



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:03 PM UTC

PDB ID : 9E1E / pdb_00009e1e
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.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

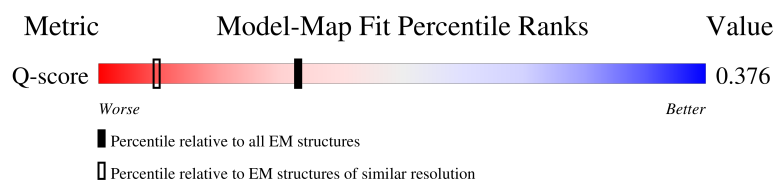
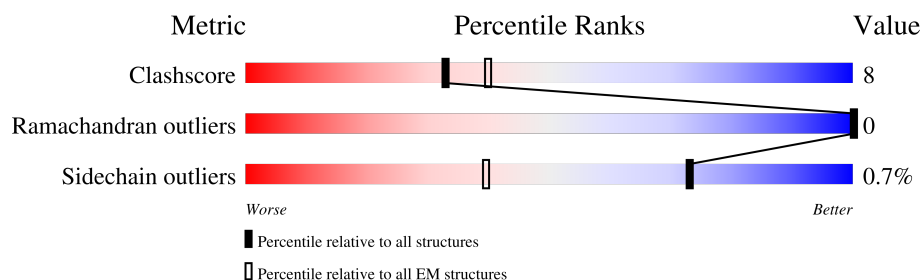
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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.



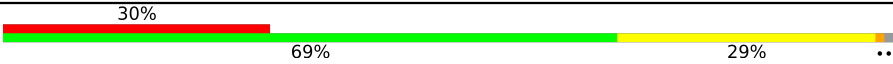
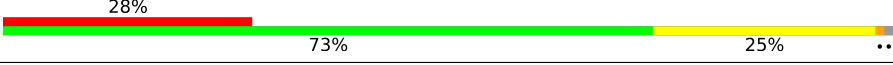
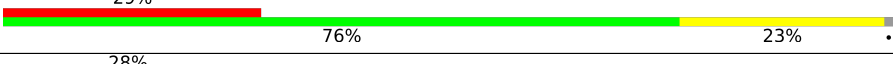
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	29% 70% 17% 13%
1	B	5037	29% 69% 18% 13%
1	C	5037	29% 69% 18% 13%
1	D	5037	29% 71% 16% 13%

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Mol	Chain	Length	Quality of chain
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.

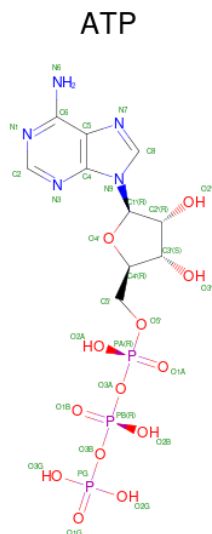
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
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).

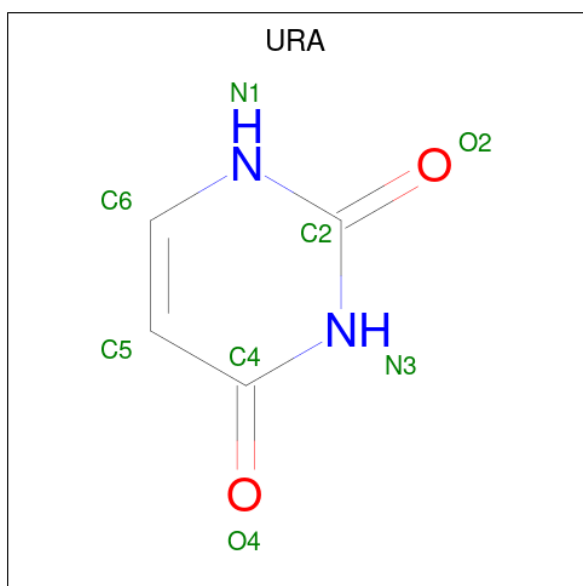
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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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 (CCD ID: URA) (formula: $C_4H_4N_2O_2$) (labeled as "Ligand of Interest" by depositor).

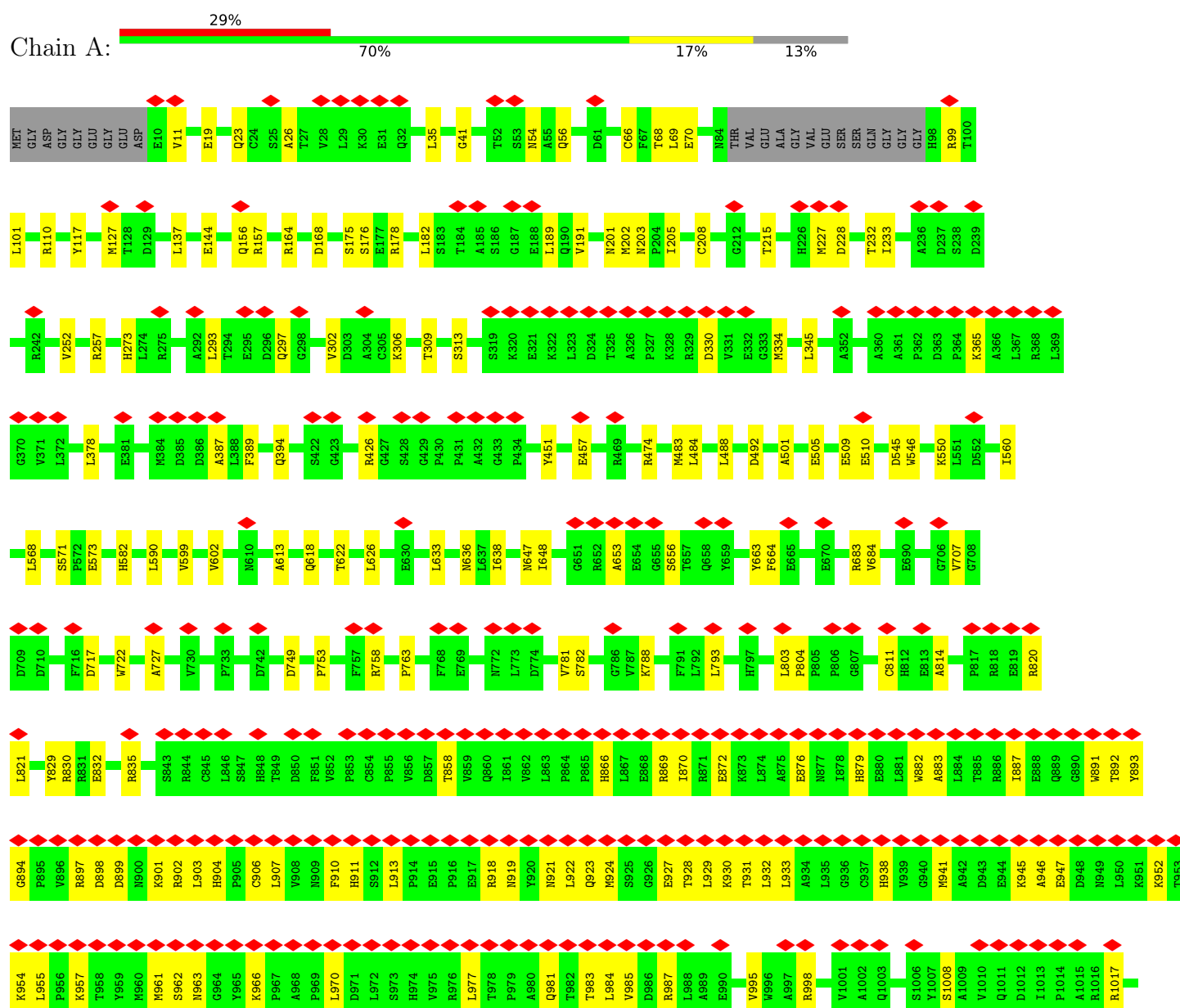


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			8	4	2	2	
6	B	1	Total	C	N	O	0
			8	4	2	2	
6	D	1	Total	C	N	O	0
			8	4	2	2	
6	C	1	Total	C	N	O	0
			8	4	2	2	

3 Residue-property plots [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.

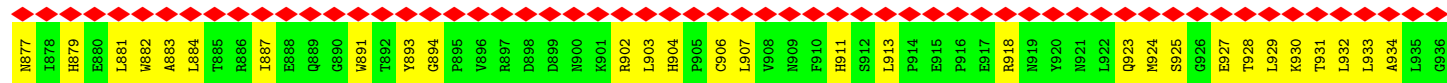
• Molecule 1: Ryanodine receptor 1





D3242	D3243	D3244	D3245	D3246	D3247	D3248	D3249	D3250	D3251	D3252	D3253	D3254	D3255	D3256	D3257	D3258	D3259	D3260	D3261	D3262	D3263	D3264	D3265	D3266	D3267	D3268	D3269	D3270	D3271	D3272	D3273	D3274	D3275	D3276	D3277	D3278	D3279	D3280	D3281	D3282	D3283	D3284	D3285	D3286	D3287	D3288	D3289	D3290	D3291	D3292	D3293	D3294	D3295	D3296	D3297	D3298	D3299	D3300	D3301	D3302				
Y3182	V3183	E3184	K3185	K3186	R3187	P3188	A3189	K3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	L3219	R3220	T3221	K3222	S3223	P3224	R3225	G3226	R3227	C3228	P3229	E3230	A3231	P3232	P3233	L3234	P3235	V3236	E3237	E3238	M3239	C3240	P3241					
ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	V3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	H3146	T3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	T3157	L3158	D3159	D3160	V3161	Q3162	G3165	V3166	R3167	T3168	L3169	T3172	V3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181								
Y3182	V3183	E3184	K3185	K3186	R3187	P3188	A3189	K3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	L3219	R3220	T3221	K3222	S3223	P3224	R3225	G3226	R3227	C3228	P3229	E3230	A3231	P3232	P3233	L3234	P3235	V3236	E3237	E3238	M3239	C3240	P3241					
M2423	H2441	Q2444	P2462	D2463	D2464	D2465	L2466	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	A2484	L2485	V2486	Q2487	S2493	F2494	V2495	H2498	K2499	M2502	E2513	N2514	D2515	D2516	L2519	H2520	D2523	V2524	G2525	F2526	L2527	F2528	D2529	M2530	R2531	A2534	S2535	L2536	D2537	T2538																		
F2541	S2542	H2546	A2547	L2550	K2564	F2569	A2570	G2571	T2572	H2573	E2574	R2575	A2576	I2577	M2578	M2582	L2583	H2584	T2585	V2586	Y2587	R2588	L2589	S2590	R2591	G2592	R2593	S2594	Q2599	R2600	I2603	E2604	E2605	C2606	L2607	M2608	C2611	I2614	R2615	F2619	L2622	R2624	R2625	L2626	V2627	F2628																		
D2629	V2630	P2631	L2632	L2633	N2634	E2635	F2636	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	N2646	H2647	A2648	I2649	C2650	Y2651	V2652	L2653	V2654	L2655	L2656	L2657	P2658	L2659	G2660	E2661	E2662	N2663	L2664	Q2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	P2679	W2680	Q2681	L2682	F2683	D2684	H2688	K2689	K2690	Y2691	D2692				
Q2693	E2694	L2695	Y2696	R2697	M2698	A2699	P2700	K2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708	A2709	L2710	H2711	P2712	D2713	Y2714	V2715	D2716	A2717	L2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	L2726	THR	THR	THR	VAL	ASP	ALA	GLU	GLY	W2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	W2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752				
S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	T2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2803	L2804	Y2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812						
L2813	K2814	A2815	W2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	A2825	A2826	R2827	E2828	G2829	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	THR	ASP	PRO	ARG	GLU	GLY	Y2855	Y2856	Q2857	Q2858	P2859	P2860	L2861	L2862	S2863	Q2864	Y2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872									
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ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	V3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	H3146	T3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	T3157	L3158	D3159	D3160	V3161	Q3162	G3165	V3166	R3167	T3168	L3169	T3172	V3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181								
Y3182	V3183	E3184	K3185	K3186	R3187	P3188	A3189	K3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	L3219	R3220	T3221	K3222	S3223	P3224	R3225	G3226	R3227	C3228	P3229	E3230	A3231	P3232	P3233	L3234	P3235	V3236	E3237	E3238	M3239	C3240	P3241					







V3139	L3140	F3144	Q3145	A3148	Q3149	H3150	Q3151	F3152	Q3153	D3154	D3155	V3156	L3158	D3159	D3160	V3161	Q3162	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3165	V3166	F3167	F3168	L3169	C3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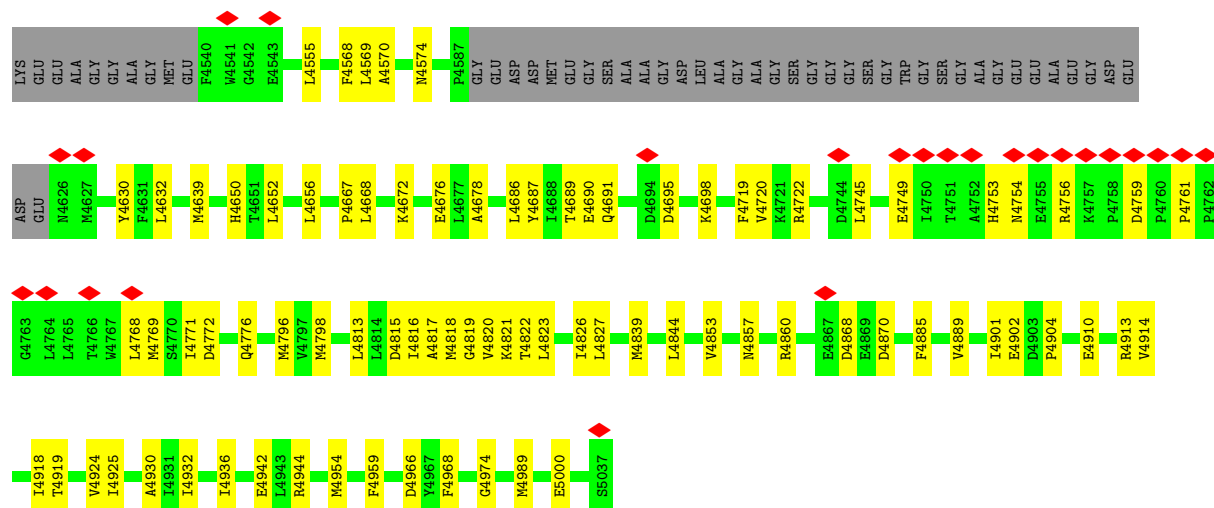




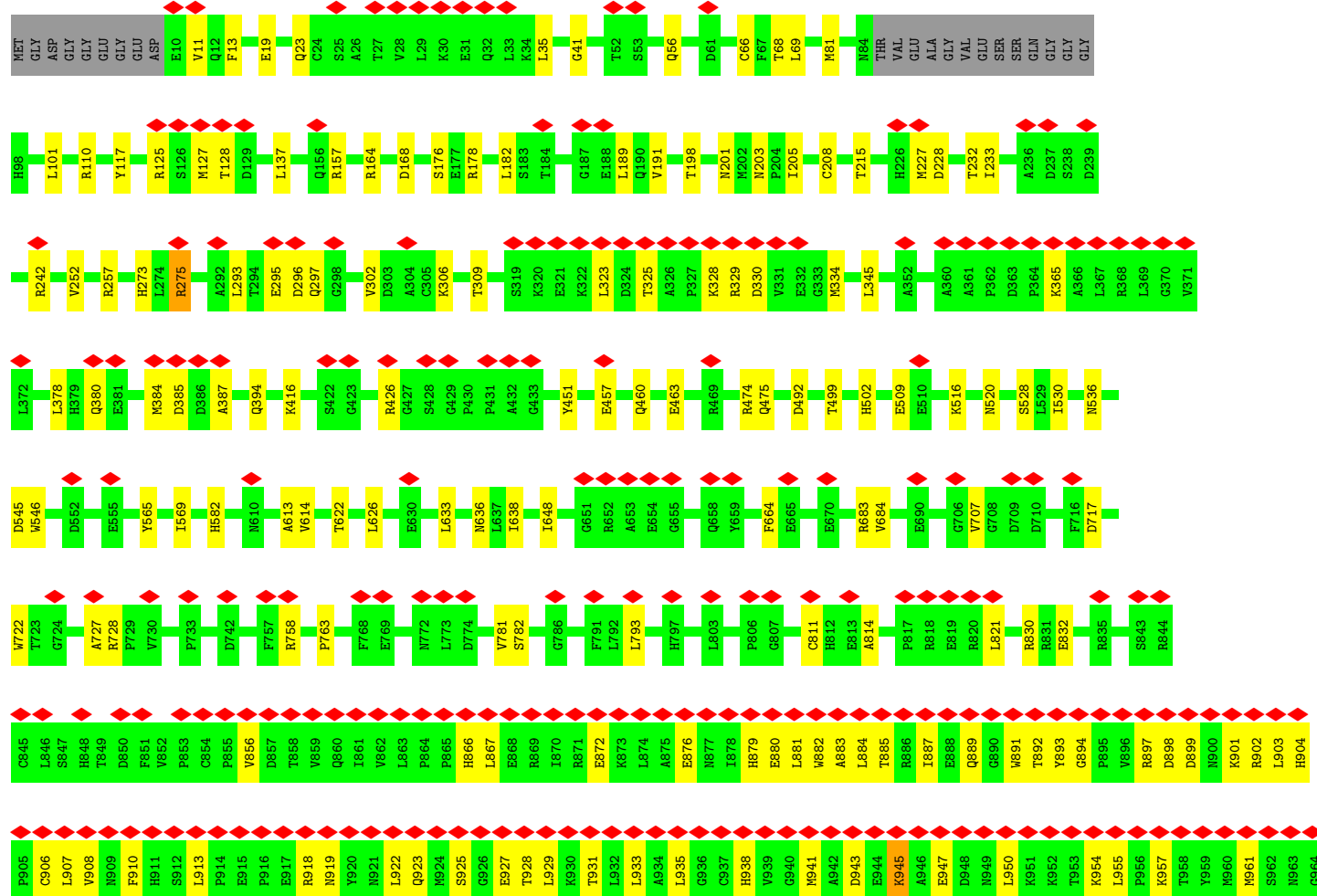


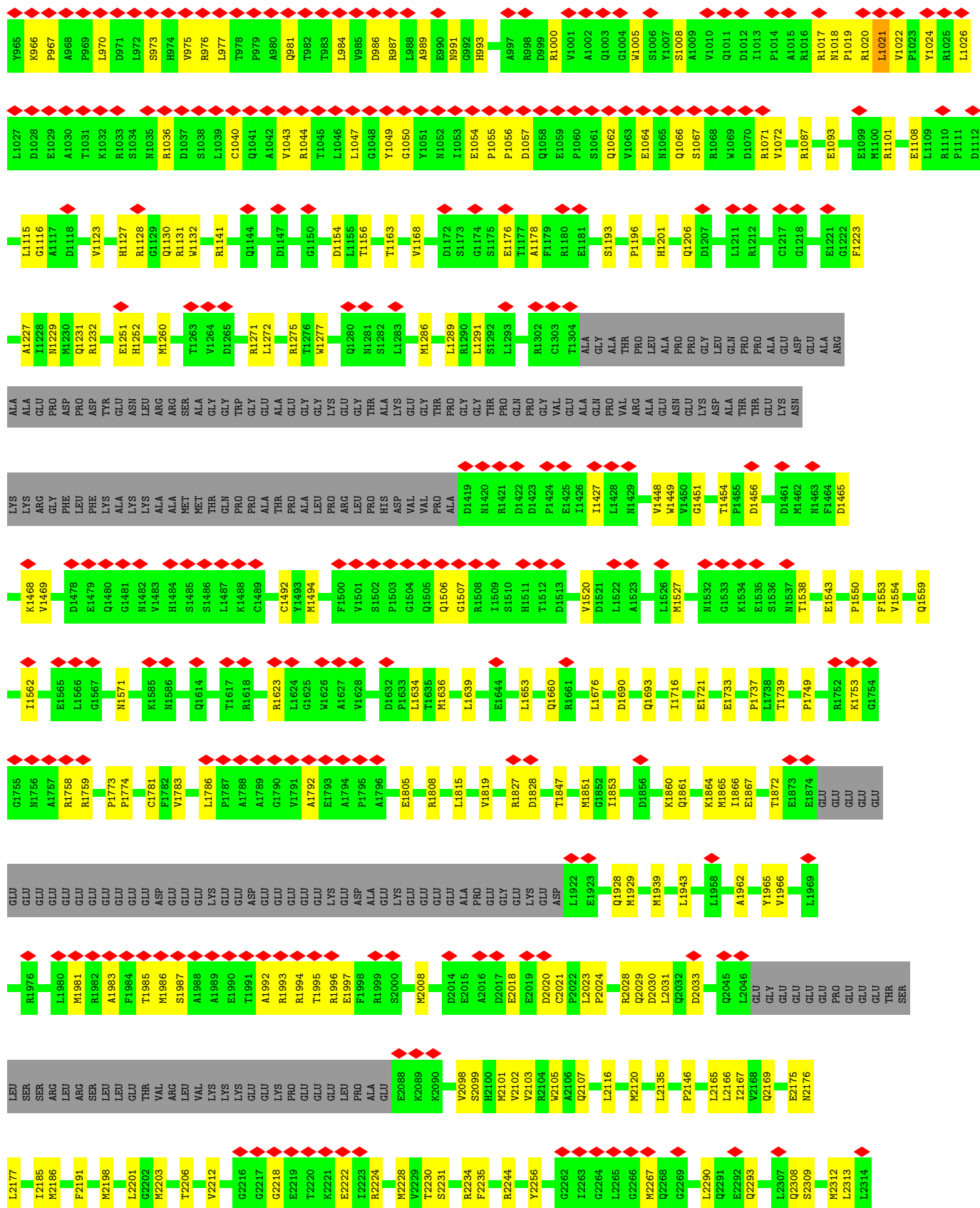


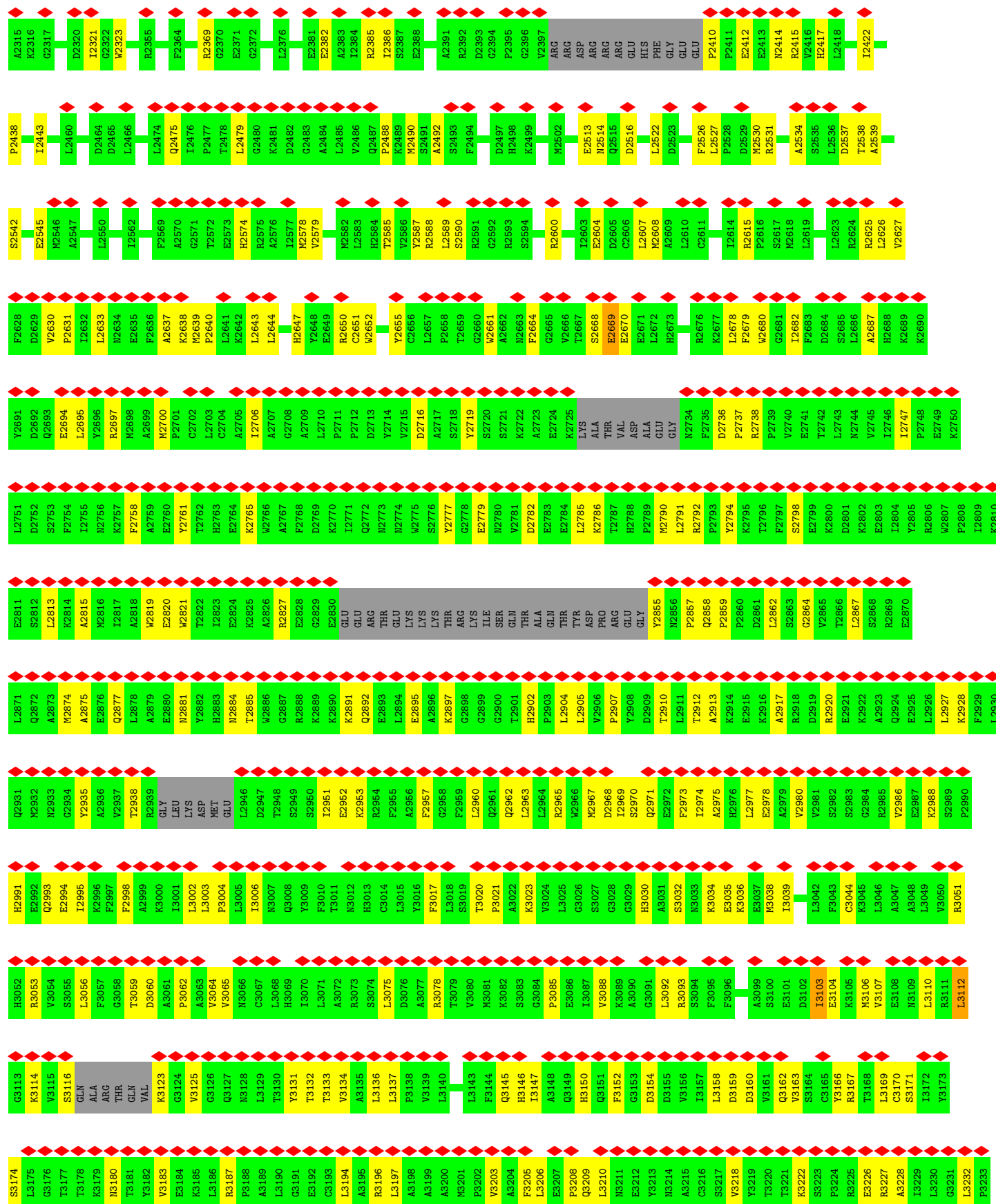




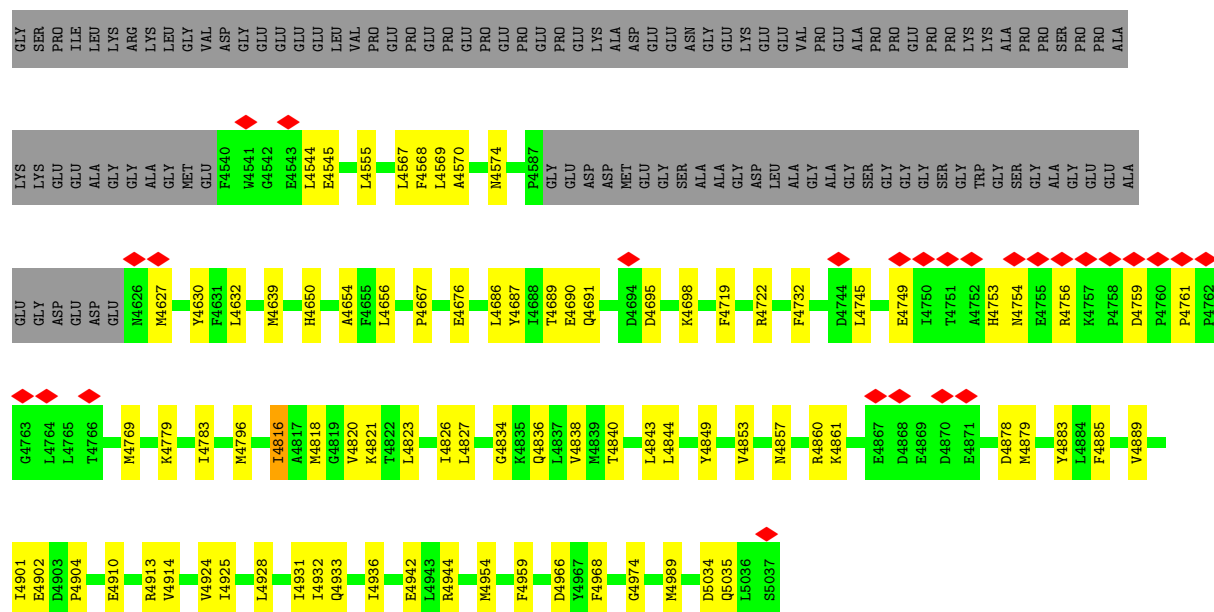
• Molecule 1: Ryanodine receptor 1



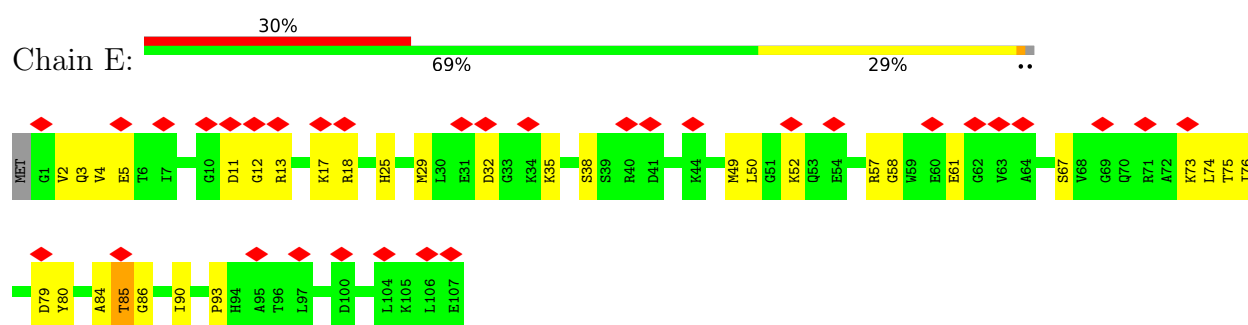




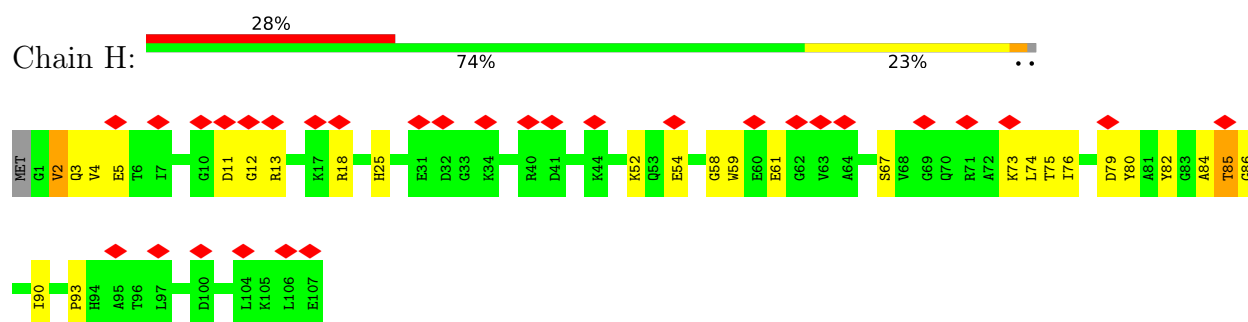




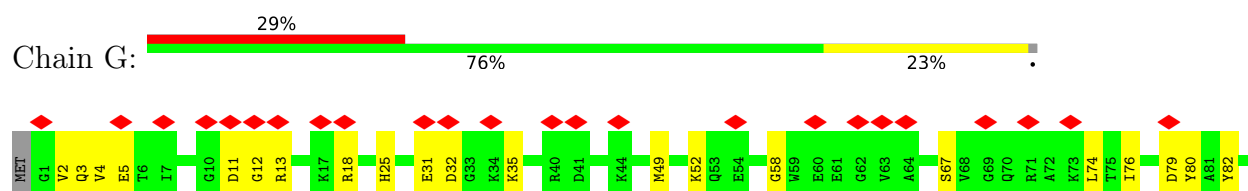
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

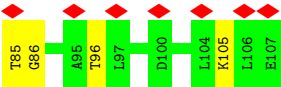


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

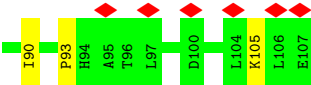
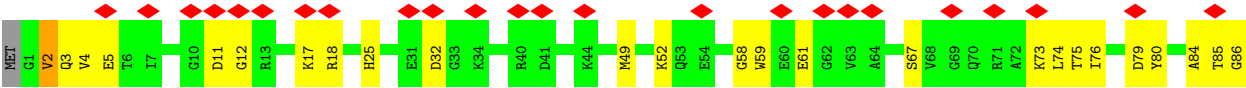


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





• 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	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, URA, 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	0.17	0/35977	0.34	2/48726 (0.0%)
1	B	0.17	0/35977	0.34	0/48726
1	C	0.16	0/35977	0.34	2/48726 (0.0%)
1	D	0.15	0/35977	0.31	1/48726 (0.0%)
2	E	0.17	0/850	0.36	0/1146
2	F	0.18	0/850	0.40	0/1146
2	G	0.18	0/850	0.39	0/1146
2	H	0.17	0/850	0.36	0/1146
All	All	0.16	0/147308	0.33	5/199488 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2669	GLU	CA-CB-CG	5.61	125.32	114.10
1	C	2971	GLN	CA-CB-CG	5.30	124.70	114.10
1	D	1783	VAL	N-CA-C	-5.25	108.16	113.20
1	A	1783	VAL	N-CA-C	-5.21	108.20	113.20
1	A	3534	MET	CB-CG-SD	5.12	128.06	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	570	0
1	B	35150	0	34797	609	0
1	C	35150	0	34797	639	0
1	D	35150	0	34797	542	0
2	E	831	0	831	19	0
2	F	831	0	831	18	0
2	G	831	0	831	16	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	2402	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 2402 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:893:TYR:HB2	1:C:961:MET:HE2	1.53	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:B:3233:PRO:HD2	1:B:3239:MET:HE1	1.59	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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%)	3812 (99%)	24 (1%)	78	92
1	B	3836/4276 (90%)	3812 (99%)	24 (1%)	78	92
1	C	3836/4276 (90%)	3817 (100%)	19 (0%)	81	93
1	D	3836/4276 (90%)	3812 (99%)	24 (1%)	78	92
2	E	89/90 (99%)	83 (93%)	6 (7%)	15	41
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	75
2	H	89/90 (99%)	85 (96%)	4 (4%)	24	56
All	All	15700/17464 (90%)	15594 (99%)	106 (1%)	73	91

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3899	PHE
1	D	1021	LEU
1	C	3103	ILE
1	B	4722	ARG
1	D	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3211	ASN
1	C	2260	ASN
1	D	949	ASN
1	C	2194	HIS
1	C	3734	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	C	5304	-	8,8,8	0.62	0	10,10,10	1.06	1 (10%)
6	URA	D	5304	-	8,8,8	0.61	0	10,10,10	1.05	1 (10%)
6	URA	A	5304	-	8,8,8	0.59	0	10,10,10	1.08	1 (10%)
3	ATP	D	5301	-	32,33,33	0.29	0	48,52,52	0.40	0
3	ATP	B	5301	-	32,33,33	0.29	0	48,52,52	0.40	0
6	URA	B	5304	-	8,8,8	0.60	0	10,10,10	1.12	1 (10%)
3	ATP	A	5301	-	32,33,33	0.29	0	48,52,52	0.40	0
3	ATP	C	5301	-	32,33,33	0.29	0	48,52,52	0.40	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
6	URA	C	5304	-	-	-	0/1/1/1
6	URA	D	5304	-	-	-	0/1/1/1
6	URA	A	5304	-	-	-	0/1/1/1
3	ATP	D	5301	-	-	8/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	9/22/38/38	0/3/3/3
6	URA	B	5304	-	-	-	0/1/1/1
3	ATP	A	5301	-	-	7/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5304	URA	C4-N3-C2	2.41	127.88	125.55
6	A	5304	URA	C4-N3-C2	2.32	127.79	125.55
6	C	5304	URA	C4-N3-C2	2.24	127.72	125.55
6	D	5304	URA	C4-N3-C2	2.21	127.69	125.55

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

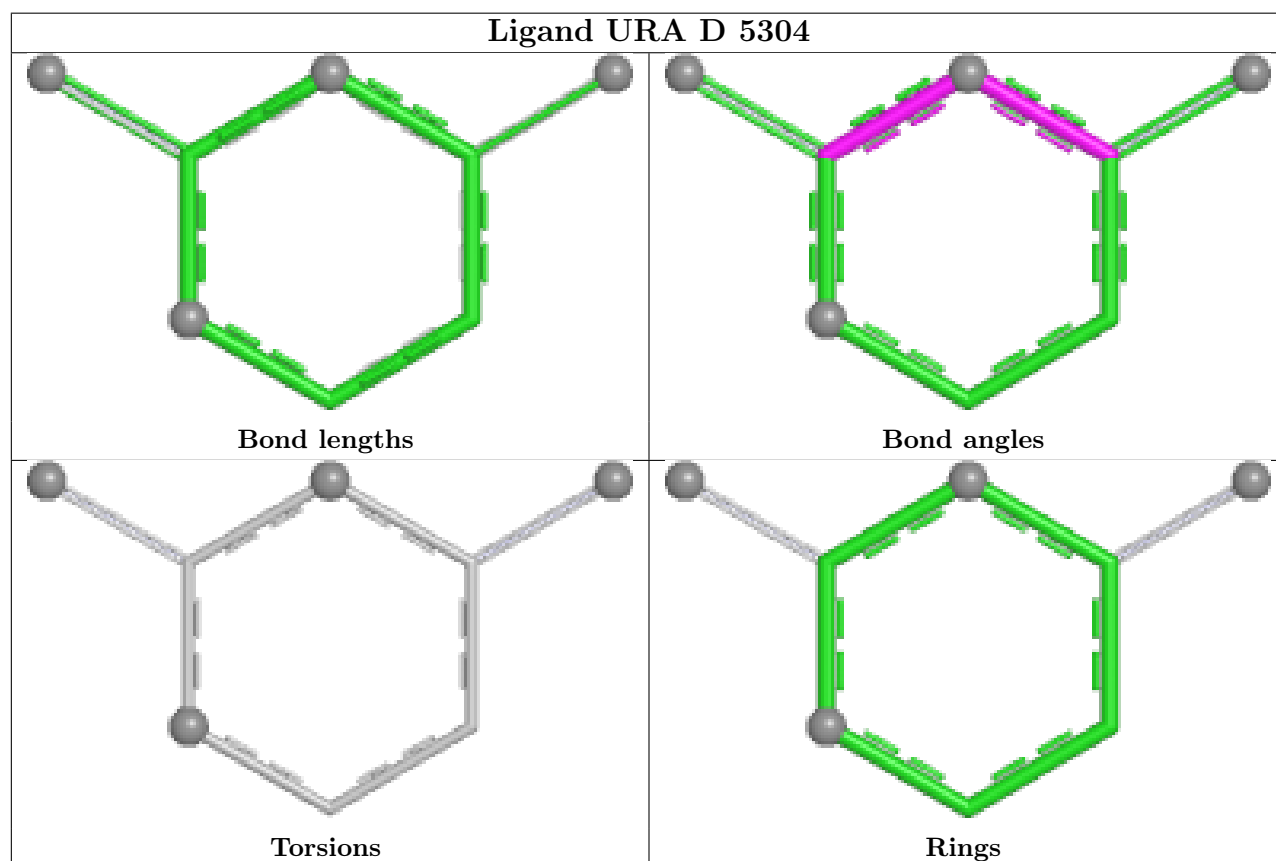
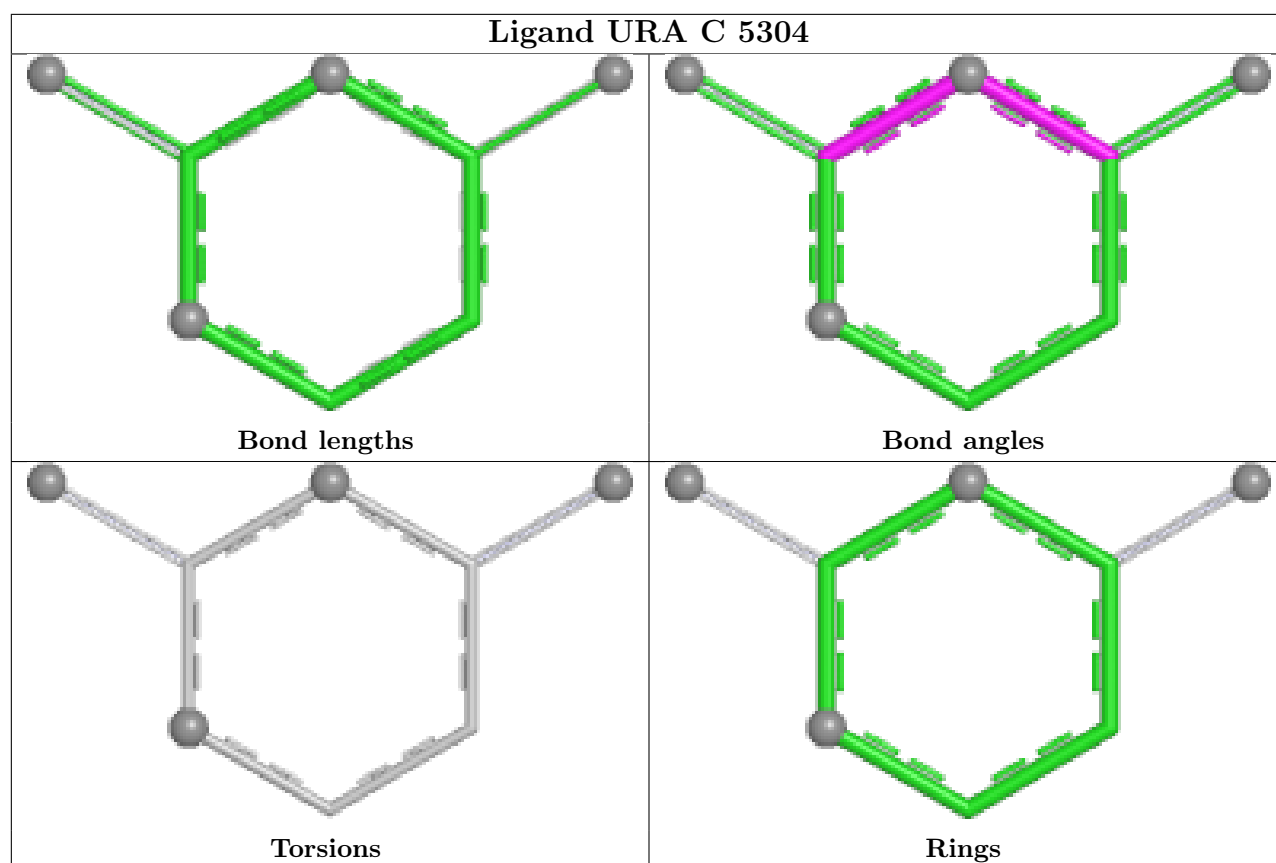
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O1A
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A

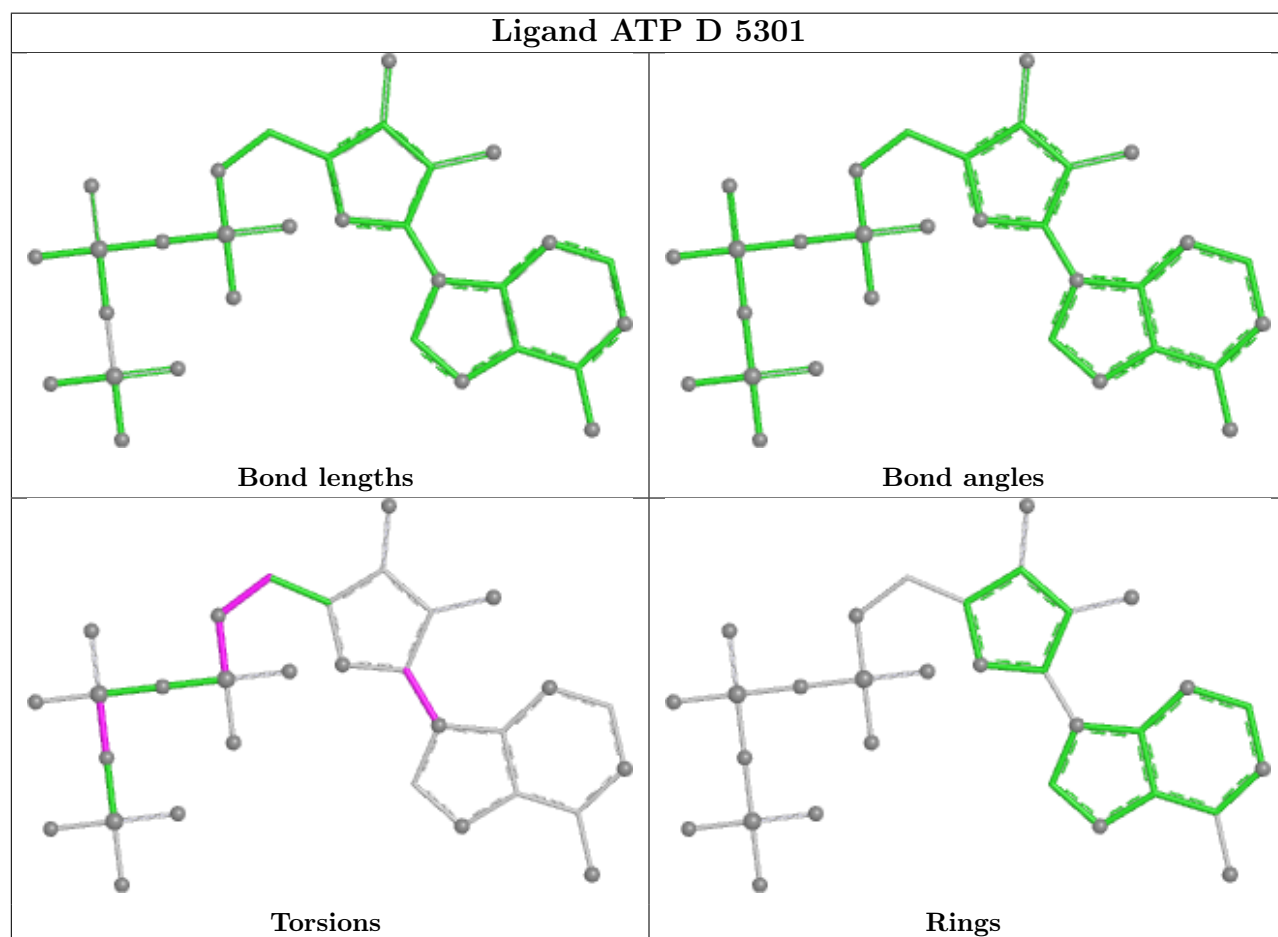
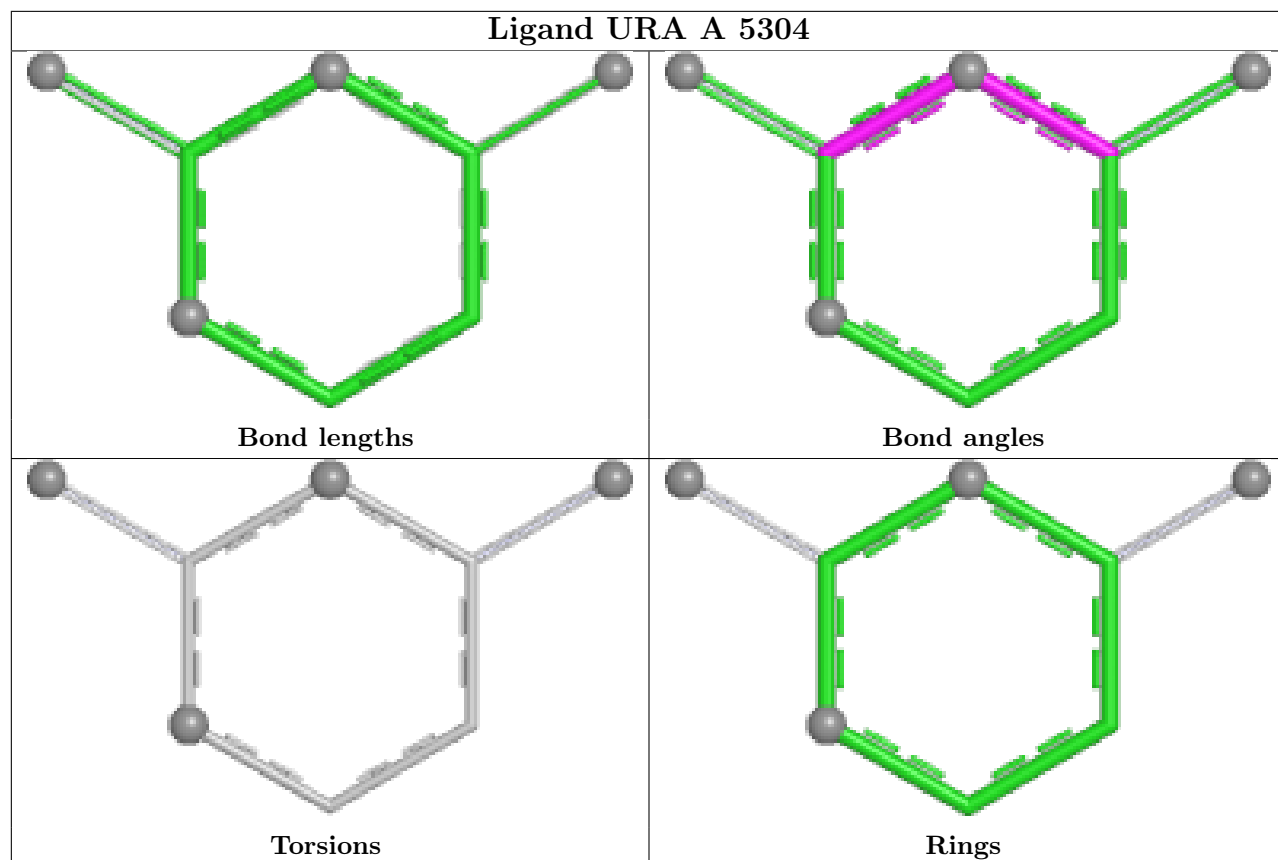
There are no ring outliers.

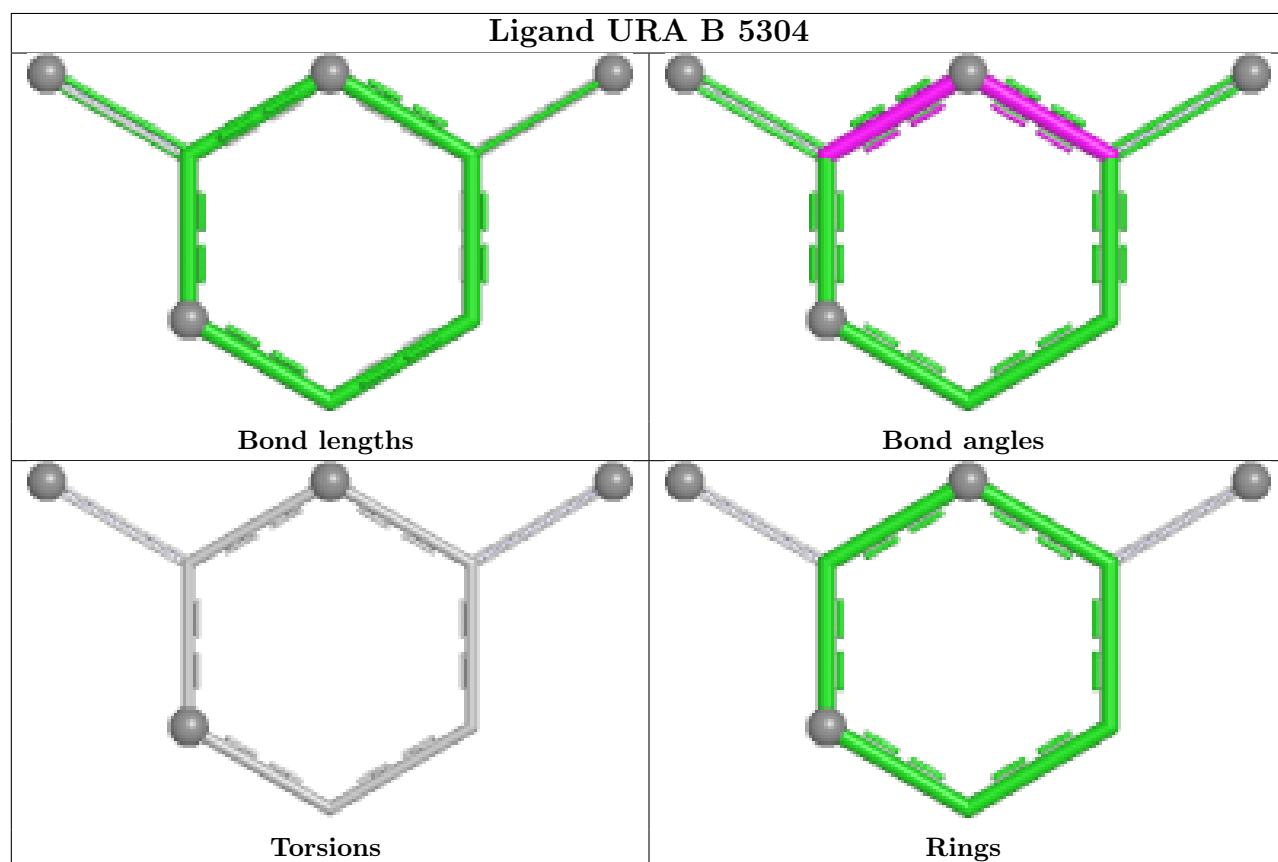
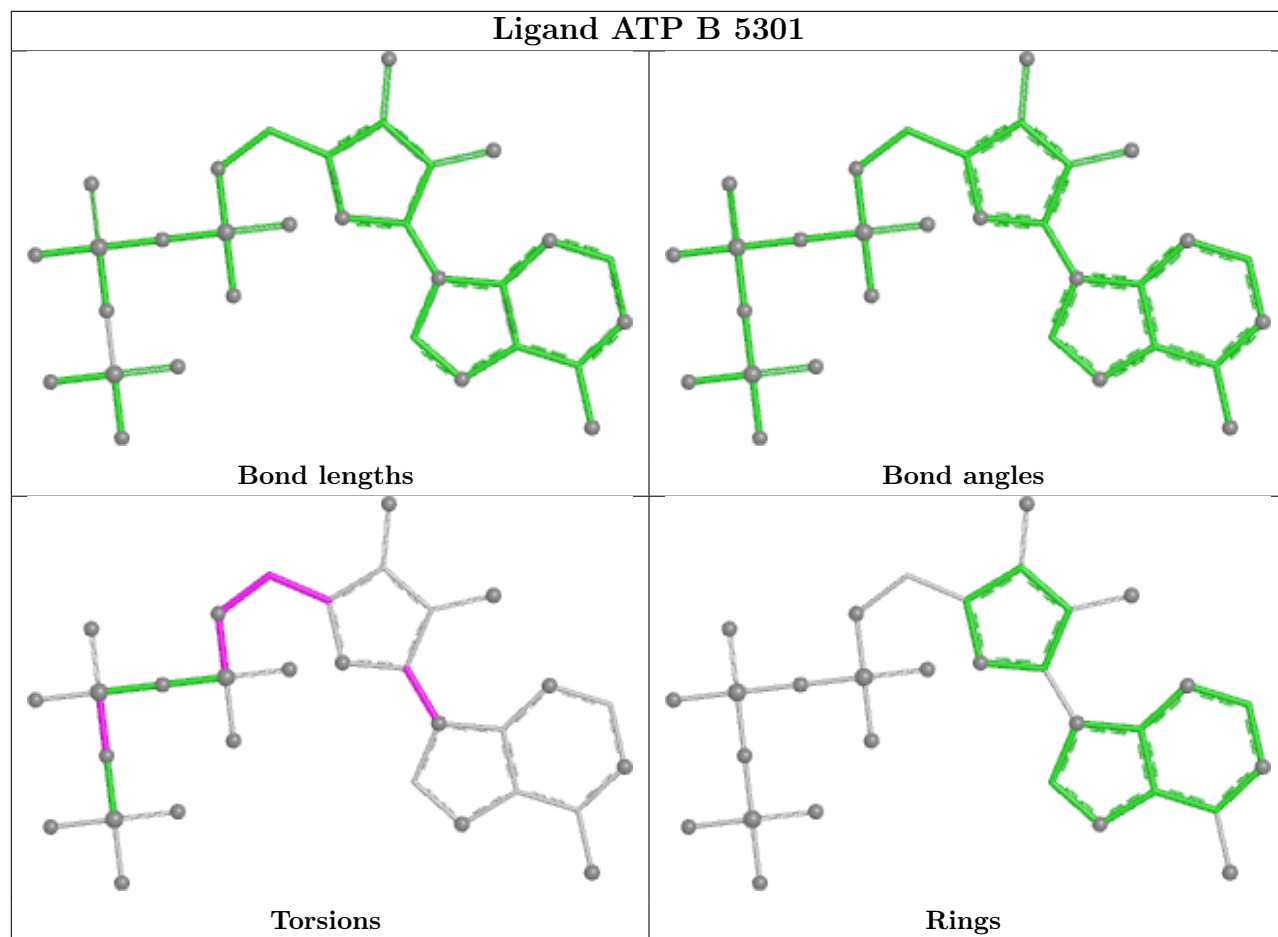
2 monomers are involved in 2 short contacts:

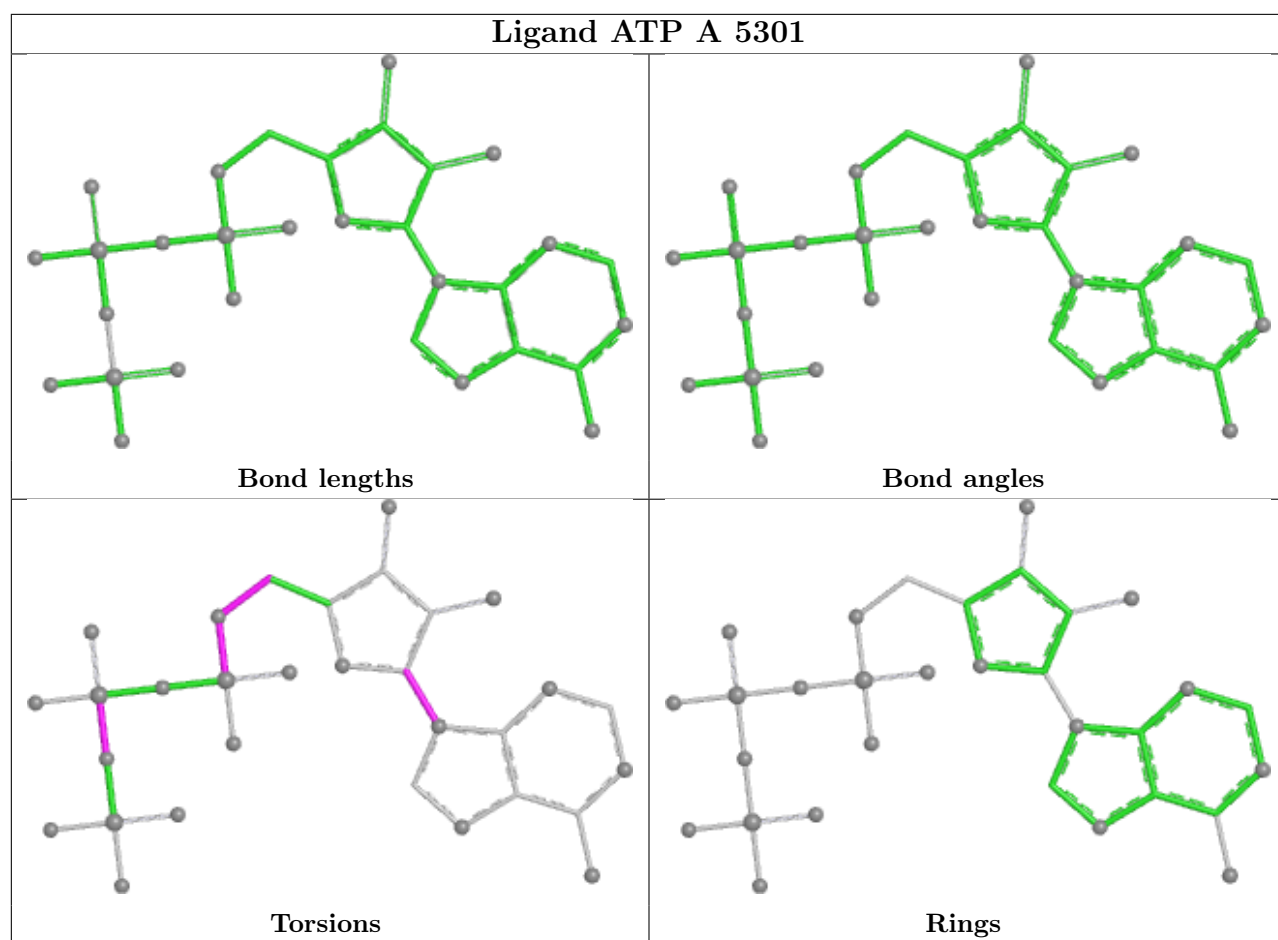
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	1	0
3	A	5301	ATP	1	0

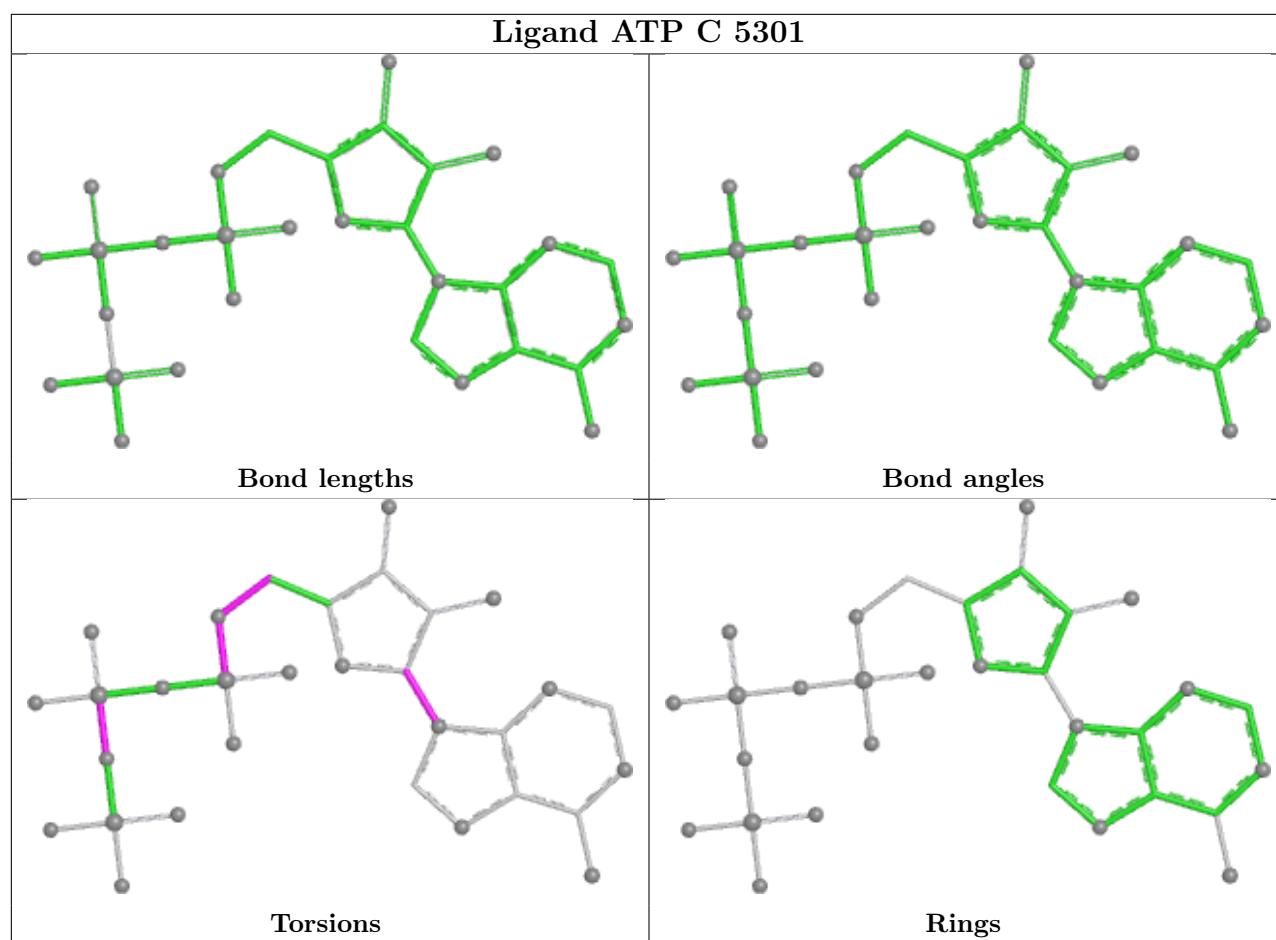
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

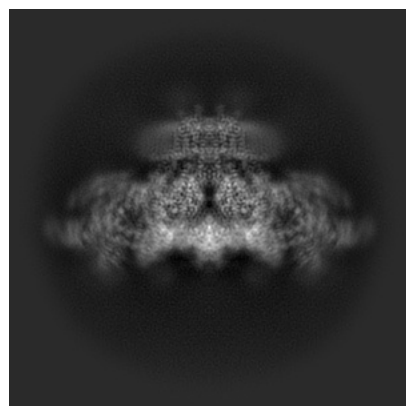
6 Map visualisation [i](#)

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.

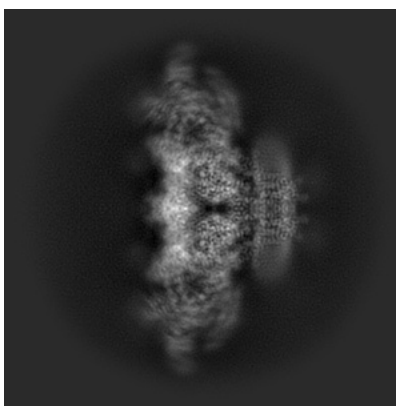
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

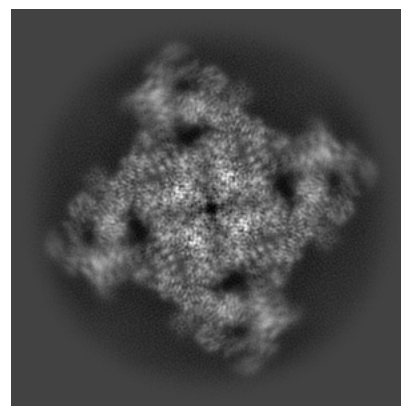
6.1.1 Primary map



X

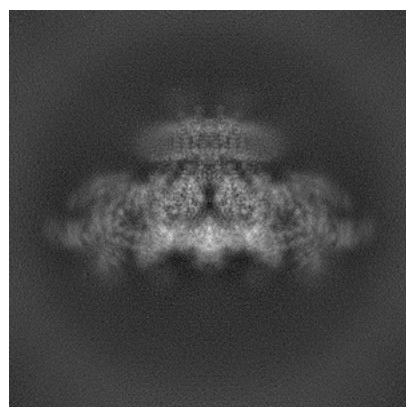


Y

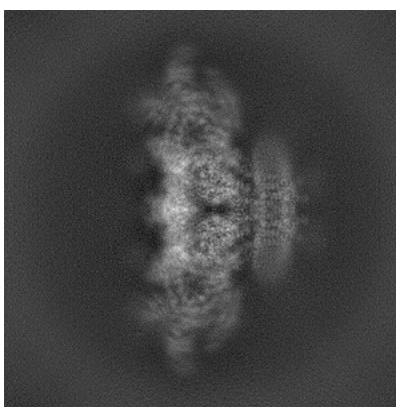


Z

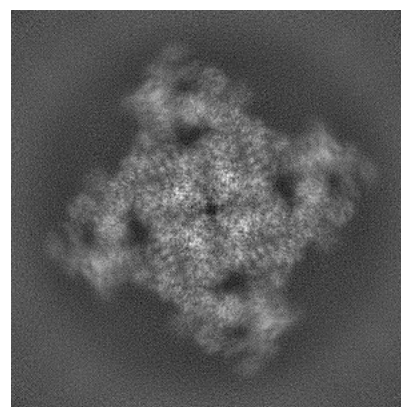
6.1.2 Raw map



X



Y

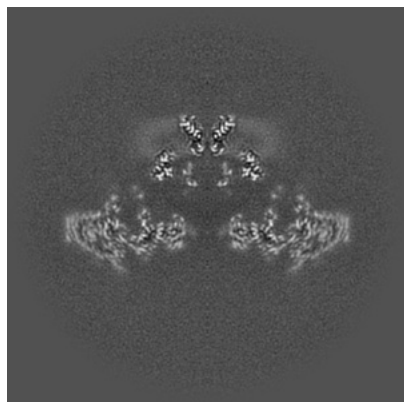


Z

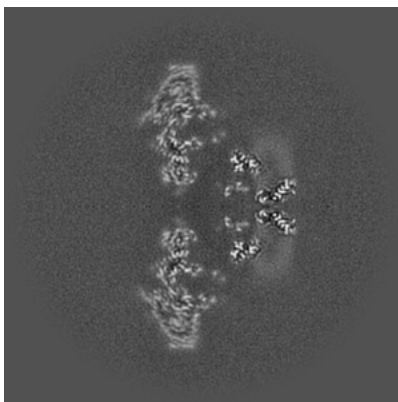
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

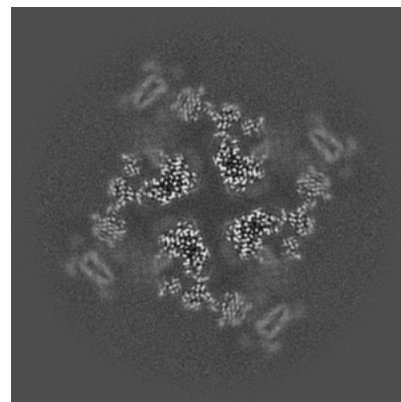
6.2.1 Primary map



X Index: 256

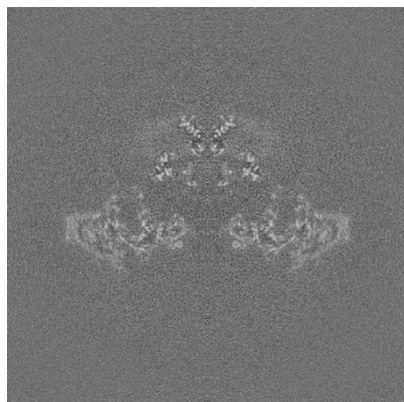


Y Index: 256

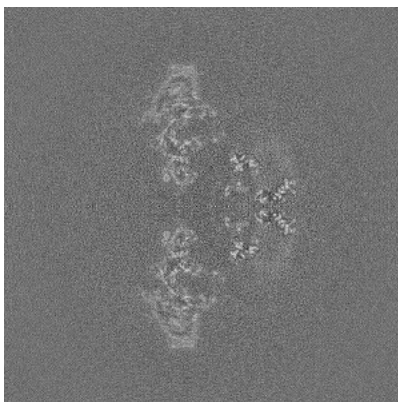


Z Index: 256

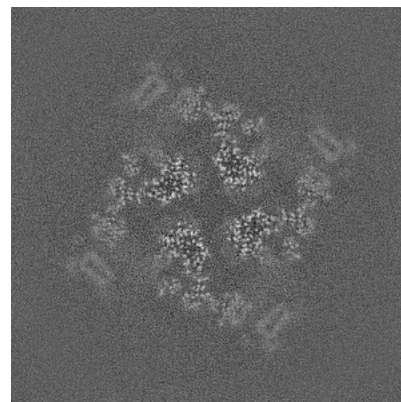
6.2.2 Raw map



X Index: 256



Y Index: 256

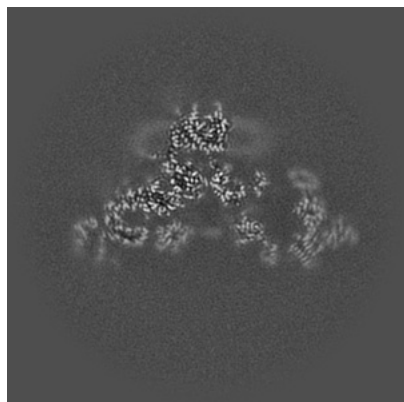


Z Index: 256

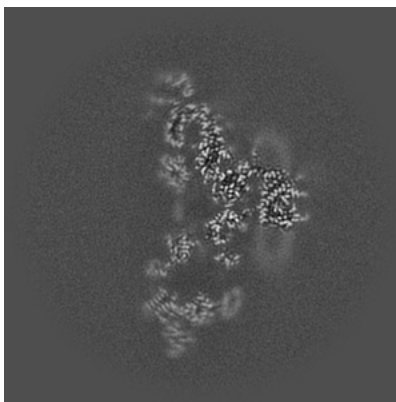
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

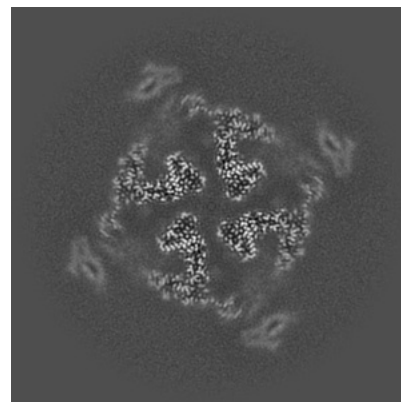
6.3.1 Primary map



X Index: 239

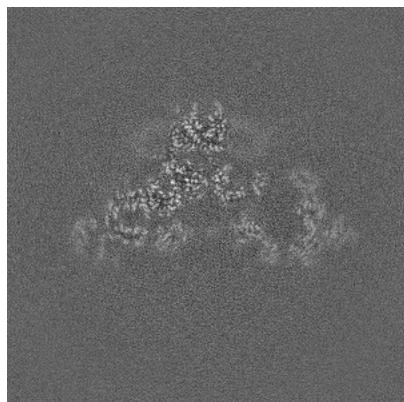


Y Index: 239

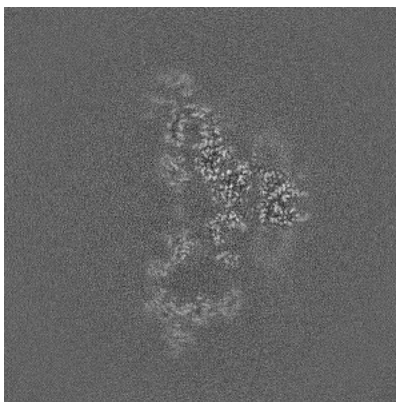


Z Index: 265

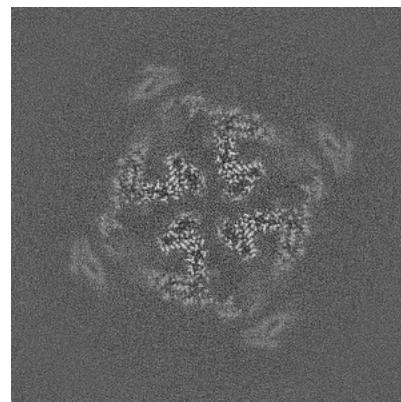
6.3.2 Raw map



X Index: 240



Y Index: 240

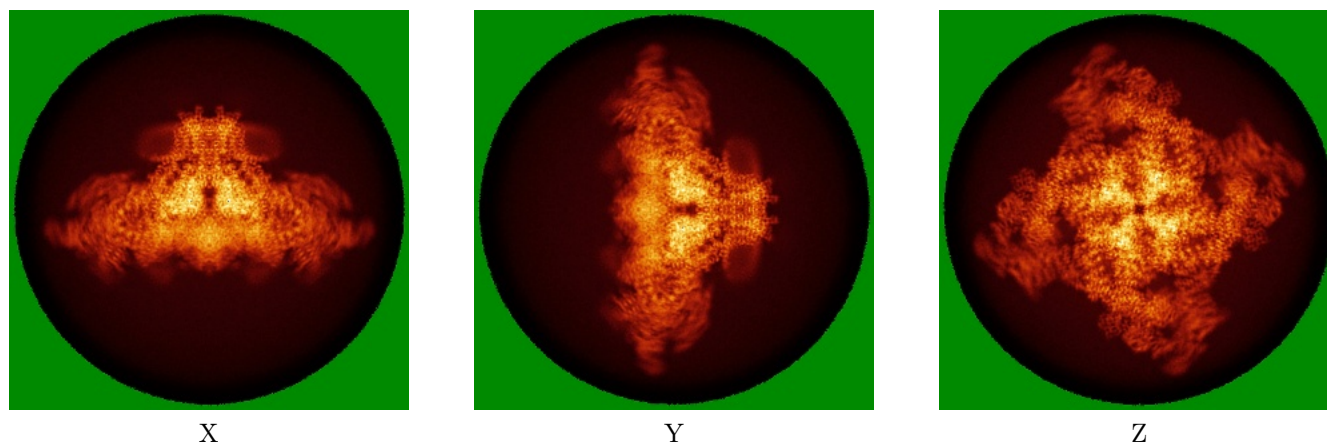


Z Index: 266

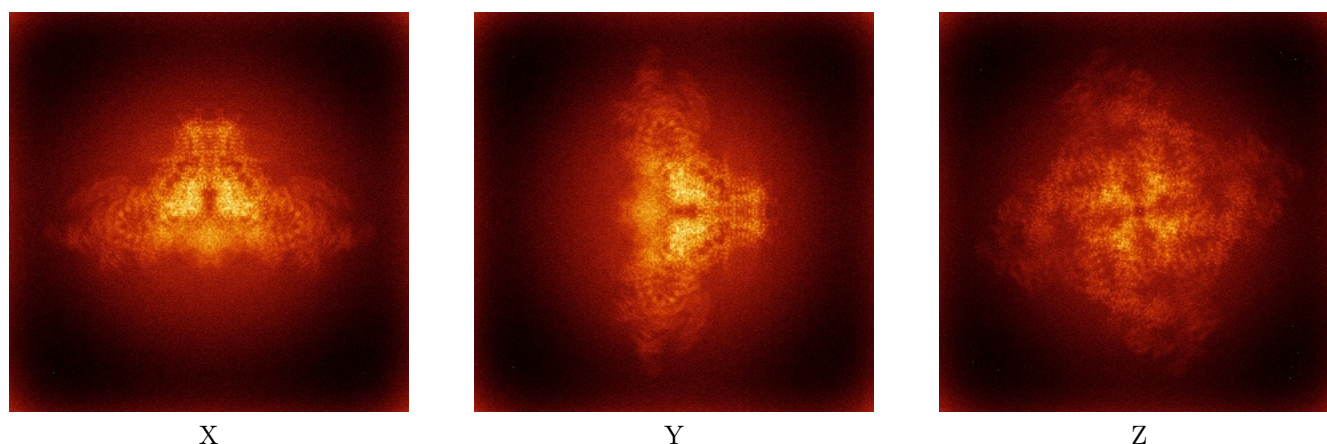
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

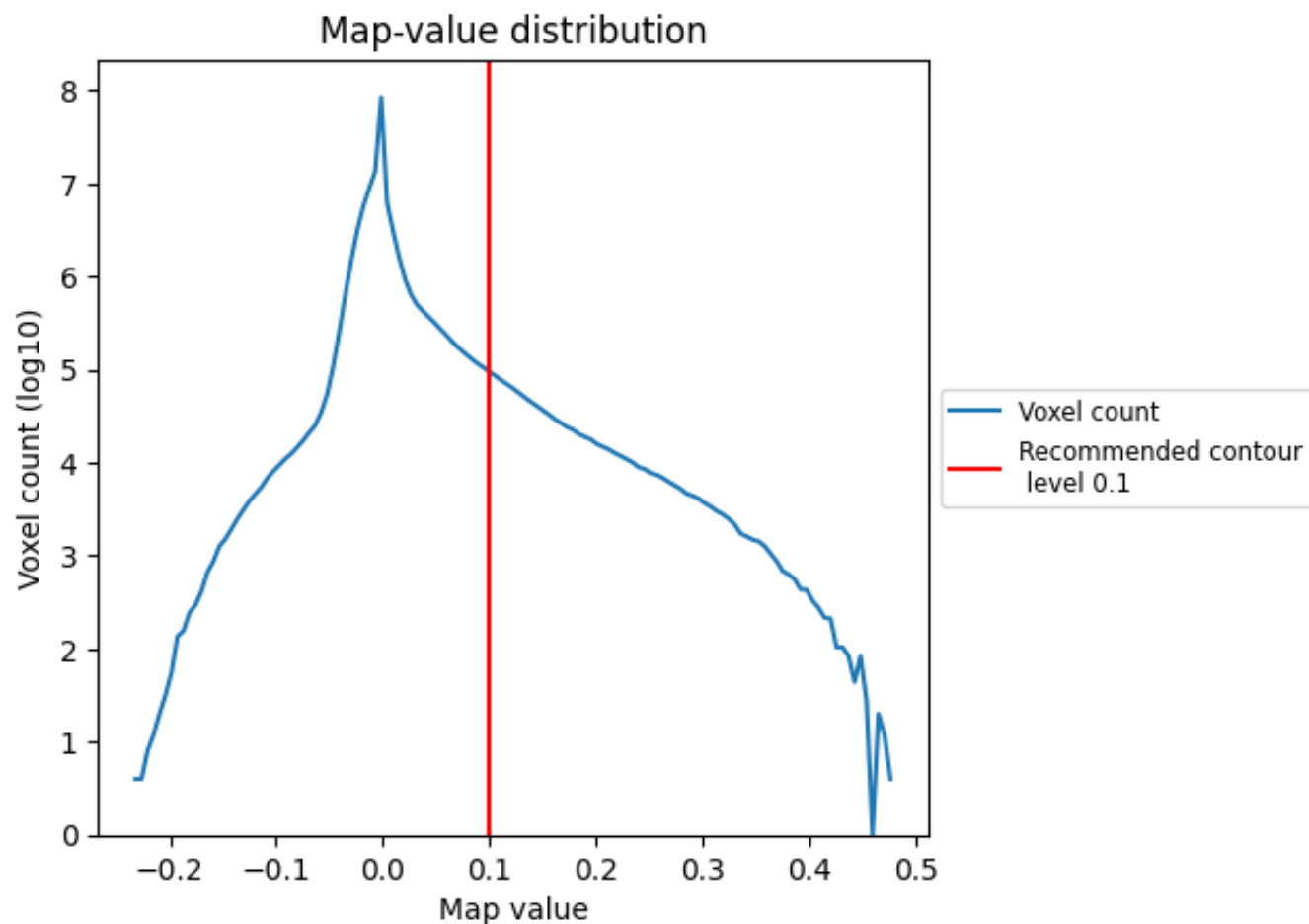
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

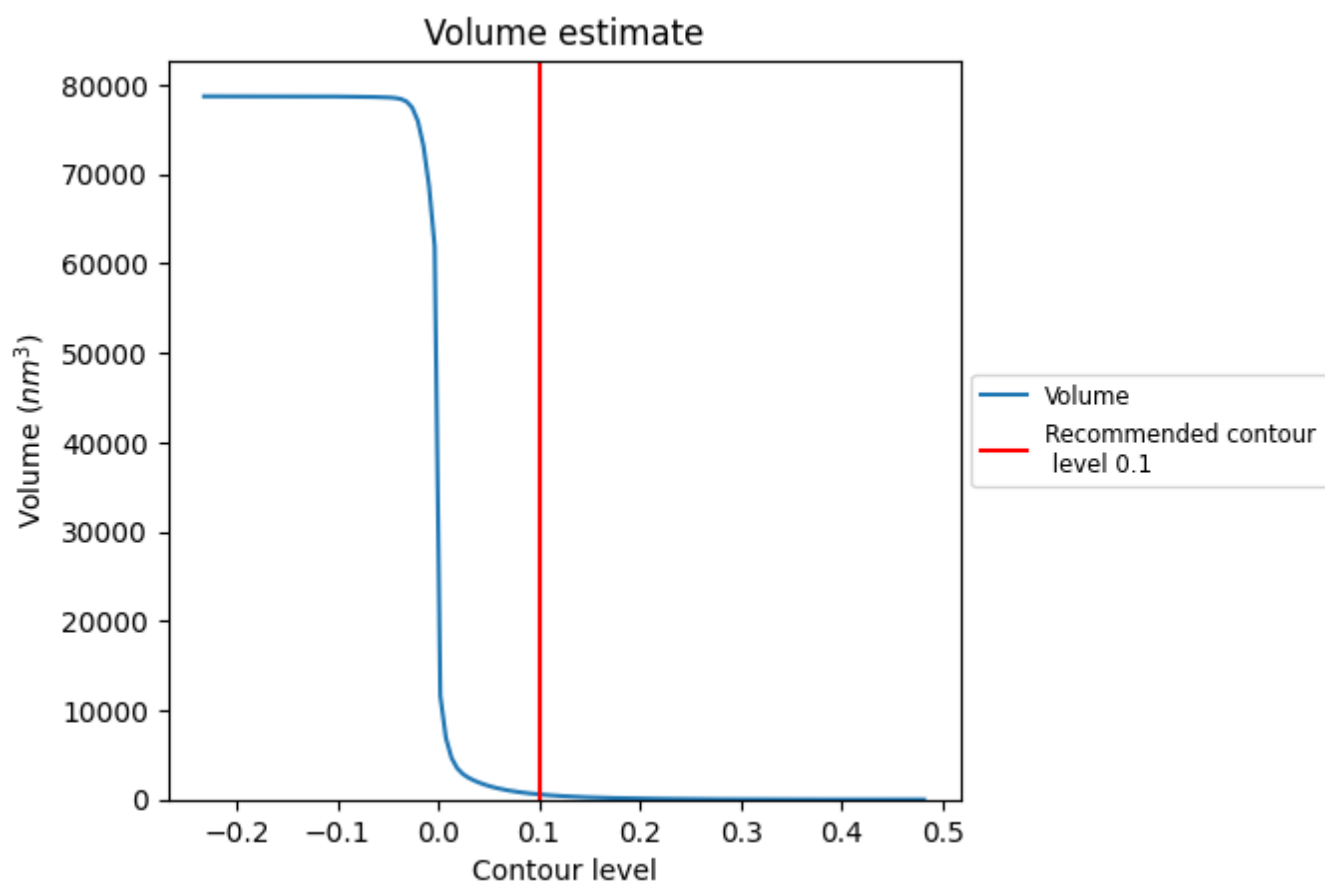
This section contains the results of statistical analysis of the map.

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.

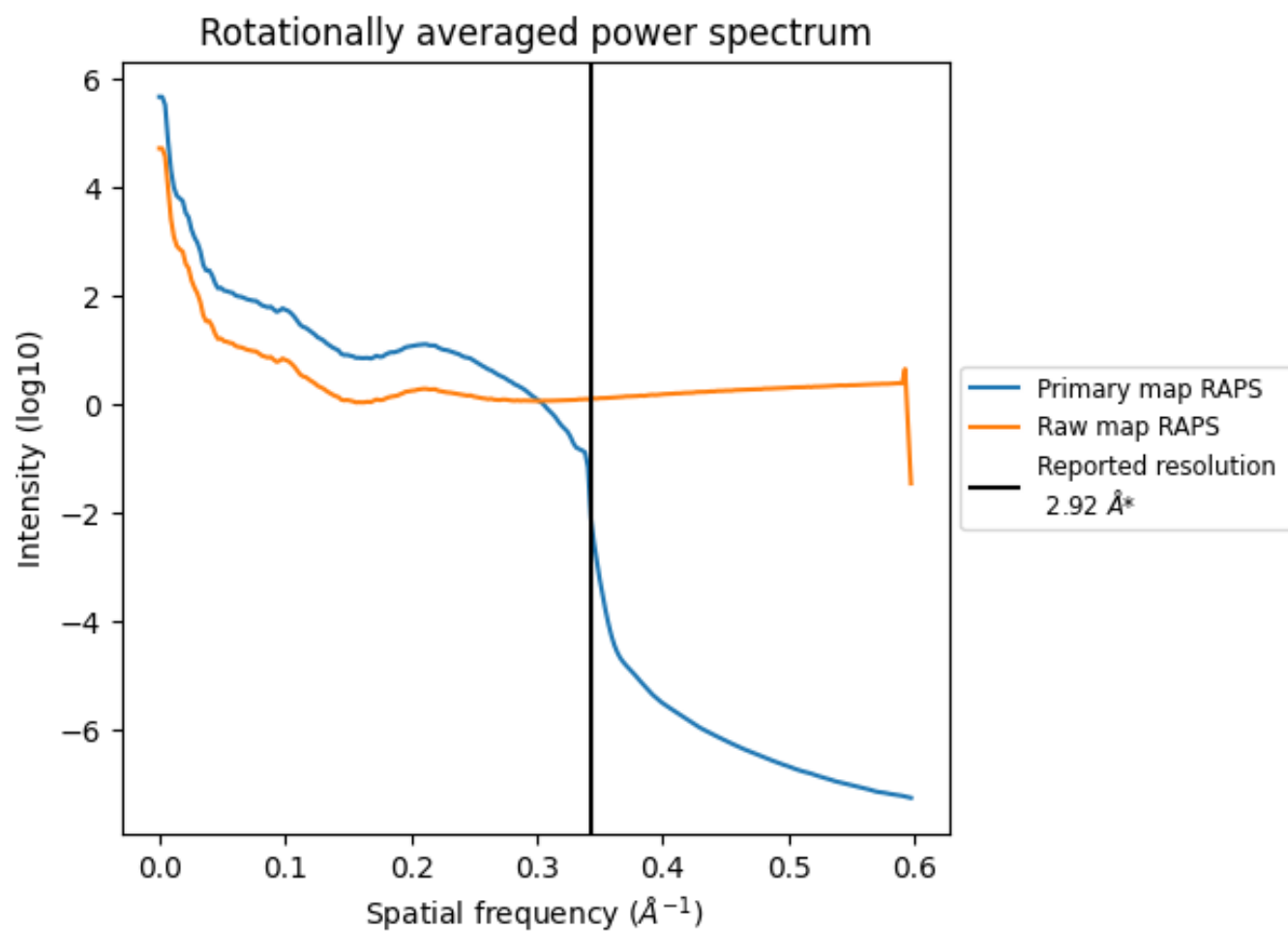
7.2 Volume estimate [i](#)



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 ⓘ

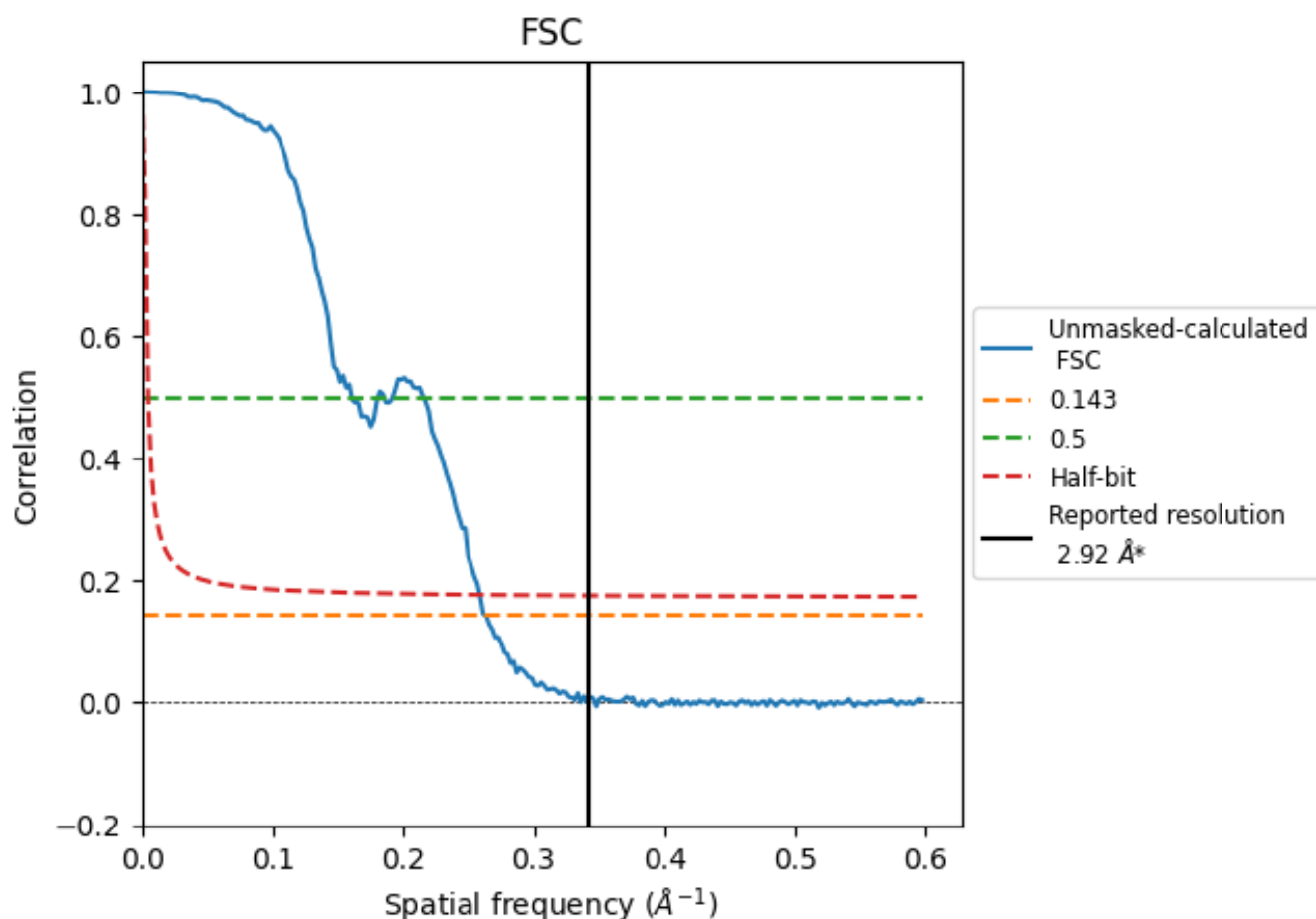


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

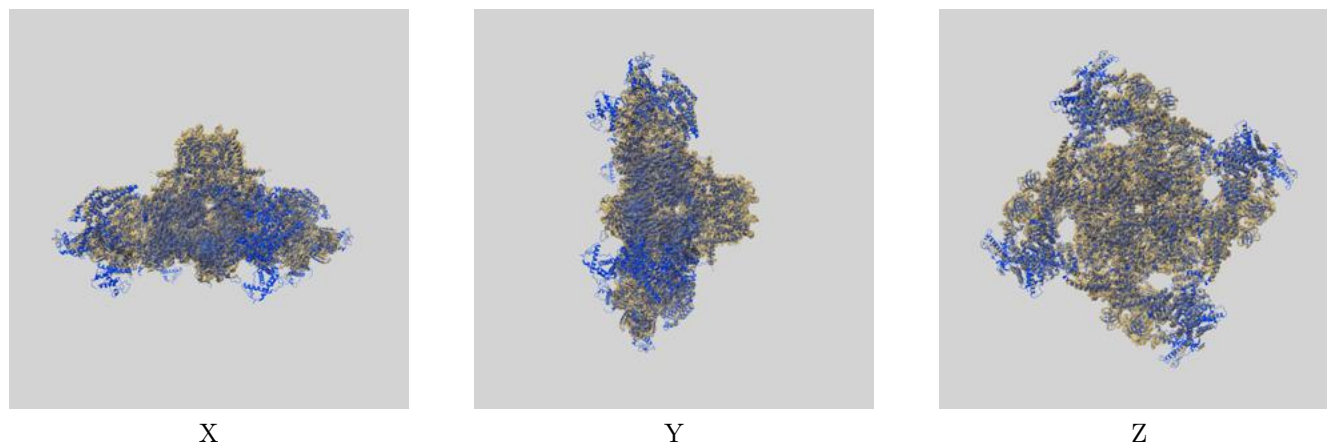
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.23	3.87

*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](#)

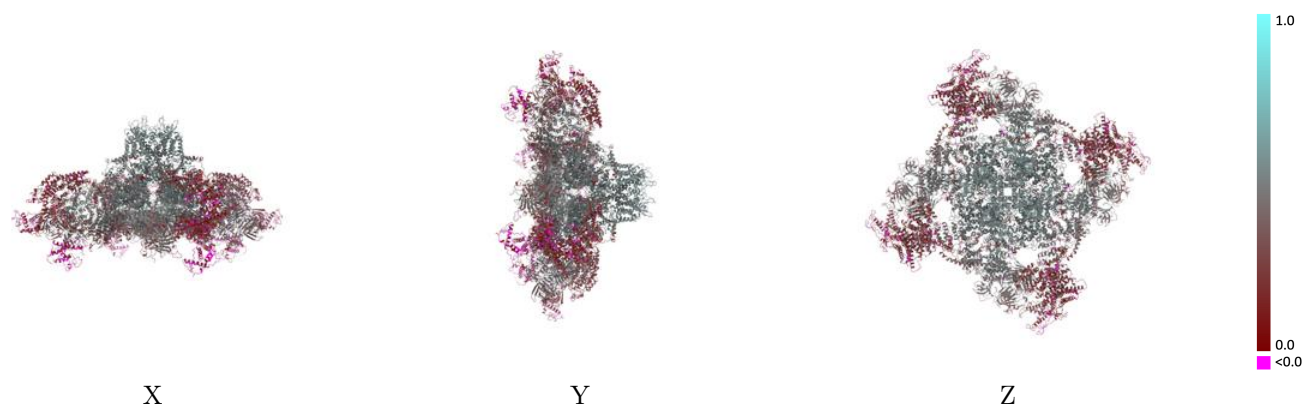
This section contains information regarding the fit between EMDB map EMD-47391 and PDB model 9E1E. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



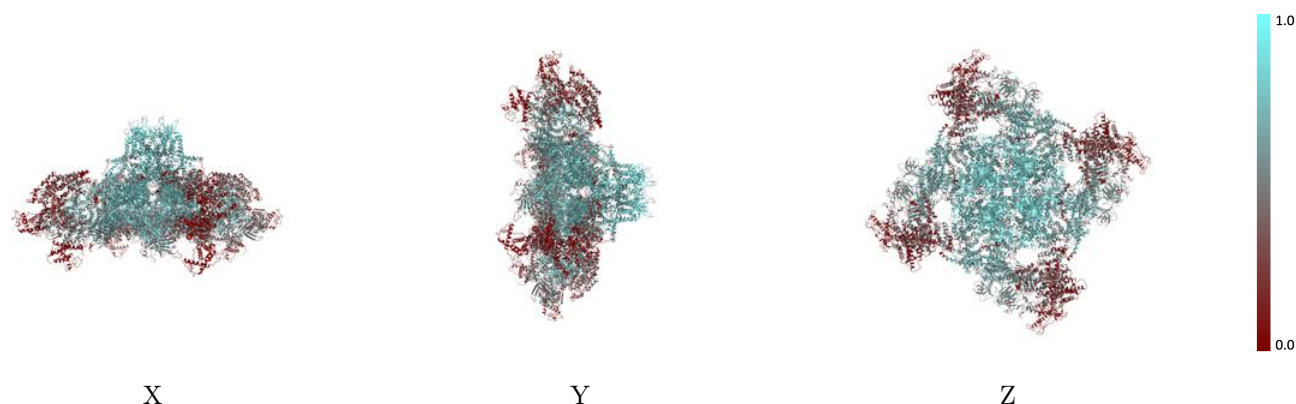
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



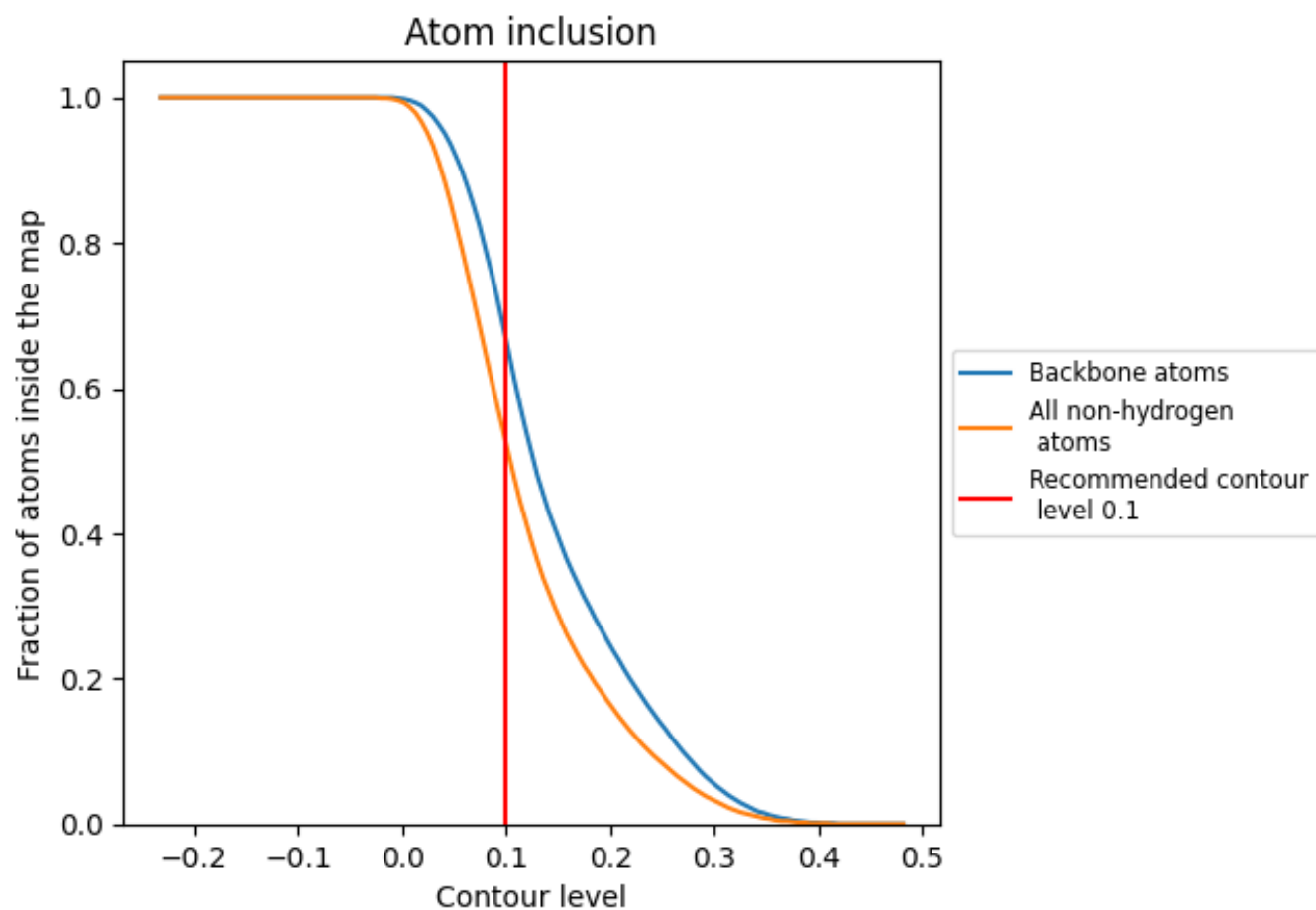
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0