



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 06:42 AM EST

PDB ID : 9E1E
EMDB ID : EMD-47391
Title : Structure of RyR1 in the primed state in the presence of uracil
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 2.92 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.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) : 2.39

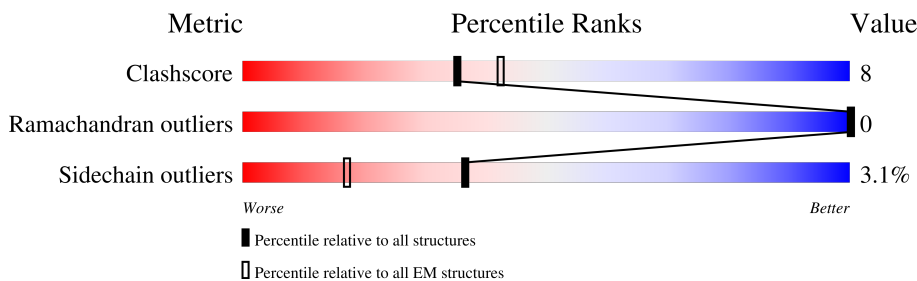
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	108	
2	F	108	
2	G	108	
2	H	108	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 144088 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

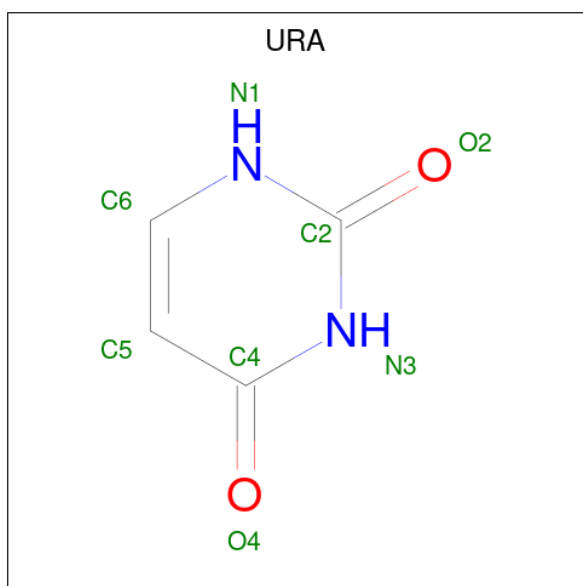
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	Total	Zn	0
			1	1	

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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 URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$) (labeled as "Ligand of Interest" by depositor).

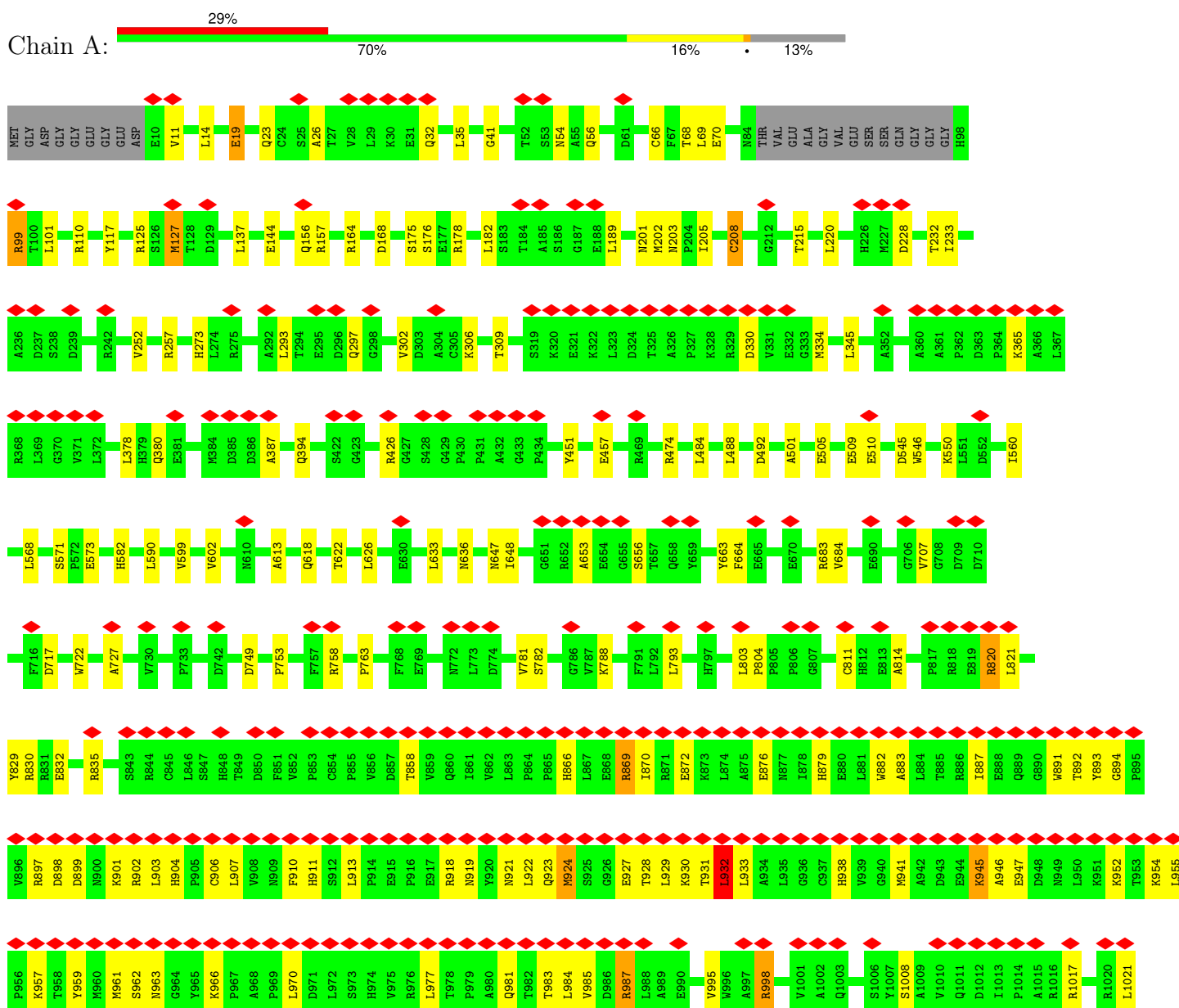


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			8	4	2	2	
6	B	1	Total	C	N	O	0
			8	4	2	2	
6	D	1	Total	C	N	O	0
			8	4	2	2	
6	C	1	Total	C	N	O	0
			8	4	2	2	

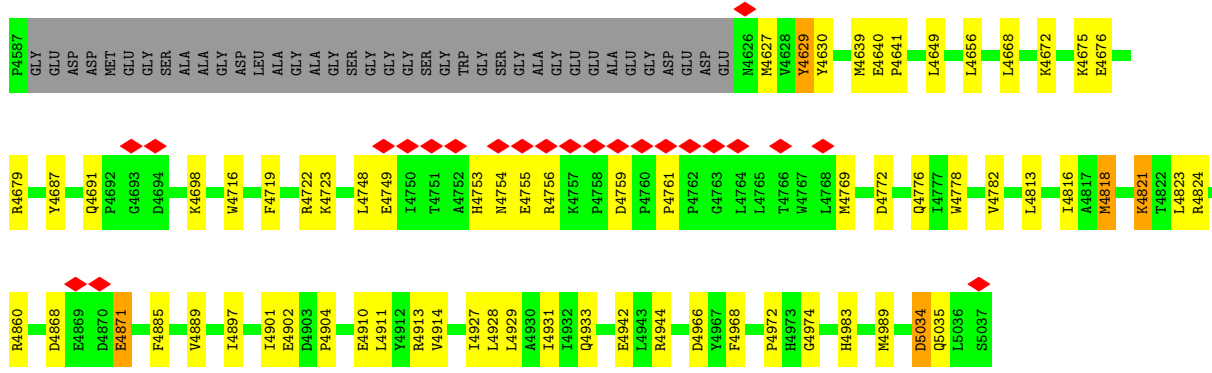
3 Residue-property plots

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.

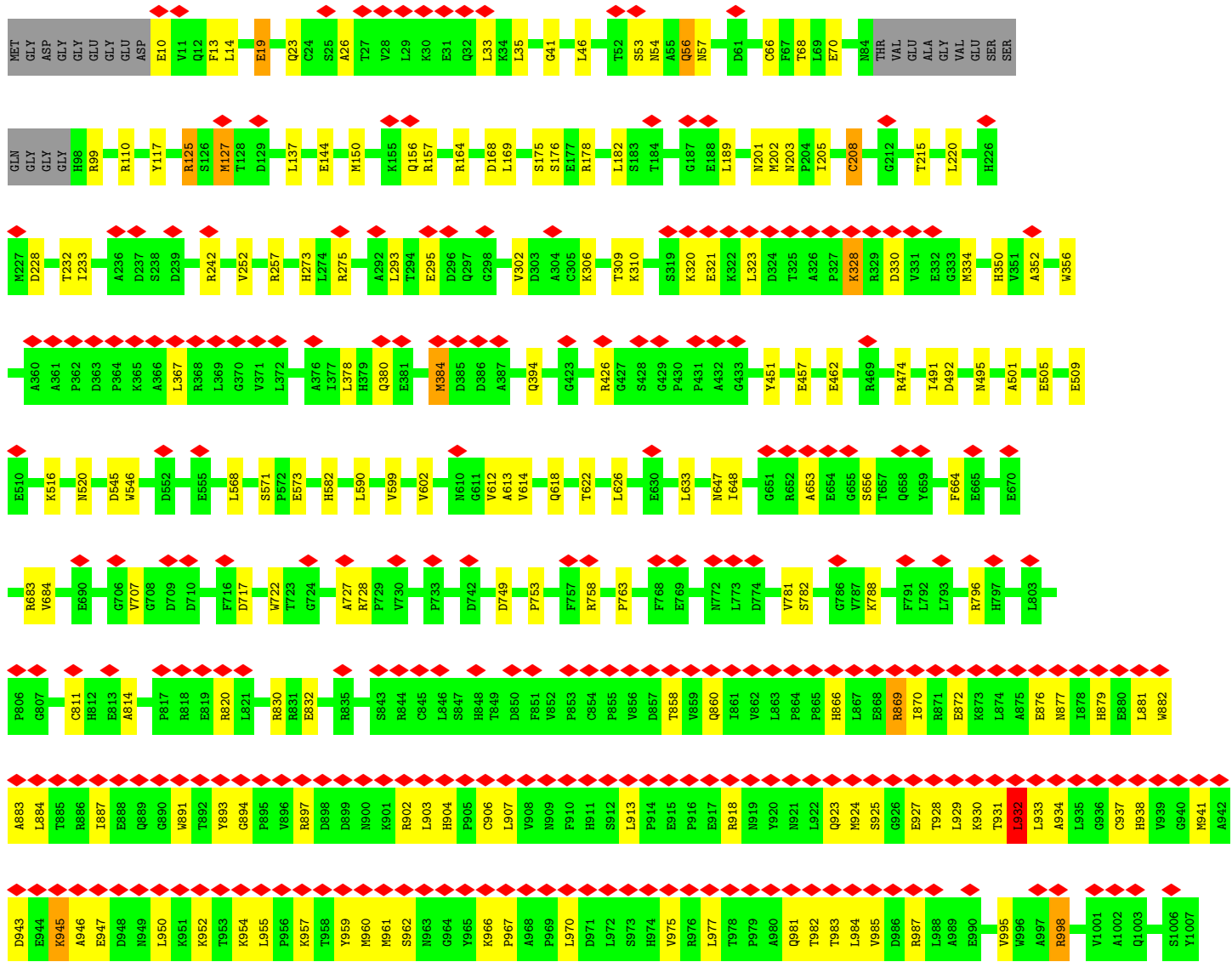
- Molecule 1: Ryanodine receptor 1

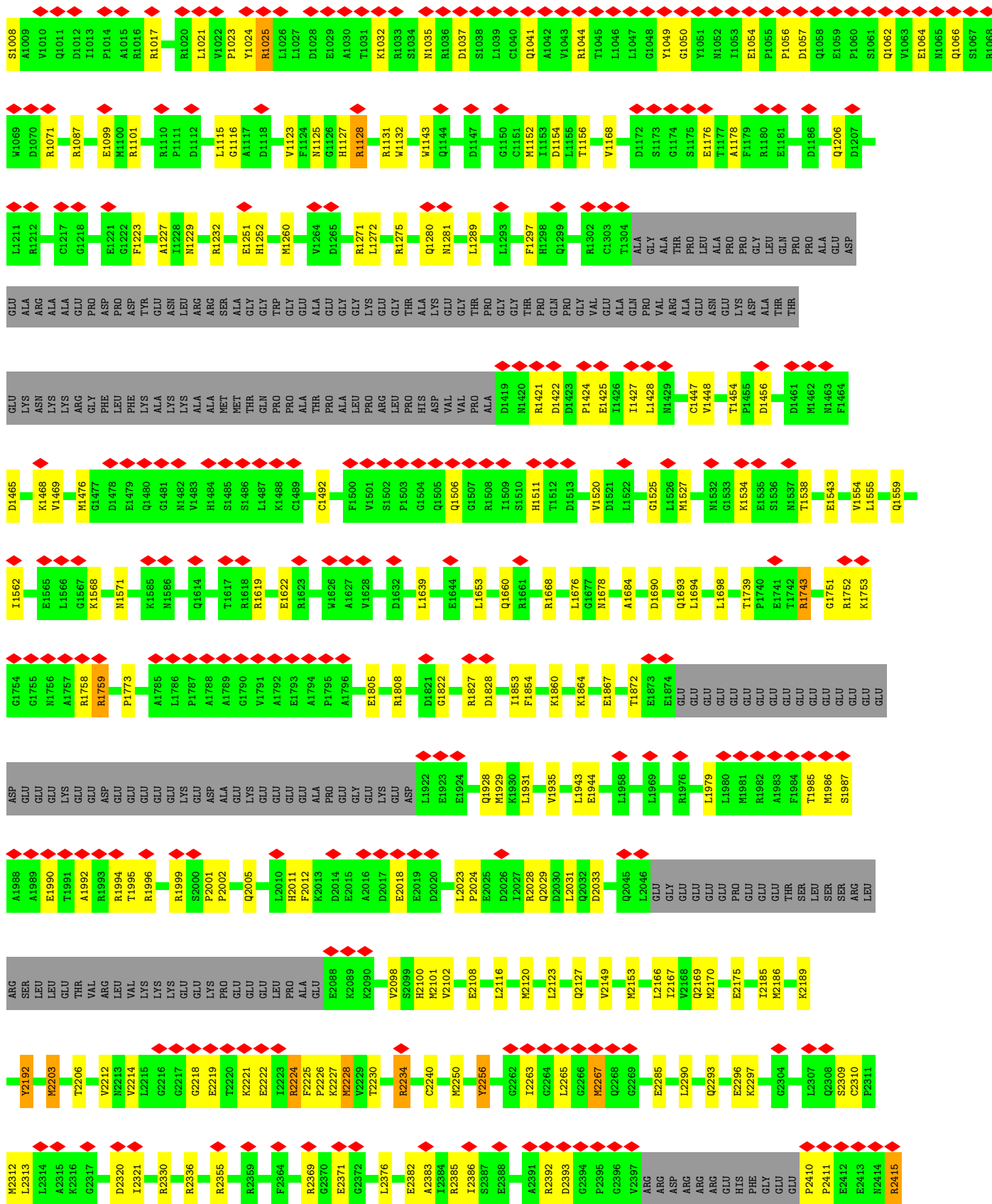


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Y3182	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	M3214	A3215	C3216	S3217	V3218	L3219	F3220	D3221	K3222	S3223	P3224	R3225	E3226	A3228	I3229	G3230	L3231	L3232	P3233	M3234	V3235	V3236	E3237	E3238	M3239	C3240	P3241	
ALA	ARG	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	V3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	S3139	L3140	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	V3161	Q3162	G3165	Y3166	R3167	T3168	L3169	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181				
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T2538	F2541	S2542	M2546	A2547	L2550	K2564	F2569	A2570	G2571	T2572	E2573	H2574	R2575	A2576	L2577	M2582	L2583	H2584	T2585	V2586	Y2587	R2588	L2589	S2590	R2591	G2592	R2593	S2594	Q2599	R2600	I2603	E2604	D2605	C2606	L2607	M2608	C2611	I2614	R2615	F2619	L2622	L2623	R2624	R2625	L2626	V2627	F2628												
D2629	V2630	P2631	L2632	L2633	N2634	E2635	F2636	K2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	H2646	H2647	H2648	R2650	C2651	Y2655	C2656	L2657	P2658	G2660	W2661	A2662	M2663	T2664	G2665	V2666	V2667	S2668	E2669	E2670	E2671	L2672	L2673	T2674	R2675	K2676	L2677	P2678	W2680	L2681	L2682	F2683	D2684	H2688	K2689	K2690	Y2691	D2692					
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L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	THR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	L2861	L2862	S2863	G2864	T2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872			
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N2933	G2934	Y2935	A2936	V2937	T2938	R2939	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	A2956	F2957	F2958	F2959	L2960	Q2961	L2963	L2964	R2965	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	F2973	L2974	A2975	H2976	L2977	E2978	A2979	V2980	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992			
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ALA	ARG	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	V3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	S3139	L3140	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	V3161	Q3162	G3165	Y3166	R3167	T3168	L3169	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181				
Y3182	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	M3214	A3215	C3216	S3217	V3218	L3219	F3220	D3221	K3222	S3223	P3224	R3225	E3226	A3228	I3229	G3230	L3231	L3232	P3233	M3234	V3235	V3236	E3237	E3238	M3239	C3240	P3241	
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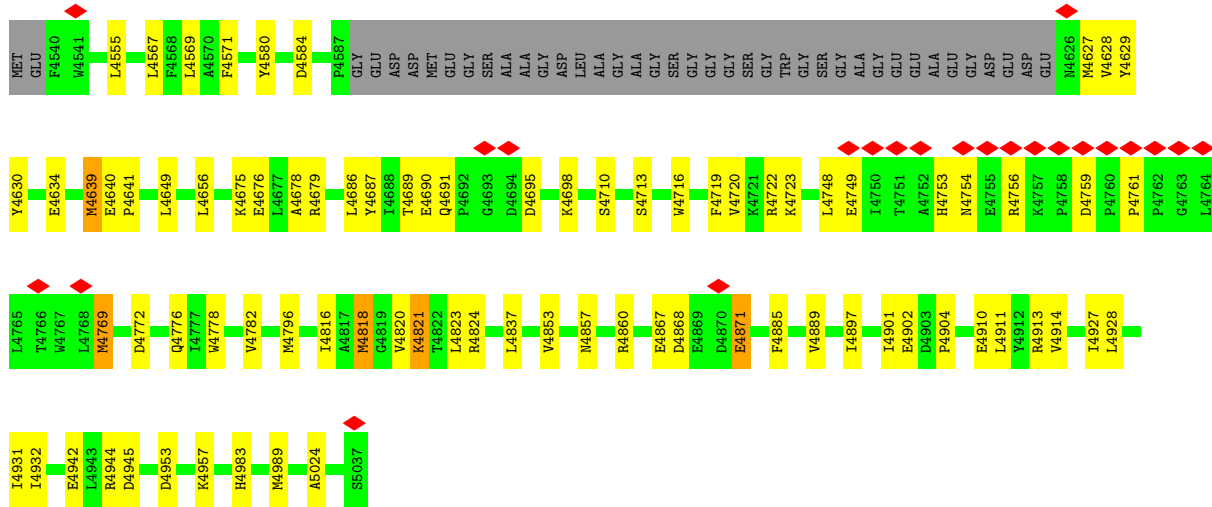


• Molecule 1: Ryanodine receptor 1

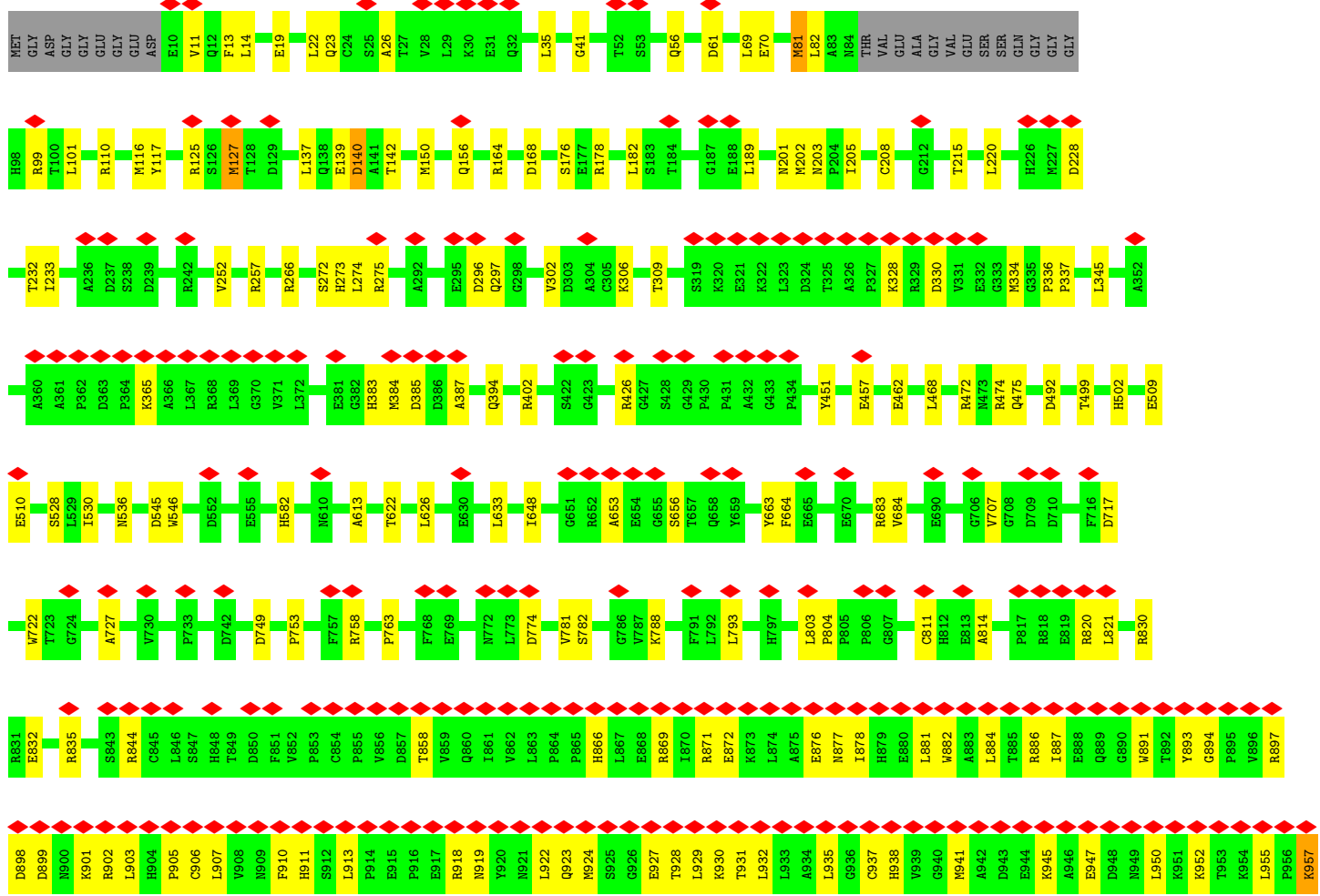




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GLY	Y2855	N2856	P2857	Q2858	P2860	D2861	L2862	G2864	V2865	T2866	L2867	S2868	R2869	L2809	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	M2884	T2885	W2886	G2887	R2888	G2889	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	L2910	T2912	A2913			
K2914	E2915	K2916	A2917	R2918	D2919	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	A2935	A2936	V2937	T2938	A2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	L2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	L2969	Q2971	E2972	F2973		
L2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	L2995	F2997	F2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	I3006	N3007	Q3008	Y3009	F3010	T3011	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	
K3034	E3035	K3036	E3037	M3038	I3039	L3042	F3043	C3044	K3045	L3046	A3047	L3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	S3061	P3062	A3063	V3064	V3065	N3066	C3067	L3068	H3069	I3070	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	L3092	F3095	F3096					
A3099	S3100	E3101	D3102	L3103	E3104	K3105	M3106	V3107	E3108	M3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	Y3131	T3132	T3133	L3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	T3157	L3158	V3159	T3220	T3221	V3161	
Q3162	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	K3179	M3180	T3181	Y3182	V3183	E3184	K3185	L3186	R3187	S3188	A3189	L3190	K3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	M3211	E3212	Y3213	N3214	A3215	C3216	S3217	L3218	V3219	T3220	T3221	K3222	
S3223	P3224	R3225	E3226	R3227	A3228	L3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240	F3241	R3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	K3250	A3251	L3252	G3253	G3254	L3255	E3256	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	H3268	V3269	L3270	E3271	L3272	T3273	L3274	F3275	M3276	L3277	C3278	S3279	V3280	L3281	P3282	R3283		

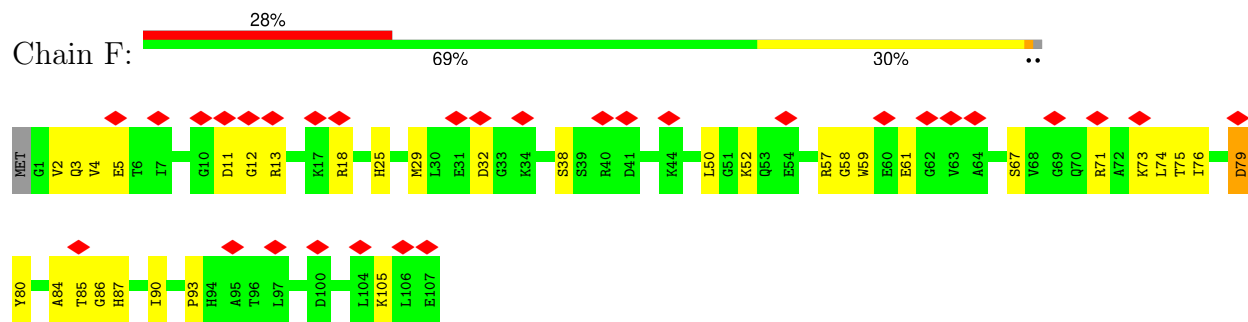


• Molecule 1: Ryanodine receptor 1



R3227	Y3166	H3038	E2978	R2918	Q2858	S2798	R2738	R2676	M2608	L2522	ARG
A3228	R3167	I3039	A2979	D2919	P2859	E2799	P2739	K2677	A2609	L2523	ARG
I3229	T3168	L3042	V2980	R2920	P2860	K2800	V2740	L2678	GLU	D2523	GLU
L3230	L3169	F3043	V2981	E2921	D2861	D2801	E2741	F2679	HIS	F2526	PHE
G3231	I3172	S3044	S2982	K2922	S2862	E2803	L2742	M2680	GLY	L2527	GLY
L3232	N3109	C3044	S2983	A2923	S2863	E2804	L2743	Q2681	GLU	P2528	GLU
P3233	L3110	L3046	G2984	Q2924	G2864	L2804	N2744	L2682	GLU	D2529	GLU
N3234	R3111	L3047	R2985	E2925	V2865	Y2805	V2745	F2683	GLU	M2530	GLU
S3235	L3112	A3048	V2986	L2926	T2866	R2806	L2746	D2684	GLU	R2531	GLU
T3236	G3113	L3049	E2987	L2927	L2867	W2807	L2747	Q2685	GLU	A2534	GLU
E3237	K3114	V3050	K2988	K2928	S2868	P2808	P2748	H2688	GLU	S2535	GLU
E3238	R3051	F2929	S2989	F2929	R2869	L2809	E2749	K2689	GLU	L2536	GLU
M3239	H3052	L2930	P2990	E2930	E2870	K2810	K2750	K2690	GLU	D2537	GLU
C3240	R3053	Q2931	H2991	L2871	L2871	E2811	L2751	Y2691	GLU	T2538	GLU
F3241	V3054	M2932	E2992	Q2872	Q2872	S2812	D2752	D2692	GLU	A2539	GLU
D3242	S3055	N2933	Q2993	A2873	A2873	L2813	S2753	E2694	GLU	F2541	GLU
I3243	L3056	G2934	E2994	M2874	M2874	K2814	F2754	L2695	GLU	S2542	GLU
P3244	F3057	Y2935	I2995	A2875	A2875	A2815	Y2755	L2696	GLU	M2546	GLU
V3245	G3058	A2936	K2996	E2876	E2876	M2816	N2756	R2697	GLU	A2547	GLU
L3246	T3059	V2937	F2997	Q2877	Q2877	L2817	K2757	Y2698	GLU	L2550	GLU
D3247	T3060	T2938	F2998	L2878	L2878	A2818	F2758	M2698	GLU	L2460	GLU
R3248	D3060	R2939	A2999	A2879	A2879	M2819	A2759	A2699	GLU	D2464	GLU
L3249	A3061	R2939	F2999	E2880	E2880	E2820	E2760	E2636	GLU	D2465	GLU
M3250	P3062	GLY	K3000	N2881	N2881	W2821	Y2761	P2636	GLU	L2466	GLU
G3251	L3128	LEU	I3001	Y2882	Y2882	T2822	T2762	A2637	GLU	F2569	GLU
D3252	L3129	LYS	I3002	H2883	H2883	L2823	H2763	A2638	GLU	G2571	GLU
I3253	T3130	ASP	L3003	Y2884	Y2884	E2824	E2764	K2639	GLU	T2572	GLU
G3254	T3131	GLU	P3004	T2885	T2885	K2825	K2765	P2640	GLU	H2574	GLU
A3257	T3132	D2946	L3005	W2886	W2886	A2826	W2766	M2639	GLU	A2576	GLU
S3258	T3133	L2947	L3006	G2887	G2887	E2828	F2768	K2638	GLU	I2577	GLU
S3259	V3134	T2948	I3007	R2888	R2888	G2829	F2769	M2638	GLU	D2580	GLU
G3260	L3135	S2949	Q3008	K2889	K2889	G2829	D2769	K2642	GLU	M2581	GLU
A3261	L3136	I2951	Y3009	K2890	K2890	E2830	K2770	L2644	GLU	M2582	GLU
A3262	L3137	E2952	F3010	R2891	R2891	GLU	I2771	L2644	GLU	M2583	GLU
R3263	P3138	E2953	T3011	G2892	G2892	ARG	P2772	L2644	GLU	M2584	GLU
Y3264	L3075	K2954	H3012	E2893	E2893	LYS	Q2773	L2644	GLU	M2585	GLU
E3265	D3076	F2955	H3013	L2894	L2894	THR	Y2774	L2644	GLU	M2587	GLU
H3268	A3077	A2956	C3014	A2895	A2895	LYS	S2776	L2644	GLU	M2588	GLU
V3269	R3078	F2957	Y3016	A2896	A2896	THR	Y2777	L2644	GLU	M2589	GLU
I3270	T3079	G2958	F3017	G2897	G2897	ARG	G2778	L2644	GLU	M2590	GLU
F3271	V3080	F2959	L3018	G2898	G2898	LYS	E2779	L2644	GLU	M2591	GLU
I3272	K3082	L2960	S3019	G2899	G2899	ILE	E2780	L2644	GLU	M2592	GLU
T3273	S3083	Q2961	P3021	G2900	G2900	SER	M2781	L2644	GLU	M2593	GLU
L3274	G3084	Q2962	A3022	T2901	T2901	THR	D2782	L2644	GLU	M2594	GLU
P3275	P3085	L2963	K3023	H2902	H2902	ALA	D2783	L2644	GLU	M2595	GLU
M3276	E3086	L2964	V3024	P2903	P2903	GLN	E2784	L2644	GLU	M2596	GLU
L3277	I3087	R2965	G3025	L2904	L2904	THR	E2785	L2644	GLU	M2597	GLU
S3278	V3088	W2966	G3026	L2905	L2905	TYR	L2785	L2644	GLU	M2598	GLU
Y3279	L3092	M2967	G3027	V2906	V2906	ASP	K2786	L2644	GLU	M2599	GLU
L3280	F3095	D2968	S3028	D2968	D2968	PRO	T2787	L2644	GLU	M2600	GLU
L3281	F3096	L2969	G3029	P2907	P2907	ARG	T2788	L2644	GLU	M2601	GLU
F3282	F3096	S2970	G3029	Q2971	Q2971	GLU	H2788	L2644	GLU	M2602	GLU
R3283	F3096	E2972	H3030	E2972	E2972	GLY	P2789	L2644	GLU	M2603	GLU
M3284	A3099	F2973	A3031	T2910	T2910	LYS	M2790	L2644	GLU	M2604	GLU
W3285	S3100	E2974	N3033	L2911	L2911	THR	L2791	L2644	GLU	M2605	GLU
E3286	E3101	L2974	K3034	T2912	T2912	ALA	L2792	L2644	GLU	M2606	GLU
R3287	D3102	A2975	K3034	A2913	A2913	GLY	Y2794	L2644	GLU	M2607	GLU
G3288	I3103	H2976	E3035	K2914	K2914	GLY	K2795	L2644	GLU	M2608	GLU
		L2977	E3037	K2916	K2916	GLY	T2796	L2644	GLU	M2609	GLU
				A2917	A2917	GLY		L2644	GLU	M2610	GLU

L3249	L3312	V3373	R3436	R3498	Q3560	L3624	GLU	E3872	E4121	GLY	ALA	SER	PRO
M3250	N3313	E3376	M3437	R3499	G3561	S3625	GLY	K3873	M4122	GLU	ALA	ASP	GLU
I3263	L3316	E3377	E3440	G3500	K3562	K3626	GLY	V3874	I4123	ALA	THR	GLU	GLY
G3264	G3317	Q3378	I3441	D3501	V3563	Q3627	ASN	M3875	Q4133	ALA	ALA	VAL	ALA
L3256	L3318	Q3379	F3442	R3502	E3564	R3628	GLY	L3890	E4134	GLU	LEU	GLY	GLY
A3257	N3319	R3380	F3443	R3503	E3565	R3629	GLU	F3899	P4135	ALA	ALA	GLY	GLY
E3258	L3320	L3381	Y3444	S3504	S3566	R3630	ALA	S3929	A4136	ALA	LEU	LEU	GLM
S3259	L3321	L3381	M3445	V3505	P3567	A3631	GLU	F3933	D4138	GLY	TRP	ALA	PRO
G3260	I3322	E3382	S3446	T3506	R3570	V3632	GLU	V3936	M4142	ALA	VAL	PRO	GLY
A3261	I3323	A3383	K3447	S3508	K3573	R3633	GLU	A3634	E4152	ALA	VAL	GLY	THR
I3263	V3324	K3384	H3449	L3509	A3574	C3635	GLU	C3635	V4154	ALA	ALA	ASP	PRO
Y3263	N3325	A3385	N3450	I3510	L3575	F3636	GLY	F3636	F4154	GLY	ALA	ARG	ALA
T3264	N3326	A3387	F3451	V3511	Y3576	R3637	GLY	R3637	D4157	ALA	GLY	ASP	GLU
E3265	L3327	E3388	K3452	A3512	R3577	M3638	GLY	M3638	P4158	ALA	ALA	ALA	PRO
E3266	G3328	E3389	E3453	T3513	Q3578	T3639	GLY	Q3578	R4161	GLY	GLY	GLY	THR
M3266	I3329	G3390	E3454	L3514	L3579	L3644	THR	L3644	E4172	VAL	VAL	ALA	PRO
P3267	D3330	E3391	E3455	K3515	P3580	P3645	ALA	P3645	E4172	ALA	ALA	GLY	GLY
H3268	E3331	L3392	Q3456	M3516	R3582	R3648	GLY	R3648	R4175	GLY	ALA	GLY	PRO
V3269	L3333	L3393	V3459	M3517	E3583	R3652	THR	M3652	F4176	ALA	ALA	GLY	TLE
I3270	T3333	V3394	V3460	L3522	E3584	H3652	THR	H3652	Y4177	ALA	THR	ASP	LEU
E3271	M3334	R3395	Q3461	N3523	E3584	H3771	ALA	H3771	G3971	ALA	ALA	ASP	LEU
T3272	M3335	D3396	N3462	M3524	D3585	L3780	ARG	L3780	P3972	ALA	LEU	GLY	LYS
T3273	K3336	E3397	E3463	C3525	D3587	Y3657	ARG	Y3657	G4185	ARG	ARG	GLY	LYS
L3274	K3337	F3398	I3464	A3526	D3588	K3658	LEU	K3658	A4186	LEU	LEU	GLY	LYS
P3275	L3338	F3399	I3466	P3527	P3589	L3663	ALA	L3663	S4187	LEU	LEU	GLY	LEU
K3276	A3339	F3400	N3466	T3528	E3590	D3666	ALA	D3666	R4188	LEU	ALA	ASP	LEU
L3277	F3341	L3401	M3467	D3529	K3591	G3661	ALA	G3661	Y4194	ALA	ALA	ASP	VAL
C3278	A3342	C3402	R3468	Q3530	L3592	E3682	ALA	E3682	E4199	ALA	ALA	GLY	ASP
L3281	K3343	R3403	S3468	D3531	V3593	E3683	ALA	M3816	M4207	GLY	GLY	GLY	GLU
P3282	P3344	D3404	F3469	L3532	K3594	Q3683	LEU	L3842	P4208	GLY	GLY	GLY	GLU
R3283	I3345	L3405	L3470	I3533	R3595	E3684	LEU	D3843	Q4209	GLY	GLY	GLY	GLU
M3284	L3346	L3406	T3471	M3534	R3596	E3685	LEU	L3844	G4226	GLY	GLY	GLY	GLU
K3285	S3347	A3407	A3472	A3536	E3597	E3686	THR	Q3850	E4227	THR	ALA	PRO	PRO
E3286	R3348	L3408	S3474	A3537	E3598	E3687	ARG	E3857	I4247	ARG	LYS	GLY	GLU
R3287	R3349	Y3409	K3475	K3537	E3688	E3688	ARG	M3858	E4253	ARG	VAL	GLY	PRO
G3288	A3349	P3410	S3476	T3538	E3689	E3689	ARG	V3859	P4254	ARG	VAL	GLY	PRO
P3289	R3350	L3411	S3477	R3539	V3690	V3690	ARG	M3858	GLU	ARG	VAL	GLY	PRO
E3290	P3351	L3412	M3478	Y3540	E3691	E3691	VAL	V3859	GLY	ARG	THR	VAL	PRO
A3291	E3352	T3413	A3479	A3541	E3692	E3692	VAL	K4063	E4253	ARG	THR	VAL	PRO
P3292	L3353	R3414	L3542	L3542	K3693	K3693	ARG	M4064	P4254	ARG	THR	VAL	PRO
P3293	H3355	D3417	K3543	K3543	R3694	R3694	ARG	K4067	GLU	ARG	THR	VAL	PRO
P3294	S3356	N3418	GLY	D3544	E3695	E3695	ARG	I4088	GLY	ARG	THR	VAL	PRO
A3295	H3357	N3419	ALA	T3545	H3699	H3699	ARG	S4089	GLY	ARG	THR	VAL	PRO
L3296	F3358	R3420	ALA	D3546	Q3700	Q3700	ARG	K4090	GLY	ARG	THR	VAL	PRO
P3297	I3359	A3421	SER	E3547	Q3715	K3715	ARG	K4091	PRO	ARG	THR	VAL	PRO
R3298	F3359	H3422	GLY	E3548	L3716	L3716	ARG	D4092	PRO	ARG	THR	VAL	PRO
A3299	I3362	G3424	SER	R3549	D3717	D3717	ARG	K4095	GLY	ARG	THR	VAL	PRO
G3299	G3363	L3424	ASP	R3550	D3727	D3727	ARG	Q4102	GLY	ARG	THR	VAL	PRO
A3300	R3364	T3425	ASP	E3551	I3728	I3728	ARG	E4119	GLY	ARG	THR	VAL	PRO
P3301	L3365	T3425	GLU	F3552	H3734	H3734	ARG	M4120	MET	ARG	THR	VAL	PRO
P3302	R3366	N3428	GLU	L3553	L3735	L3735	ARG			ARG	THR	VAL	PRO
P3303	K3367	A3429	THR	Q3554	E3736	E3736	ARG			ARG	THR	VAL	PRO
C3304	R3368	A3430	LYS	N3555			ARG			ARG	THR	VAL	PRO
T3305	A3369	A3431	LYS	N3556			ARG			ARG	THR	VAL	PRO
A3306	G3370	E3432	LYS	L3557			ARG			ARG	THR	VAL	PRO
V3307	K3371	E3433	LYS	L3557			ARG			ARG	THR	VAL	PRO
T3308	V3372	L3434	LYS	L3559			ARG			ARG	THR	VAL	PRO
S3309	F3435	P3435	LYS	L3559			ARG			ARG	THR	VAL	PRO



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33584	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	0.482	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: CA, URA, ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/35977	0.50	4/48726 (0.0%)
1	B	0.28	0/35977	0.50	1/48726 (0.0%)
1	C	0.28	0/35977	0.51	3/48726 (0.0%)
1	D	0.27	0/35977	0.49	3/48726 (0.0%)
2	E	0.29	0/850	0.53	0/1146
2	F	0.30	0/850	0.55	0/1146
2	G	0.30	0/850	0.54	0/1146
2	H	0.29	0/850	0.53	0/1146
All	All	0.28	0/147308	0.50	11/199488 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3603	LEU	CA-CB-CG	7.34	132.17	115.30
1	A	1979	LEU	CA-CB-CG	6.30	129.79	115.30
1	D	3666	ASP	CB-CG-OD2	6.20	123.88	118.30
1	D	3542	LEU	CA-CB-CG	5.87	128.79	115.30
1	C	3542	LEU	CA-CB-CG	5.64	128.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35150	0	34797	529	0
1	B	35150	0	34797	555	0
1	C	35150	0	34797	580	0
1	D	35150	0	34797	492	0
2	E	831	0	831	17	0
2	F	831	0	831	16	0
2	G	831	0	831	15	0
2	H	831	0	831	17	0
3	A	31	0	12	1	0
3	B	31	0	12	1	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	8	0	3	0	0
6	B	8	0	3	0	0
6	C	8	0	3	0	0
6	D	8	0	3	0	0
All	All	144088	0	142572	2194	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 8.

The worst 5 of 2194 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:2647:HIS:HE2	1:C:2655:TYR:HH	1.18	0.89
1:C:3254:GLY:HA2	1:C:3318:ASN:HD21	1.40	0.86
1:D:957:LYS:H	1:D:957:LYS:HD2	1.41	0.84
1:D:3573:MET:HB3	1:D:3577:ARG:HH21	1.43	0.81
1:D:3550:ARG:HD3	1:D:3594:ARG:HH22	1.44	0.81

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%)	4260 (97%)	125 (3%)	0	100	100
1	B	4385/5037 (87%)	4251 (97%)	134 (3%)	0	100	100
1	C	4385/5037 (87%)	4264 (97%)	121 (3%)	0	100	100
1	D	4385/5037 (87%)	4272 (97%)	113 (3%)	0	100	100
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	17960/20580 (87%)	17447 (97%)	513 (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%)	3719 (97%)	117 (3%)	35	68
1	B	3836/4276 (90%)	3714 (97%)	122 (3%)	34	67
1	C	3836/4276 (90%)	3716 (97%)	120 (3%)	35	68
1	D	3836/4276 (90%)	3720 (97%)	116 (3%)	36	69
2	E	89/90 (99%)	84 (94%)	5 (6%)	17	46
2	F	89/90 (99%)	79 (89%)	10 (11%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	89/90 (99%)	82 (92%)	7 (8%)	10	29
2	H	89/90 (99%)	80 (90%)	9 (10%)	6	19
All	All	15700/17464 (90%)	15194 (97%)	506 (3%)	37	67

5 of 506 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3185	LYS
1	C	2482	ASP
1	D	957	LYS
1	C	2330	ARG
1	C	3449	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1558	HIS
1	C	56	GLN
1	C	3318	ASN
1	C	3268	HIS
1	B	56	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
6	URA	D	5304	-	8,8,8	0.61	0	10,10,10	1.05	1 (10%)
3	ATP	C	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
6	URA	A	5304	-	8,8,8	0.59	0	10,10,10	1.08	1 (10%)
6	URA	C	5304	-	8,8,8	0.62	0	10,10,10	1.06	1 (10%)
3	ATP	B	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
6	URA	B	5304	-	8,8,8	0.60	0	10,10,10	1.12	1 (10%)
3	ATP	A	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
3	ATP	D	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (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
6	URA	D	5304	-	-	-	0/1/1/1
3	ATP	C	5301	-	-	6/18/38/38	0/3/3/3
6	URA	A	5304	-	-	-	0/1/1/1
6	URA	C	5304	-	-	-	0/1/1/1
3	ATP	B	5301	-	-	8/18/38/38	0/3/3/3
6	URA	B	5304	-	-	-	0/1/1/1
3	ATP	A	5301	-	-	6/18/38/38	0/3/3/3
3	ATP	D	5301	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	C4'-O4'-C1'	-4.28	106.00	109.92
3	D	5301	ATP	C4'-O4'-C1'	-4.27	106.02	109.92
3	C	5301	ATP	C4'-O4'-C1'	-4.27	106.02	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5301	ATP	C4'-O4'-C1'	-4.23	106.05	109.92
6	B	5304	URA	C4-N3-C2	2.41	127.88	125.55

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

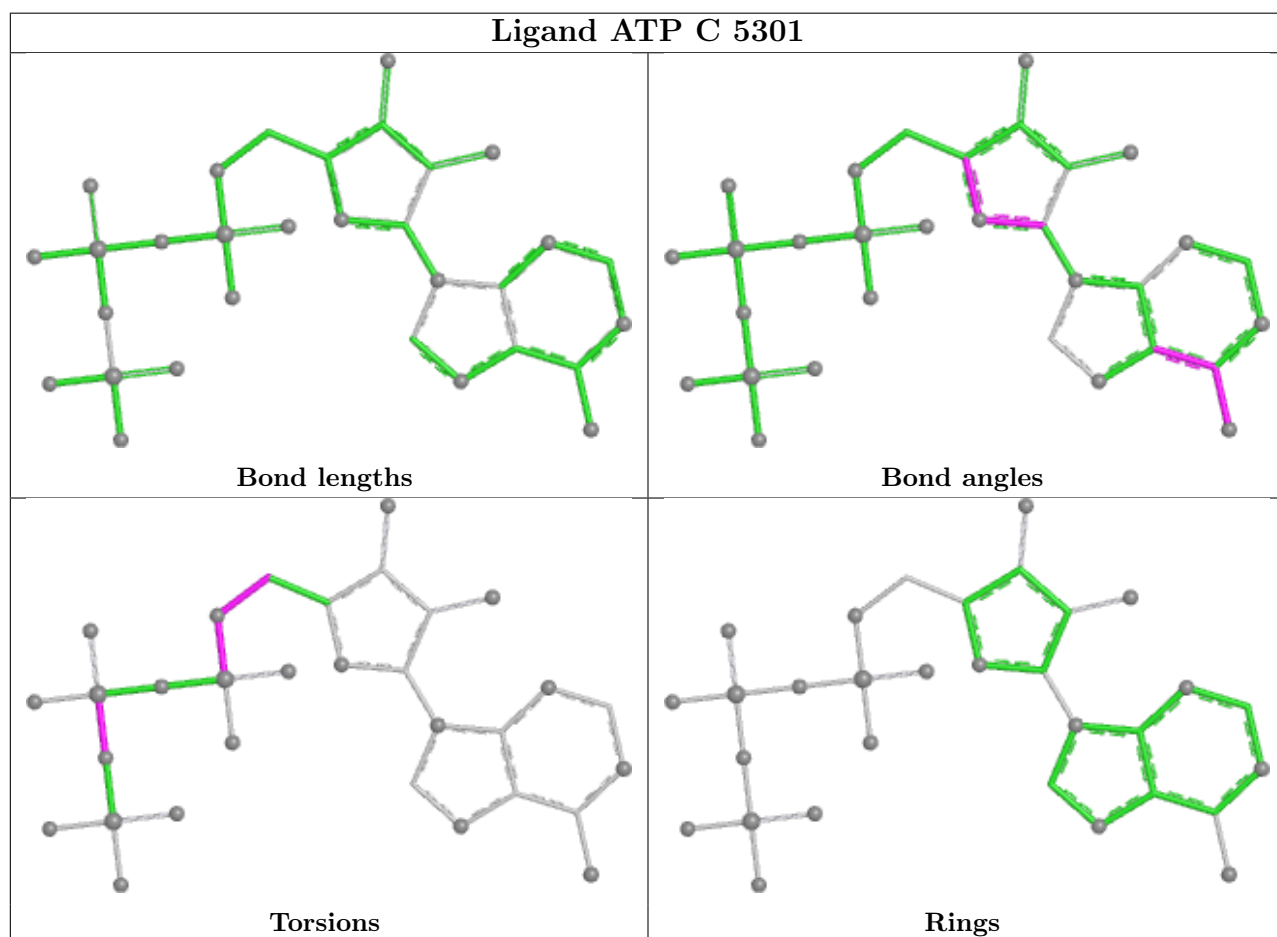
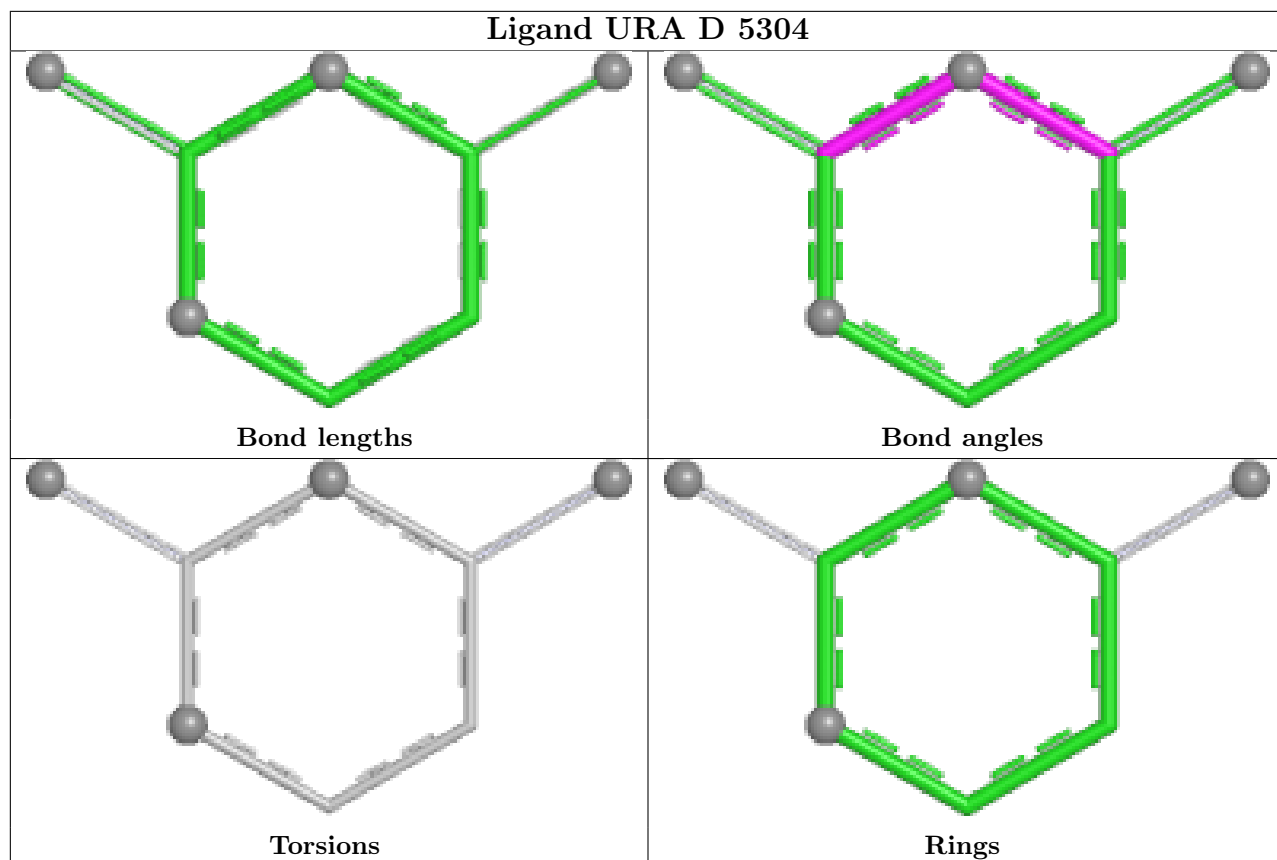
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O1A
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A

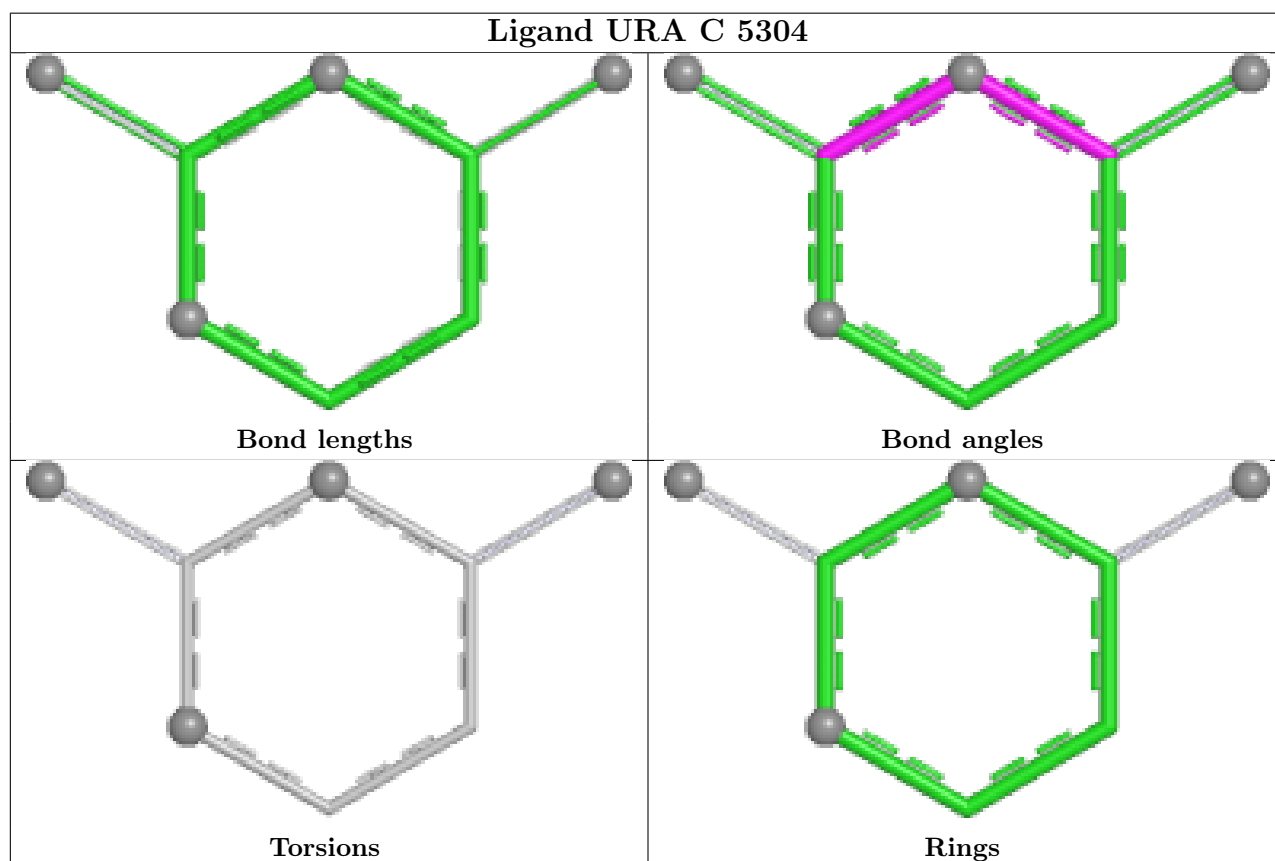
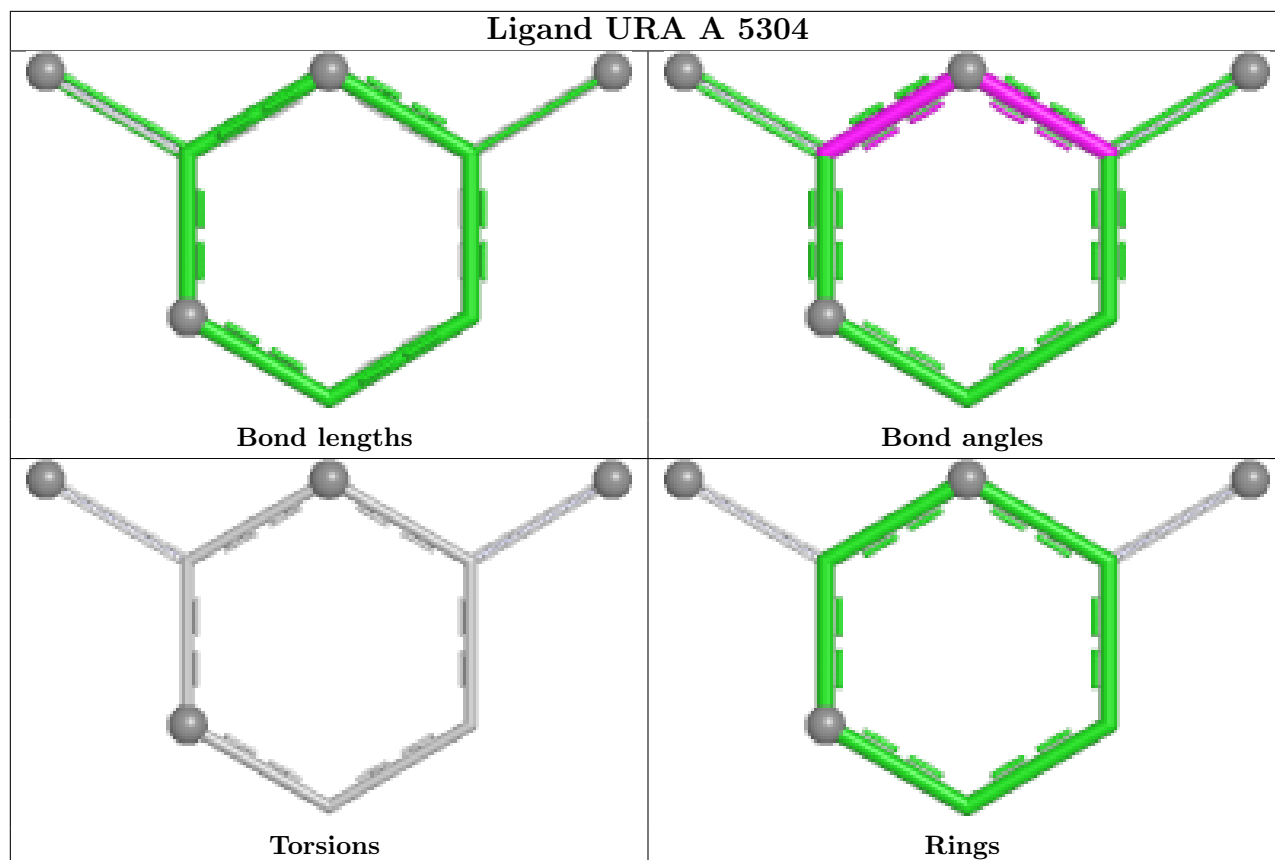
There are no ring outliers.

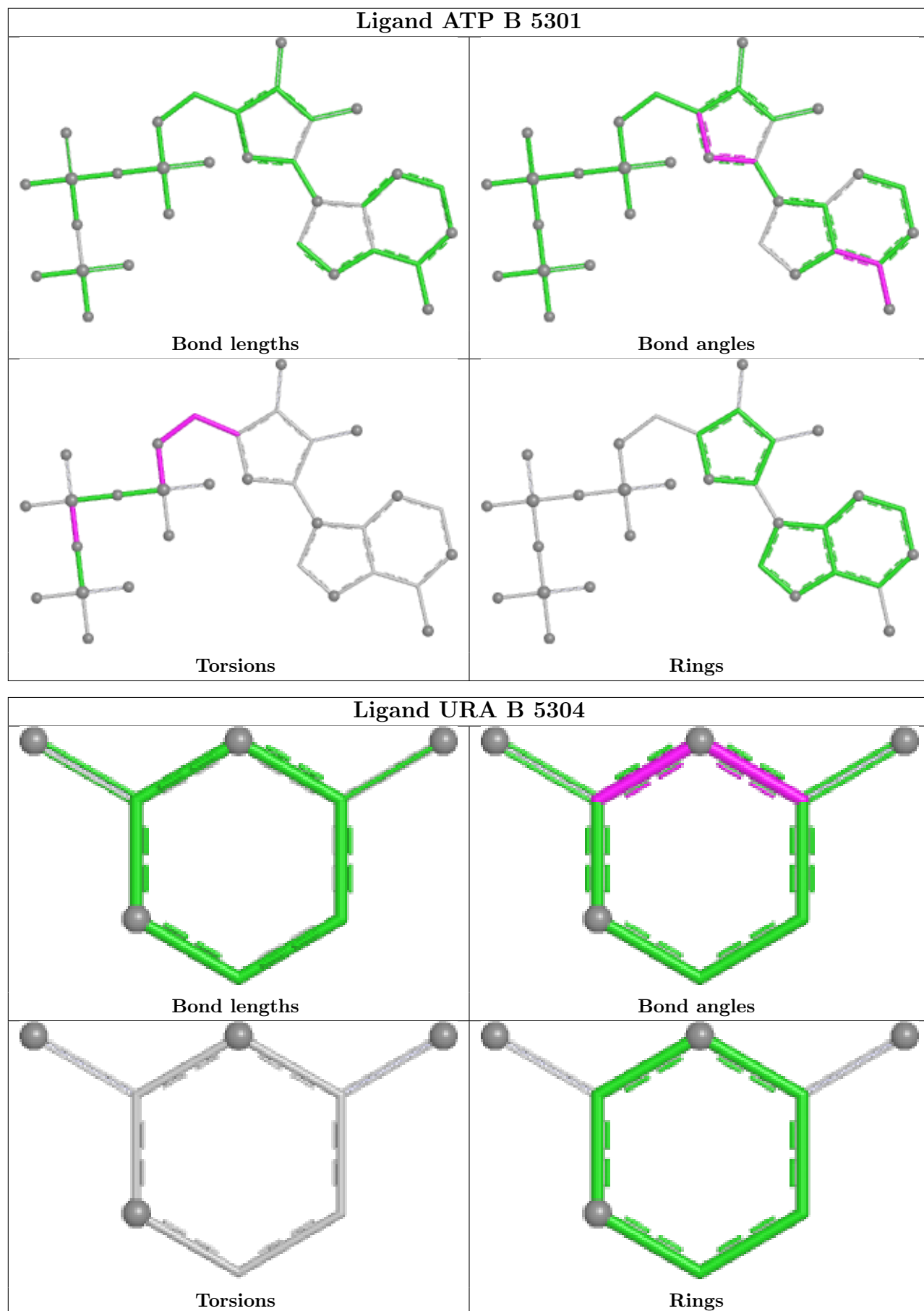
2 monomers are involved in 2 short contacts:

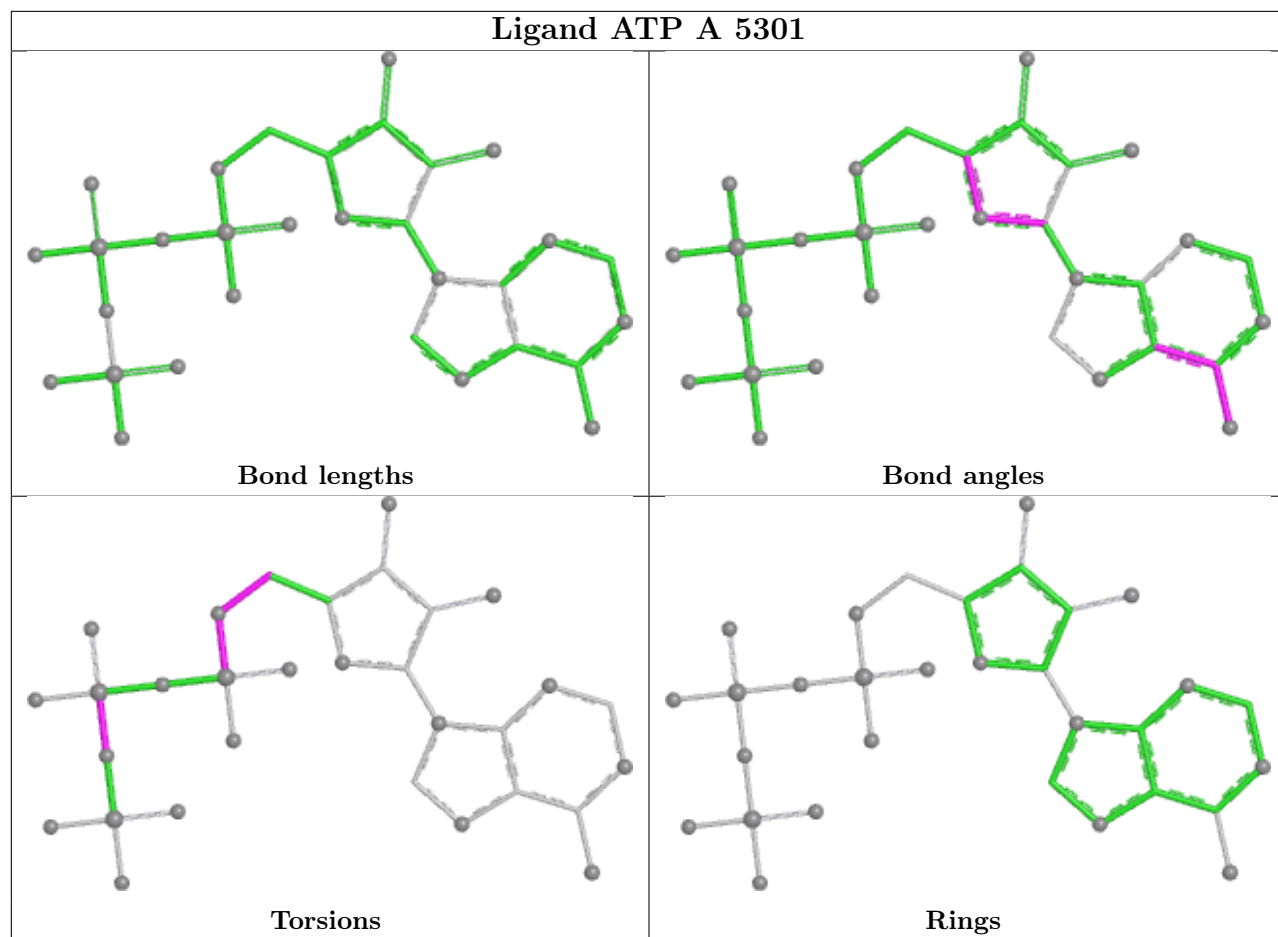
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	1	0
3	A	5301	ATP	1	0

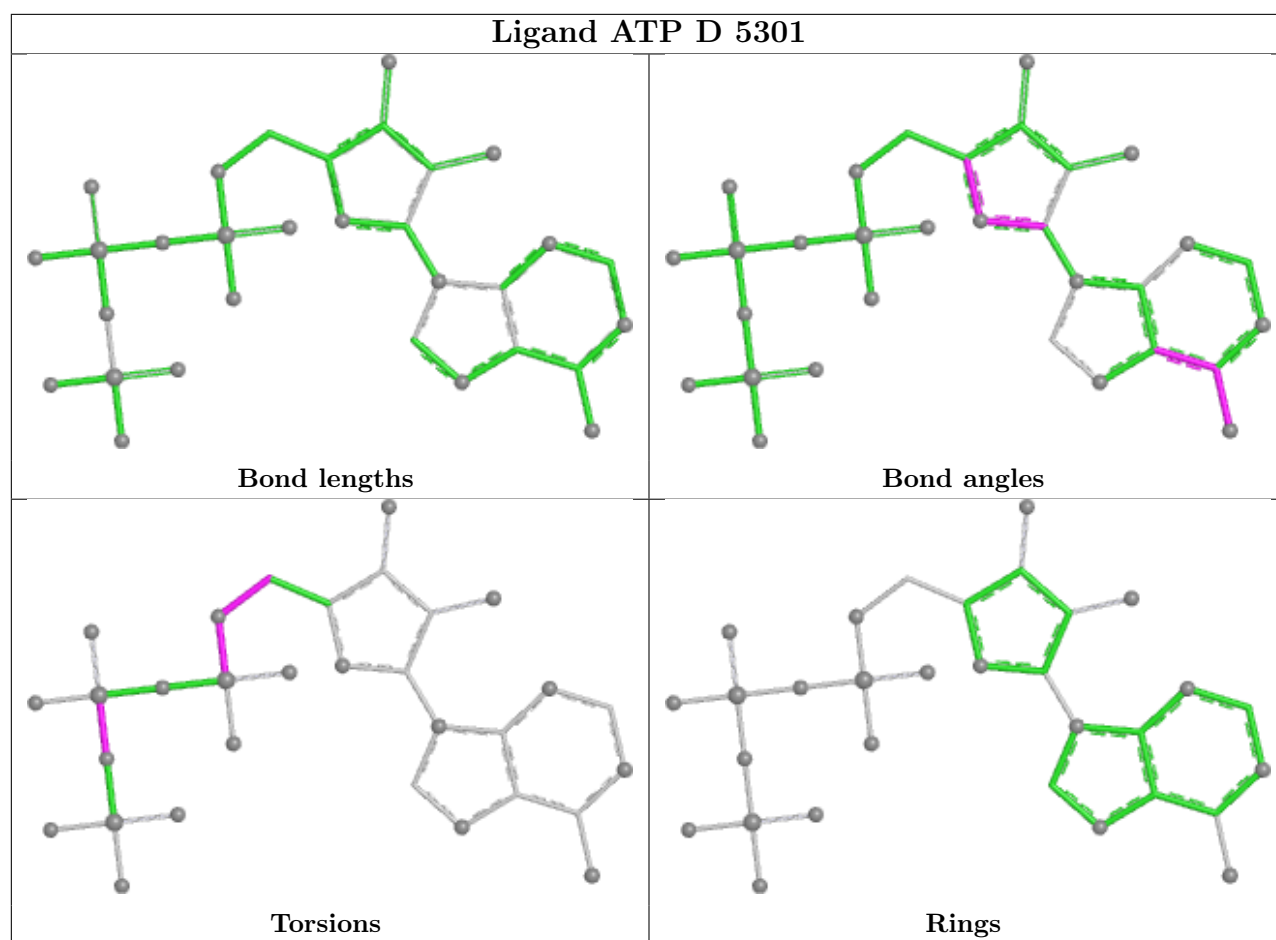
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

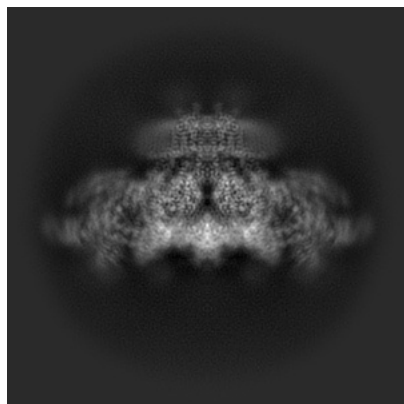
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47391. These allow visual inspection of the internal detail of the map and identification of artifacts.

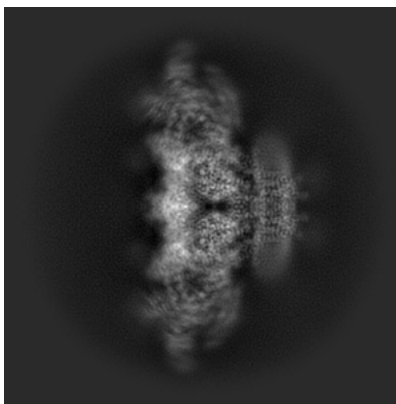
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

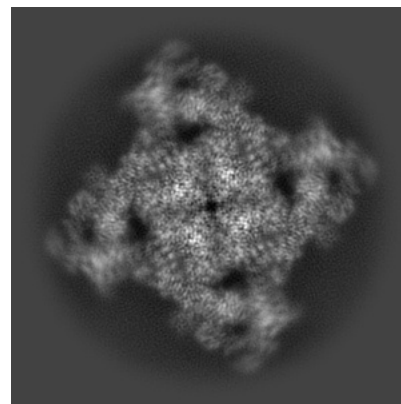
6.1.1 Primary map



X

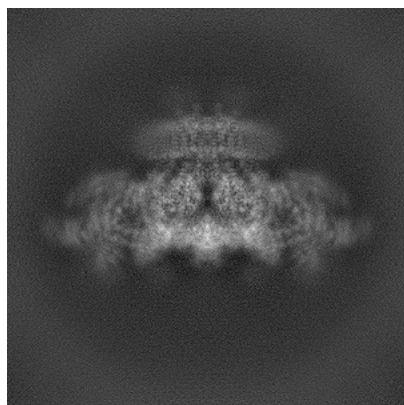


Y

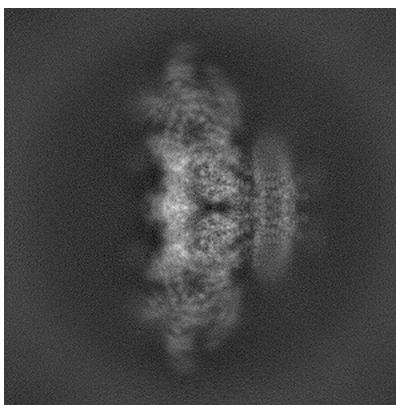


Z

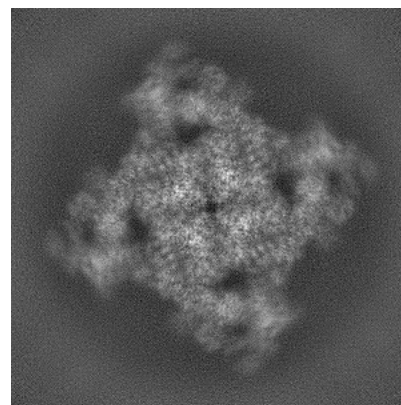
6.1.2 Raw map



X



Y

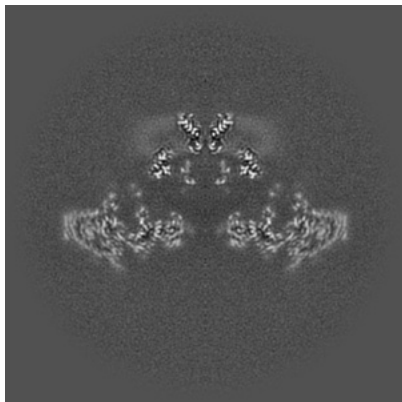


Z

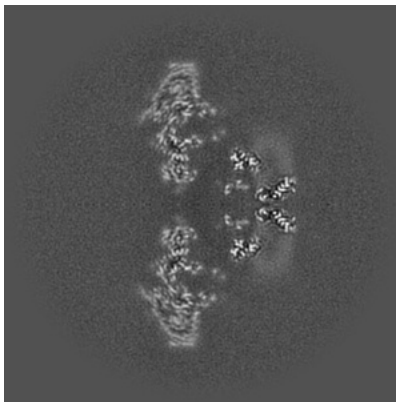
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

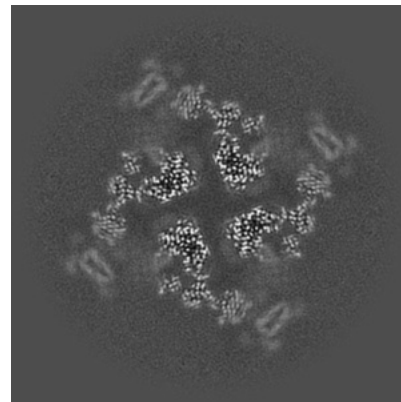
6.2.1 Primary map



X Index: 256

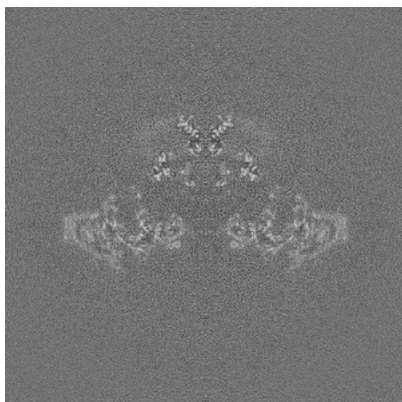


Y Index: 256

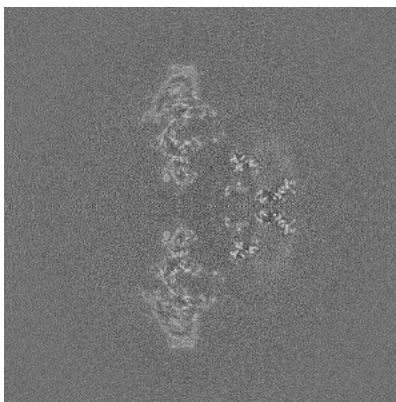


Z Index: 256

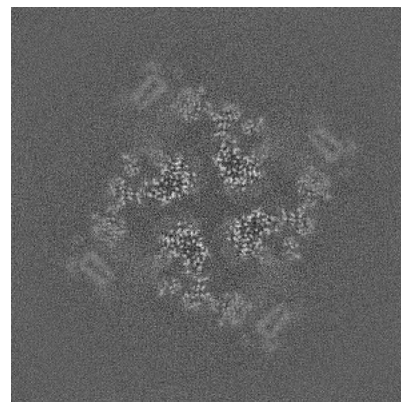
6.2.2 Raw map



X Index: 256



Y Index: 256

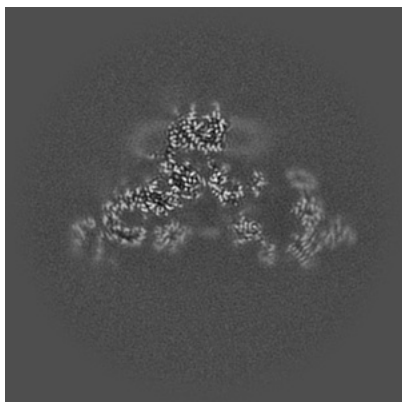


Z Index: 256

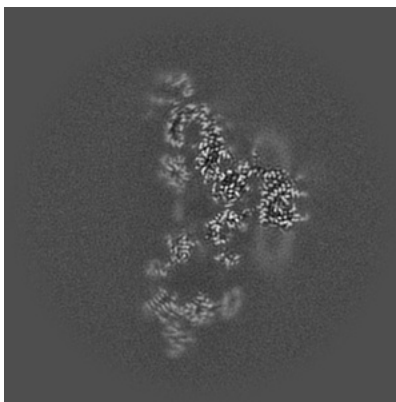
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

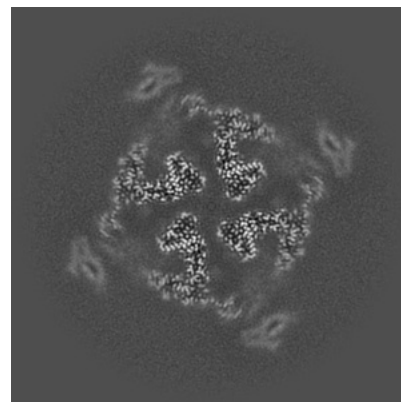
6.3.1 Primary map



X Index: 239

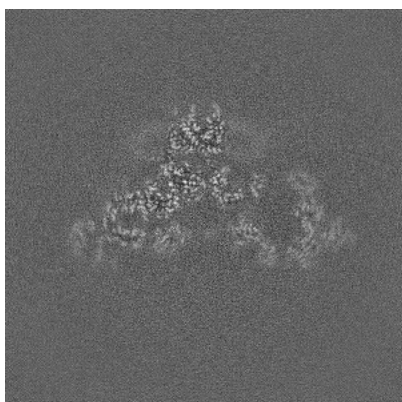


Y Index: 239

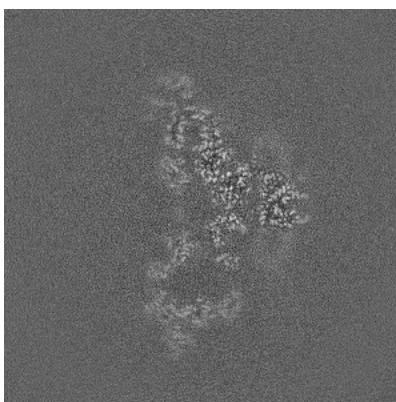


Z Index: 265

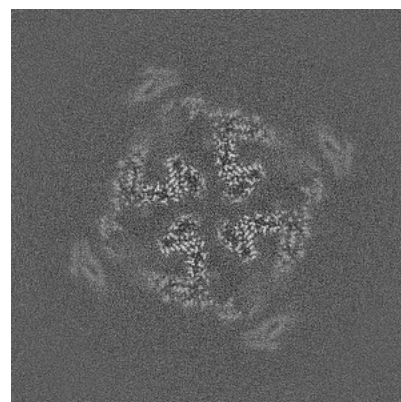
6.3.2 Raw map



X Index: 240



Y Index: 240

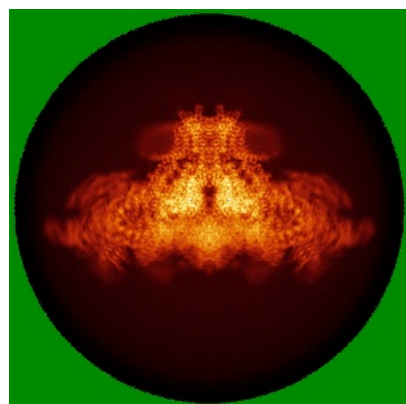


Z Index: 266

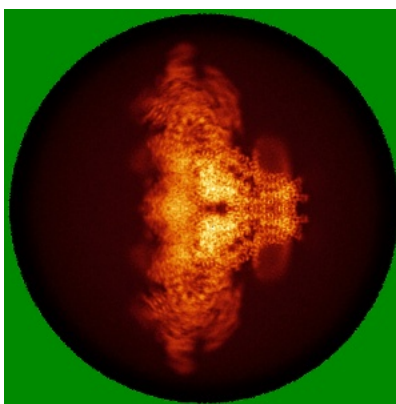
The images above show the largest variance slices of the map in three orthogonal directions.

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

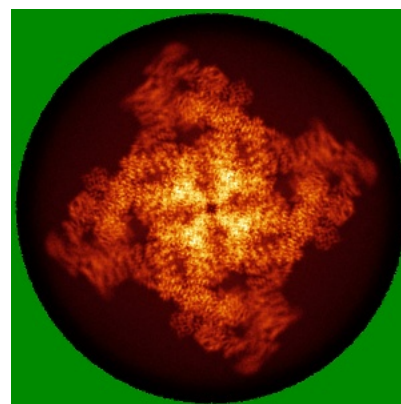
6.4.1 Primary map



X

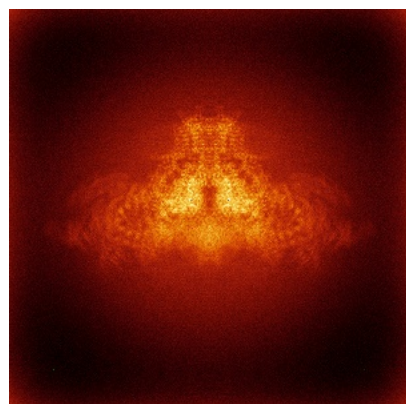


Y

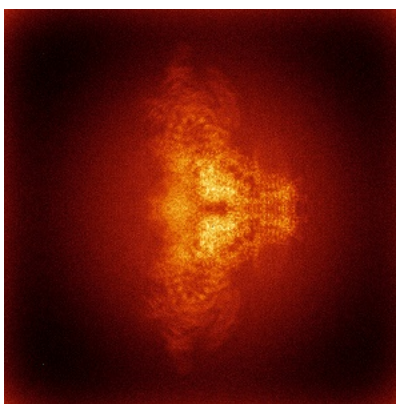


Z

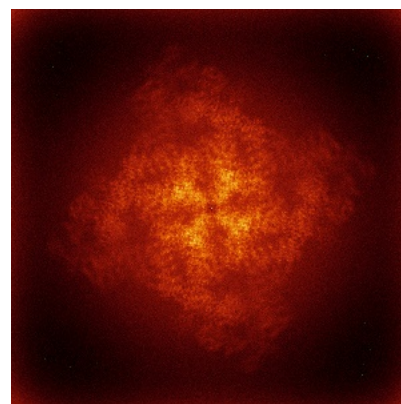
6.4.2 Raw map



X



Y

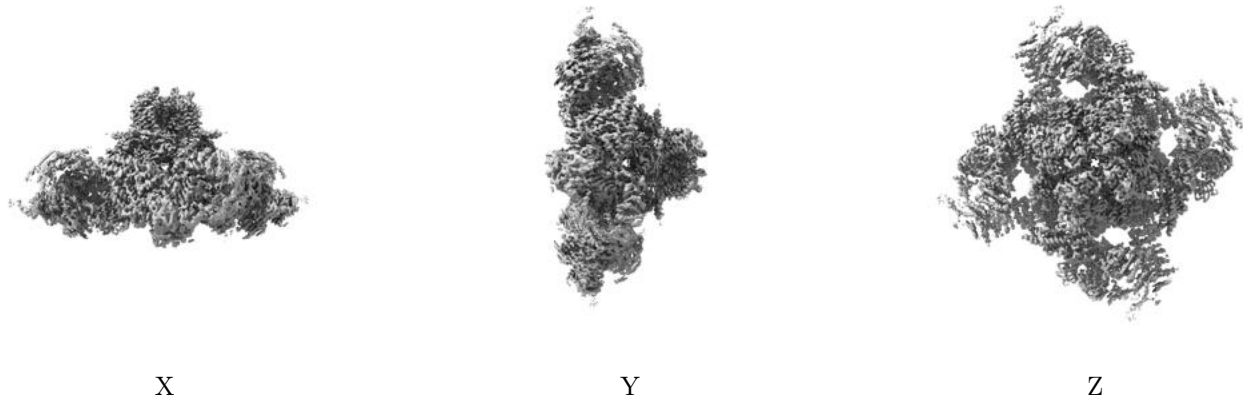


Z

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.

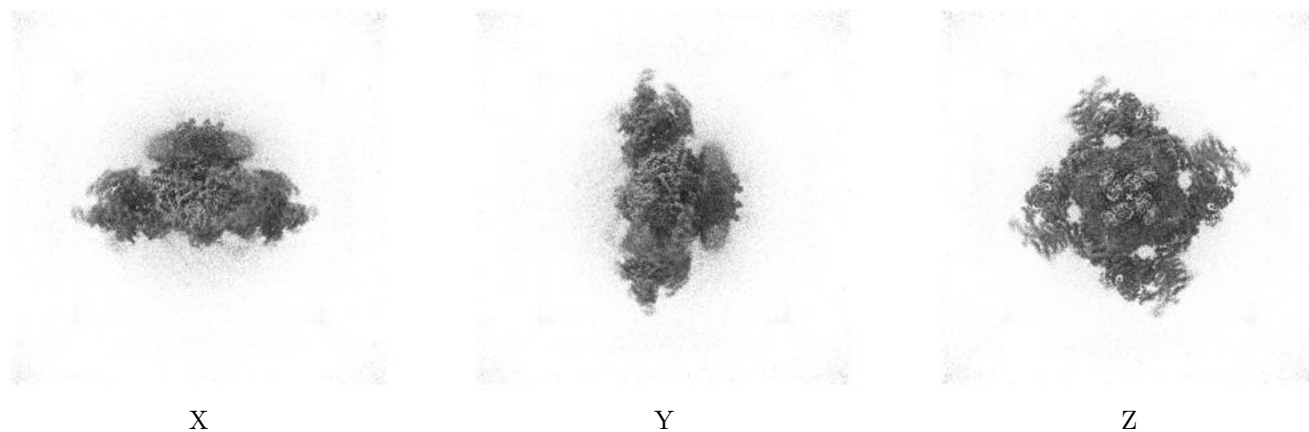
6.5 Orthogonal surface views [i](#)

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.

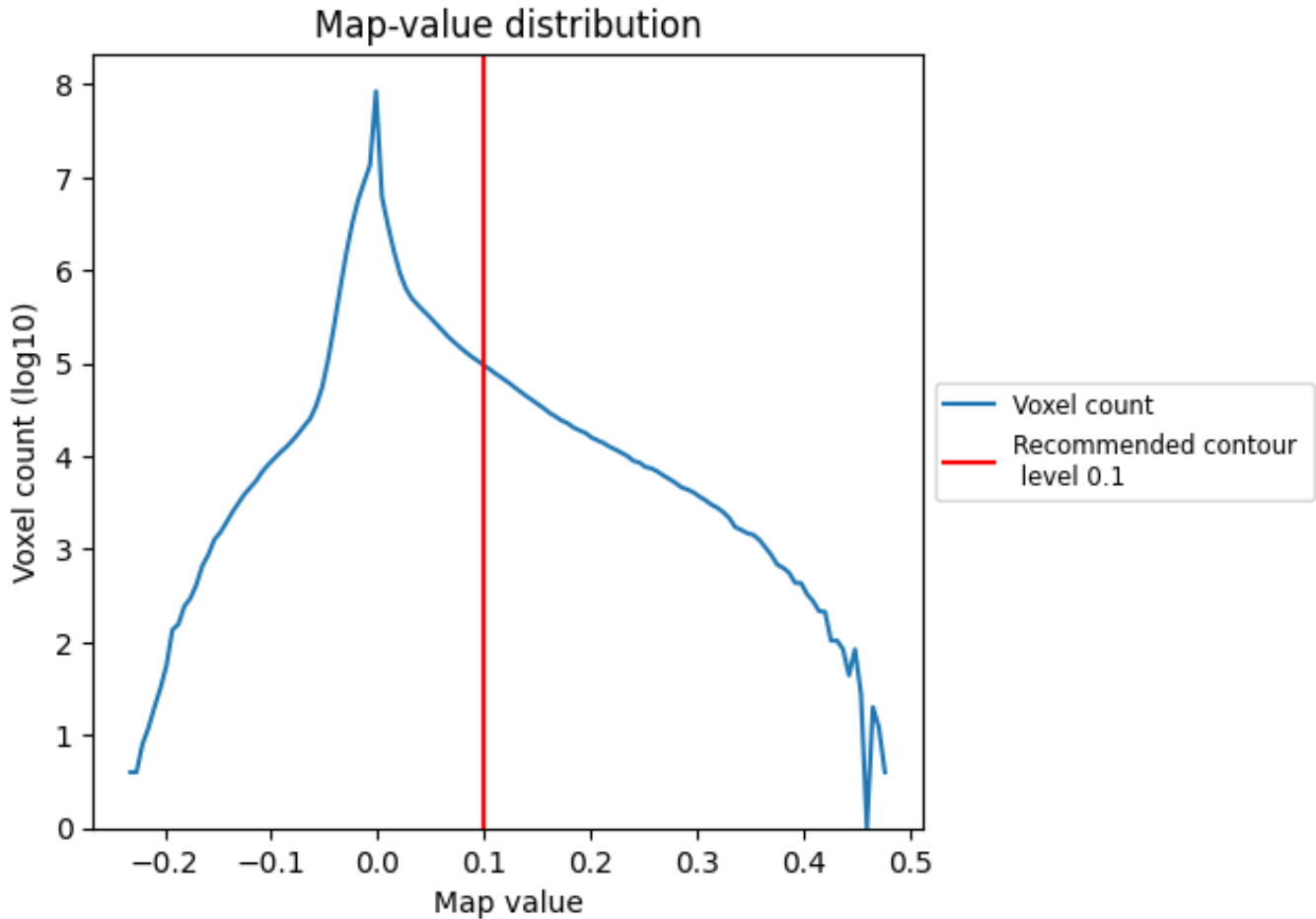
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

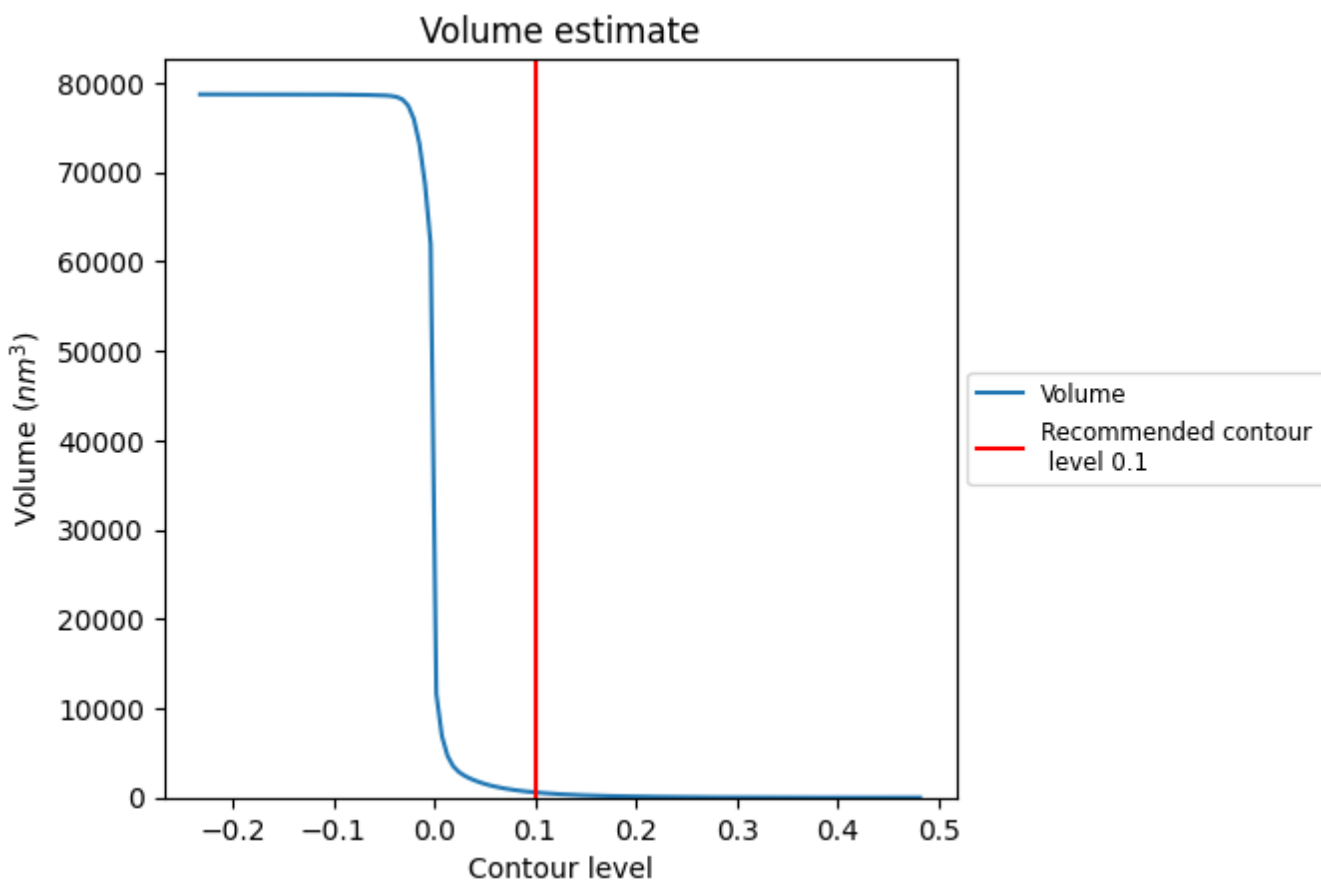
This section contains the results of statistical analysis of the map.

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.

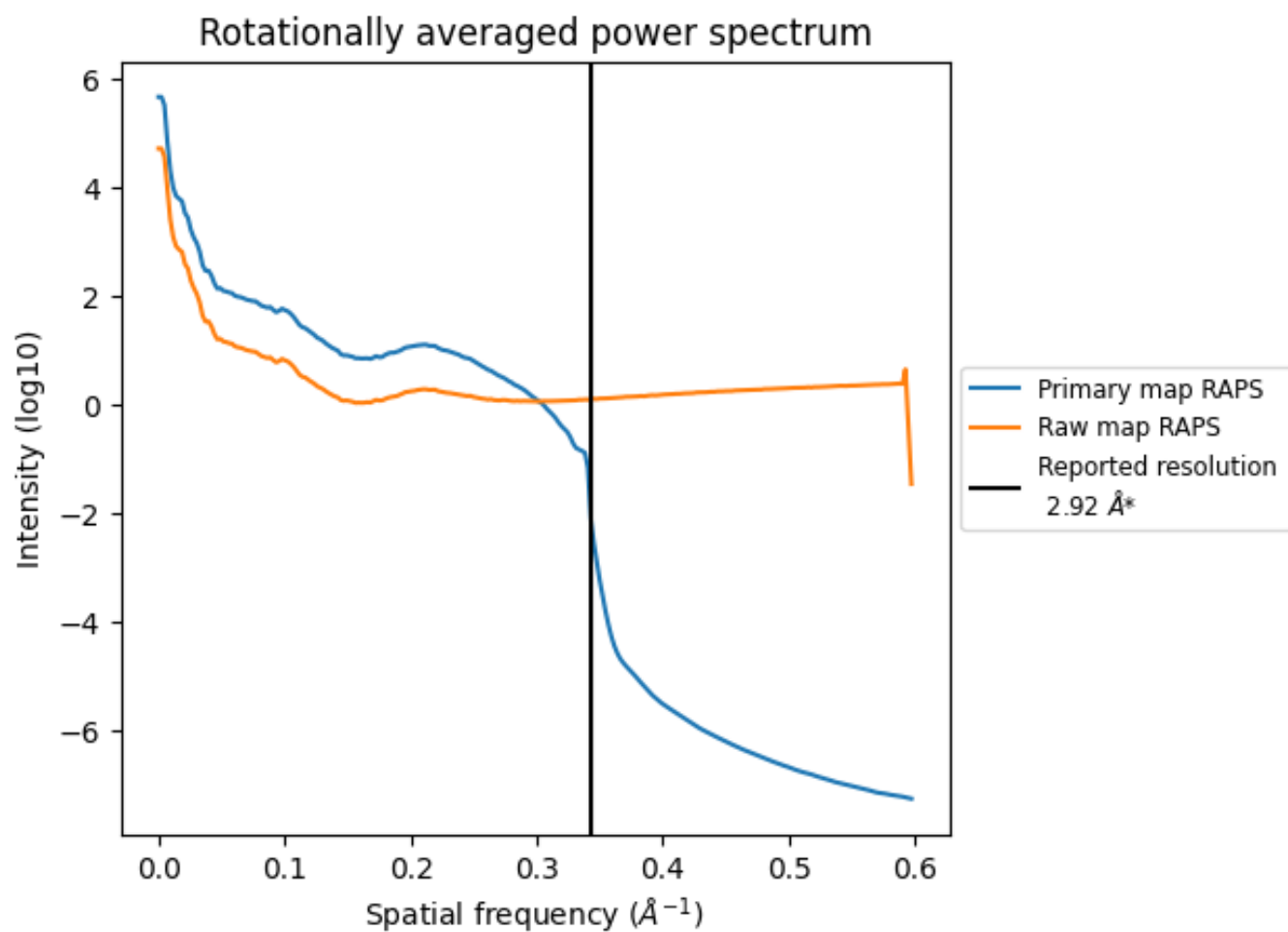
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 584 nm³; this corresponds to an approximate mass of 528 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

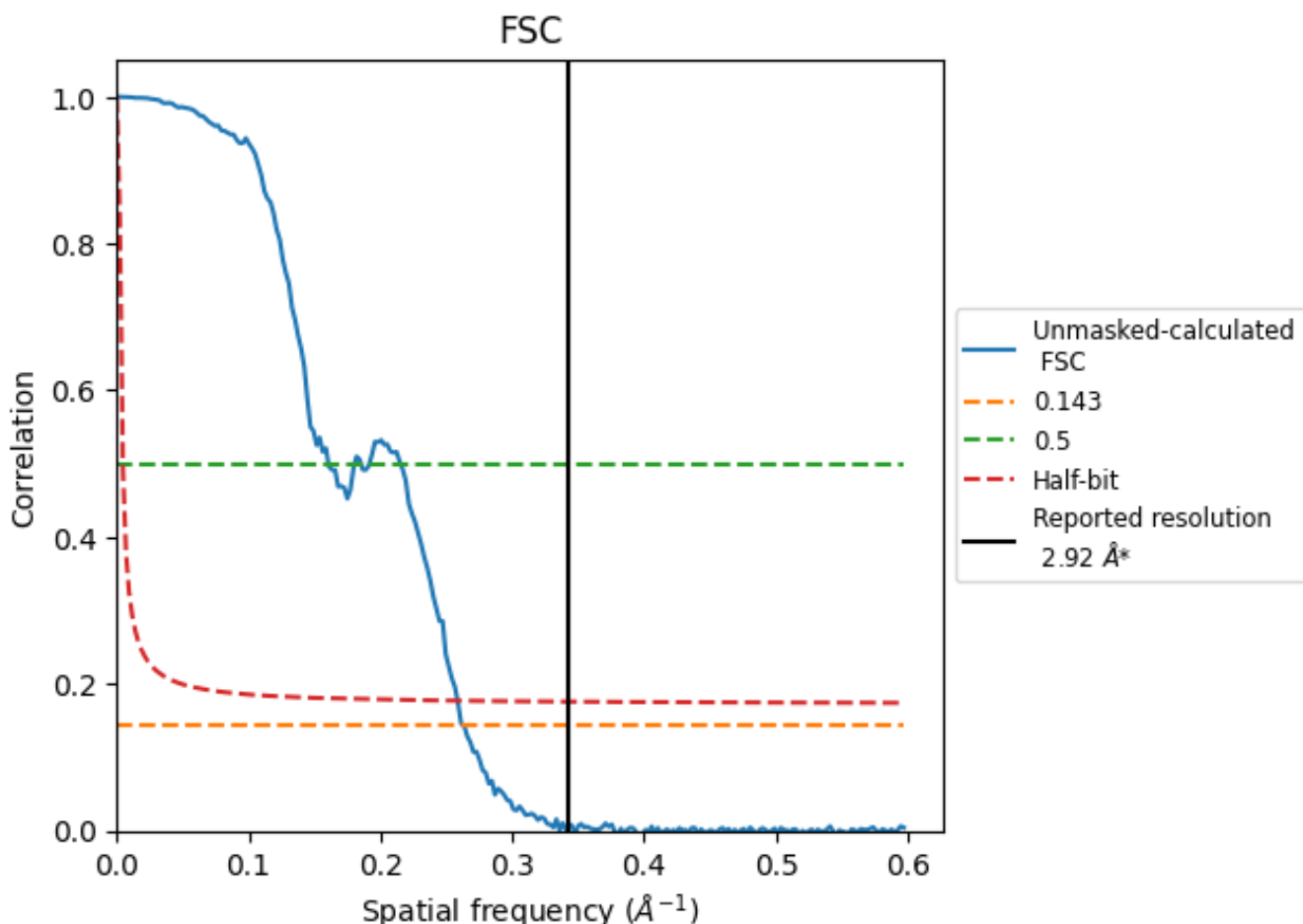


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

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 0.342 \AA^{-1}

8.2 Resolution estimates [i](#)

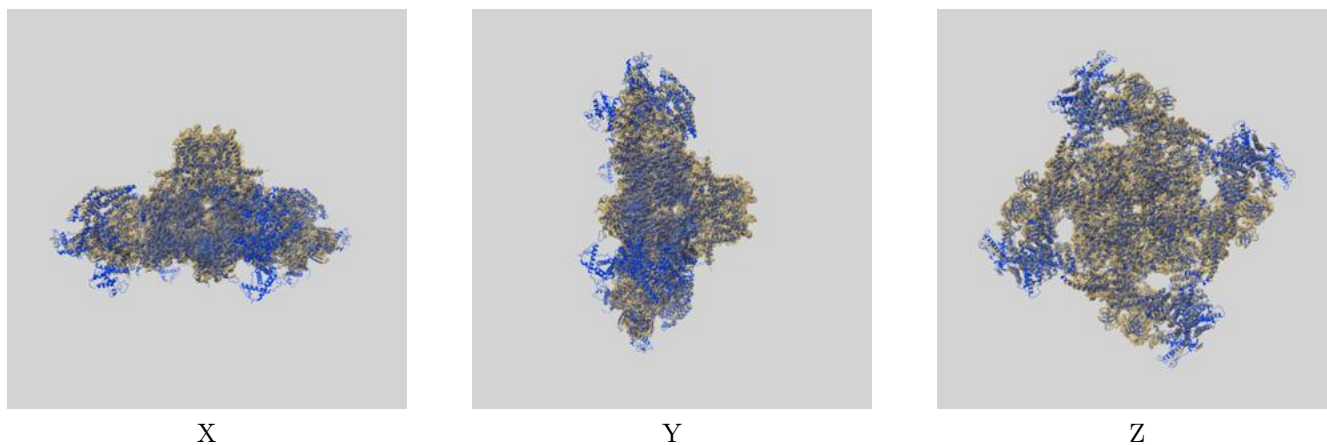
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.23	3.87

*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 3.80 differs from the reported value 2.92 by more than 10 %

9 Map-model fit [i](#)

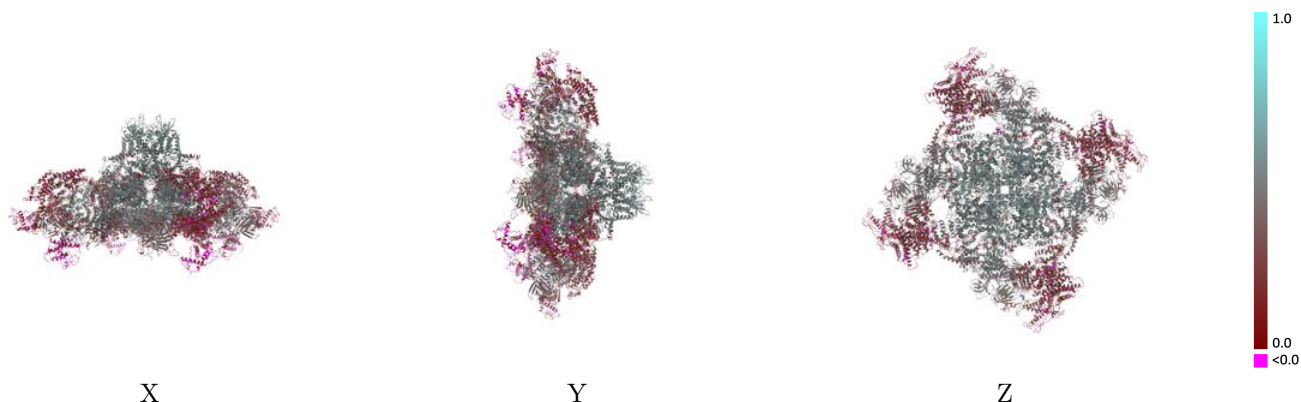
This section contains information regarding the fit between EMDB map EMD-47391 and PDB model 9E1E. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



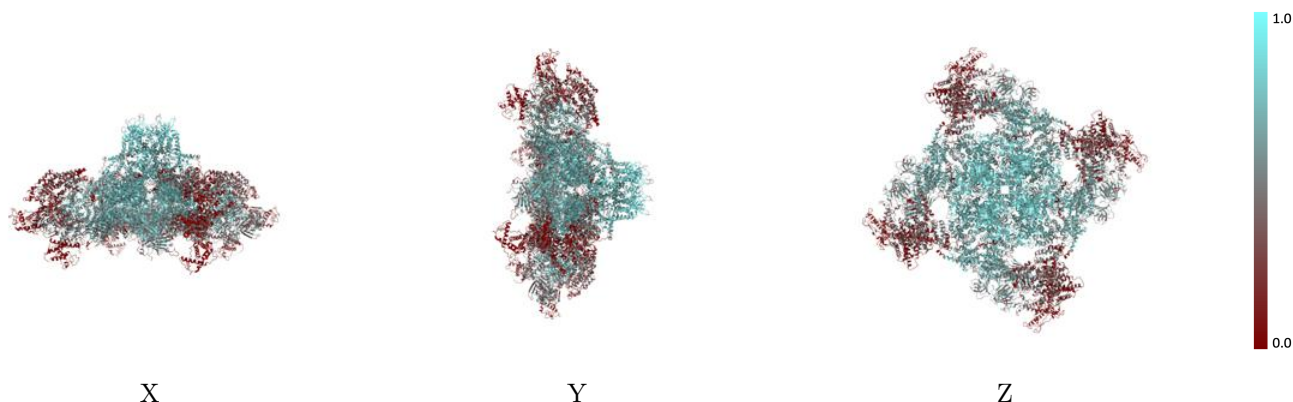
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



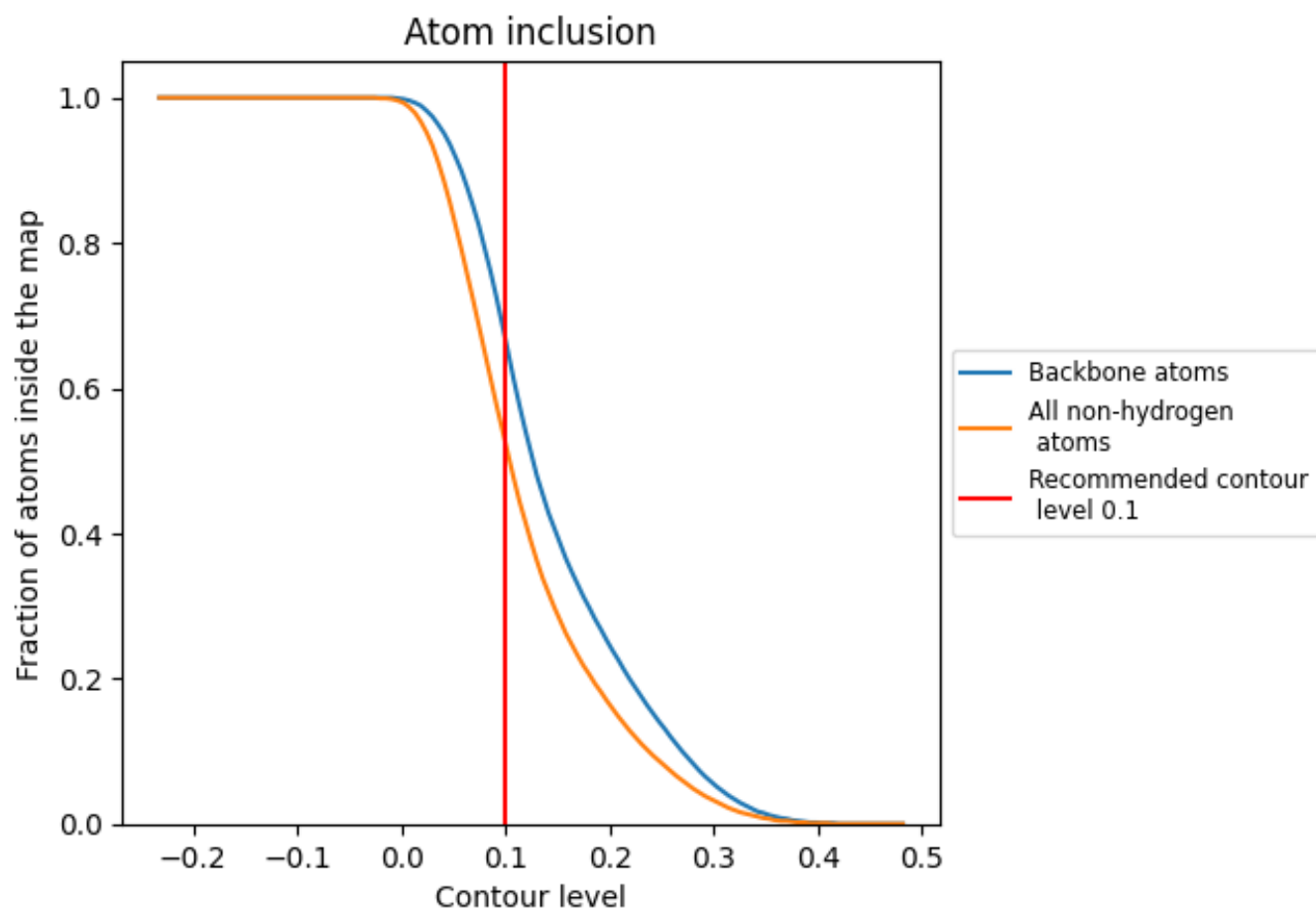
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



















9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 52% 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	 0.5250	 0.3760
A	 0.5260	 0.3740
B	 0.5260	 0.3740
C	 0.5240	 0.3730
D	 0.5270	 0.3750
E	 0.4910	 0.4340
F	 0.4930	 0.4290
G	 0.4920	 0.4280
H	 0.4930	 0.4300

