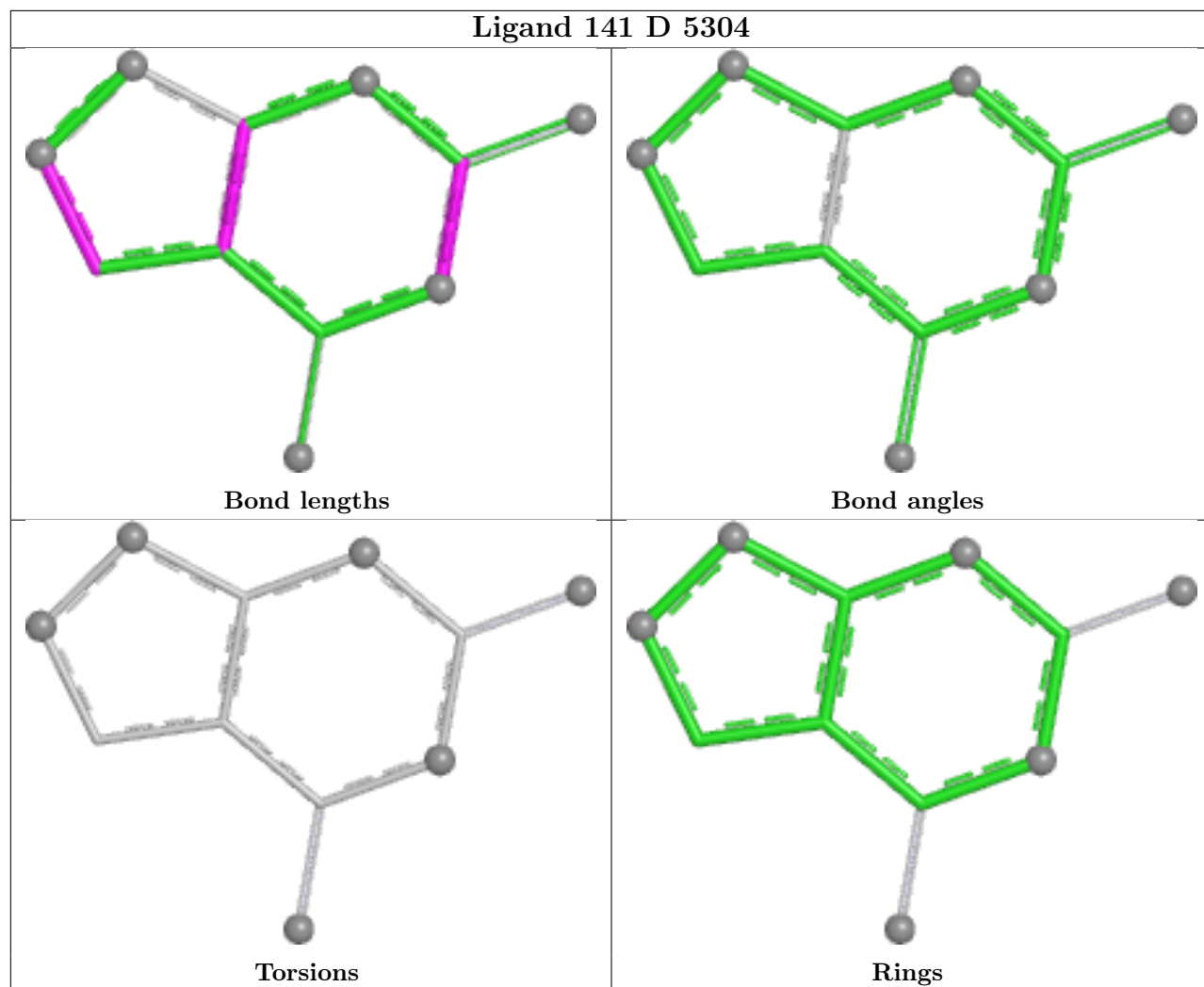
There are no ring outliers.

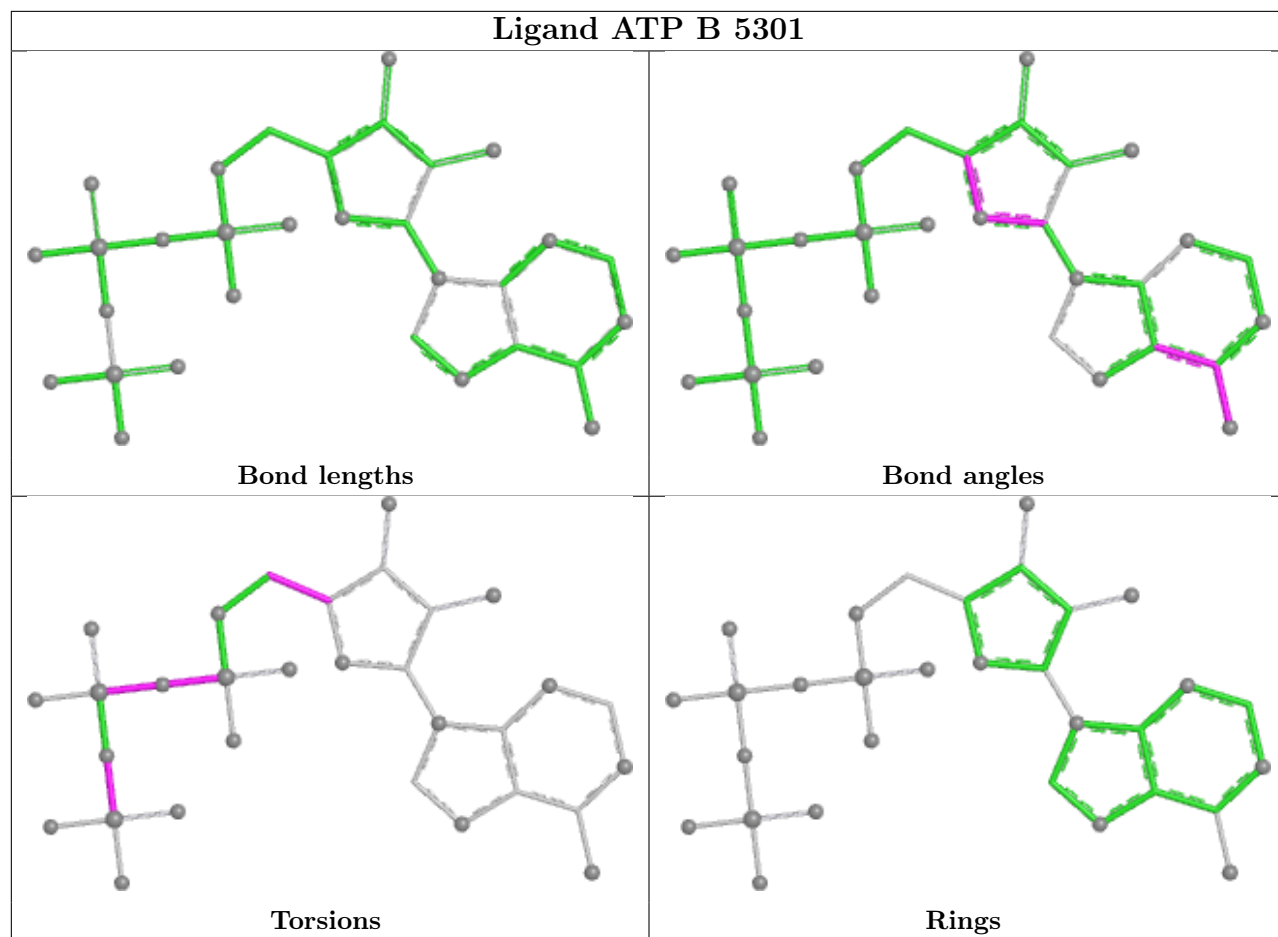
No monomer is involved in short contacts.

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.

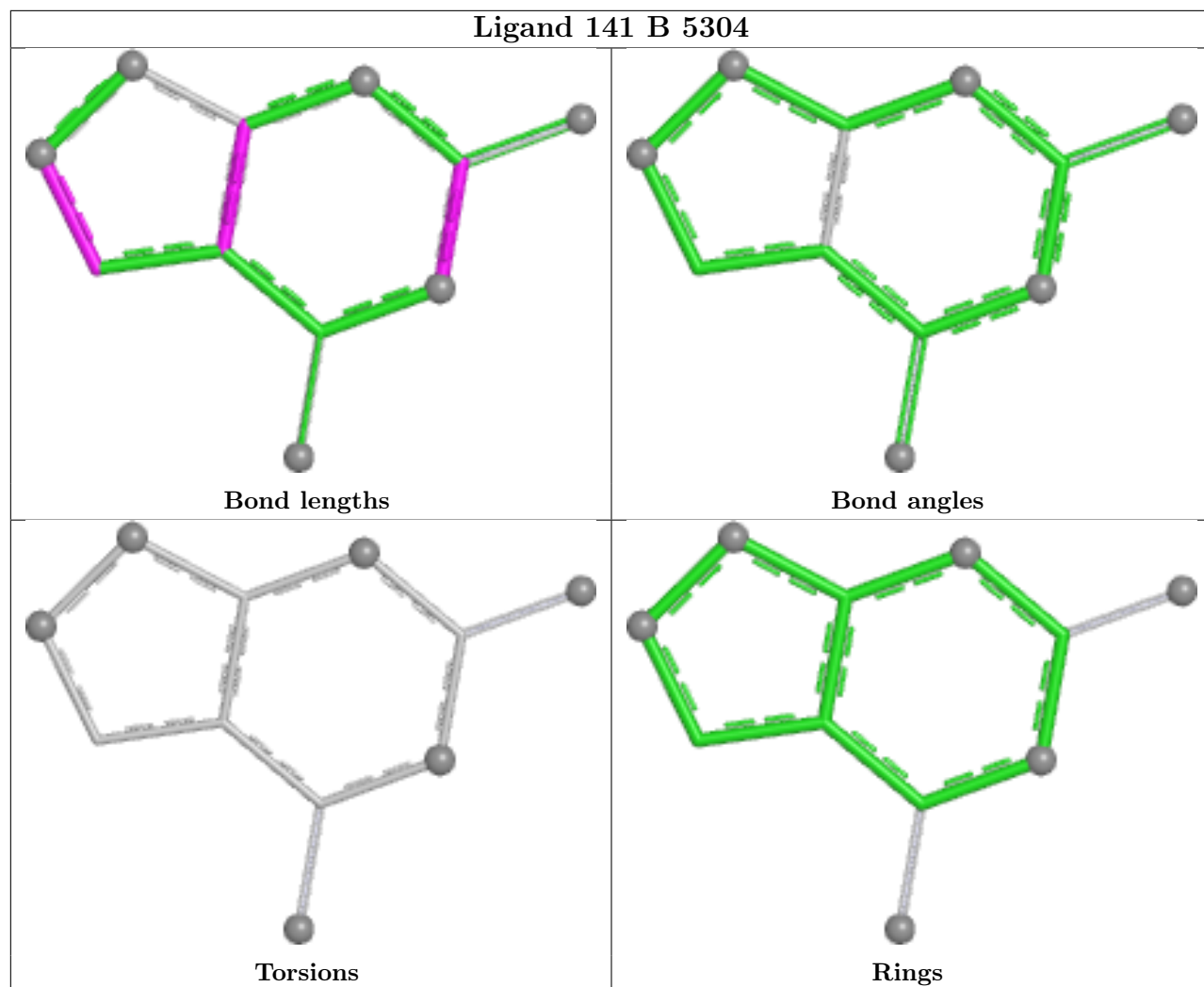


Ligand 141 D 5304

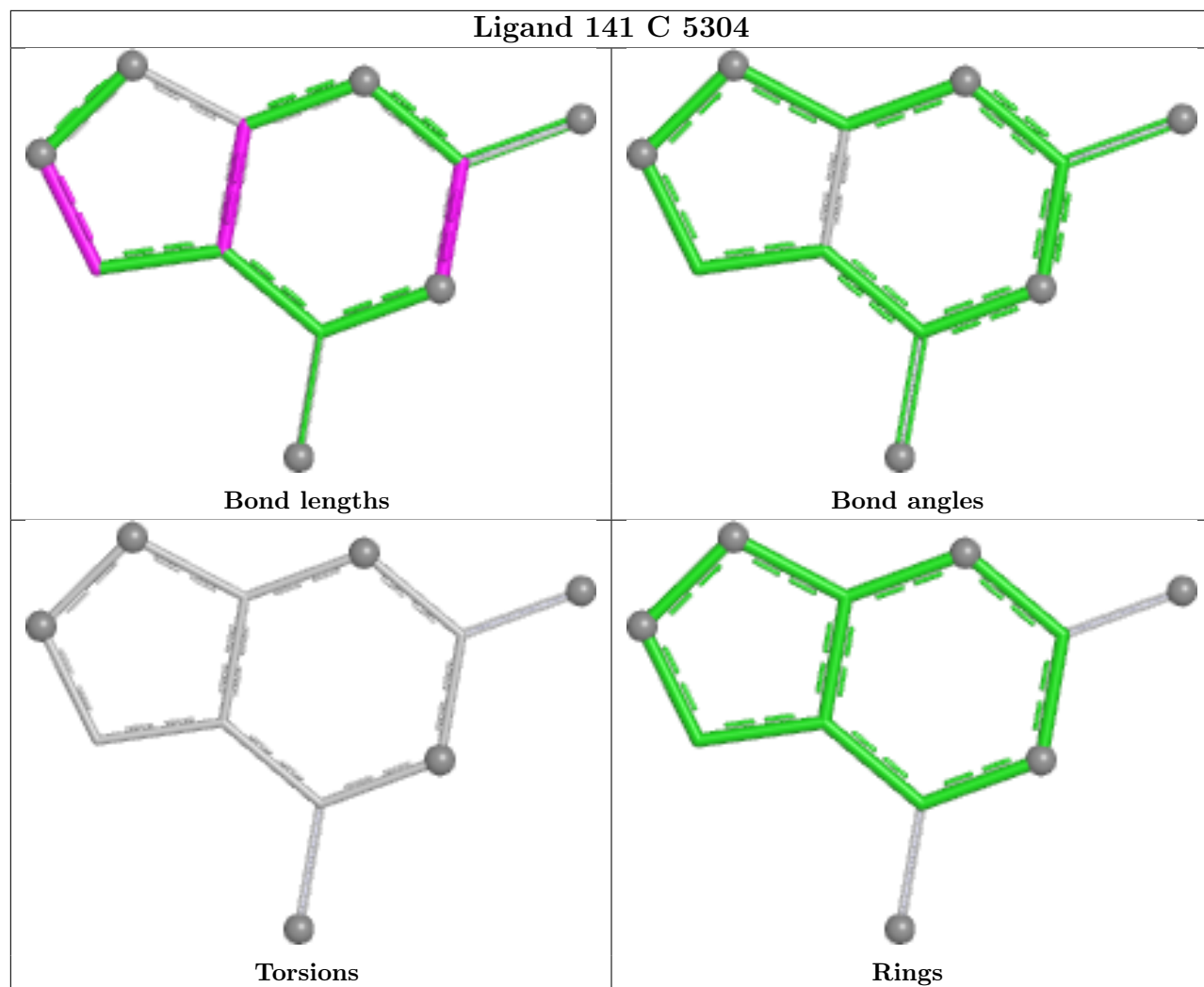


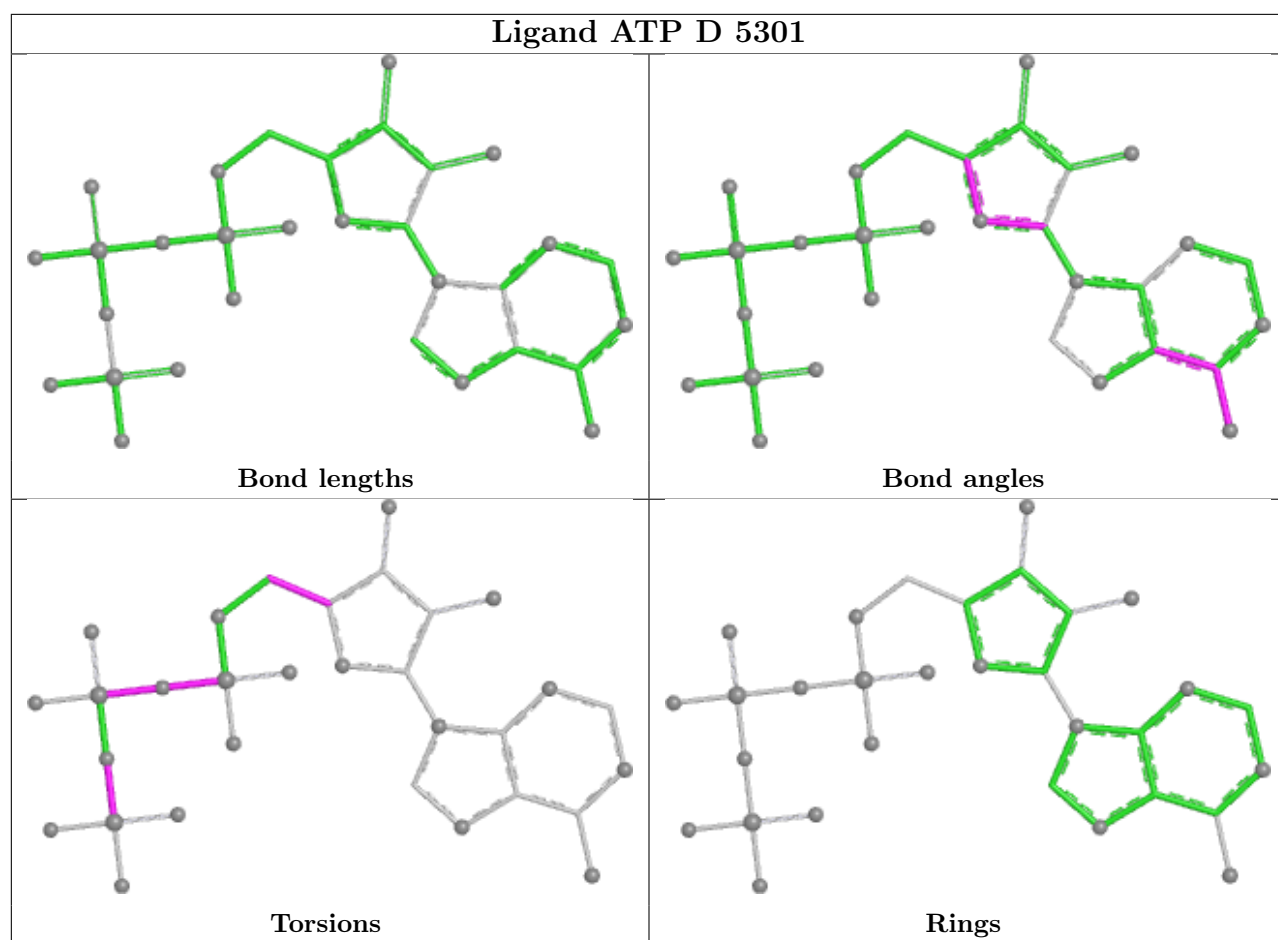


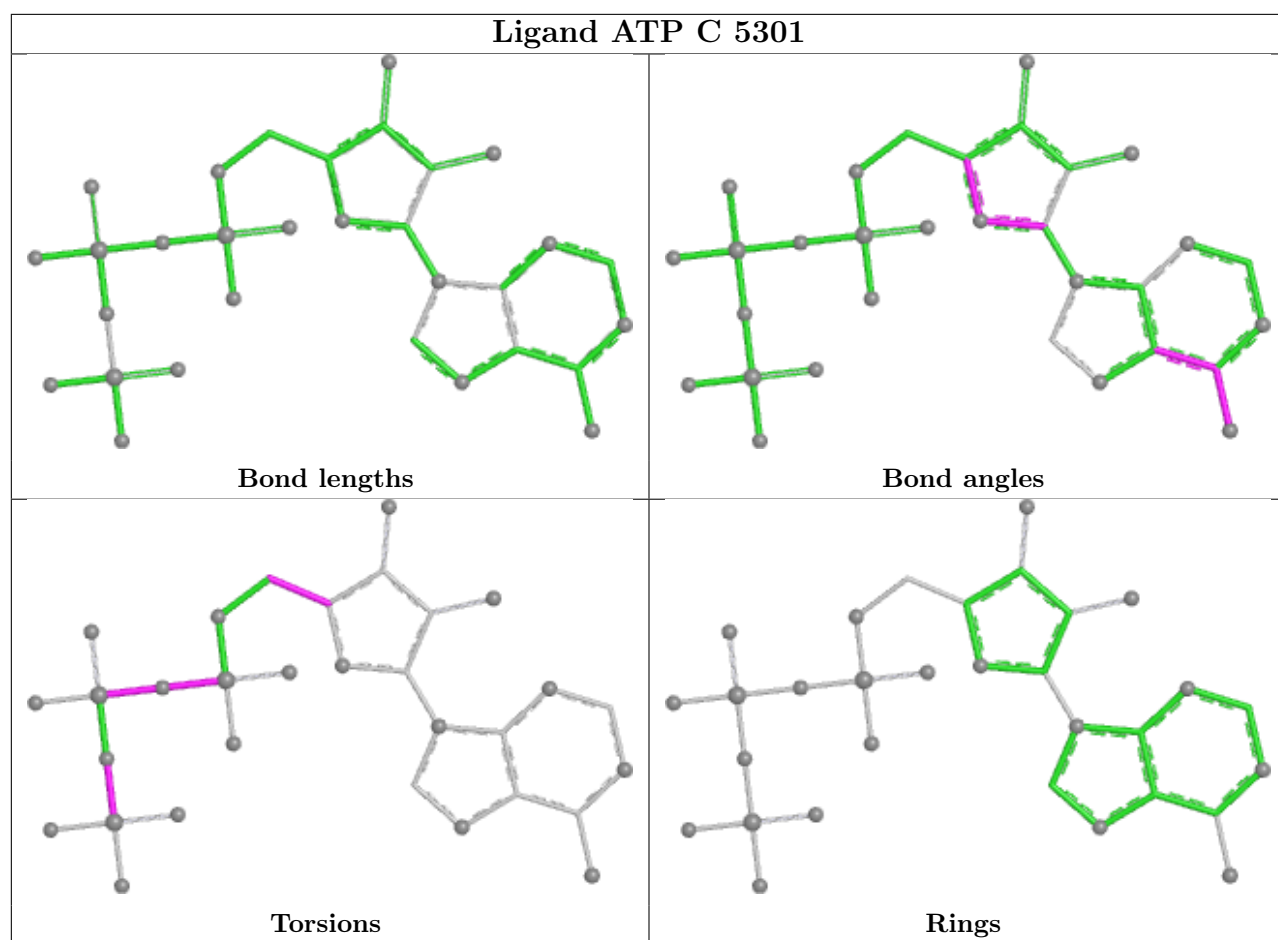
Ligand 141 B 5304

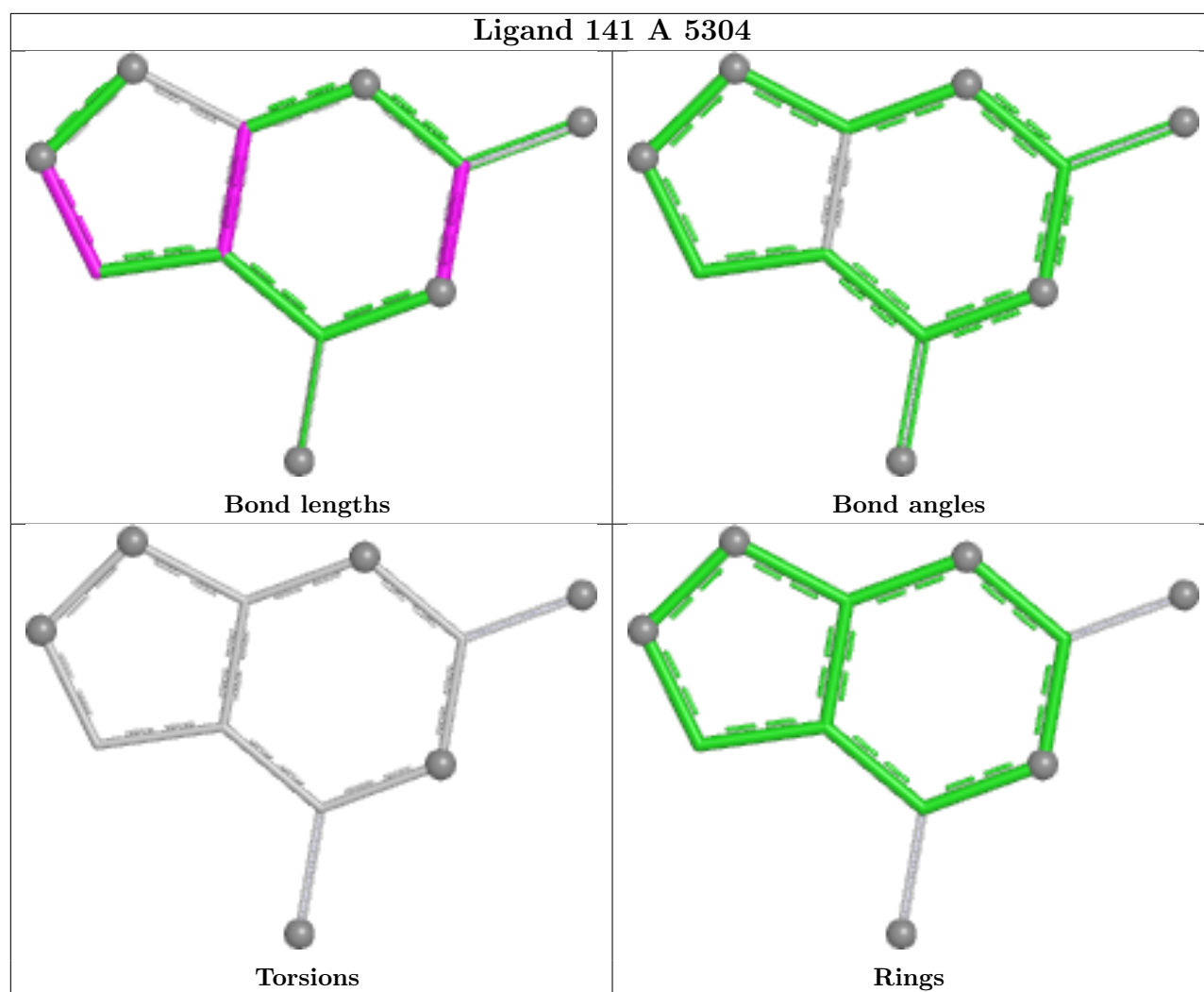


Ligand 141 C 5304









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.

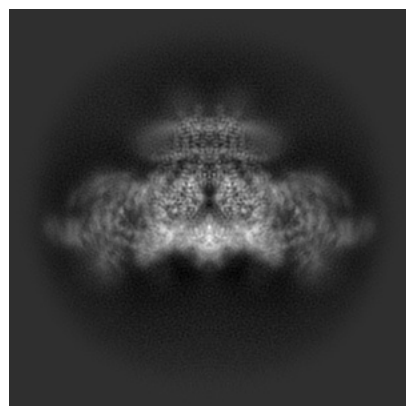
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47393. These allow visual inspection of the internal detail of the map and identification of artifacts.

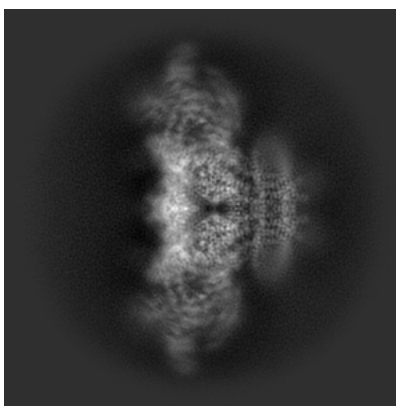
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

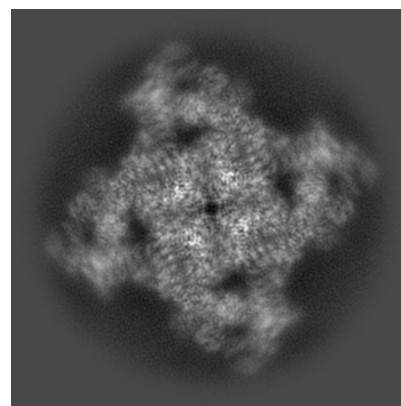
6.1.1 Primary map



X

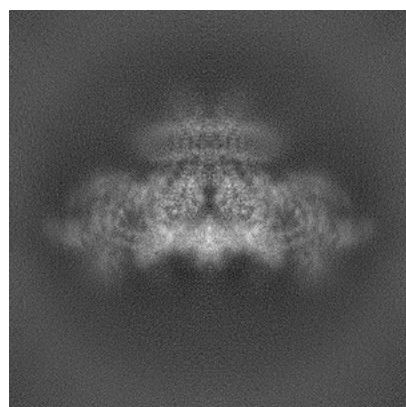


Y

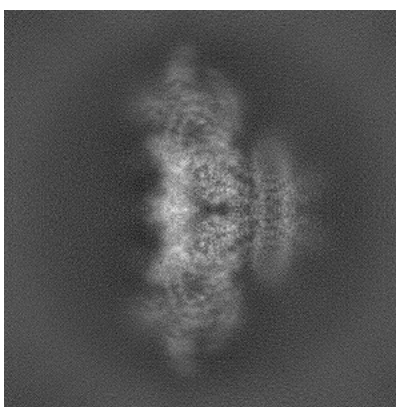


Z

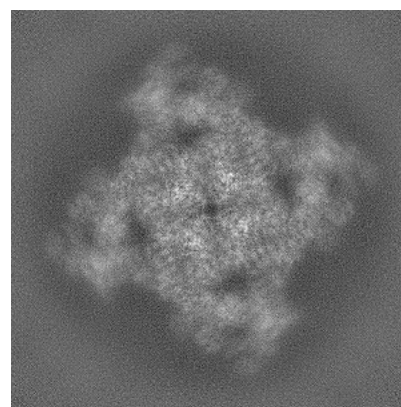
6.1.2 Raw map



X



Y

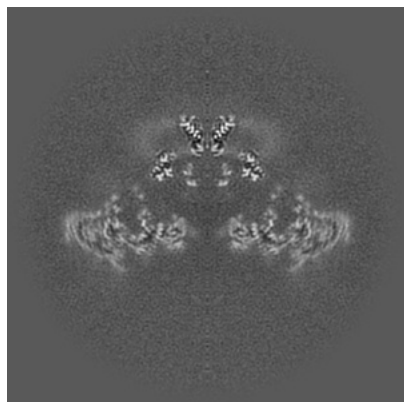


Z

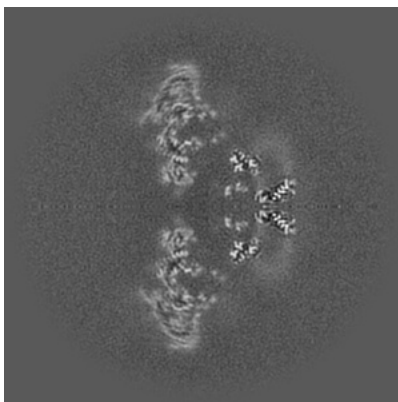
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

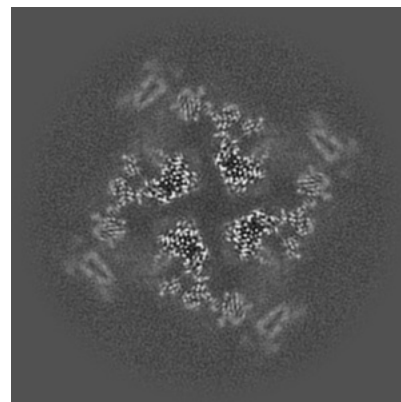
6.2.1 Primary map



X Index: 256

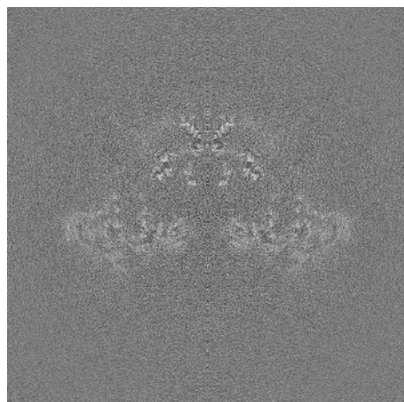


Y Index: 256

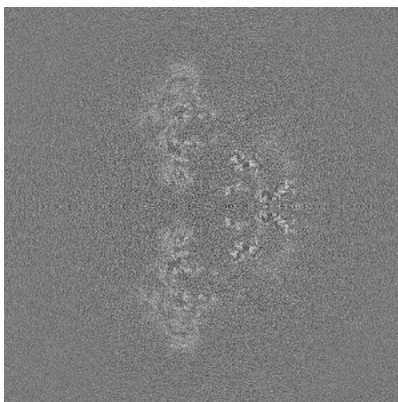


Z Index: 256

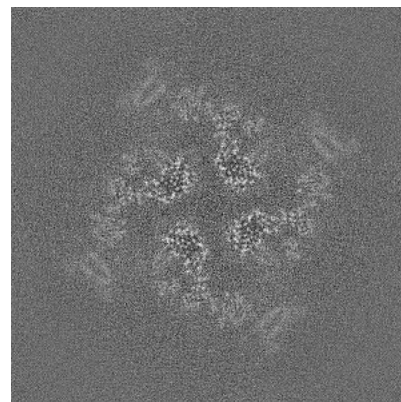
6.2.2 Raw map



X Index: 256



Y Index: 256

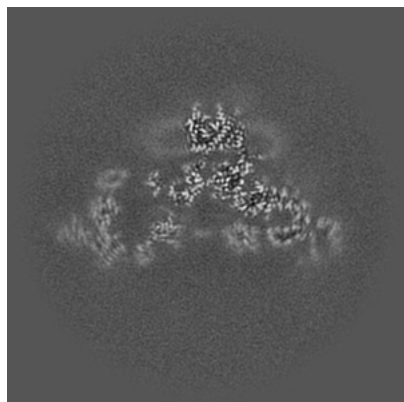


Z Index: 256

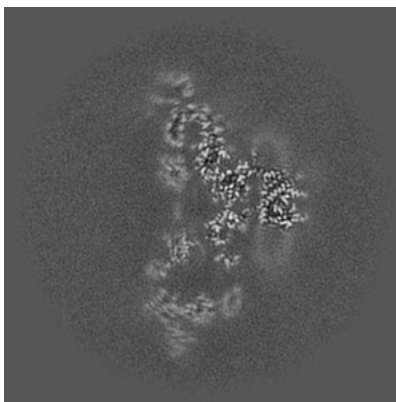
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

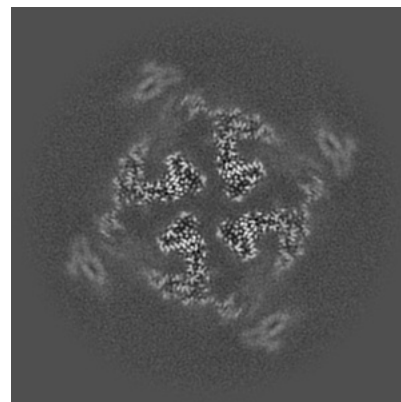
6.3.1 Primary map



X Index: 273

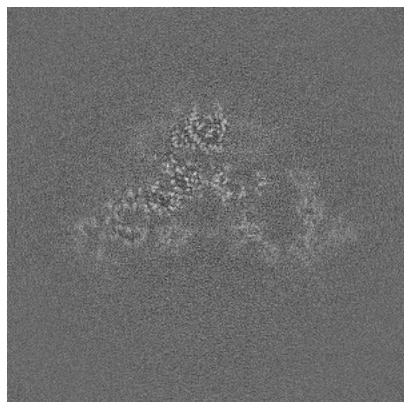


Y Index: 239

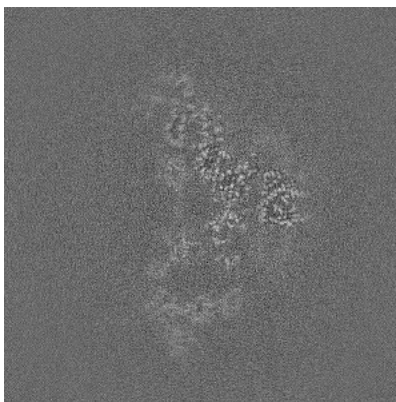


Z Index: 265

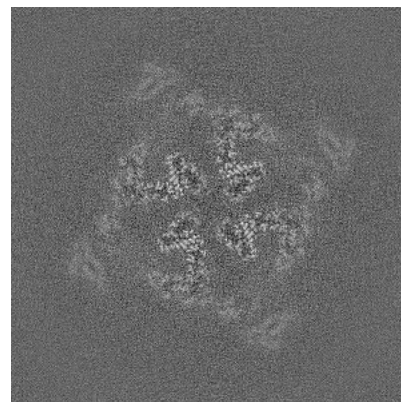
6.3.2 Raw map



X Index: 239



Y Index: 239

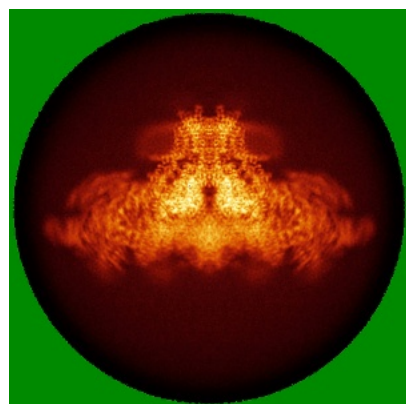


Z Index: 266

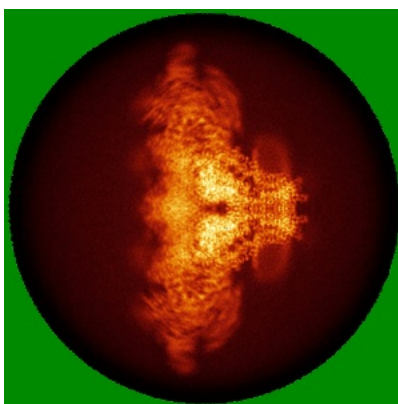
The images above show the largest variance slices of the map in three orthogonal directions.

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

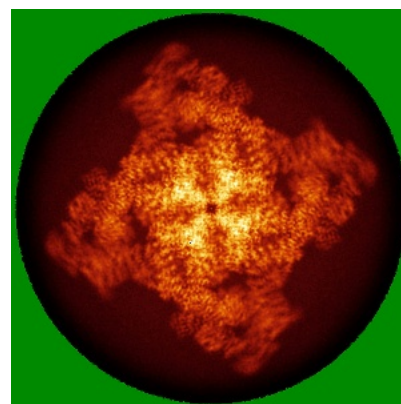
6.4.1 Primary map



X

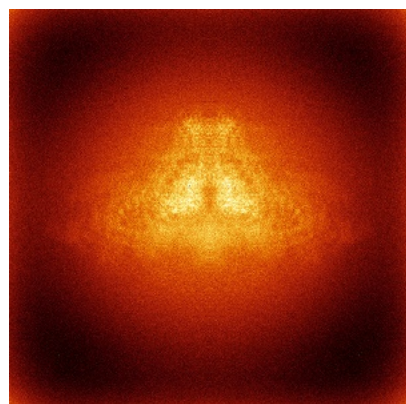


Y

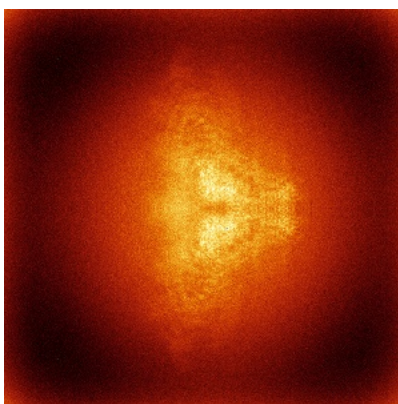


Z

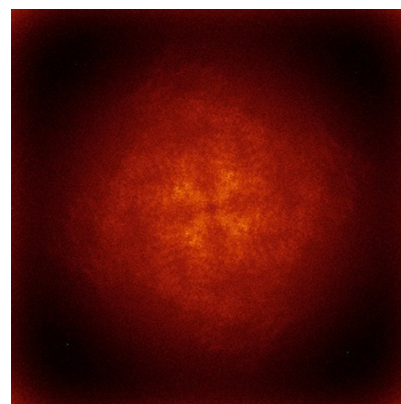
6.4.2 Raw map



X



Y

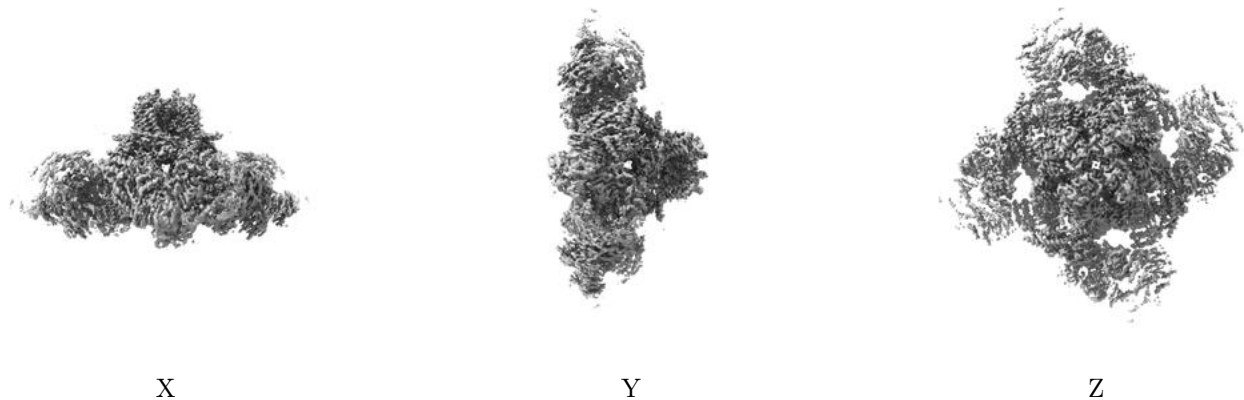


Z

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.

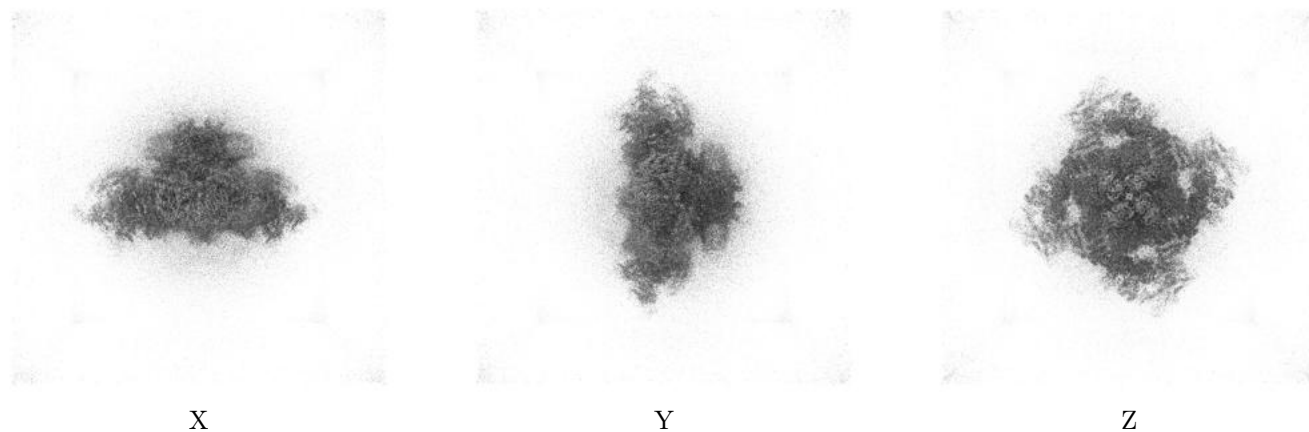
6.5 Orthogonal surface views [i](#)

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.

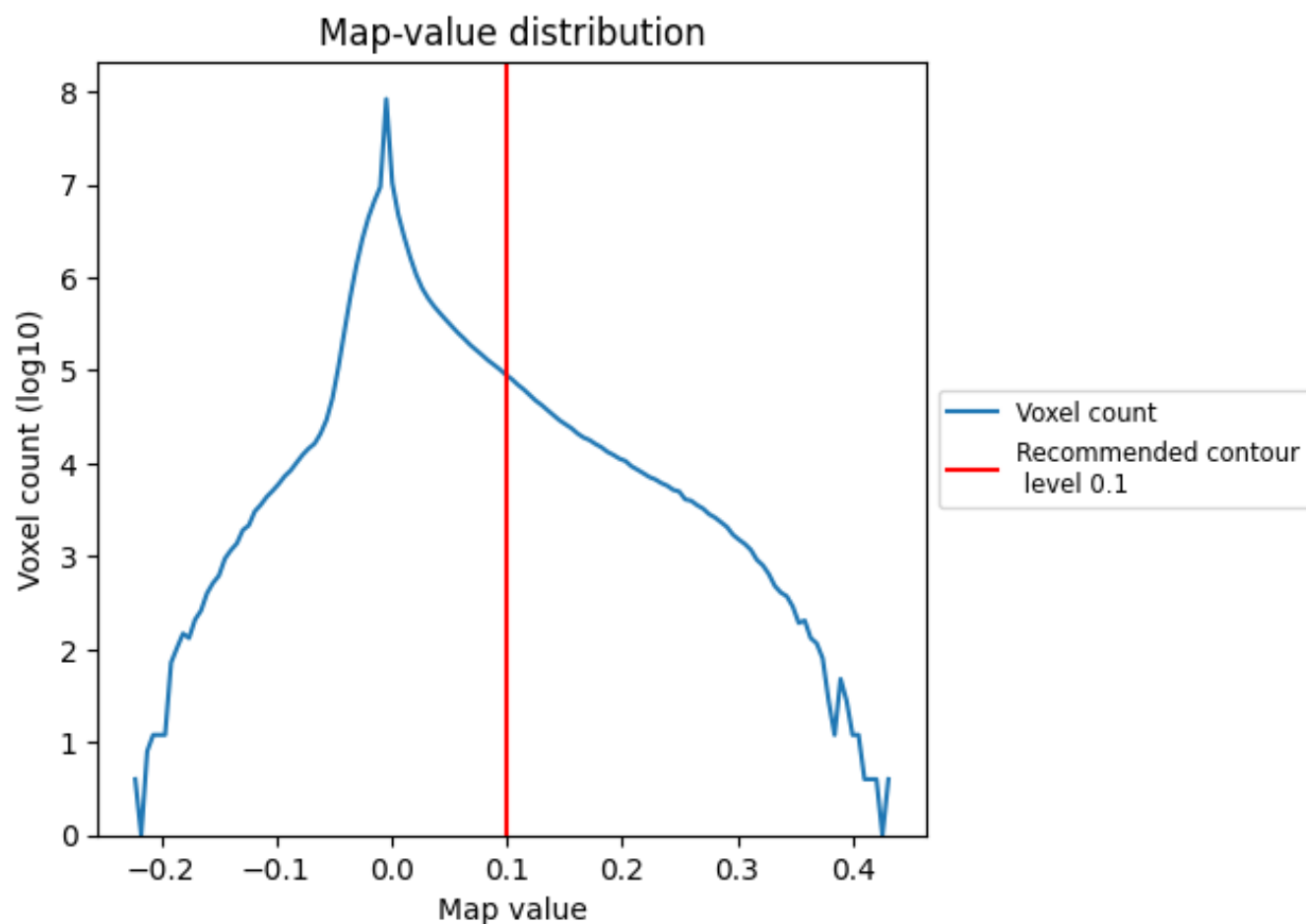
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

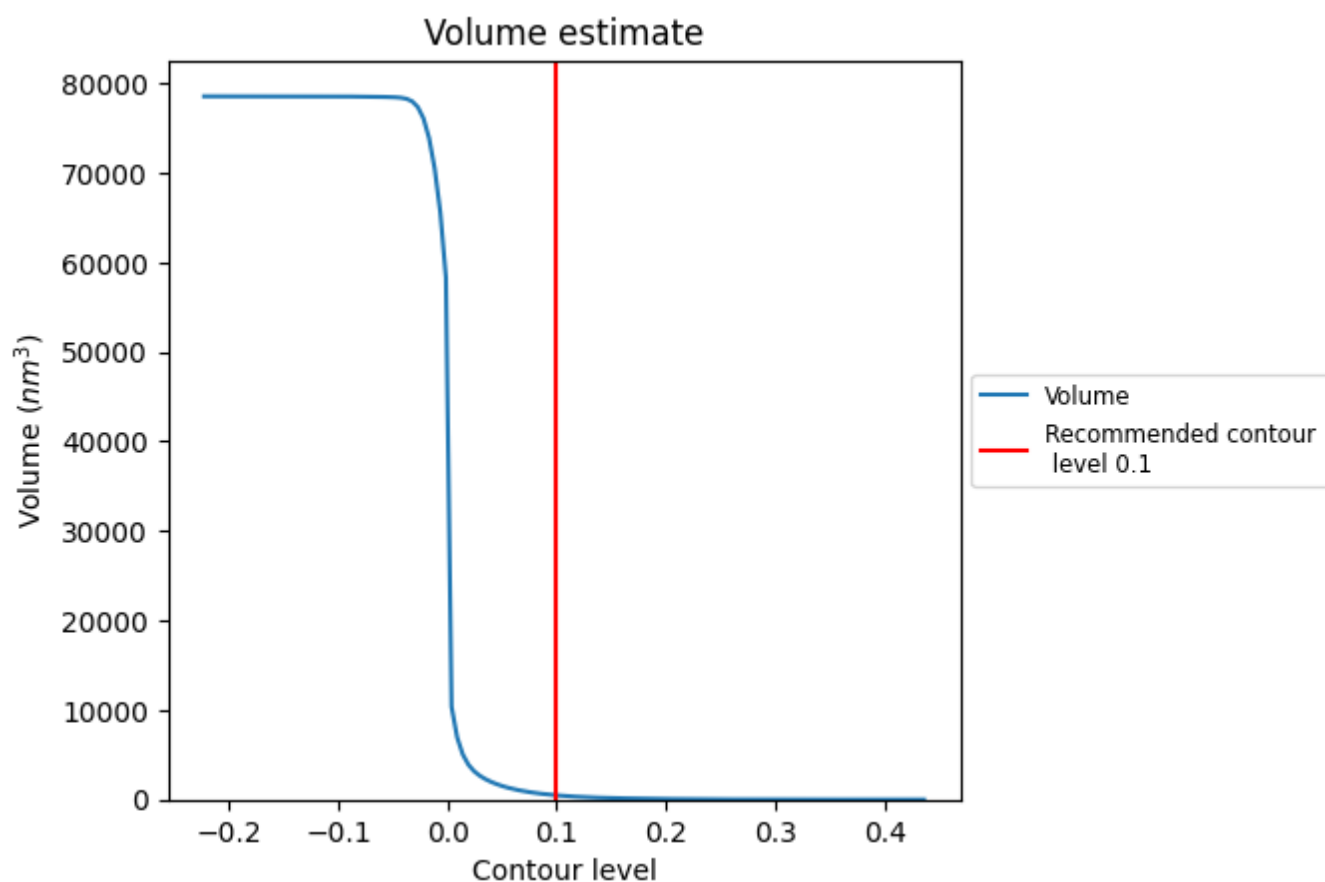
This section contains the results of statistical analysis of the map.

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.

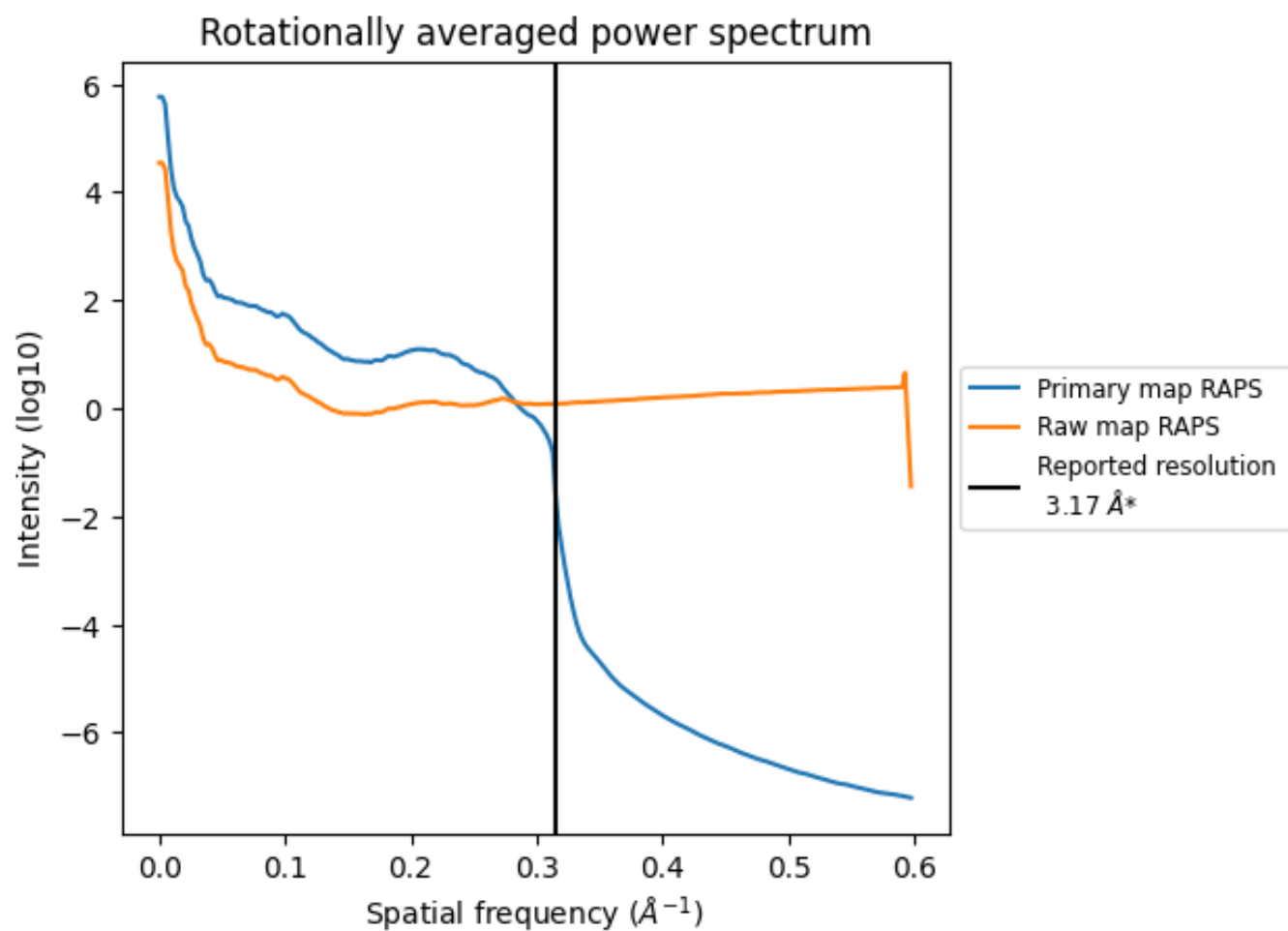
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm³; this corresponds to an approximate mass of 431 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 ⓘ

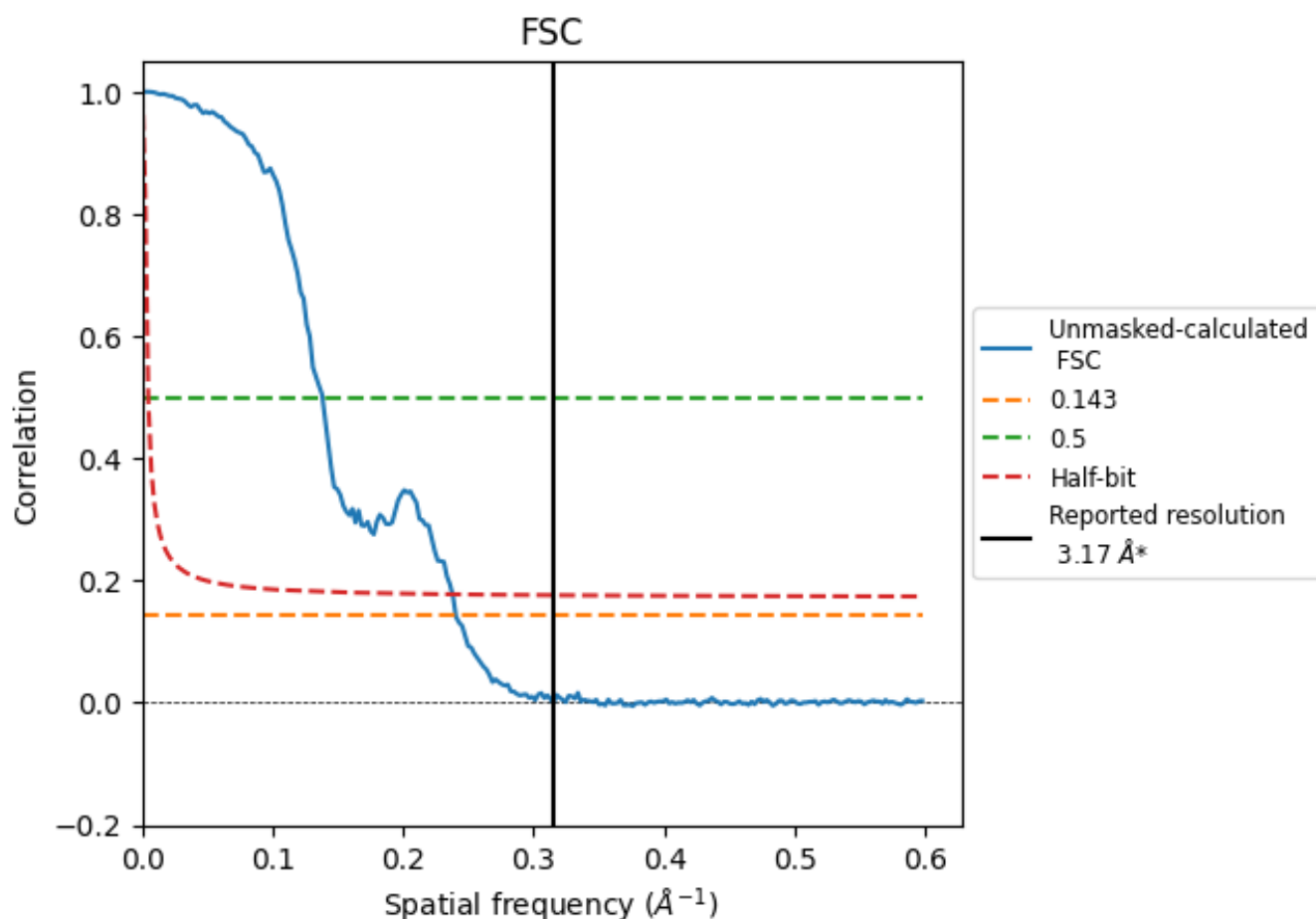


*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

8.2 Resolution estimates [i](#)

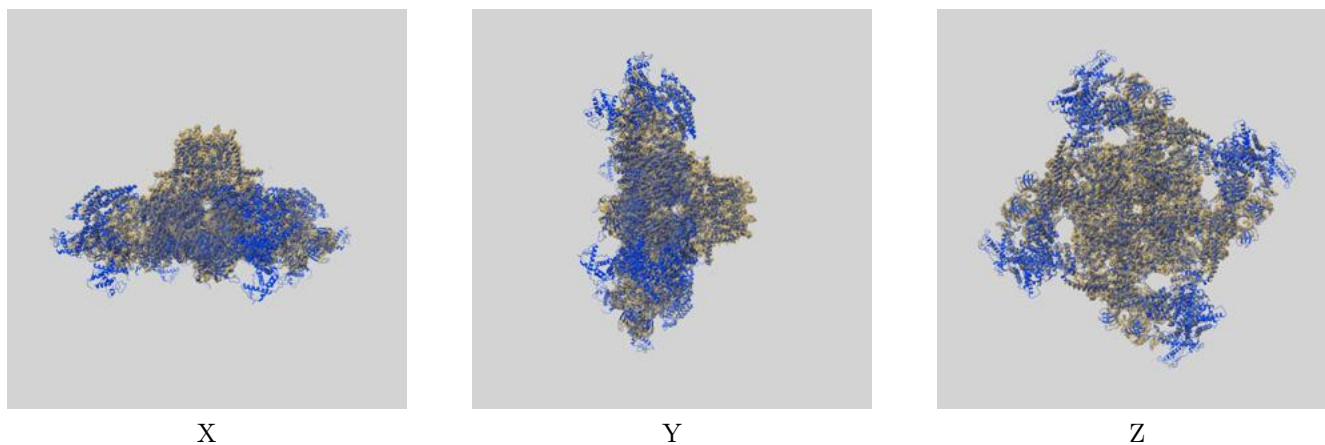
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.24	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

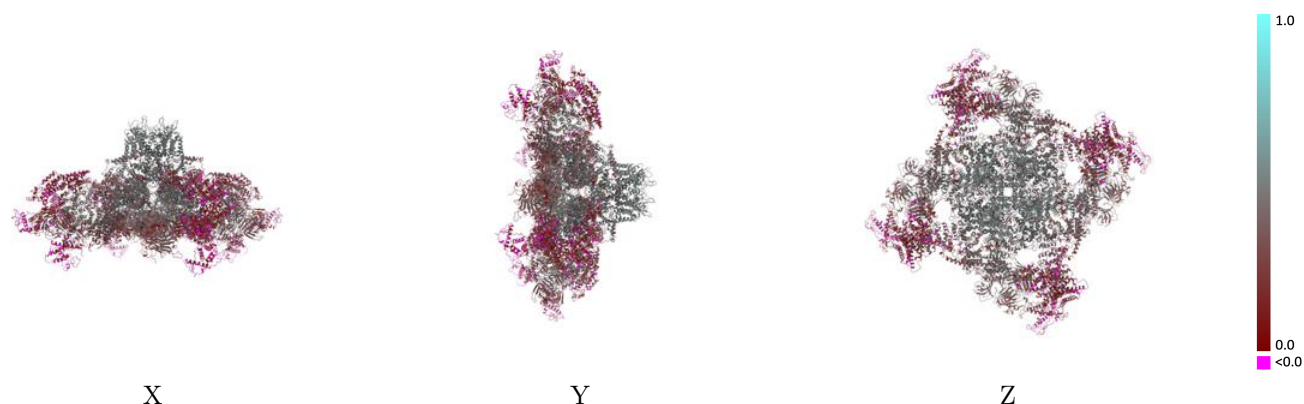
This section contains information regarding the fit between EMDB map EMD-47393 and PDB model 9E1G. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



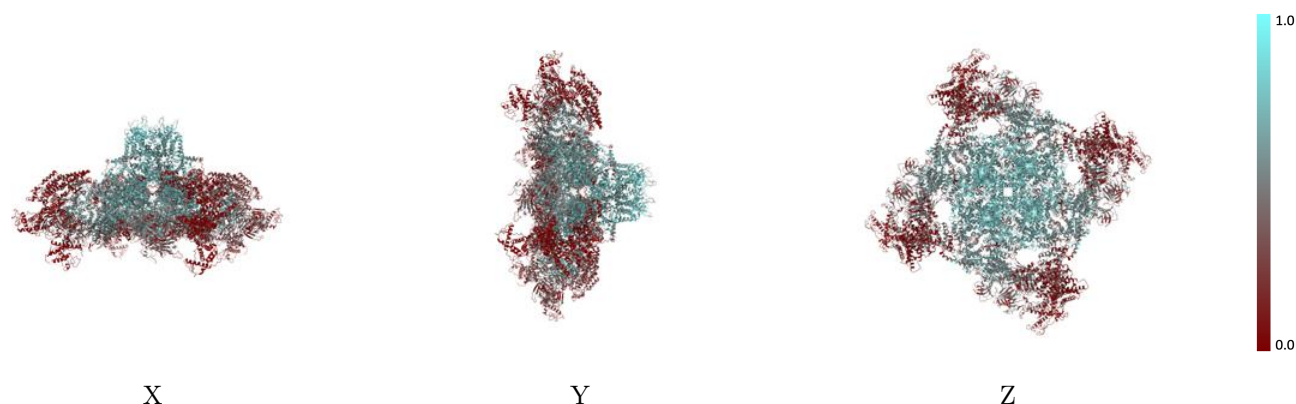
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



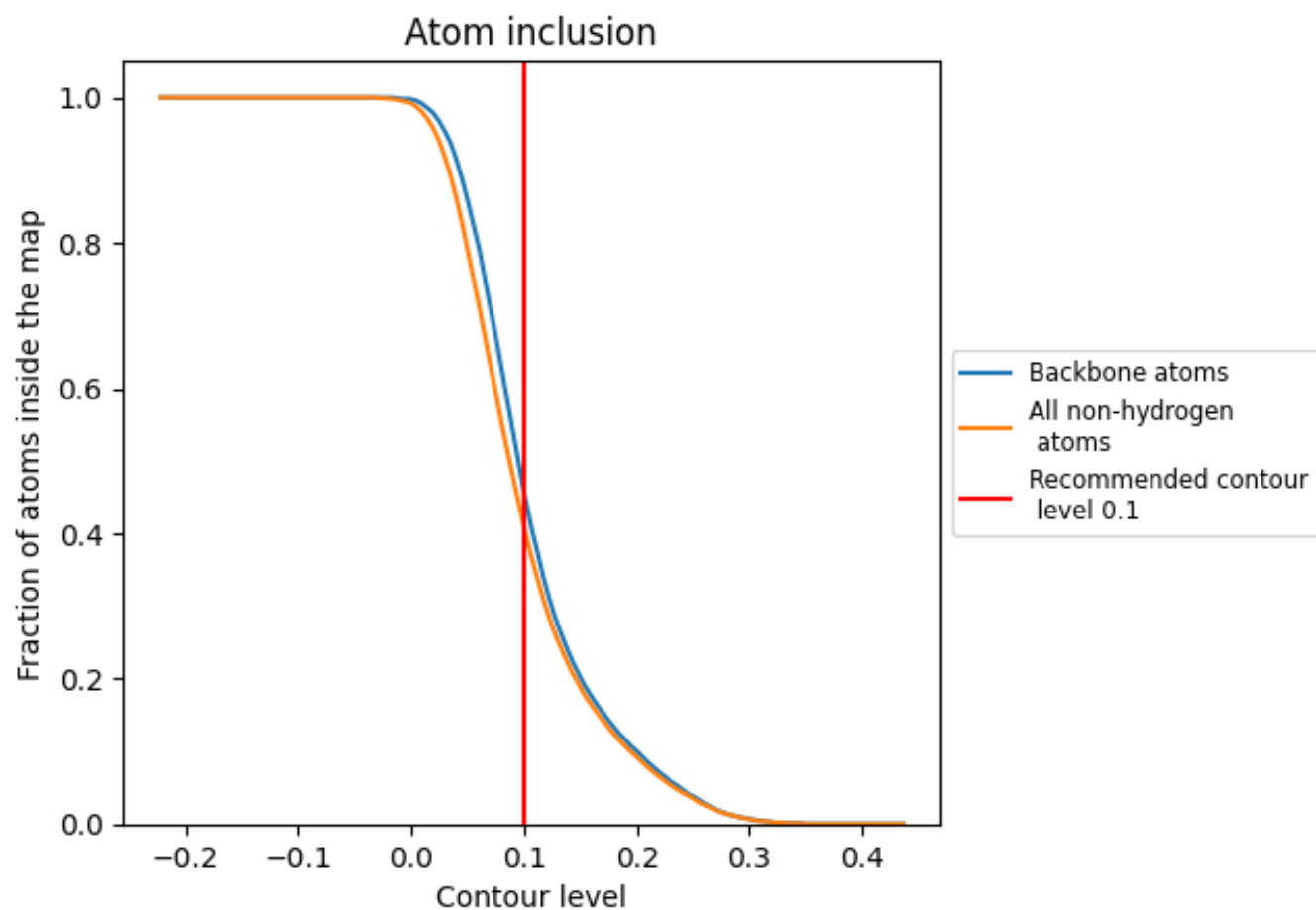
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 46% of all backbone atoms, 41% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4080	<div></div> 0.3230
A	<div></div> 0.4200	<div></div> 0.3260
B	<div></div> 0.4200	<div></div> 0.3210
C	<div></div> 0.4200	<div></div> 0.3210
D	<div></div> 0.4200	<div></div> 0.3210
E	<div></div> 0.2860	<div></div> 0.3640
F	<div></div> 0.2850	<div></div> 0.3620
G	<div></div> 0.2850	<div></div> 0.3570
H	<div></div> 0.2860	<div></div> 0.3640

1.0

0.0

<0.0