



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 03:45 PM UTC

PDB ID : 8UXE / pdb_00008uxe
EMDB ID : EMD-42761
Title : Structure of PKA phosphorylated human RyR2-R420Q in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.53 Å(reported)
Based on initial model : 7UA5

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:

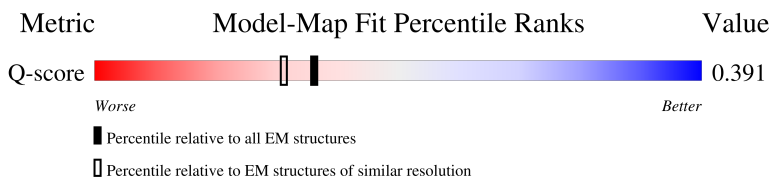
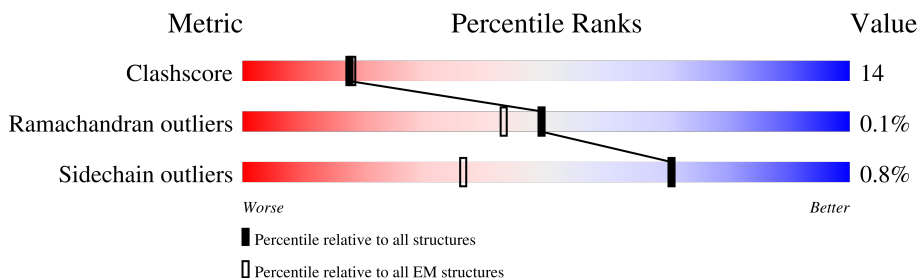
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.53 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	12947 (3.03 - 4.02)

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	E	108	 73% 24% ..
1	F	108	 74% 23% ..
1	G	108	 73% 24% ..
1	H	108	 74% 23% ..

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Mol	Chain	Length	Quality of chain
2	A	4967	
2	B	4967	
2	C	4967	
2	D	4967	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 138692 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
2	B	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
2	C	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
2	D	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		

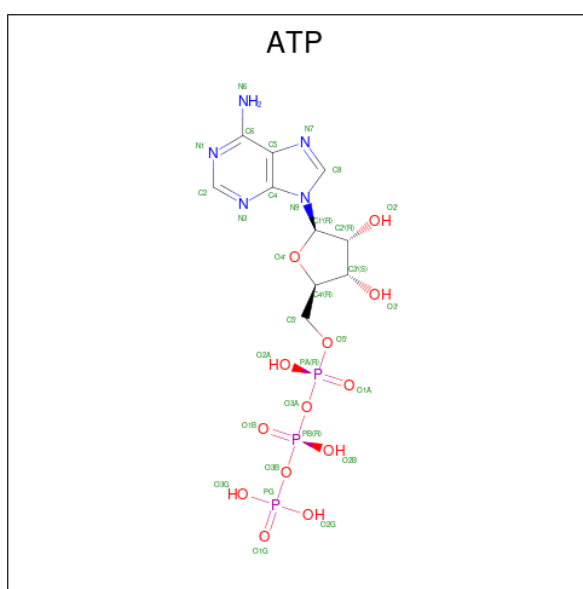
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	conflict	UNP Q92736
B	420	GLN	ARG	conflict	UNP Q92736
C	420	GLN	ARG	conflict	UNP Q92736
D	420	GLN	ARG	conflict	UNP Q92736

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



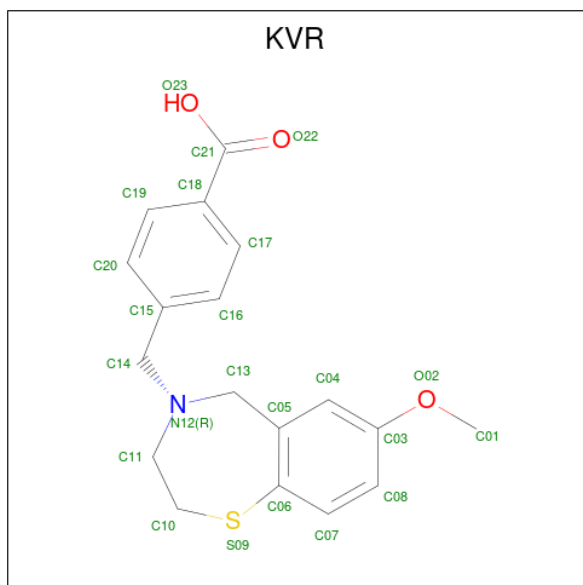
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

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

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: C₁₈H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).

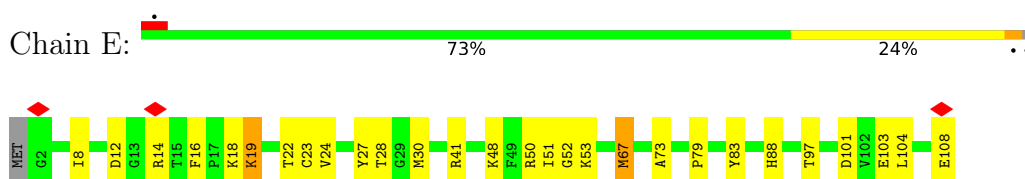


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	23	18	1	3	1	0
5	B	1	23	18	1	3	1	0
5	C	1	23	18	1	3	1	0
5	D	1	23	18	1	3	1	0

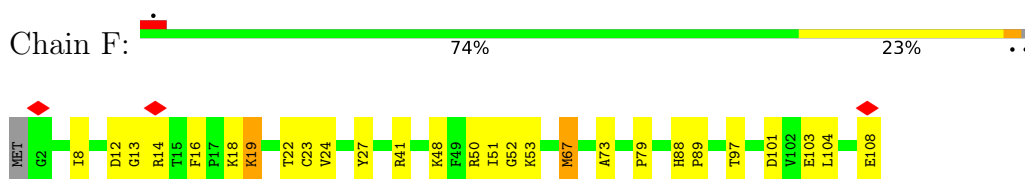
3 Residue-property plots

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.

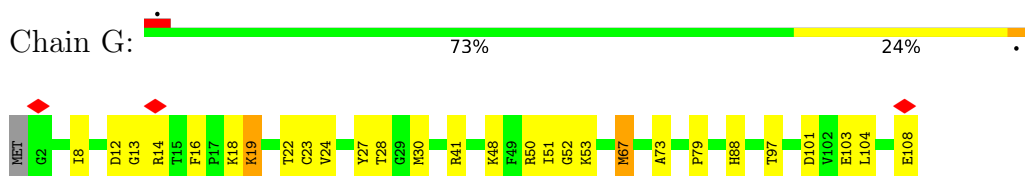
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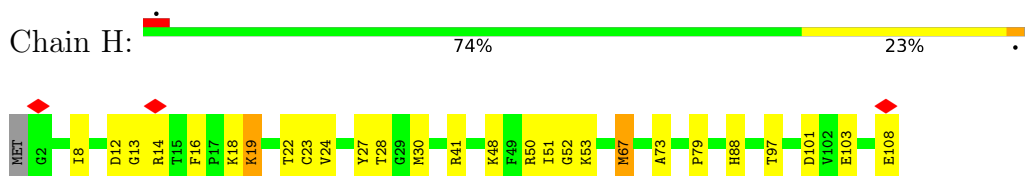
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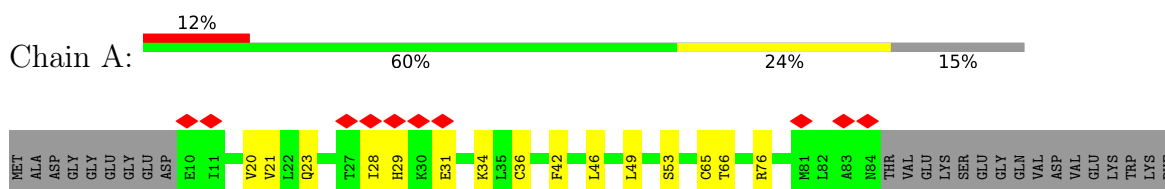
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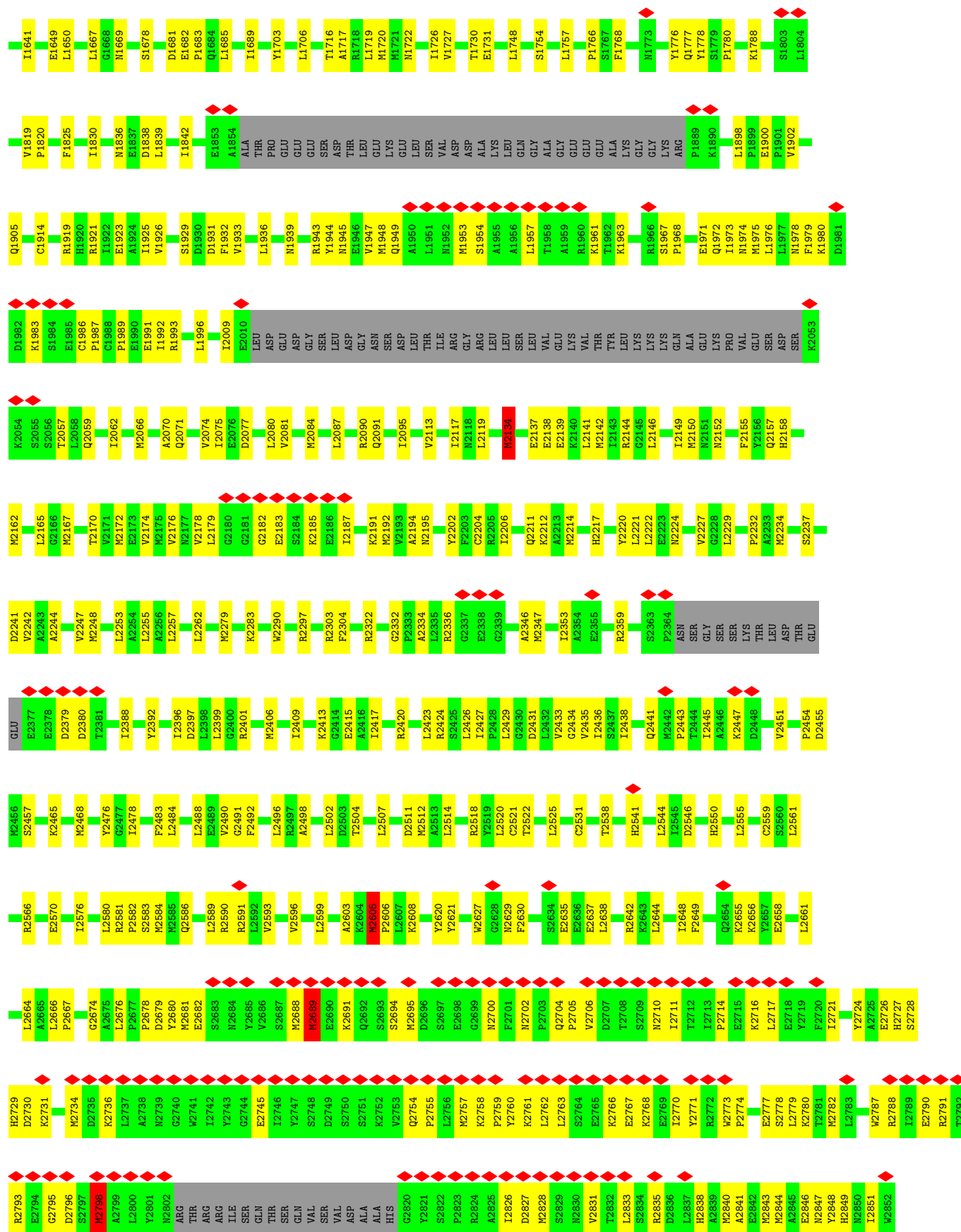
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 2

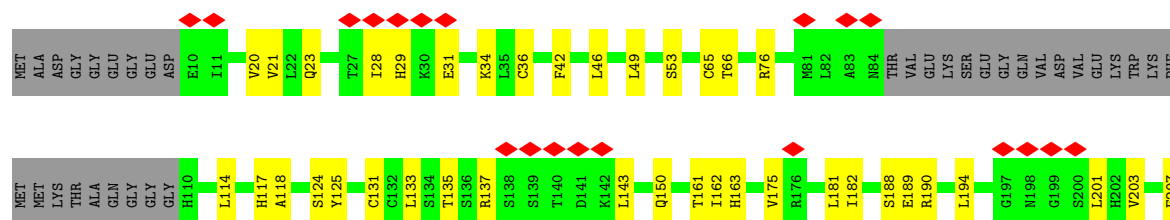








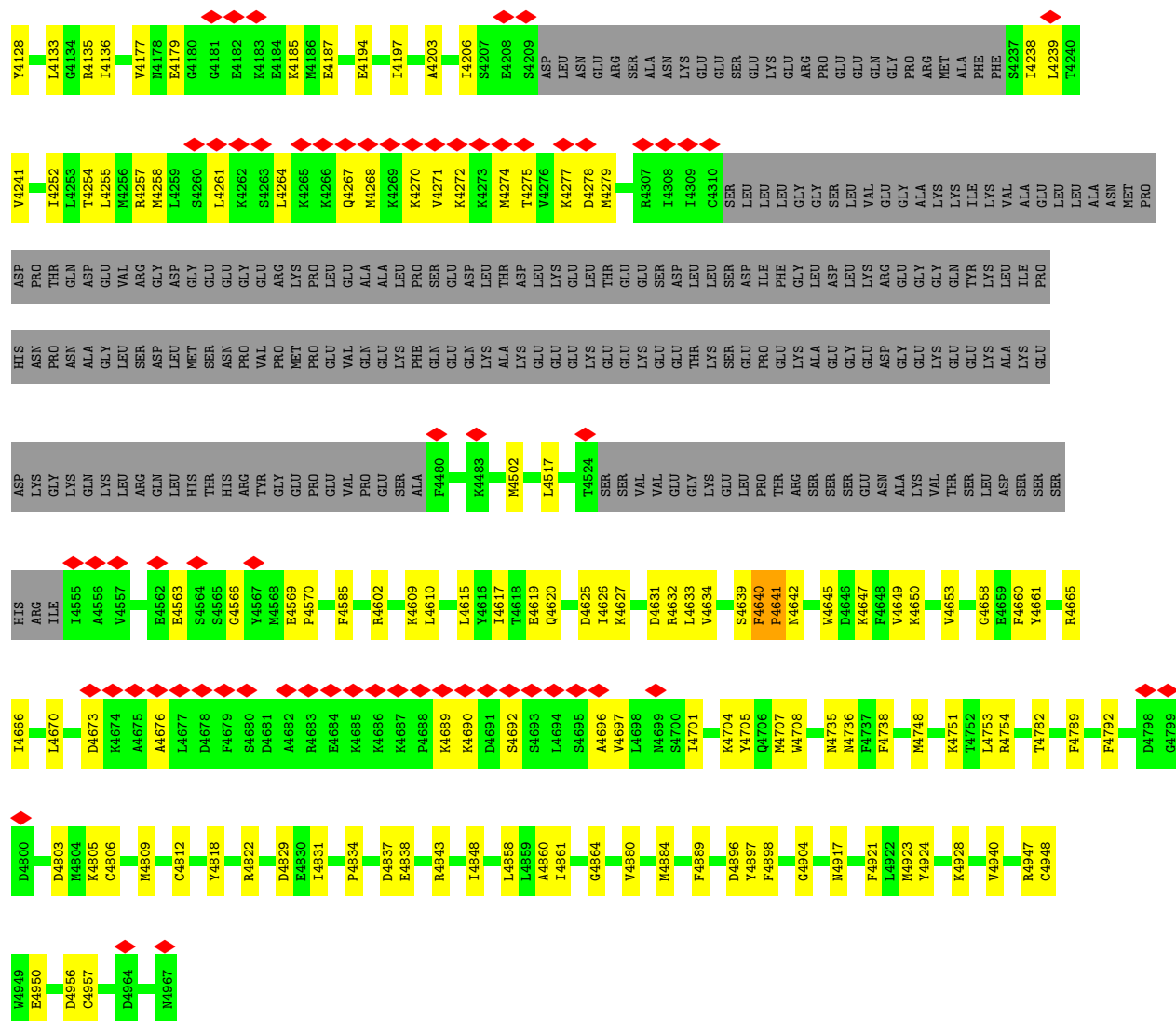
- Molecule 2: Ryanodine receptor 2



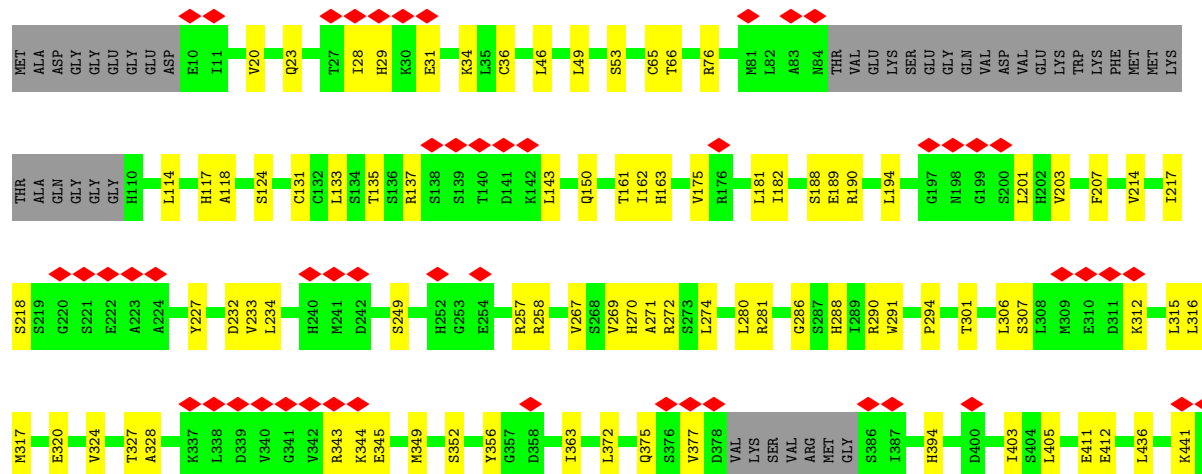


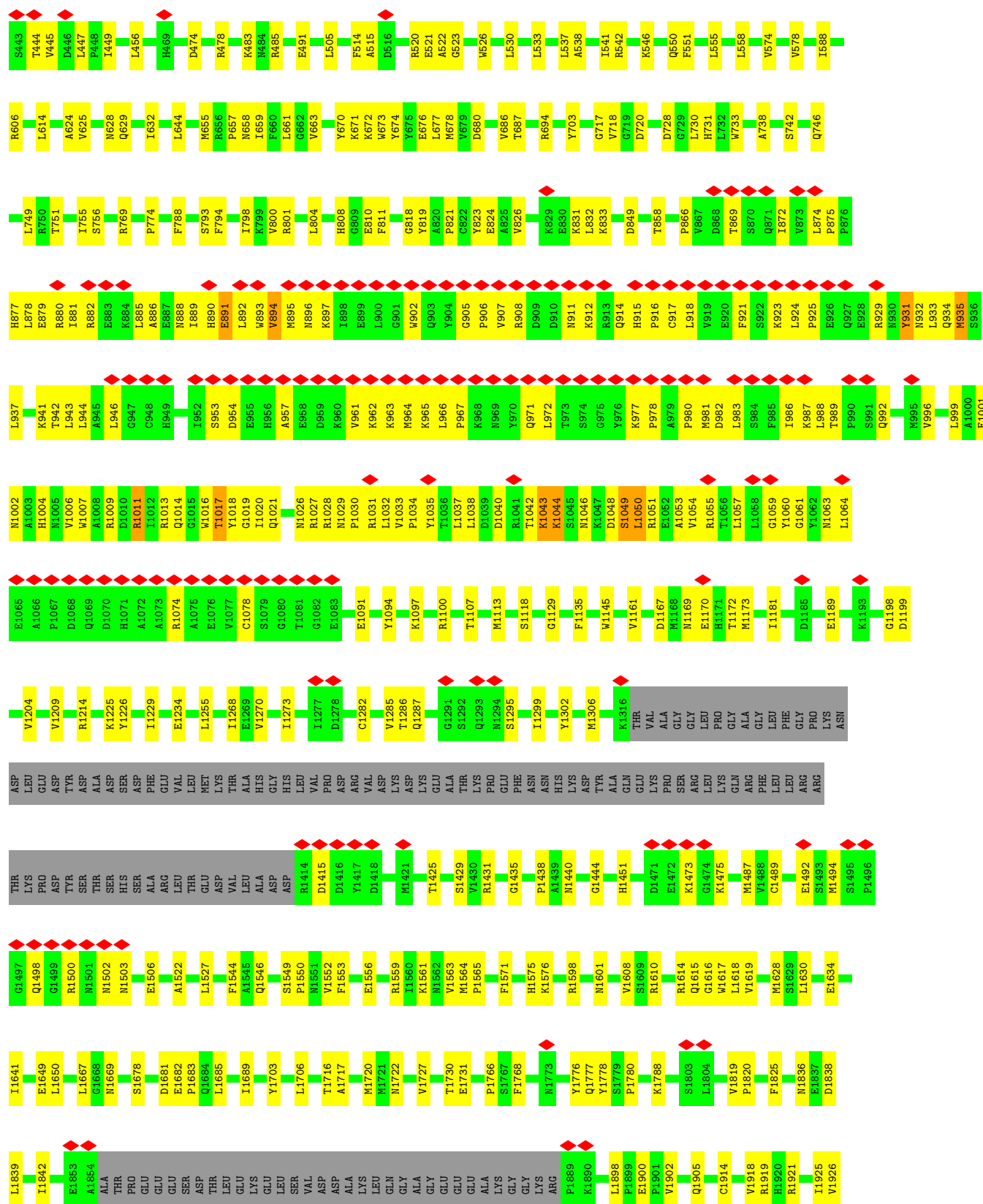






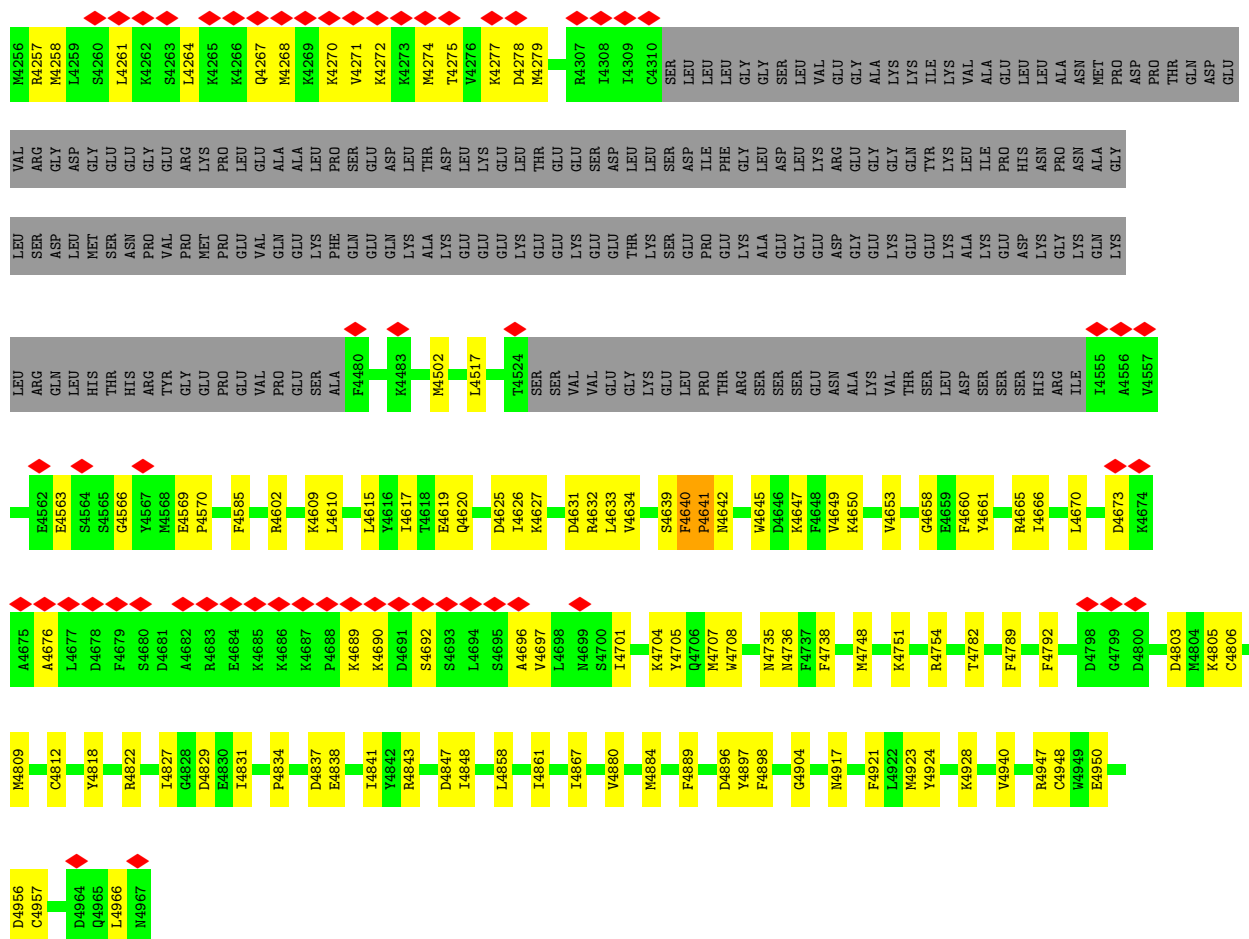
• Molecule 2: Ryanodine receptor 2



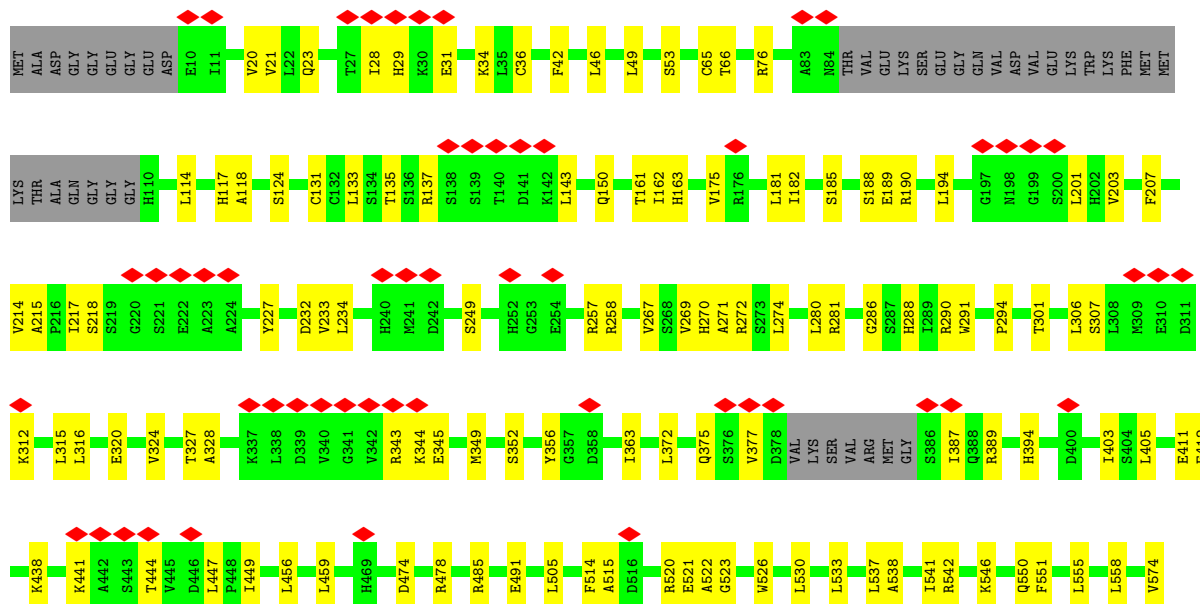


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Y2874	D2875	T2876	L2877	E2881	K2882	K2883	K2884	D2885	R2886	E2887	K2888	A2889	Q2890	D2891	I2892	L2893	K2894	F2895	L2896	Q2897	L2898	Y2901	A2902	V2903	S2904	R2905	G2906	F2907	D2908	K2909	L2910	E2911	L2912	D2913	T2914	P2915	S2916	L2917	R2920	F2921	A2922	Y2923	L2926	Q2927	L2928	L2929	I2930	R2931	Y2932	Y2933	H2937	I2940						
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V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438	Q2441	M2442	P2443	T2444	I2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477	I2478	F2483	L2484	L2488	E2489												
V2490	G2491	F2492	L2496	R2497	A2498	L2502	E2415	T2504	L2417	R2420	L2423	R2424	S2425	L2426	P2427	F2428	G2430	D2431	L2432	V2433	G2434	I2436	S2437	I2438																																		





• Molecule 2: Ryanodine receptor 2





L3014	V3015	R3016	R3017	R3018	L3021	F3022	G3023	N3024	D3025	A3026	T3027	S3028	I3029	H3034	L3035	G3037	Q3038	T3039	L3040	D3041	A3042	R3043	T3044	V3045	K3046	V3047	L3050	V3053	K3054	L3057	R3058	L3061	A3064	L3068	E3069	K3070	T3071	K3072	E3073	N3074	L3075	K3076	Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG									
Q2928	L2929	R3016	R3017	R3018	H2937	L2940	F2943	D2944	T2945	G2946	S2947	R2948	G2949	K2950	Q3038	Q2961	E2952	H2953	F2954	P2955	A2964	K2965	V2966	V2967	L2968	Y2974	F2975	K2976	H2978	R2979	L2980	Y2981	F2982	L2983	S2984	A2985	G2986	F2987	R2988	D2989	L2990	P2991	S2992	G2993	G2994	K3001	E3002	M3003	L3007	V3013									
S2862	K2863	G2864	G2865	G2866	G2867	H2868	P2869	L2870	L2871	Y2874	D2875	T2876	L2877	E2881	K2882	A2883	D2884	D2885	D2886	E2887	K2888	A2889	Q2890	D2891	L2892	L2893	K2894	F2895	L2896	Q2897	T2898	Y2901	A2902	V2903	S2904	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	S2916	I2917	R2920	F2921	A2922	Y2923	L2926	Q2927					
L2800	Y2801	H2802	ARG	THR	ARG	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	M2828	S2829	N2830	V2831	T2832	L2833	S2834	R2835	D2836	L2837	H2838	A2839	M2840	A2841	E2842	M2843	M2844	A2845	E2846	N2847	Y2848	H2849	H2850	L2851	K2854	K2855	H2858	E2859	L2860	E2861		
A2738	N2739	G2740	V2741	I2742	G2743	E2745	I2746	S2747	S2748	D2749	S2750	S2751	K2752	V2753	P2754	L2756	M2757	K2758	P2759	Y2760	K2761	L2762	L2763	S2764	E2765	E2766	E2767	K2768	E2769	I2770	Y2771	R2772	S2773	P2774	E2777	S2778	L2779	K2780	T2781	M2782	L2783	A2784	V2787	R2788	I2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	S2797	H2798	A2799				
L2600	Y2601	H2602	ARG	THR	ARG	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	ASP	ALA	ALA	HIS	G2620	Y2621	S2622	P2623	R2624	A2625	I2626	D2627	M2628	S2629	N2630	V2631	T2632	L2633	S2634	R2635	D2636	L2637	H2638	A2639	M2640	A2641	M2642	M2643	M2644	A2645	E2646	N2647	Y2648	H2649	Q2654	E2658	L2661	L2664	A2665	L2666	P2667	G2674	A2675	L2676
P2677	F2678	D2679	Y2680	M2681	Q2682	S2683	N2684	Y2685	L2686	R2687	S2688	N2689	R2690	L2691	L2692	V2693	V2696	L2699	A2603	K2604	K2605	P2606	L2607	K2608	K2619	Y2620	Y2621	G2626	G2628	N2629	G2630	E2635	E2636	E2637	R2642	K2643	L2644	I2648	F2649	Q2654	E2658	L2661	L2664	A2665	L2666	P2667	G2674	A2675	L2676										
K2581	P2582	S2583	M2584	Q2585	Q2586	L2589	R2590	L2591	L2592	V2593	V2596	L2599	A2603	K2604	K2605	P2606	L2607	K2608	K2619	Y2620	Y2621	G2626	G2628	N2629	G2630	E2635	E2636	E2637	R2642	K2643	L2644	I2648	F2649	Q2654	E2658	L2661	L2664	A2665	L2666	P2667	G2674	A2675	L2676																
F2478	F2483	L2484	L2488	E2489	V2490	G2491	F2492	L2496	L2497	A2498	L2502	D2503	T2504	L2507	D2511	M2512	A2513	L2514	L2520	G2521	L2525	C2531	T2538	H2541	L2544	D2545	H2560	Y2563	R2564	L2565	K2567	G2568	S2569	L2571	R2572	L2573	P2714	E2715	K2716	L2717	E2718	Y2719	F2720	I2721	Y2724	A2725	E2726	H2727	S2728	H2729	D2730	K2731	H2732	S2733	N2734	D2735	K2736	L2737	
L2388	Y2392	I2396	L2397	L2398	L2399	G2400	R2401	M2406	I2409	K2413	G2414	E2415	A2416	L2417	L2423	R2424	S2425	L2426	I2427	F2428	L2429	G2430	L2432	V2433	G2434	I2436	S2437	L2438	Q2441	M2442	P2443	T2444	L2445	A2446	K2447	D2448	V2451	P2454	D2455	M2456	S2457	K2465	M2468	Y2476	G2477														
L2253	A2254	L2255	A2256	L2257	L2262	M2279	K2283	G2284	Y2285	W2290	R2297	E2298	R2303	F2304	R2322	G2332	P2333	A2334	L2335	G2337	A2346	M2347	I2353	A2354	E2355	R2359	S2363	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	D2378	D2379	D2380	T2381	I2382														
T2057	L2058	Q2059	I2062	M2066	A2070	Q2071	V2074	I2075	E2076	D2077	L2080	V2081	M2084	L2087	Q2090	Q2091	V2113	I2117	N2118	L2119	M2134	E2137	E2138	E2139	K2140	L2141	M2142	I2143	R2144	G2145	L2146	I2149	M2150	N2151	N2152	F2155	Y2156	Q2157	H2158	M2162	M2167	T2170																	
V2171	M2172	E2173	V2174	M2175	V2176	M2177	V2178	L2179	G2180	G2181	G2182	E2183	S2184	E2185	E2186	I2187	K2191	M2192	V2193	A2194	N2195	Y2202	F2203	R2204	K2205	I2206	Q2211	A2213	M2214	H2217	Y2220	L2221	N2224	V2227	G2228	L2229	F2232	A2233	M2234	S2237	D2241	V2242	A2243	A2244	V2247	M2248													
L2253	A2254	L2255	A2256	L2257	L2262	M2279	K2283	G2284	Y2285	W2290	R2297	E2298	R2303	F2304	R2322	G2332	P2333	A2334	L2335	G2337	A2346	M2347	I2353	A2354	E2355	R2359	S2363	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	E2377	D2378	D2379	D2380	T2381	I2382														



F4921	K4751	K4649	GLU	GLY	LEU	LYS
L4922	R4754	K4650	ASN	GLU	LYS	ILE
M4923			ALA	ASP	ARG	LYS
Y4924	T4782	V4653	LYS	GLY	GLU	VAL
L4925			VAL	GLU	GLY	ALA
	F4789	G4658	THR	LYS	GLU	GLU
		F4659	SER	GLU	LEU	LEU
	F4792	F4660	LEU	GLU	TYR	LEU
		Y4661	ASP	LYS	ALA	ASP
			SER	LYS	ASN	MET
	D4798	R4665	SER	GLU	ILE	PRO
G4799		I4666	SER	ASP	LEU	PRO
D4800			HIS	LYS	HIS	ASP
		L4670	ARG	LYS	ASN	PRO
			ILE	GLY	PRO	THR
	D4673	I4555	LYS	GLY	ASN	GLN
	K4674	A4556	GLN	LYS	ALA	ASP
	A4675	V4557	LYS	GLN	GLY	GLU
	A4676		LEU	LEU	VAL	VAL
	L4677	E4562	ARG	ARG	SER	ARG
	D4678	E4563	GLN	GLN	ASP	GLY
	F4679	S4564	LEU	HIS	LEU	ASP
	S4680		THR	THR	MET	GLY
	D4681	Y4567	HIS	HIS	SER	GLU
	A4682	M4568	ARG	ARG	ASN	GLU
	R4683	E4569	TYR	TYR	PRO	GLY
	F4684	P4570	GLY	GLY	VAL	GLU
	K4685	F4585	PRO	PRO	MET	LYS
	K4686		GLU	GLU	PRO	PRO
	K4687	R4602	VAL	VAL	GLU	LEU
	P4688	K4609	PRO	PRO	ALA	GLU
	K4689	L4610	GLU	GLU	GLU	ALA
	K4690	L4615	SER	ALA	LYS	LEU
	D4691	Y4616	ALA	F4480	GLN	SER
	S4692	I4617	LYS	K4483	GLU	GLU
	L4694	E4619	LEU	M4502	ASP	ASP
	S4695	Q4620	THR	L4517	LYS	THR
	A4696		ALA		LYS	ASP
	V4697	D4625	GLU	T4524	GLU	LEU
	L4698	I4626	LYS	SER	GLU	GLU
	M4699	K4627	THR	VAL	LYS	THR
	S4700		SER	GLU	GLU	GLU
	I4701	D4631	LYS	VAL	LYS	GLU
	K4704	R4632	GLU	GLY	GLU	ASP
	Y4705	L4633	LYS	LYS	THR	LEU
	Q4706	V4634	GLU	LYS	LYS	LEU
	M4707	S4639	THR	GLU	SER	SER
	V4708	F4640	ARG	PRO	GLU	ASP
		P4641	THR	THR	PRO	ILE
		M4642	ARG	ARG	GLU	PHE
	M4726	V4645	SER	SER	LYS	GLY
	M4735	D4646	SER	SER	ALA	LEU
	M4736	K4647	SER	SER	ALA	ASP
	F4737	F4648	SER	SER		
	F4738					
	M4748					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.660	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	426.752, 426.752, 426.752	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8335, 0.8335, 0.8335	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.21	0/834	0.44	0/1123
1	F	0.21	0/834	0.44	0/1123
1	G	0.21	0/834	0.44	0/1123
1	H	0.21	0/834	0.44	0/1123
2	A	0.19	0/34509	0.44	6/46612 (0.0%)
2	B	0.20	0/34509	0.44	6/46612 (0.0%)
2	C	0.20	0/34509	0.44	6/46612 (0.0%)
2	D	0.20	0/34509	0.44	6/46612 (0.0%)
All	All	0.20	0/141372	0.44	24/190940 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3262	GLU	CA-CB-CG	7.61	129.31	114.10
2	B	3262	GLU	CA-CB-CG	7.60	129.30	114.10
2	D	3262	GLU	CA-CB-CG	7.60	129.30	114.10
2	C	3262	GLU	CA-CB-CG	7.58	129.25	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2605	MET	CB-CG-SD	6.62	132.57	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	4640	PHE	Peptide
2	B	4640	PHE	Peptide
2	C	4640	PHE	Peptide
2	D	4640	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	818	0	821	21	0
1	F	818	0	821	22	0
1	G	818	0	821	19	0
1	H	818	0	821	18	0
2	A	33769	0	33450	938	0
2	B	33769	0	33450	922	0
2	C	33769	0	33450	925	0
2	D	33769	0	33450	927	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	3	0
4	B	62	0	24	3	0
4	C	62	0	24	3	0
4	D	62	0	24	3	0
5	A	23	0	0	2	0
5	B	23	0	0	2	0
5	C	23	0	0	2	0
5	D	23	0	0	2	0
All	All	138692	0	137180	3736	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 14.

The worst 5 of 3736 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1031:ARG:HH21	2:B:1038:LEU:HD11	1.24	1.02
2:A:1031:ARG:HH21	2:A:1038:LEU:HD11	1.24	1.02
2:D:1031:ARG:HH21	2:D:1038:LEU:HD11	1.24	1.00
2:C:1031:ARG:HH21	2:C:1038:LEU:HD11	1.24	1.00
2:C:894:VAL:HG21	2:C:972:LEU:HD22	1.48	0.95

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	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	48	79
2	B	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	48	79
2	C	4198/4967 (84%)	4061 (97%)	132 (3%)	5 (0%)	48	79
2	D	4198/4967 (84%)	4060 (97%)	133 (3%)	5 (0%)	48	79
All	All	17212/20300 (85%)	16655 (97%)	537 (3%)	20 (0%)	49	79

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3927	PRO

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Mol	Chain	Res	Type
2	A	4641	PRO
2	B	3927	PRO
2	B	4641	PRO
2	C	3927	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/89 (99%)	86 (98%)	2 (2%)	44	64
1	F	88/89 (99%)	86 (98%)	2 (2%)	44	64
1	G	88/89 (99%)	86 (98%)	2 (2%)	44	64
1	H	88/89 (99%)	86 (98%)	2 (2%)	44	64
2	A	3708/4358 (85%)	3680 (99%)	28 (1%)	73	77
2	B	3708/4358 (85%)	3680 (99%)	28 (1%)	73	77
2	C	3708/4358 (85%)	3680 (99%)	28 (1%)	73	77
2	D	3708/4358 (85%)	3680 (99%)	28 (1%)	73	77
All	All	15184/17788 (85%)	15064 (99%)	120 (1%)	70	77

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2689	MET
2	D	2134	MET
2	C	935	MET
2	D	1050	LEU
2	D	3819	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	3115	HIS

Continued on next page...

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Mol	Chain	Res	Type
2	D	896	ASN
2	C	3770	ASN
2	C	4579	HIS
2	D	1917	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, 4 are monoatomic - leaving 12 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	$\# Z > 2$
5	KVR	B	5004	-	24,25,25	0.49	0	31,34,34	0.82	2 (6%)
4	ATP	A	5003	-	32,33,33	0.54	0	48,52,52	0.57	0
4	ATP	C	5003	-	32,33,33	0.54	0	48,52,52	0.57	0
5	KVR	C	5004	-	24,25,25	0.52	0	31,34,34	0.83	2 (6%)
5	KVR	D	5004	-	24,25,25	0.50	0	31,34,34	0.83	2 (6%)
5	KVR	A	5004	-	24,25,25	0.51	0	31,34,34	0.83	2 (6%)
4	ATP	A	5002	-	32,33,33	0.31	0	48,52,52	0.37	0
4	ATP	D	5003	-	32,33,33	0.56	0	48,52,52	0.57	0
4	ATP	B	5002	-	32,33,33	0.31	0	48,52,52	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	D	5002	-	32,33,33	0.31	0	48,52,52	0.37	0
4	ATP	C	5002	-	32,33,33	0.32	0	48,52,52	0.37	0
4	ATP	B	5003	-	32,33,33	0.55	0	48,52,52	0.57	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
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	A	5003	-	-	6/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	6/22/38/38	0/3/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	A	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	A	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	6/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5004	KVR	C10-S09-C06	3.24	107.30	102.71
5	D	5004	KVR	C10-S09-C06	3.23	107.28	102.71
5	A	5004	KVR	C10-S09-C06	3.22	107.28	102.71
5	B	5004	KVR	C10-S09-C06	3.18	107.21	102.71
5	B	5004	KVR	C14-N12-C11	2.12	114.54	111.09

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O2A

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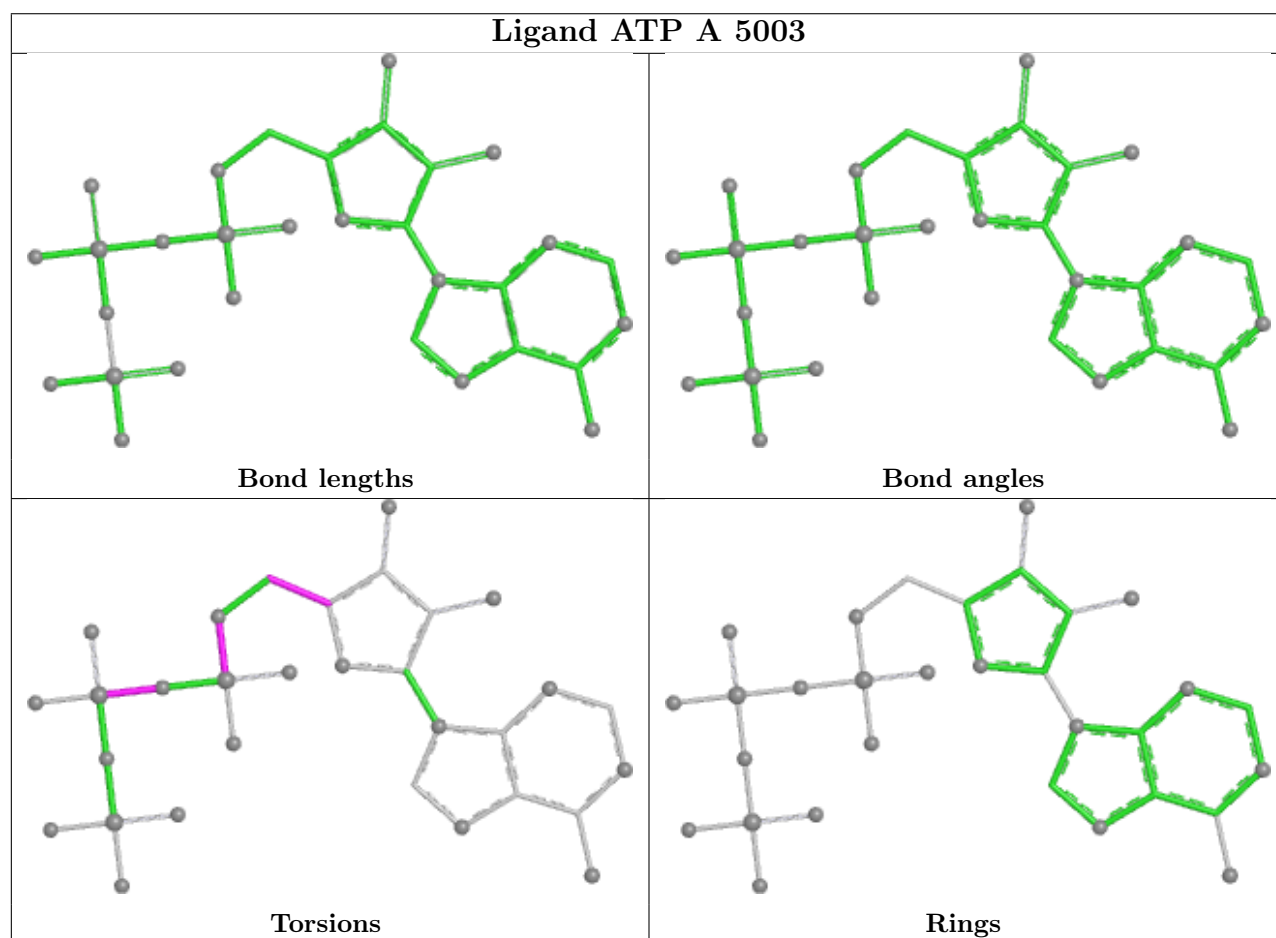
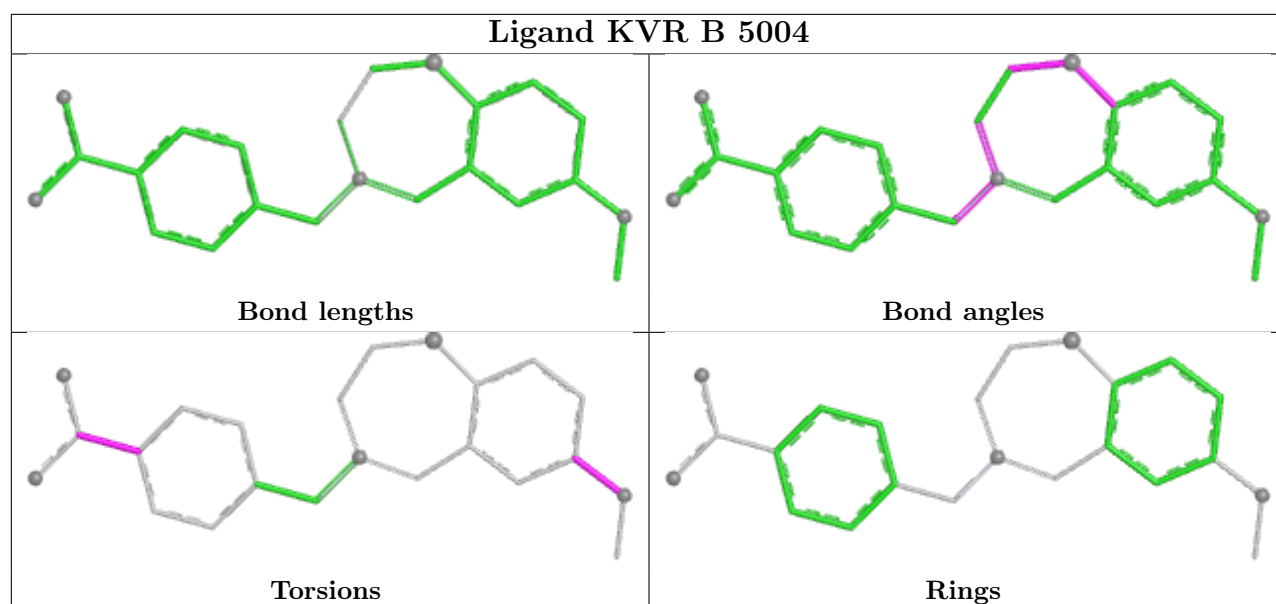
Mol	Chain	Res	Type	Atoms
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	C5'-O5'-PA-O2A

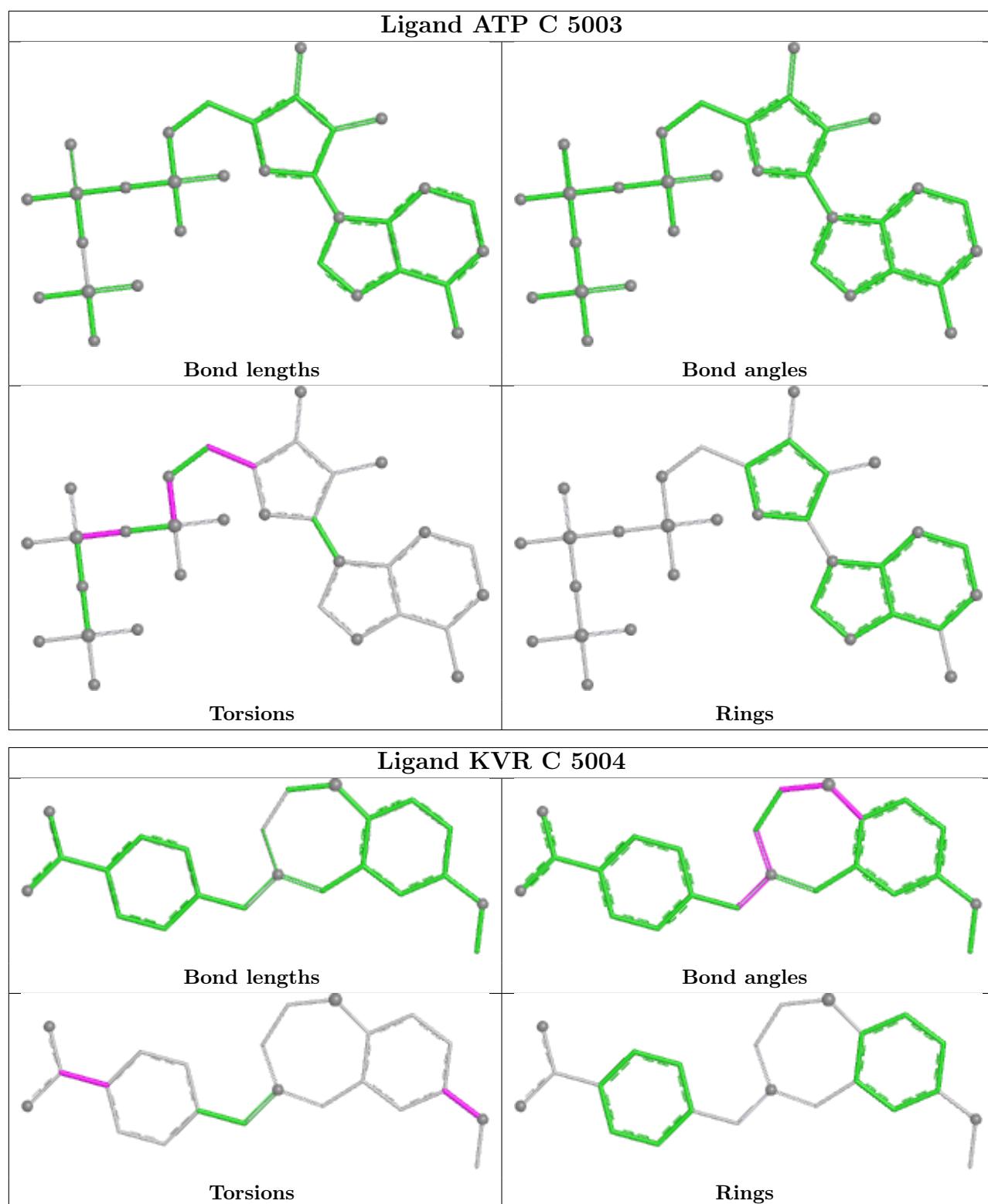
There are no ring outliers.

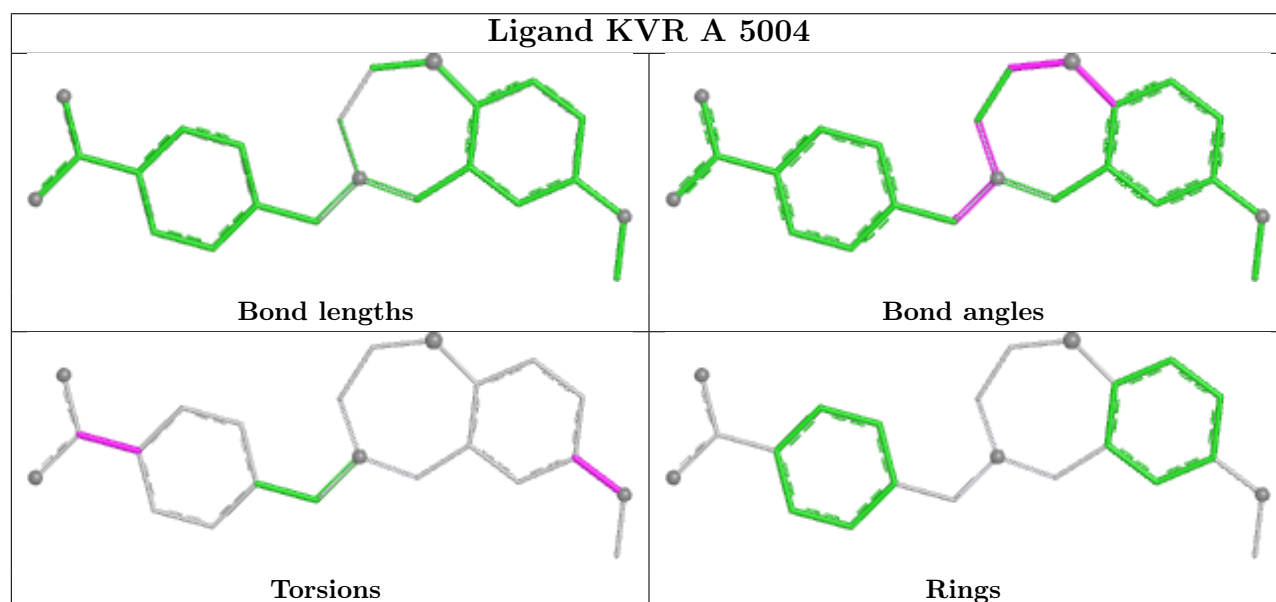
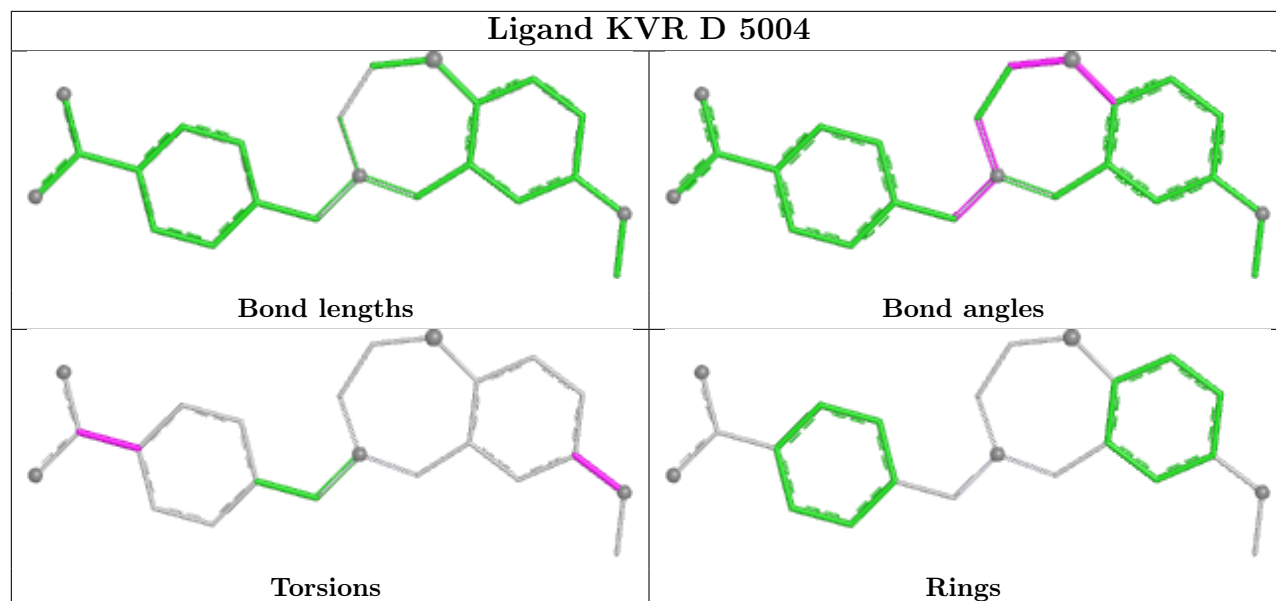
8 monomers are involved in 16 short contacts:

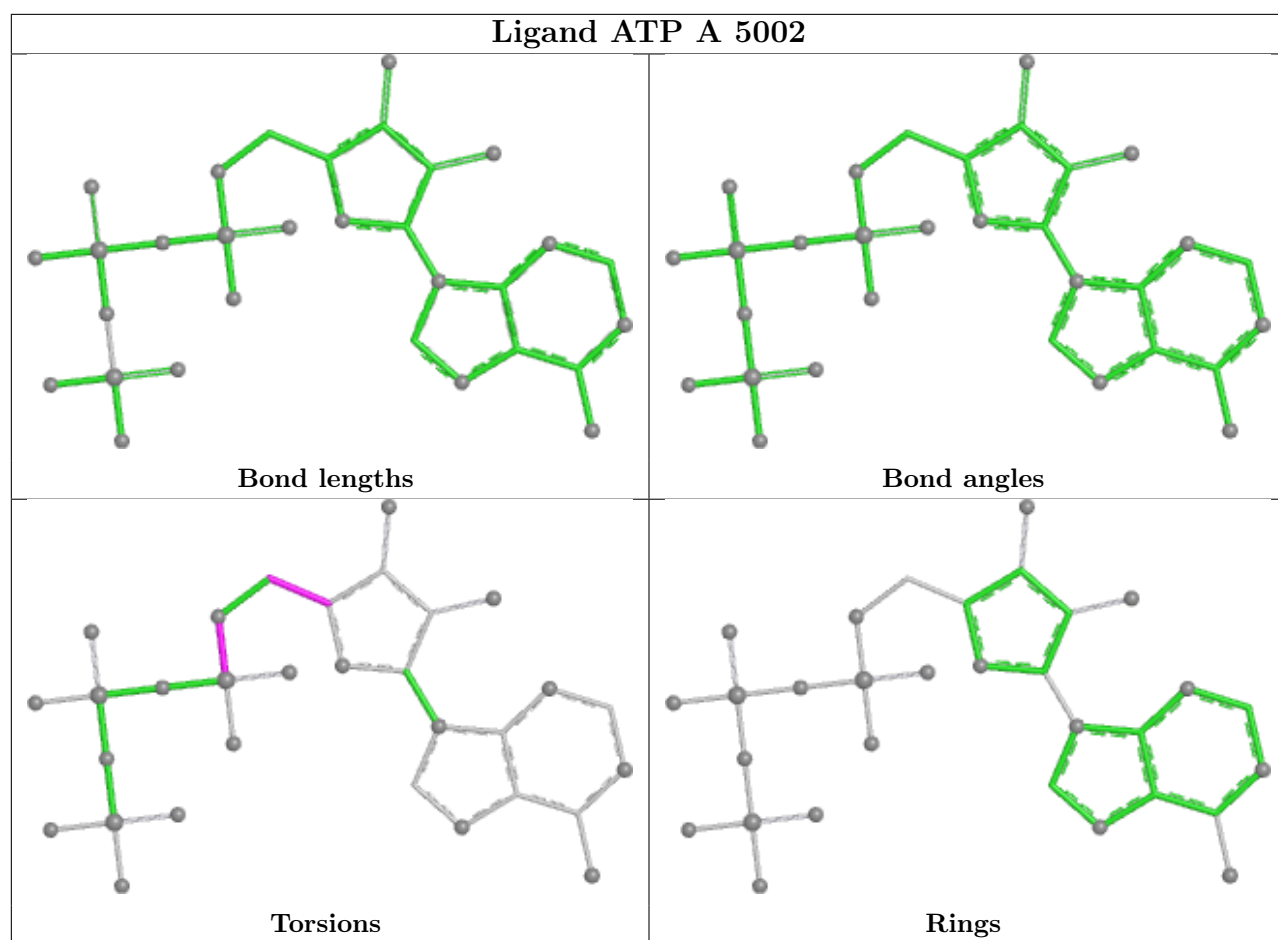
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5004	KVR	2	0
4	A	5003	ATP	3	0
4	C	5003	ATP	3	0
5	C	5004	KVR	2	0
5	D	5004	KVR	2	0
5	A	5004	KVR	2	0
4	D	5003	ATP	3	0
4	B	5003	ATP	3	0

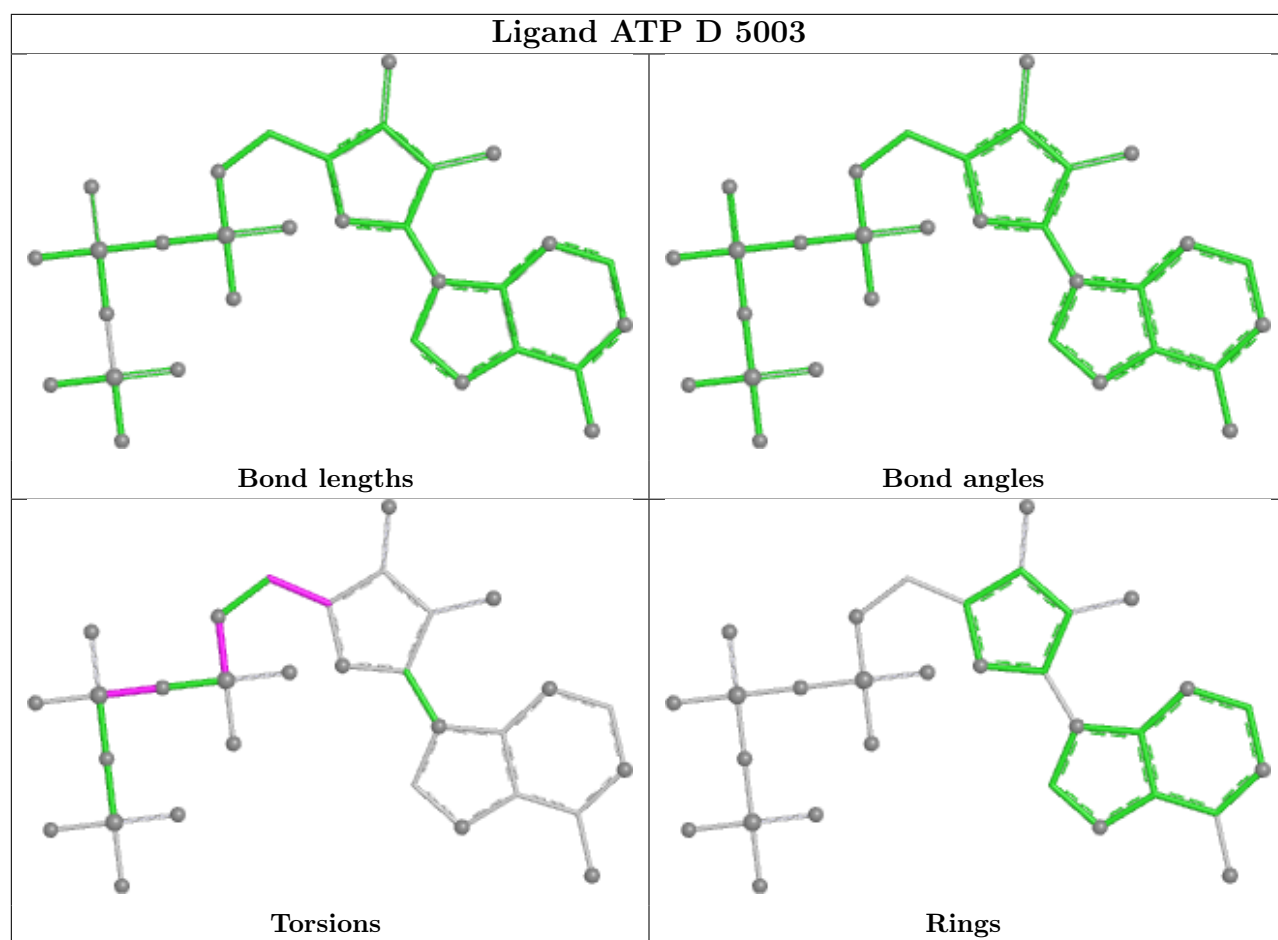
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

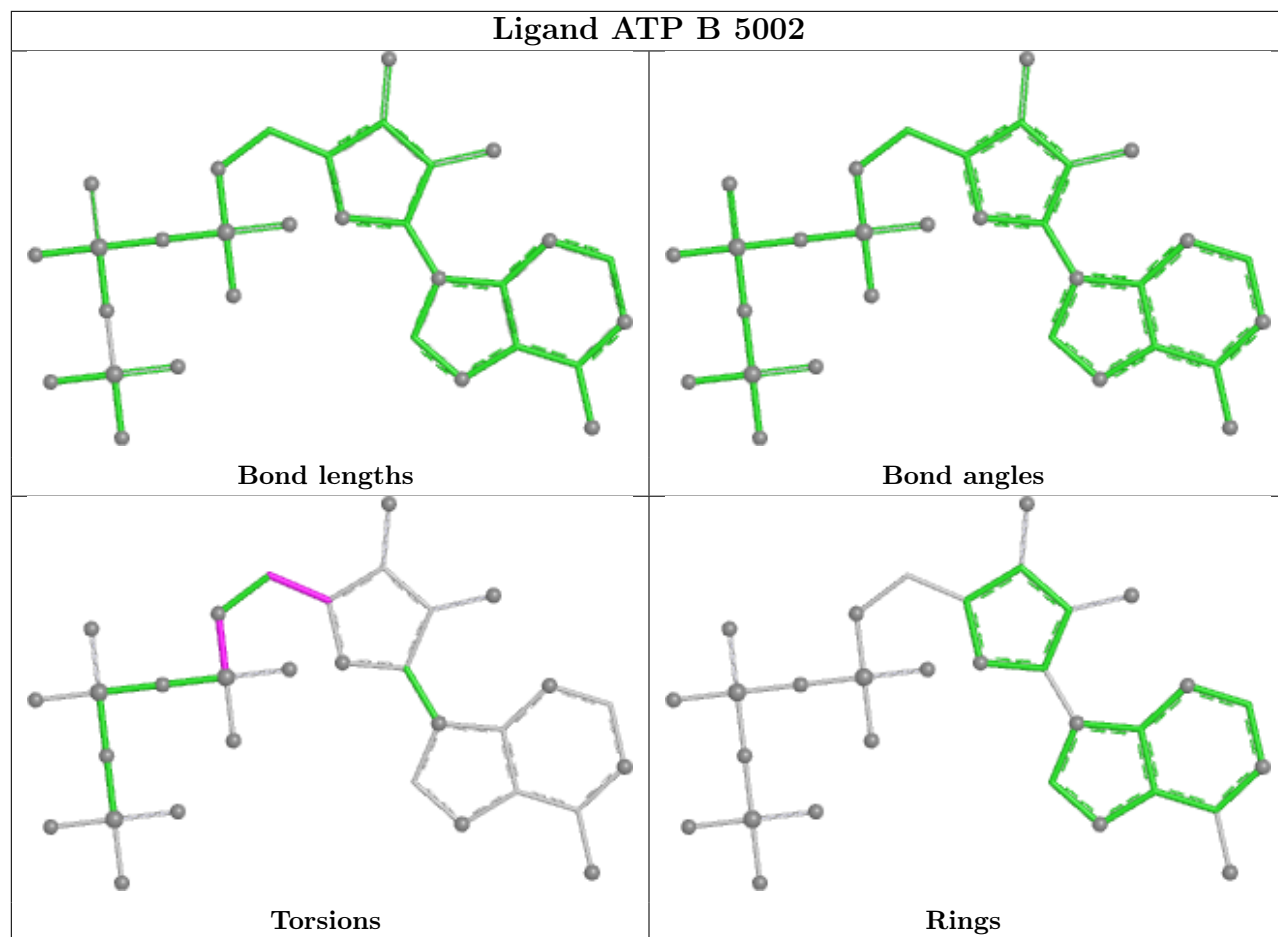


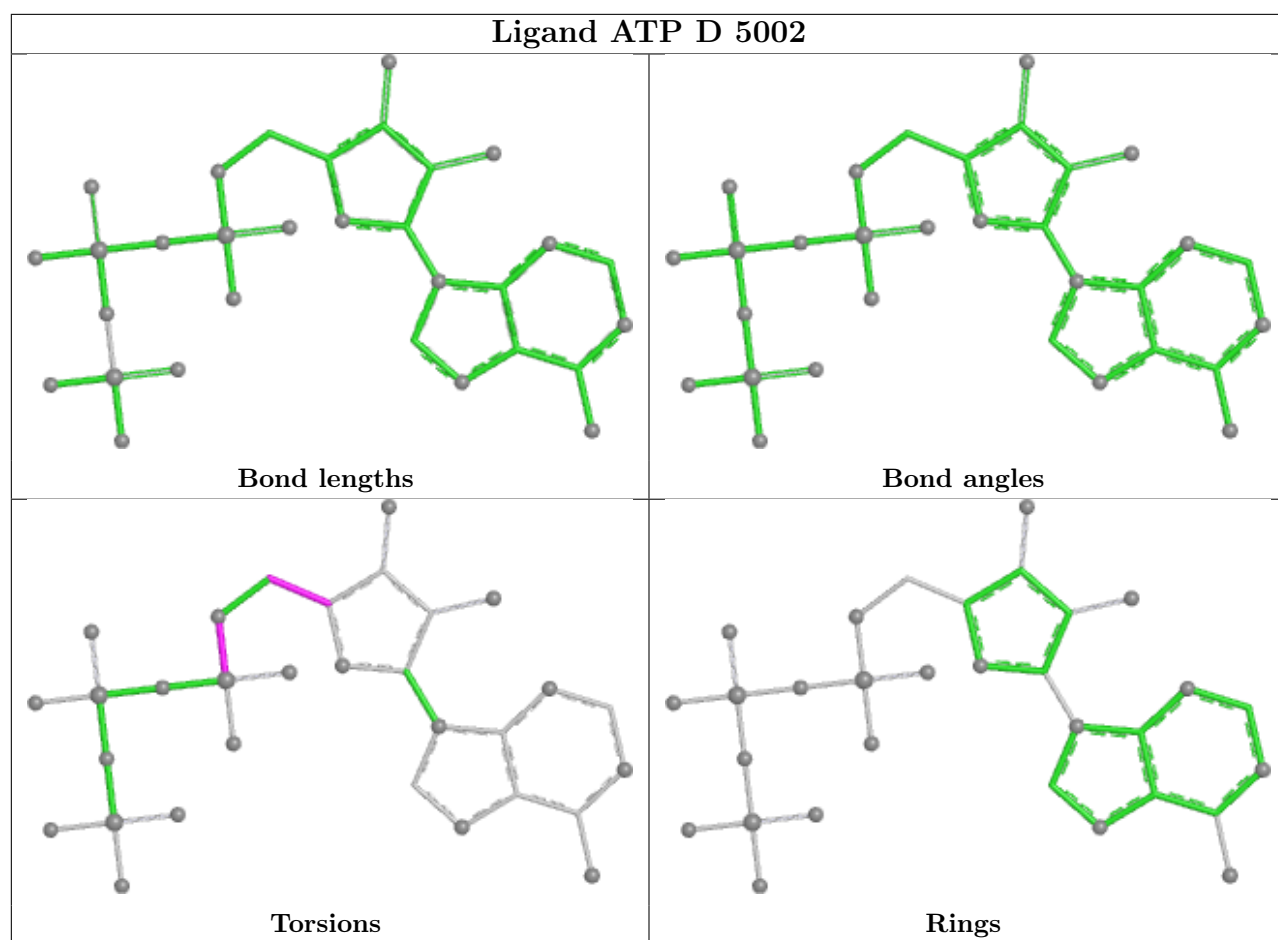


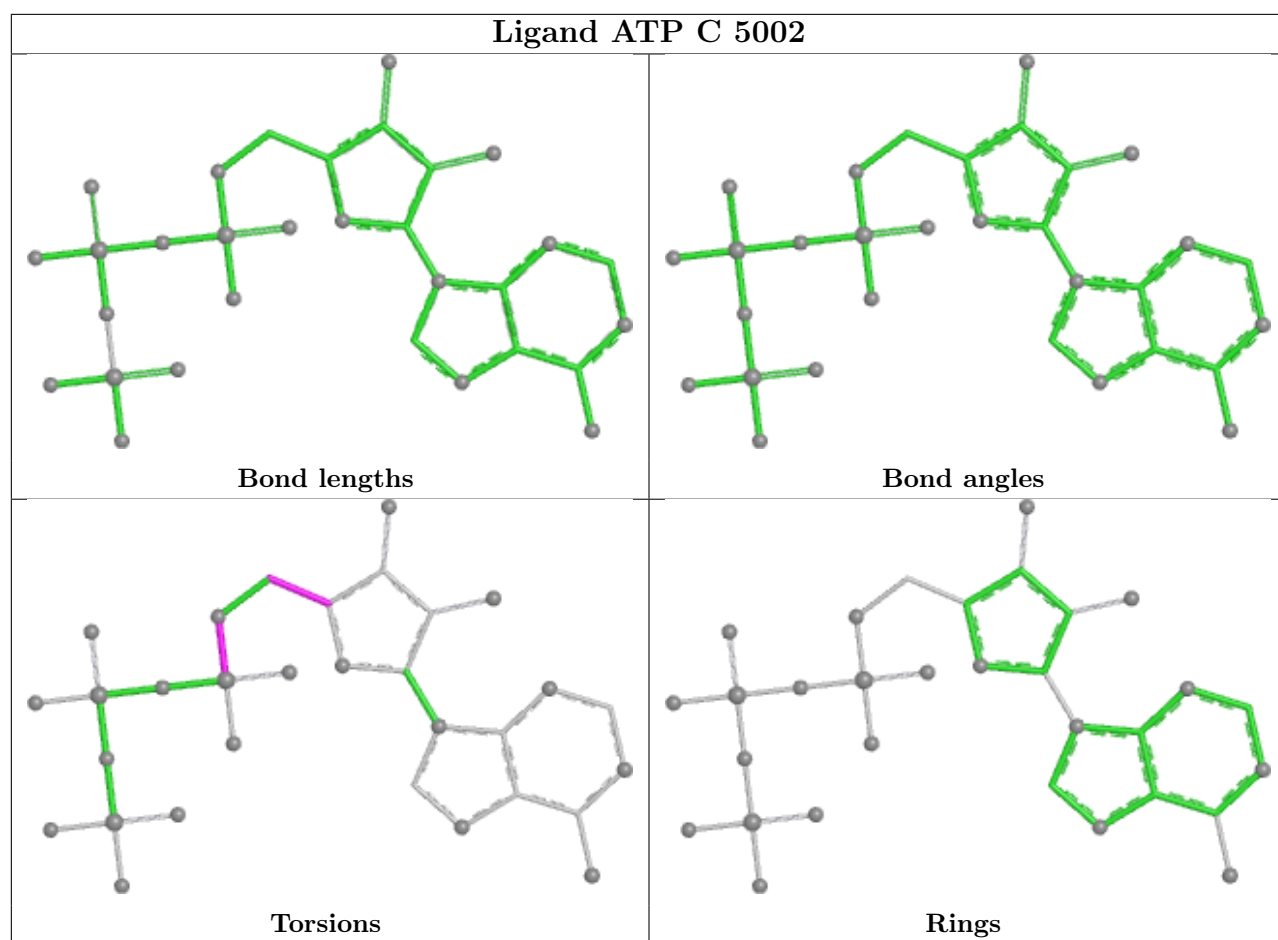


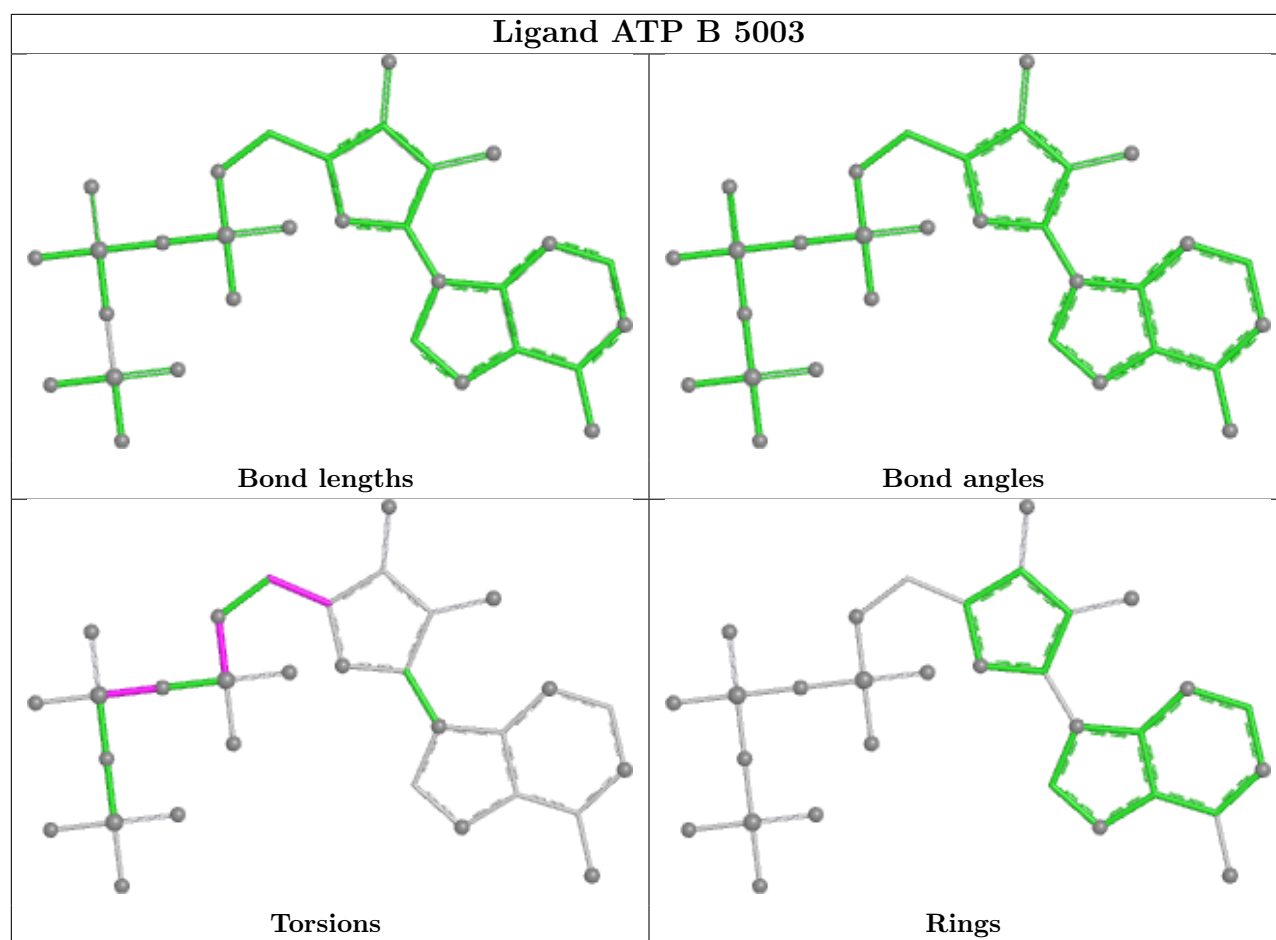












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

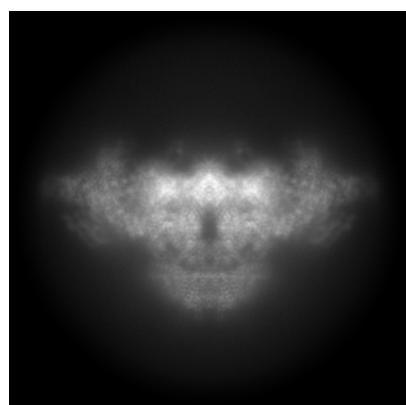
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42761. These allow visual inspection of the internal detail of the map and identification of artifacts.

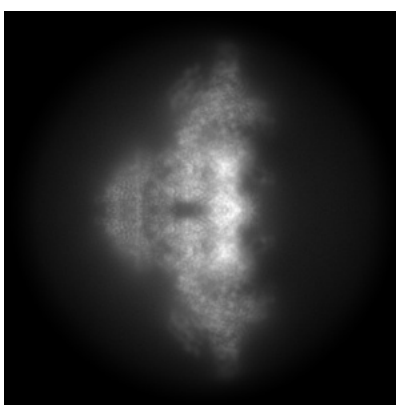
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

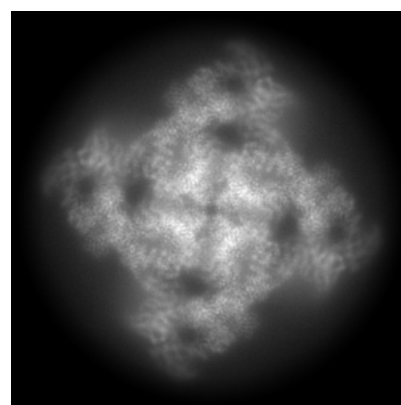
6.1.1 Primary map



X



Y

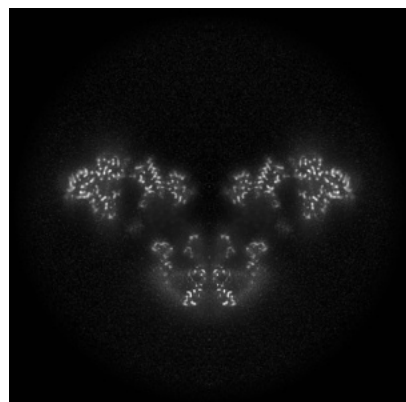


Z

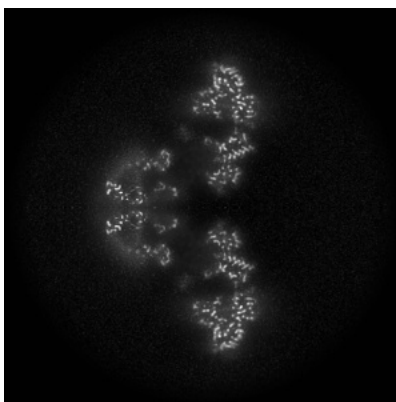
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

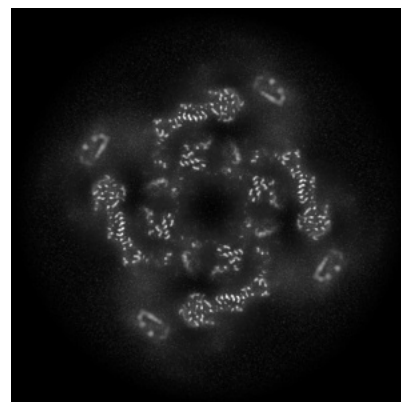
6.2.1 Primary map



X Index: 256



Y Index: 256

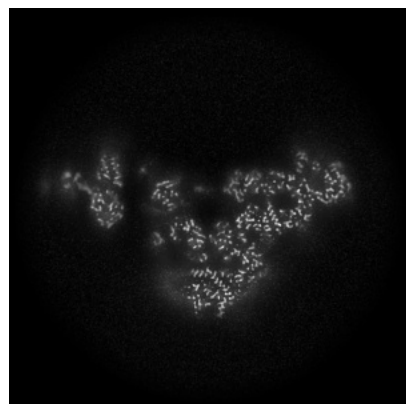


Z Index: 256

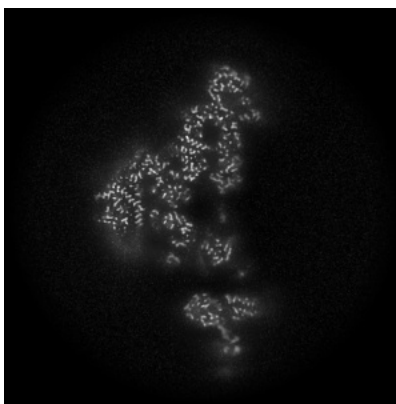
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

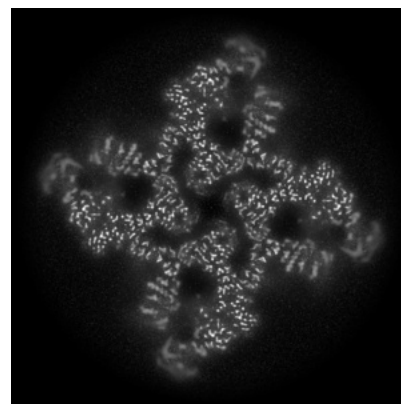
6.3.1 Primary map



X Index: 238



Y Index: 274



Z Index: 282

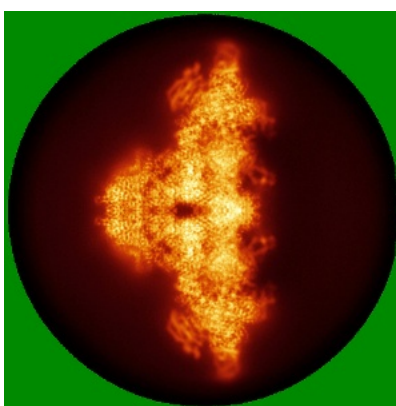
The images above show the largest variance slices of the map in three orthogonal directions.

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

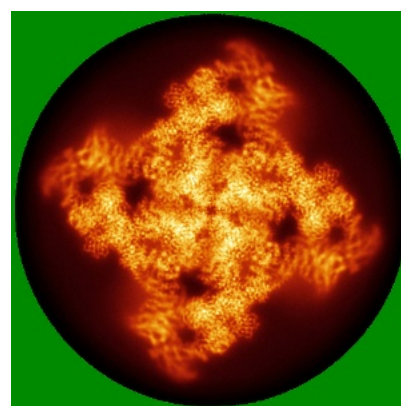
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

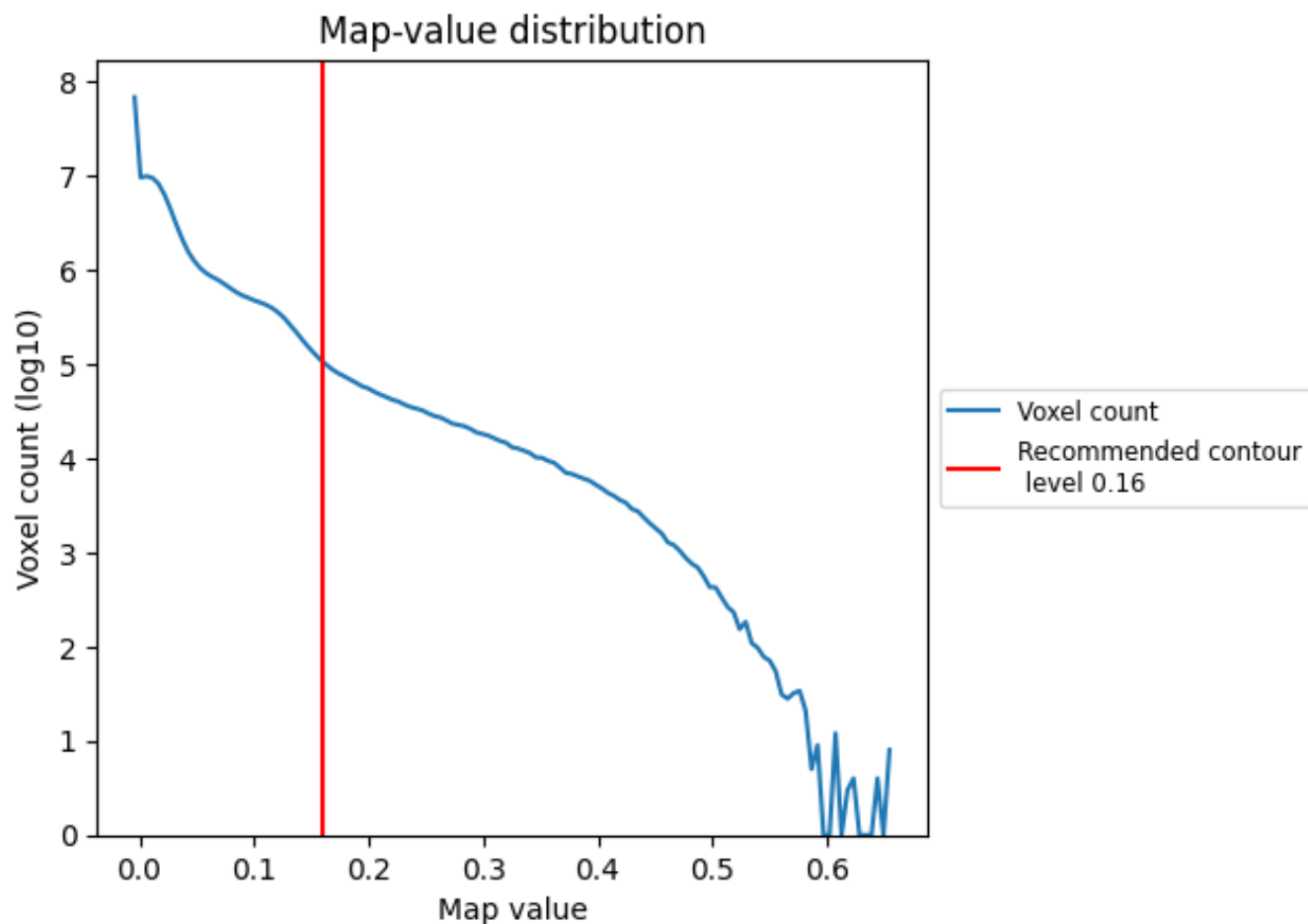
6.6 Mask visualisation

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

7 Map analysis [i](#)

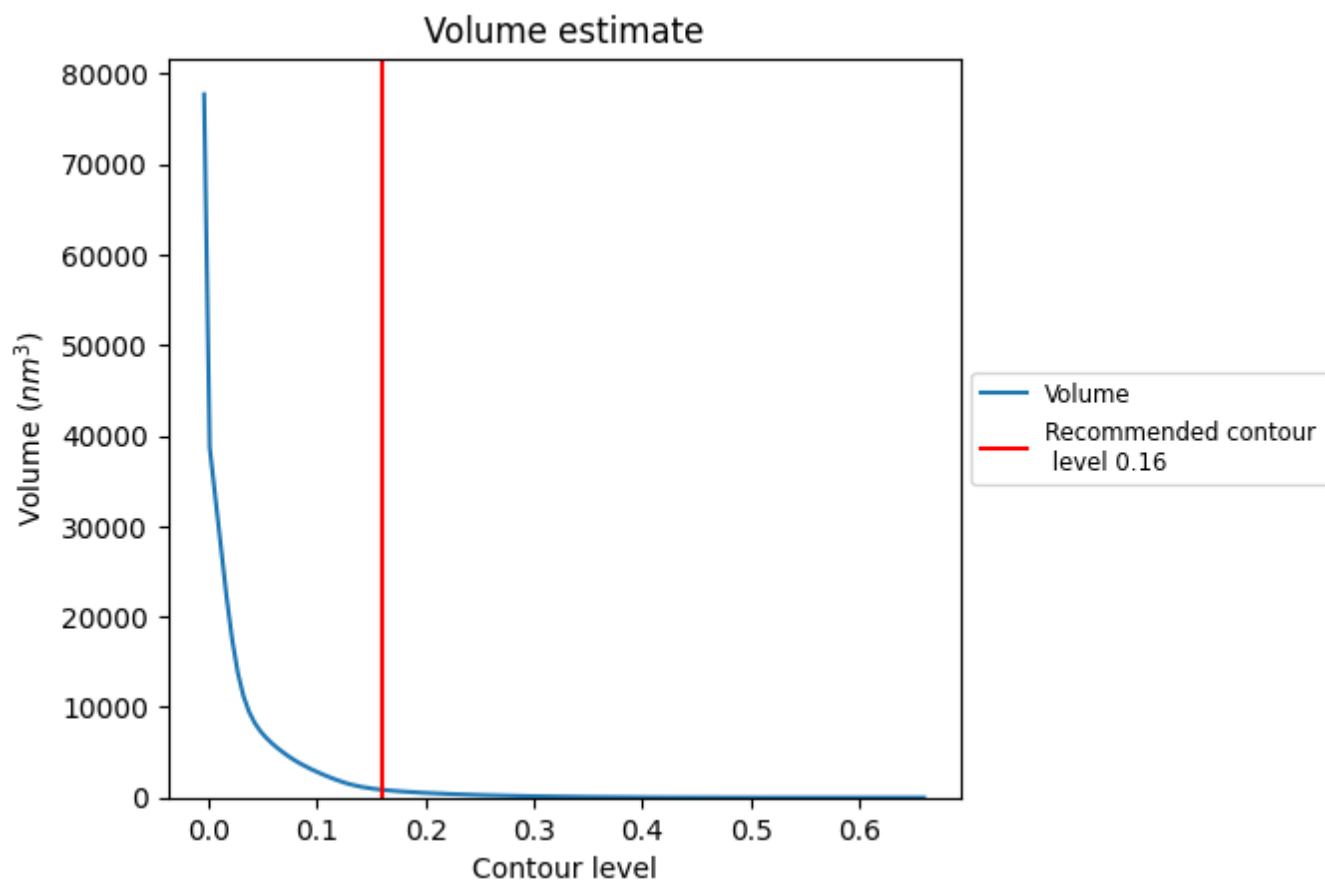
This section contains the results of statistical analysis of the map.

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.

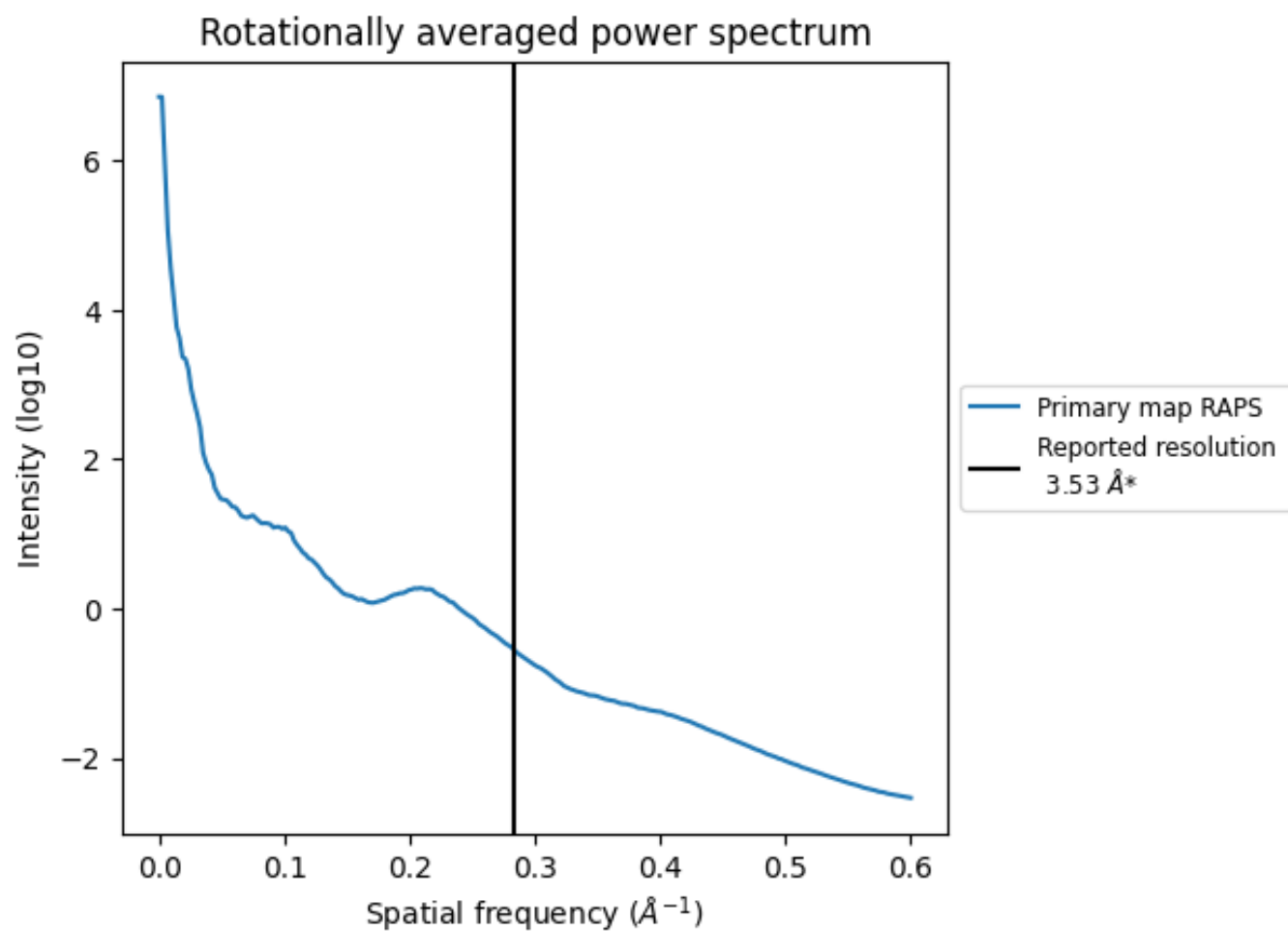
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 858 nm^3 ; this corresponds to an approximate mass of 775 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 0.283 Å⁻¹

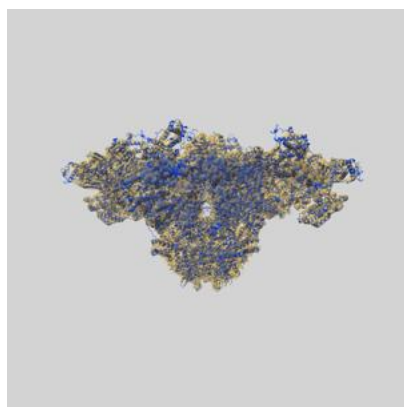
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

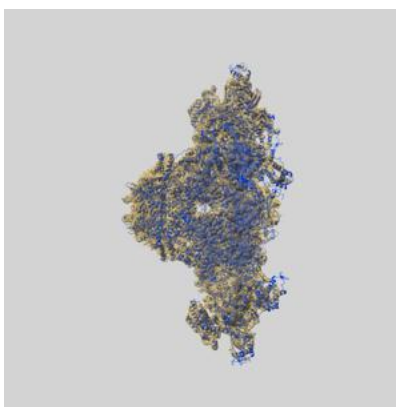
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42761 and PDB model 8UXE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

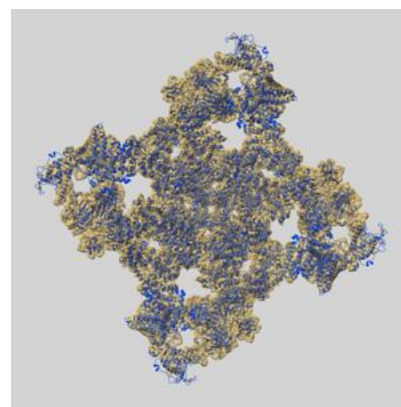
9.1 Map-model overlay [i](#)



X



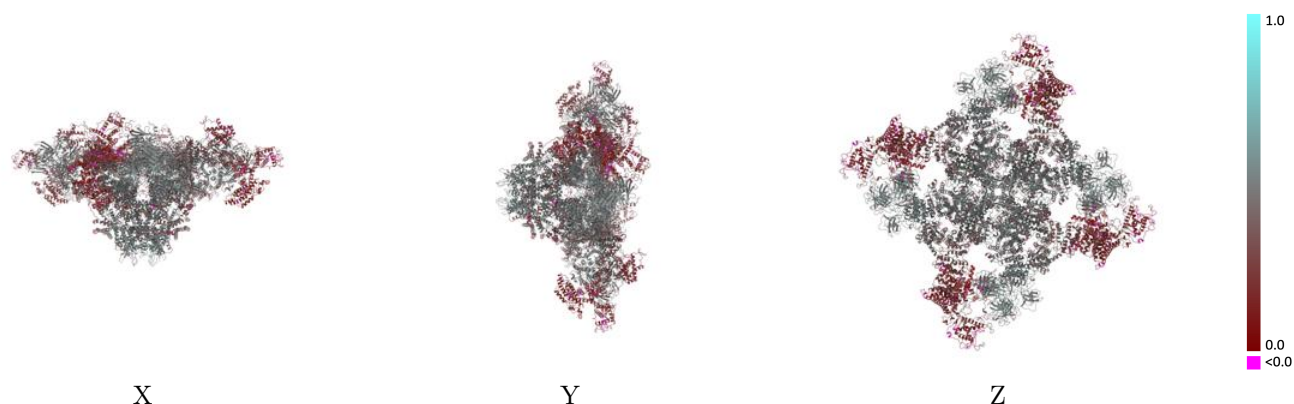
Y



Z

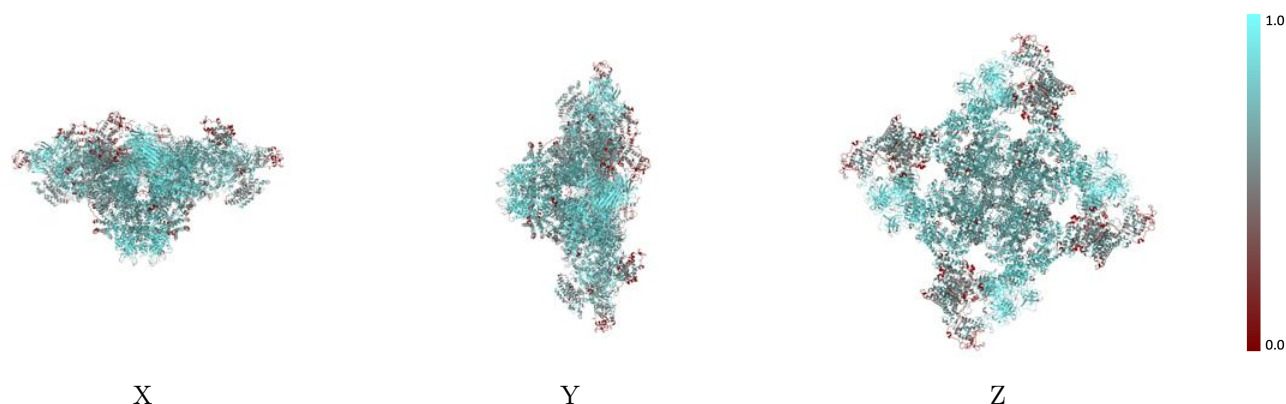
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



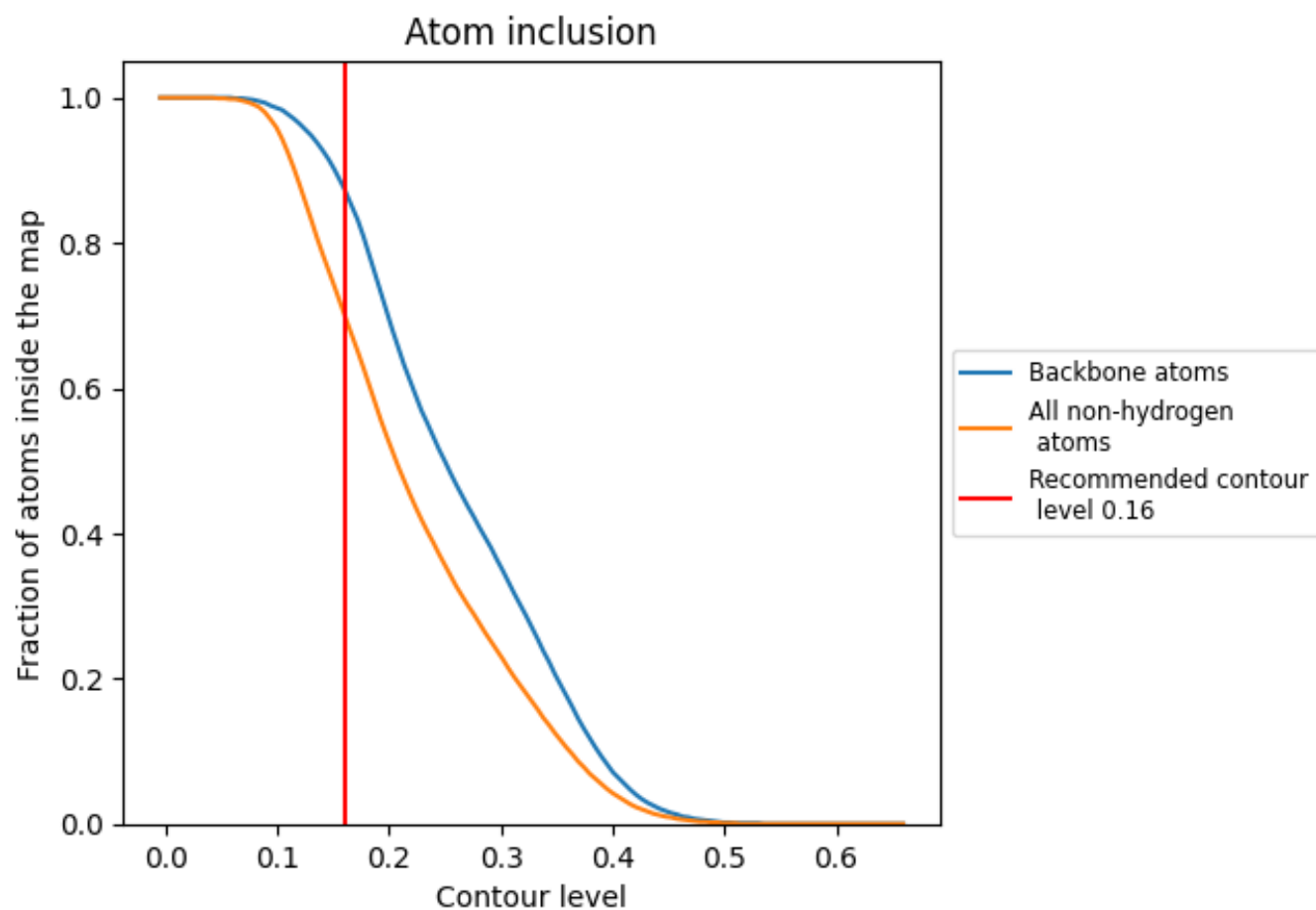
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.3910
A	0.6990	0.3870
B	0.7000	0.3900
C	0.7000	0.3900
D	0.7000	0.3900
E	0.8190	0.4810
F	0.8090	0.4800
G	0.8180	0.4790
H	0.8230	0.4800

1.0

0.0

<0.0