



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 09:05 AM UTC

PDB ID : 7UA9 / pdb_00007ua9
EMDB ID : EMD-26416
Title : Structure of dephosphorylated human RyR2 in the open state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 3.59 Å (reported)
Based on initial model : 7U9Q

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:

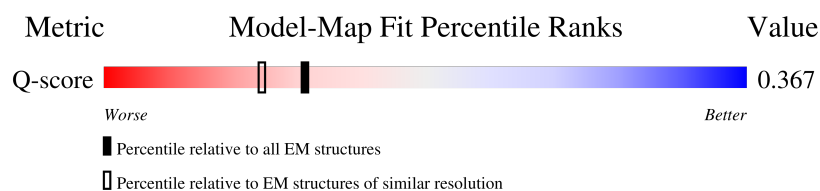
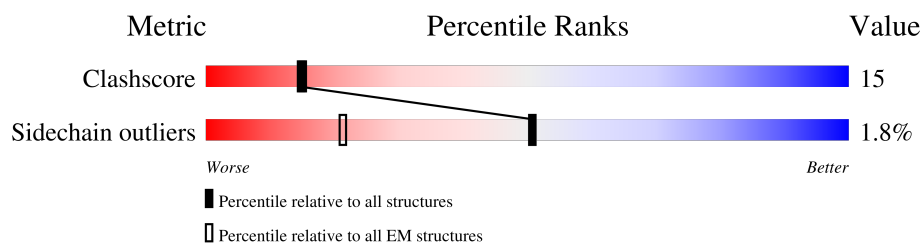
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.59 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12565 (3.09 - 4.09)

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	 81% 15% . .
1	F	108	 78% 18% . .
1	G	108	 76% 19% . .
1	H	108	 75% 21% . .
2	A	4967	 15% 59% 25% . 15%

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Mol	Chain	Length	Quality of chain
2	B	4967	15% 59% 25% • 15%
2	C	4967	15% 59% 25% • 15%
2	D	4967	15% 59% 25% • 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 138656 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		

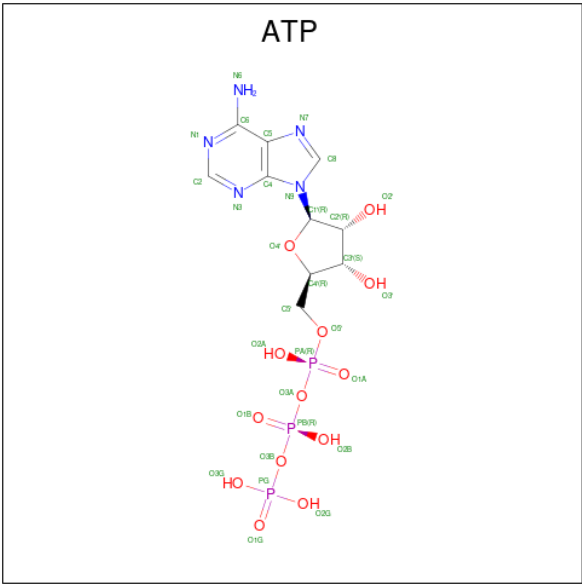
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

- 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: C₁₀H₁₆N₅O₁₃P₃) (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	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

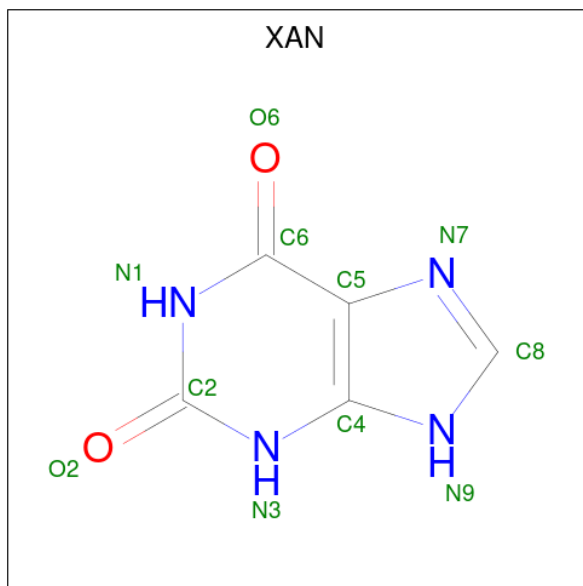
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

- Molecule 6 is XANTHINE (CCD ID: XAN) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).

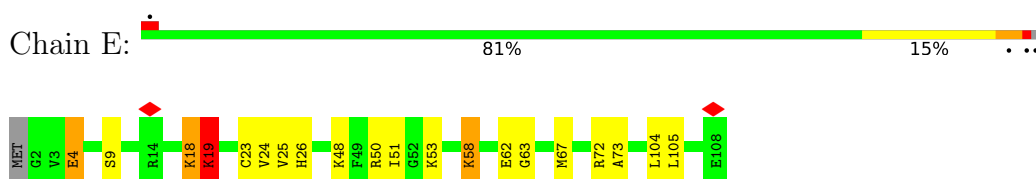


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			11	5	4	2	
6	B	1	Total	C	N	O	0
			11	5	4	2	
6	C	1	Total	C	N	O	0
			11	5	4	2	
6	D	1	Total	C	N	O	0
			11	5	4	2	

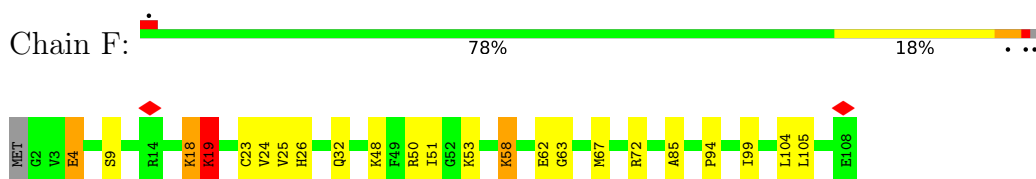
3 Residue-property plots [i](#)

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

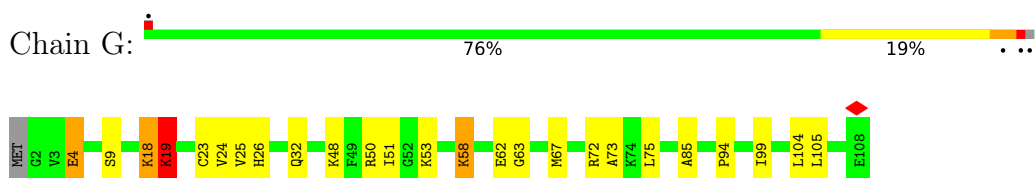
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



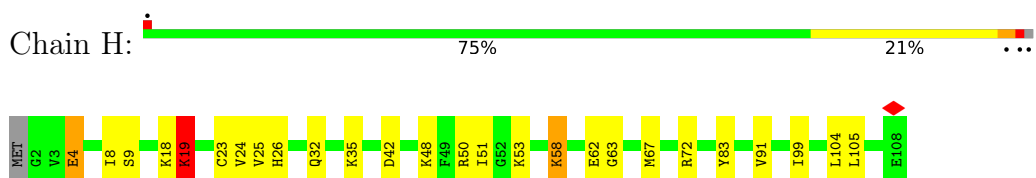
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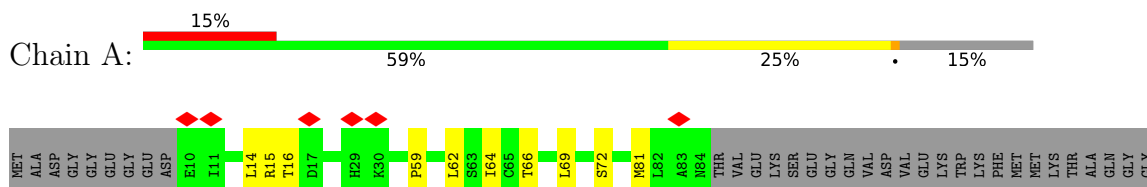
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



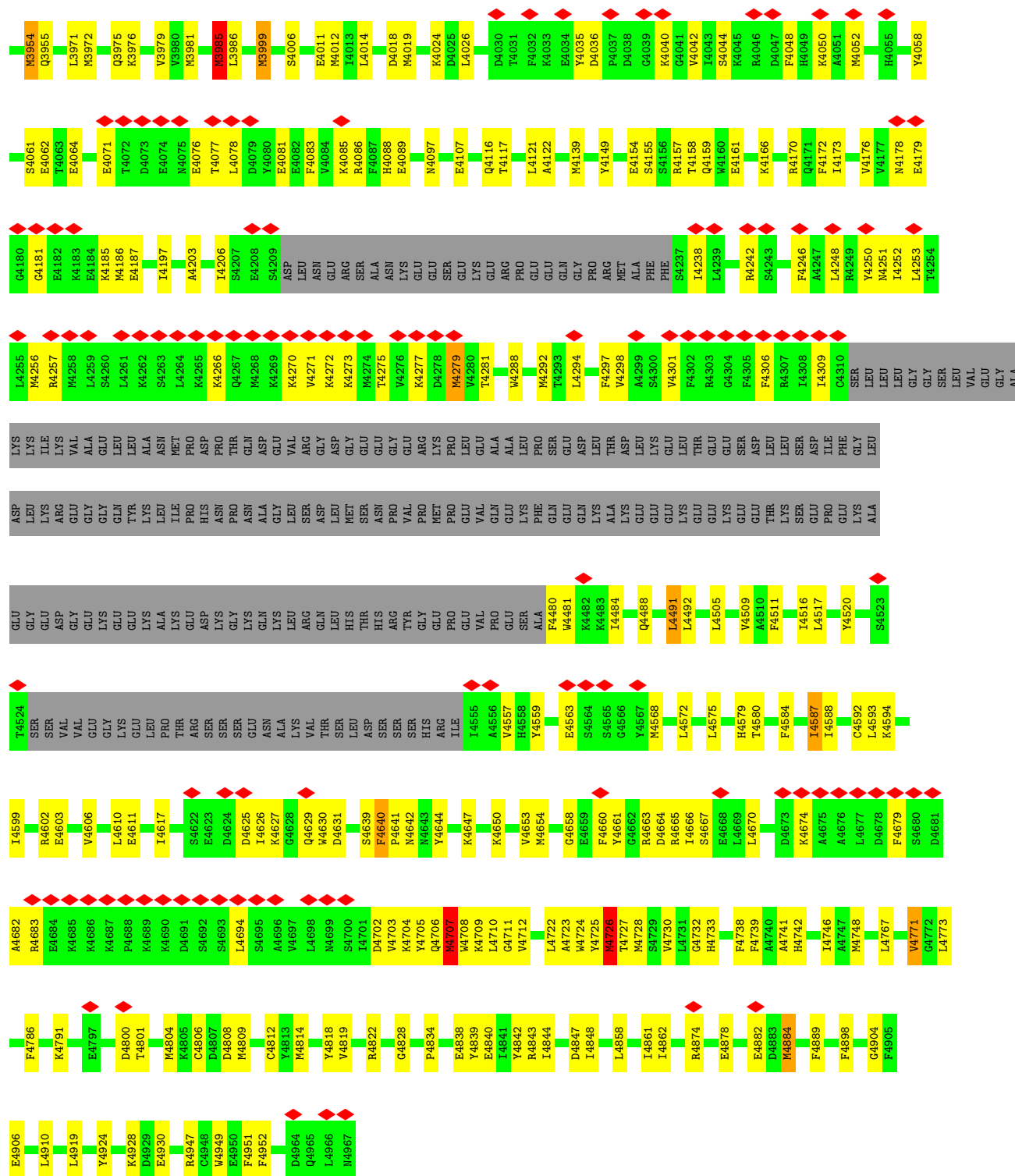
- Molecule 2: Ryanodine receptor 2



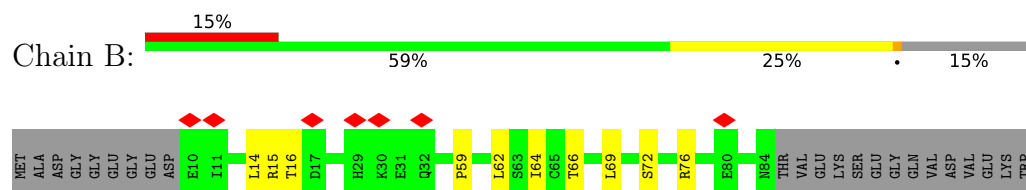








- Molecule 2: Ryanodine receptor 2











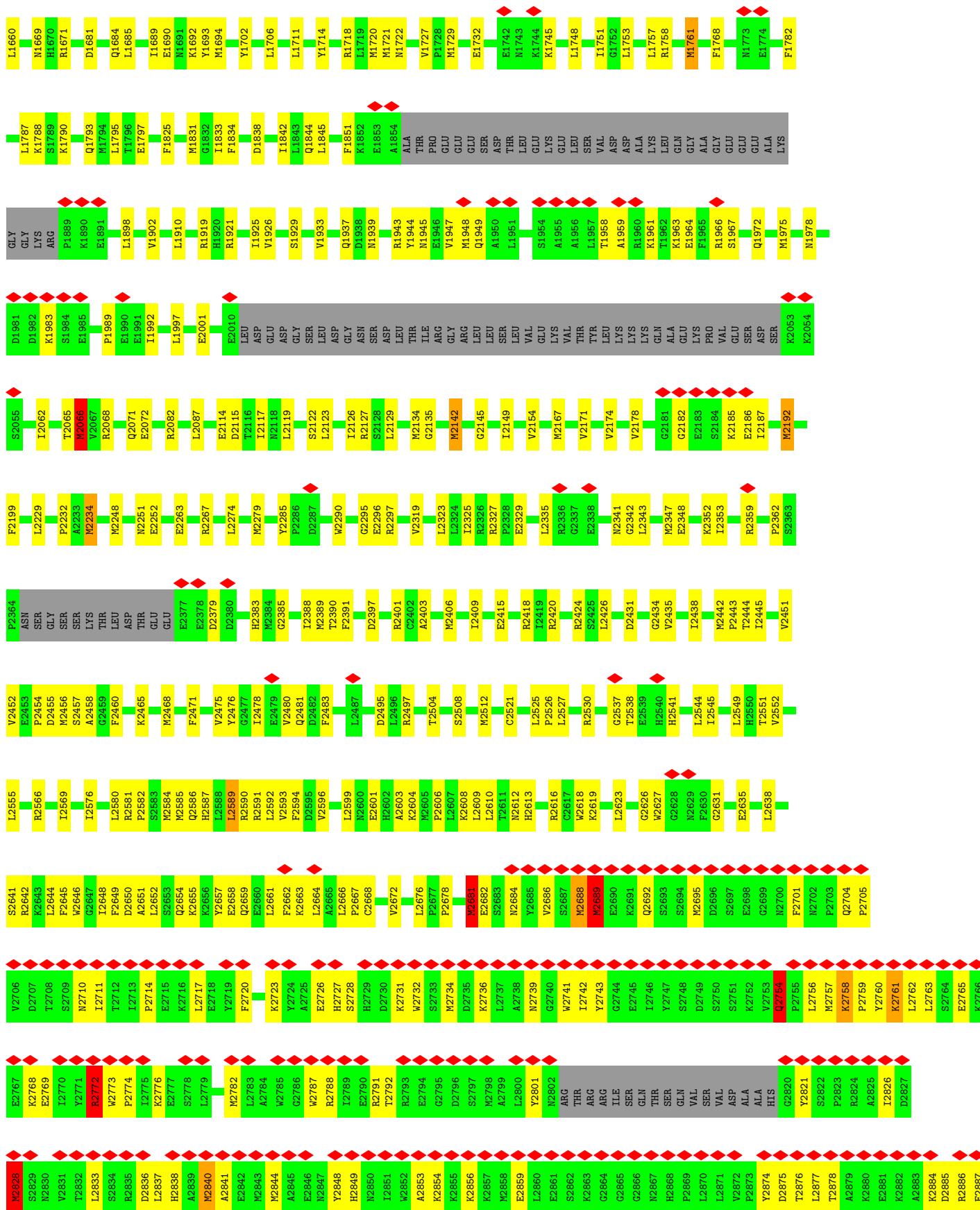


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P2714	E2715	K2716	L2717	E2718	Y2719	F2720	L2721	N2722	K2723	Y2724	K2725	A2726	H2727	S2728	H2729	D2730	K2731	W2732	M2733	D2735	K2736	A2738	N2739	G2740	I2741	I2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	M2750	S2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759	K2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	K2768	E2769	I2770	Y2771	R2772	W2773		
P2774	L2775	K2776	E2777	K2780	T2781	M2782	L2783	A2784	W2785	G2786	W2787	R2788	L2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	L2826	D2827	R2828	S2829	N2830	V2831	T2832	L2833	S2834	
P2714	E2715	K2716	L2717	E2718	Y2719	F2720	L2721	N2722	K2723	Y2724	K2725	A2726	H2727	S2728	H2729	D2730	K2731	W2732	M2733	D2735	K2736	A2738	N2739	G2740	I2741	I2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	M2750	S2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759	K2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	K2768	E2769	I2770	Y2771	R2772	W2773		
R2581	P2582	S2583	M2584	Q2585	Q2586	H2587	L2588	L2589	R2590	R2591	L2592	L2593	F2594	L2595	L2596	L2599	N2600	E2601	H2602	A2603	K2604	M2605	L2606	K2608	L2609	L2610	T2611	N2612	H2613	R2616	W2618	K2619	Y2620	L2623	G2626	W2627	G2631	A2632	E2635	L2638	S2641	R2642	K2643	L2644	F2645	W2646	G2647	L2648	F2649										
B2650	A2651	L2652	S2653	Q2654	K2655	K2656	E2657	E2658	Q2659	Q2660	L2661	F2662	K2663	L2664	L2665	L2666	L2667	P2667	C2668	V2672	L2676	F2677	P2678	Y2680	K2681	E2682	S2683	M2684	Y2685	V2686	S2687	M2688	K2689	E2690	K2691	S2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	H2700	F2701	H2702	L2703	Q2704	P2705	P2706	D2707	T2708	S2709	N2710	L2711	T2712	L2713		
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B2650	A2651	L2652	S2653	Q2654	K2655	K2656	E2657	E2658	Q2659	Q2660	L2661	F2662	K2663	L2664	L2665	L2666	L2667	P2667	C2668	V2672	L2676	F2677	P2678	Y2680	K2681	E2682	S2683	M2684	Y2685	V2686	S2687	M2688	K2689	E2690	K2691	S2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	H2700	F2701	H2702	L2703	Q2704	P2705	P2706	D2707	T2708	S2709	N2710	L2711	T2712	L2713		
P2714	E2715	K2716	L2717	E2718	Y2719	F2720	L2721	N2722	K2723	Y2724	K2725	A2726	H2727	S2728	H2729	D2730	K2731	W2732	M2733	D2735	K2736	A2738	N2739	G2740	I2741	I2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	M2750	S2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759	K2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	K2768	E2769	I2770	Y2771	R2772	W2773		
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K2066	V2067	R2068	Q2071	E2072	R2082	L2087	E2114	D2115	T2116	I2117	L2118	L2119	S2122	L2123	I2126	R2127	S2128	L2129	M2134	G2135	M2142	G2145	I2149	V2154	M2167	V2171	V2174	V2178	G2181	G2182	E2183	S2184	E2186	I2187	M2192	F2199	L2229	P2232																					
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LYS	THR	ASP	THR	GLU	E2377	E2378	D2379	D2380	H2383	M2384	G2385	I2388	M2389	T2390	F2391	D2397	R2401	C2402	A2403	M2406	I2409	E2415	R2418	I2419	R2420	R2424	S2425	L2426	D2431	G2434	V2435	I2438	M2442	P2443	T2444	I2445	V2451	V2452	E2453	P2454	D2455	M2456	S2457																
A2458	G2459	F2460	K2465	W2468	F2471	V2475	Y2476	G2477	I2478	E2479	W2480	Q2481	D2482	F2483	D2495	R2497	T2504	S2508	M2512	C2521	L2525	P2526	L2527	R2530	G2537	T2538	H2541	L2544	L2545	L2549	T2551	V2552	L2555	R2556	L2569	T2576	L2580																						
R2581	P2582	S2583	M2584	Q2585	Q2586	H2587	L2588	L2589	R2590	R2591	L2592	L2593	F2594	L2595	L2596	L2599	N2600	E2601	H2602	A2603	K2604	M2605	L2606	K2608	L2609	L2610	T2611	N2612	H2613	R2616	W2618	K2619	Y2620	L2623	G2626	W2627	G2631	A2632	E2635	L2638	S2641	R2642	K2643	L2644	F2645	W2646	G2647	L2648	F2649										
B2650	A2651	L2652	S2653	Q2654	K2655	K2656	E2657	E2658	Q2659	Q2660	L2661	F2662	K2663	L2664	L2665	L2666	L2667	P2667	C2668	V2672	L2676	F2677	P2678	Y2680	K2681	E2682	S2683	M2684	Y2685	V2686	S2687	M2688	K2689	E2690	K2691	S2692	S2693	S2694	M2695	D2696	S2697	E2698	G2699	H2700	F2701	H2702	L2703	Q2704	P2705	P2706	D2707	T2708	S2709	N2710	L2711	T2712	L2713		
P2714	E2715	K2716	L2717	E2718	Y2719	F2720	L2721	N2722	K2723	Y2724	K2725	A2726	H2727	S2728	H2729	D2730	K2731	W2732	M2733	D2735	K2736	A2738	N2739	G2740	I2741	I2742	Y2743	G2744	E2745	L2746	Y2747	S2748	D2749	M2750	S2751	K2752	V2753	Q2754	P2755	L2756	M2757	K2758	P2759	K2760	K2761	L2762	L2763	S2764	E2765	K2766	E2767	K2768	E2769	I2770	Y2771	R2772	W2773		
P2774	L2775	K2776	E2777	K2780	T2781	M2782	L2783	A2784	W2785	G2786	W2787	R2788	L2789	E2790	R2791	T2792	R2793	E2794	G2795	D2796	S2797	M2798	A2799	L2800	Y2801	N2802	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	L2826	D2827	R2828	S2829	N2830	V2831	T2832	L2833	S2834	

L3803	D3804	L3805	F3808	G3816	L3817	G3818	M3819	V3820	F3821	E3822	E3823	G3824	S3825	G3826	E3827	K3828	V3829	D3833	D3838	Q3844	L3845	L3846	N3851	F3854	Q3855	L3858	N3864	S3884	Y3891	Y3892	F3906	S3907	K3908	E3922	G3926	F3927	C3928	R3939	V3945	V3950	M3954																			
K3697	S3698	C3699	H3700	D3701	E3702	GLU	ASP	ASP	ASP	GLY	GLU	GLU	E3710	K3711	K3712	E3715	E3716	L3725	Y3726	Q3727	Q3728	A3729	R3730	L3731	H3732	D3733	R3734	E3837	D3838	K3839	M3754	A3757	K3760	I3763	A3764	N3770	K3776	M3777	L3778	K3782	E3783	K3784	K3785	D3786	V3787	F3790	L3796													
GLN	ARG	LYS	ARG	ALA	V3599	V3600	A3601	C3602	F3603	R3604	M3605	A3606	L3608	Y3609	N3610	L3611	R3612	R3613	V3617	S3627	W3628	E3633	H3634	E3637	D3638	K3639	A3649	E3650	P3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	R3660	L3664	H3665	T3668	T3677	E3678	K3679	E3684	L3687	Y3688	M3689												
LEU	PRO	ASN	THR	ASP	ASP	THR	SER	ASP	PRO	GLY	LYS	THR	VAL	GLU	VAL	LEU	ASP	ALA	ASN	VAL	PHE	HIS	LEU	GLN	LYS	SER	LYS	ARG	GLY	ILE	ARG	ASN	PRO	GLY	ILE	ARG	LYS	THR	LEU	GLN	THR	ALA	ILE	THR	GLN	ASP														
ARG	GLU	GLN	GLY	ASN	PHE	VAL	VAL	VAL	ASN	GLN	ILE	ASP	MET	ALA	PHE	LEU	ILE	THR	ASP	THR	LYS	SER	LYS	MET	LYS	ALA	ALA	ALA	LYS	TRP	VAL	SER	GLN	ASP	GLN	TYR	SER	MET	VAL	TYR	SER	GLU	VAL	LEU	LEU															
LEU	ILE	ASP	GLU	THR	PHE	THR	THR	THR	ALA	ALA	ARG	ASP	TYR	PRO	LEU	LEU	ILE	THR	ASP	ILE	ILE	ASP	PHE	VAL	LYS	ASP	LYS	ASP	LYS	GLN	PRO	GLU	ILE	ARG	ASN	PRO	GLU	THR	ILE	THR	TRP	ASN	LYS																	
A3294	W3295	M3296	K3297	R3298	L3299	A3300	V3301	F3302	S3303	Q3304	I3306	I3307	M3308	K3309	V3310	K3311	P3312	Q3313	L3314	L3315	K3316	T3317	H3318	S3319	F3320	L3320	P3321	L3322	M3323	E3324	K3325	L3326	A3327	K3328	K3329	A3330	A3331	T3332	V3333	V3334	S3335	E3336	E3337	ASP	HIS	LEU	LYS	ALA	ALA	ALA	ARG	ASP	SER	GLU	ALA	LEU	LEU	LEU	LEU	M3231
P3232	H3233	V3234	K3235	V3237	I3238	L3239	P3240	K3241	K3242	C3243	S3244	Y3245	K3246	S3247	R3248	W3249	E3250	E3251	G3252	G3253	P3254	E3255	N3256	N3257	P3258	E3259	R3260	A3261	E3262	K3263	C3264	C3265	T3266	A3267	L3268	N3269	S3270	E3271	H3272	K3273	N3274	T3275	L3276	L3277	G3278	N3279	T3280	L3281	K3282	I3283	I3284	L3288	G3289	D3291	Q3293					
E3172	T3173	H3174	L3175	D3176	K3177	H3178	N3179	I3180	S3182	Y3181	I3183	Y3184	N3185	T3186	K3187	S3188	S3189	R3190	E3191	R3192	A3193	A3194	L3195	S3196	L3197	P3198	T3199	N3200	V3201	E3202	D3203	V3204	C3205	P3206	N3207	I3208	P3209	S3210	L3211	E3212	K3213	L3214	M3215	E3216	E3217	I3218	V3219	E3220	L3221	A3222	E3223	S3224	G3225	R3227	F3228	T3229	Q3230	M3231		
H3111	I3112	G3113	Q3114	H3115	Q3116	F3117	G3118	E3119	D3120	L3121	I3122	L3123	E3124	D3125	V3126	Q3127	V3128	S3129	C3130	Y3131	R3132	I3133	L3134	L3137	Y3138	A3139	L3140	G3141	T3142	S3143	K3144	S3145	I3146	Y3147	V3148	E3149	R3150	Q3151	R3152	S3153	A3154	L3155	G3156	E3157	C3158	L3159	A3160	A3161	F3162	A3163	A3165	F3166	P3167	V3168	F3170	L3171				
I3035	L3036	T3039	L3040	D3041	Q3042	R3043	V3044	M3046	K3047	G3049	L3050	K3054	R3058	A3059	F3060	A3064	A3065	E3066	D3067	L3068	E3069	K3070	T3071	R3072	E3073	N3074	L3075	K3076	Q3077	G3078	Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	G3089	V3090	T3091	Q3092	L3093	I3094	A3100	M3104	F3109	E3110										
F2895	L2896	Q2897	L2898	K2899	Q2900	Y2901	A2902	V2903	S2904	R2905	G2906	F2907	K2908	D2909	L2910	E2911	L2912	D2913	T2914	P2915	E2918	K2919	L2920	F2921	A2922	Y2923	S2924	F2925	L2926	Q2927	Q2928	L2929	I2930	R2931	E2935	A2936	H2937	Q2938	Y2939	I2940	F2943	I2944	G2945	G2946	S2947	R2948	T3027	G2949	S3028	K2950	G2951	E2952	H2953	F2954	Y2955	L2956	I2960			

[illegible]









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36491	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	0.549	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: CA, XAN, ZN, 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	0.15	0/834	0.53	1/1123 (0.1%)
1	F	0.15	0/834	0.53	1/1123 (0.1%)
1	G	0.15	0/834	0.53	1/1123 (0.1%)
1	H	0.15	0/834	0.53	1/1123 (0.1%)
2	A	0.39	8/34511 (0.0%)	0.50	25/46614 (0.1%)
2	B	0.39	8/34511 (0.0%)	0.50	23/46614 (0.0%)
2	C	0.39	8/34511 (0.0%)	0.50	23/46614 (0.0%)
2	D	0.39	8/34511 (0.0%)	0.50	24/46614 (0.1%)
All	All	0.39	32/141380 (0.0%)	0.50	99/190948 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	7
2	B	0	7
2	C	0	7
2	D	0	7
All	All	0	28

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3117	PHE	CD1-CE1	29.31	2.26	1.38
2	D	3117	PHE	CD1-CE1	29.31	2.26	1.38
2	A	3117	PHE	CD1-CE1	29.28	2.26	1.38
2	C	3117	PHE	CD1-CE1	29.26	2.26	1.38
2	B	3117	PHE	CD2-CE2	27.68	2.21	1.38

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3043	ARG	CD-NE-CZ	21.97	155.15	124.40
2	B	3043	ARG	CD-NE-CZ	21.96	155.15	124.40
2	D	3043	ARG	CD-NE-CZ	21.95	155.13	124.40
2	C	3043	ARG	CD-NE-CZ	21.95	155.13	124.40
2	B	3043	ARG	CG-CD-NE	11.05	136.30	112.00

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2754	GLN	Peptide
2	A	2772	ARG	Sidechain
2	A	2828	MET	Peptide
2	A	3043	ARG	Sidechain
2	A	469	HIS	Peptide

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	E	818	0	821	14	0
1	F	818	0	821	15	0
1	G	818	0	821	17	0
1	H	818	0	821	19	0
2	A	33771	0	33453	1038	0
2	B	33771	0	33453	1035	0
2	C	33771	0	33453	1032	0
2	D	33771	0	33453	1039	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	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	11	0	4	0	0
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
All	All	138656	0	137208	4129	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 15.

The worst 5 of 4129 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:D:3117:PHE:CG	2:D:3117:PHE:CD1	1.80	1.67
2:B:3117:PHE:CD2	2:B:3117:PHE:CG	1.78	1.66
2:B:3117:PHE:CG	2:B:3117:PHE:CD1	1.80	1.66
2:D:3117:PHE:CG	2:D:3117:PHE:CD2	1.78	1.63
2:C:3117:PHE:CD2	2:C:3117:PHE:CG	1.78	1.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	E	88/89 (99%)	84 (96%)	4 (4%)	24	51
1	F	88/89 (99%)	84 (96%)	4 (4%)	24	51
1	G	88/89 (99%)	84 (96%)	4 (4%)	24	51
1	H	88/89 (99%)	84 (96%)	4 (4%)	24	51
2	A	3675/4358 (84%)	3610 (98%)	65 (2%)	51	68
2	B	3708/4358 (85%)	3643 (98%)	65 (2%)	51	68
2	C	3708/4358 (85%)	3643 (98%)	65 (2%)	51	68
2	D	3708/4358 (85%)	3643 (98%)	65 (2%)	51	68
All	All	15151/17788 (85%)	14875 (98%)	276 (2%)	51	68

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	2066	MET
2	D	2406	MET
2	D	3981	MET
2	B	1729	MET
2	B	1564	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1178	ASN
2	D	2211	GLN
2	D	3811	GLN
2	B	2118	ASN
2	B	1905	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 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
6	XAN	A	5004	-	12,12,12	1.78	5 (41%)	14,17,17	2.32	6 (42%)
4	ATP	A	5005	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	B	5005	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	C	5005	-	32,33,33	0.25	0	48,52,52	0.30	0
4	ATP	D	5005	-	32,33,33	0.25	0	48,52,52	0.30	0
6	XAN	C	5004	-	12,12,12	1.78	5 (41%)	14,17,17	2.32	6 (42%)
6	XAN	D	5004	-	12,12,12	1.78	5 (41%)	14,17,17	2.31	6 (42%)
4	ATP	D	5002	-	32,33,33	0.25	0	48,52,52	0.27	0
6	XAN	B	5004	-	12,12,12	1.78	5 (41%)	14,17,17	2.31	6 (42%)
4	ATP	B	5002	-	32,33,33	0.25	0	48,52,52	0.27	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	XAN	A	5004	-	-	-	0/2/2/2
4	ATP	A	5005	-	-	6/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	B	5005	-	-	6/22/38/38	0/3/3/3
4	ATP	C	5005	-	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	5005	-	-	6/22/38/38	0/3/3/3
6	XAN	C	5004	-	-	-	0/2/2/2
6	XAN	D	5004	-	-	-	0/2/2/2
4	ATP	D	5002	-	-	9/22/38/38	0/3/3/3
6	XAN	B	5004	-	-	-	0/2/2/2
4	ATP	B	5002	-	-	9/22/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5004	XAN	C6-N1	-3.27	1.32	1.38
6	B	5004	XAN	C6-N1	-3.26	1.32	1.38
6	C	5004	XAN	C6-N1	-3.26	1.32	1.38
6	D	5004	XAN	C6-N1	-3.25	1.32	1.38
6	B	5004	XAN	O6-C6	-2.47	1.18	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5004	XAN	C6-N1-C2	-4.62	120.00	126.37
6	A	5004	XAN	C6-N1-C2	-4.62	120.01	126.37
6	D	5004	XAN	C6-N1-C2	-4.61	120.03	126.37
6	B	5004	XAN	C6-N1-C2	-4.58	120.06	126.37
6	A	5004	XAN	N9-C8-N7	-4.28	108.01	112.98

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O2G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	PB-O3B-PG-O2G
4	B	5002	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 8 short contacts:

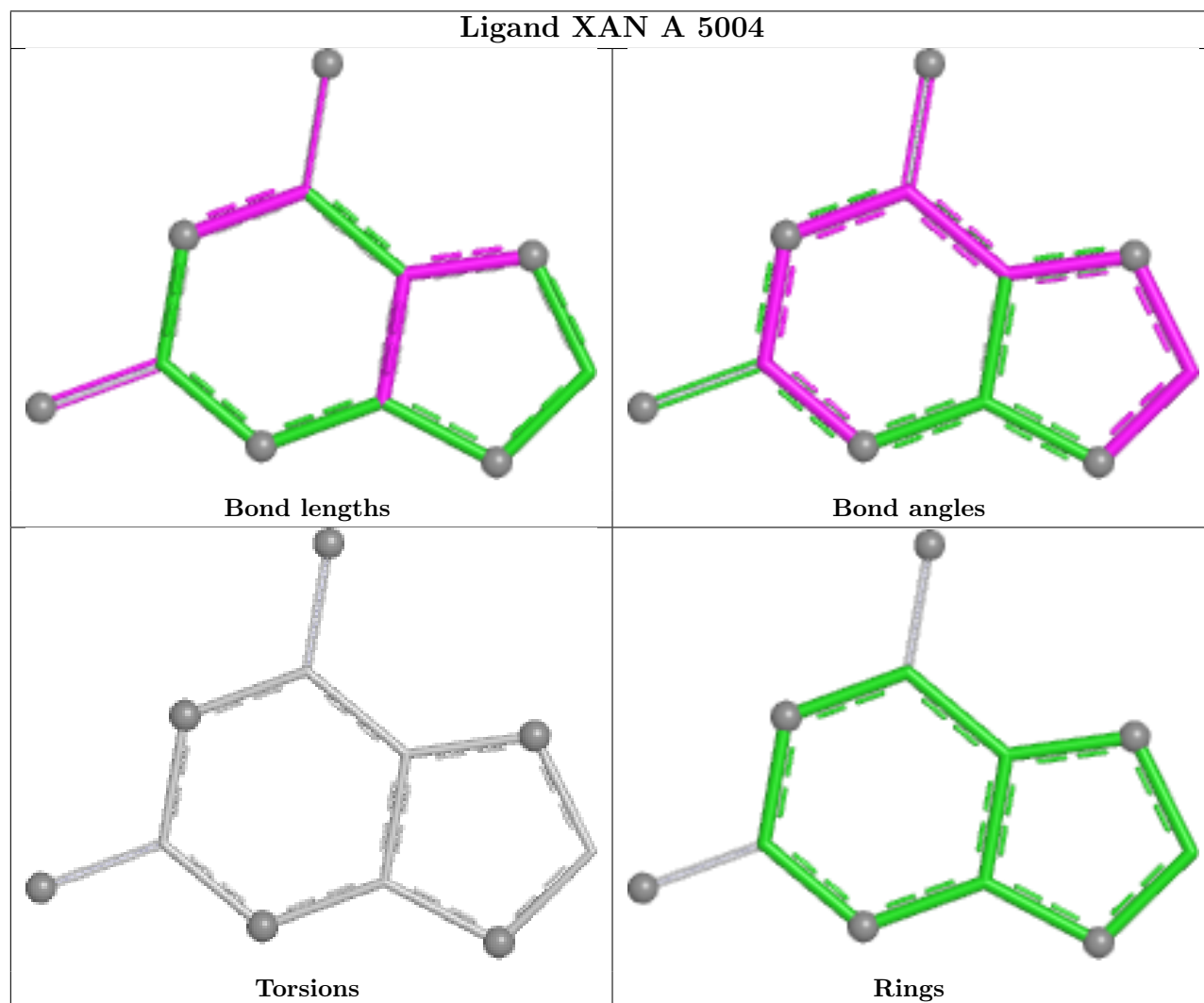
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5005	ATP	2	0

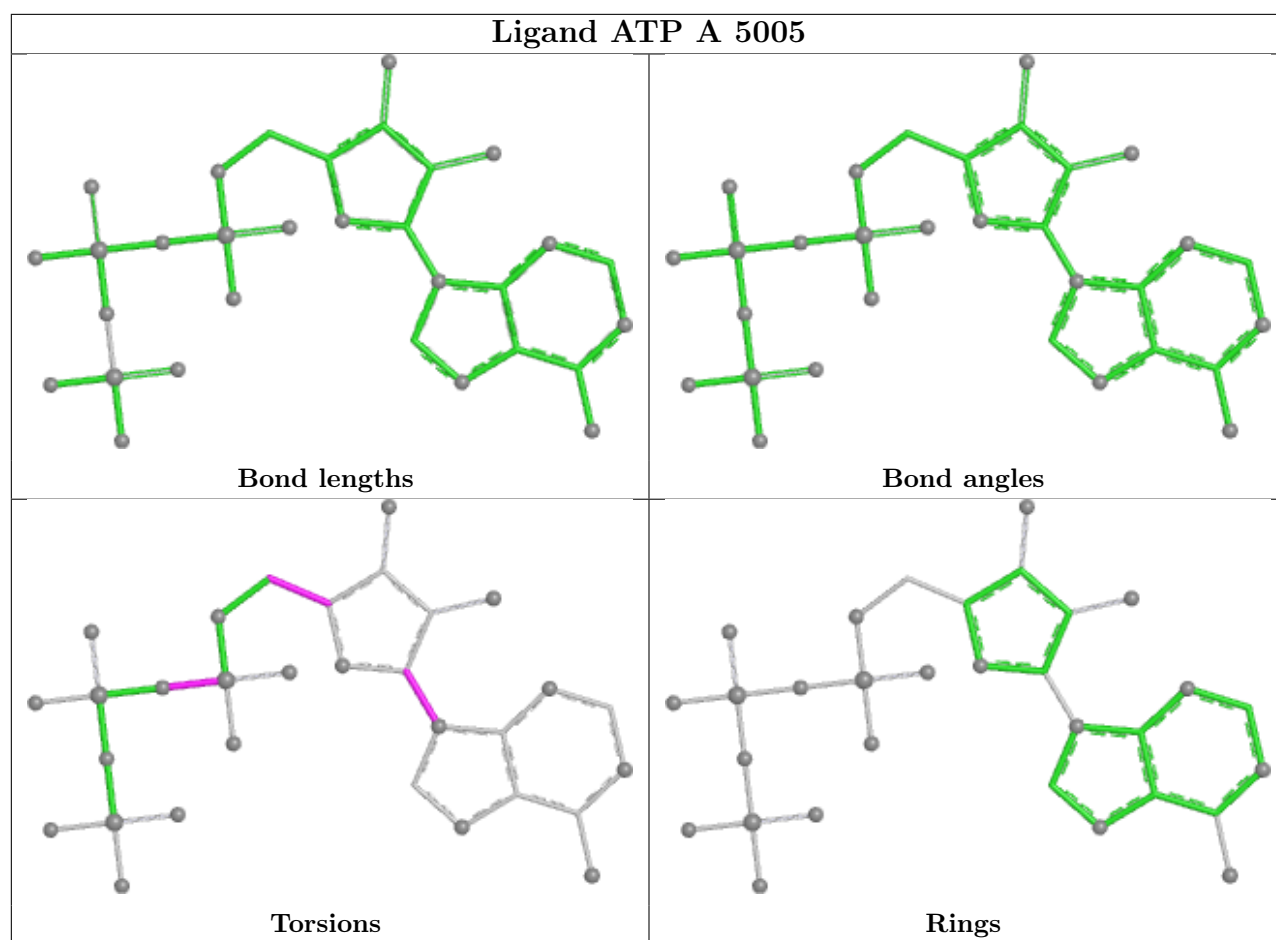
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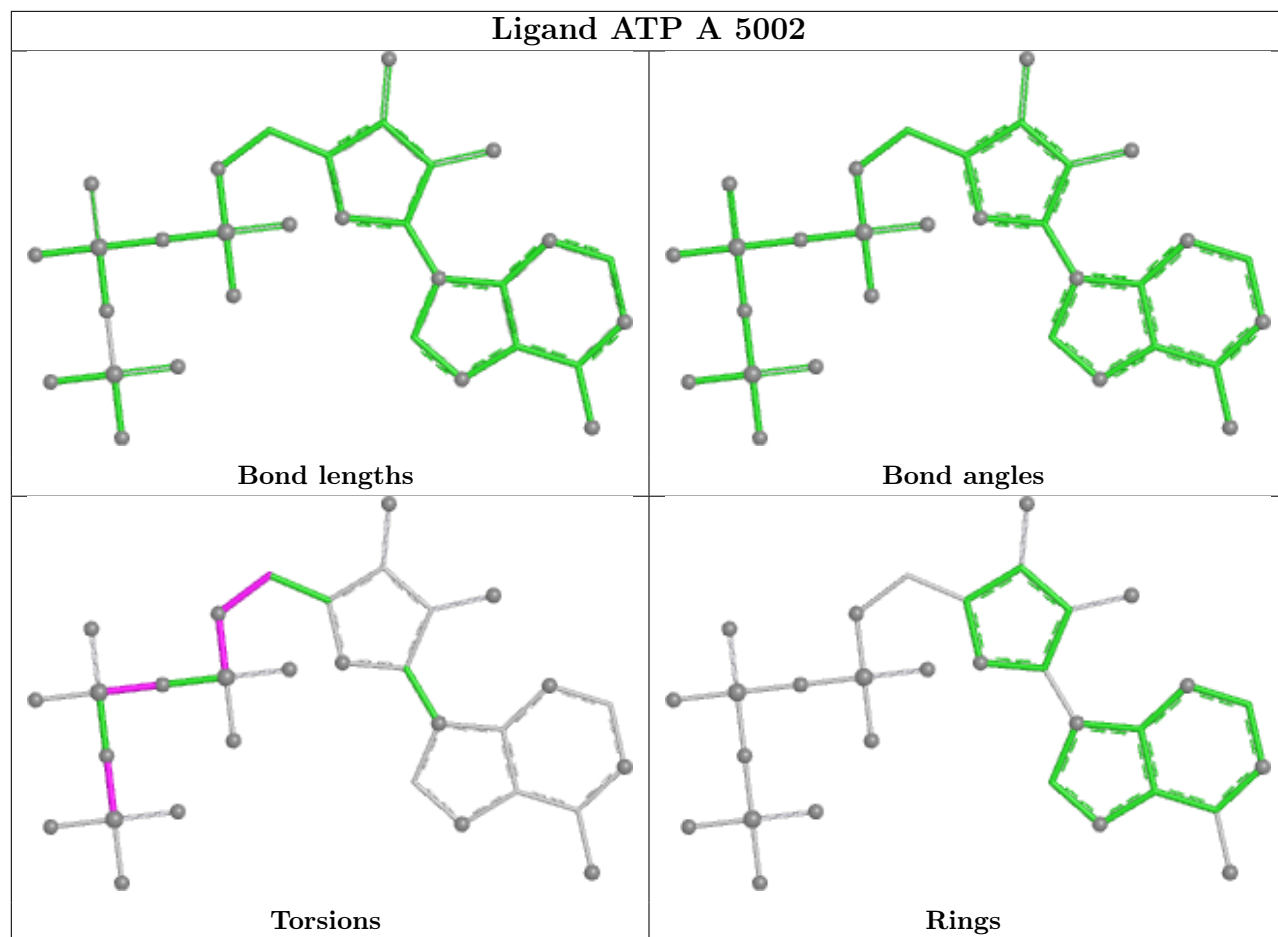
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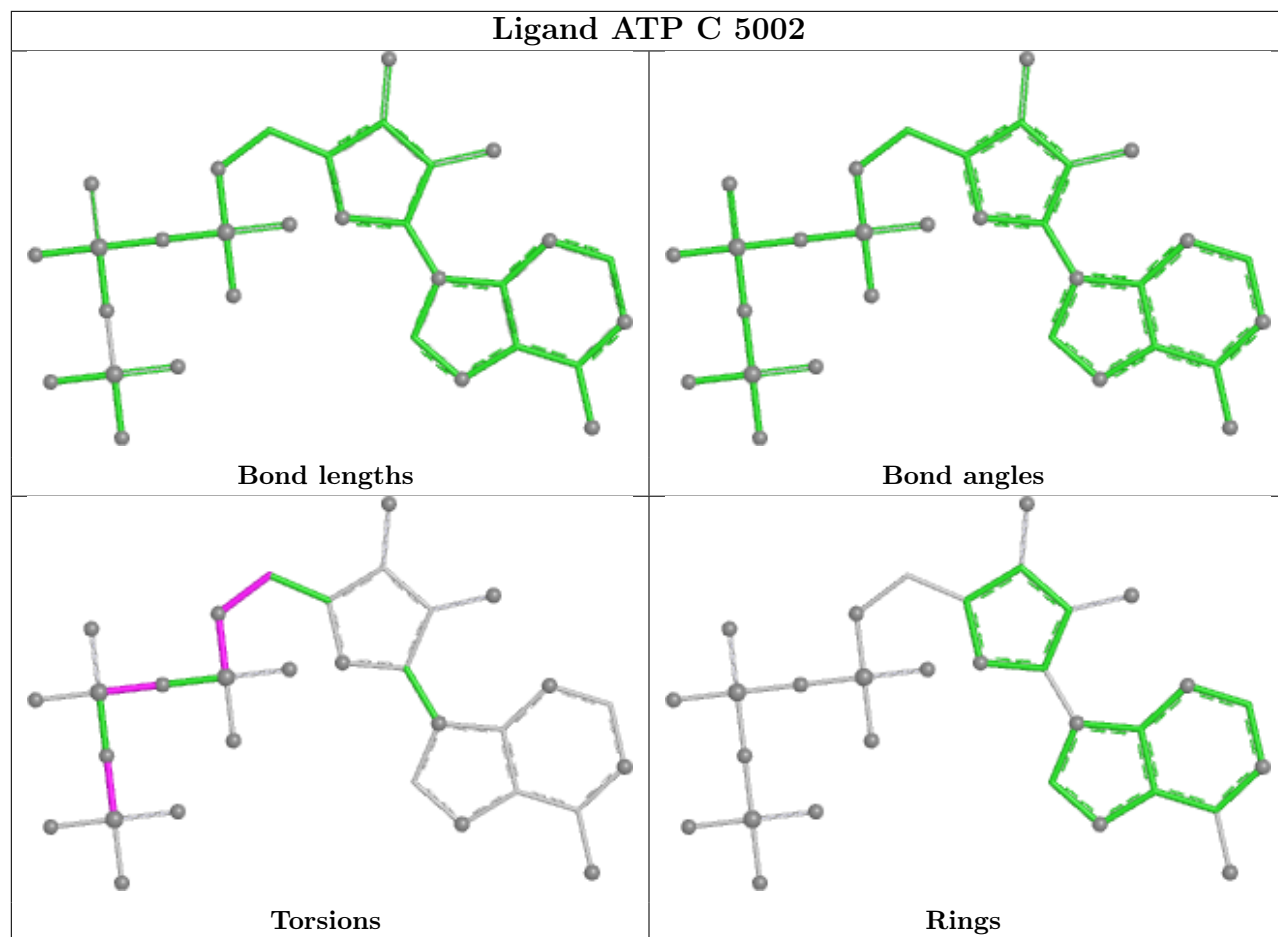
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5005	ATP	2	0
4	C	5005	ATP	2	0
4	D	5005	ATP	2	0

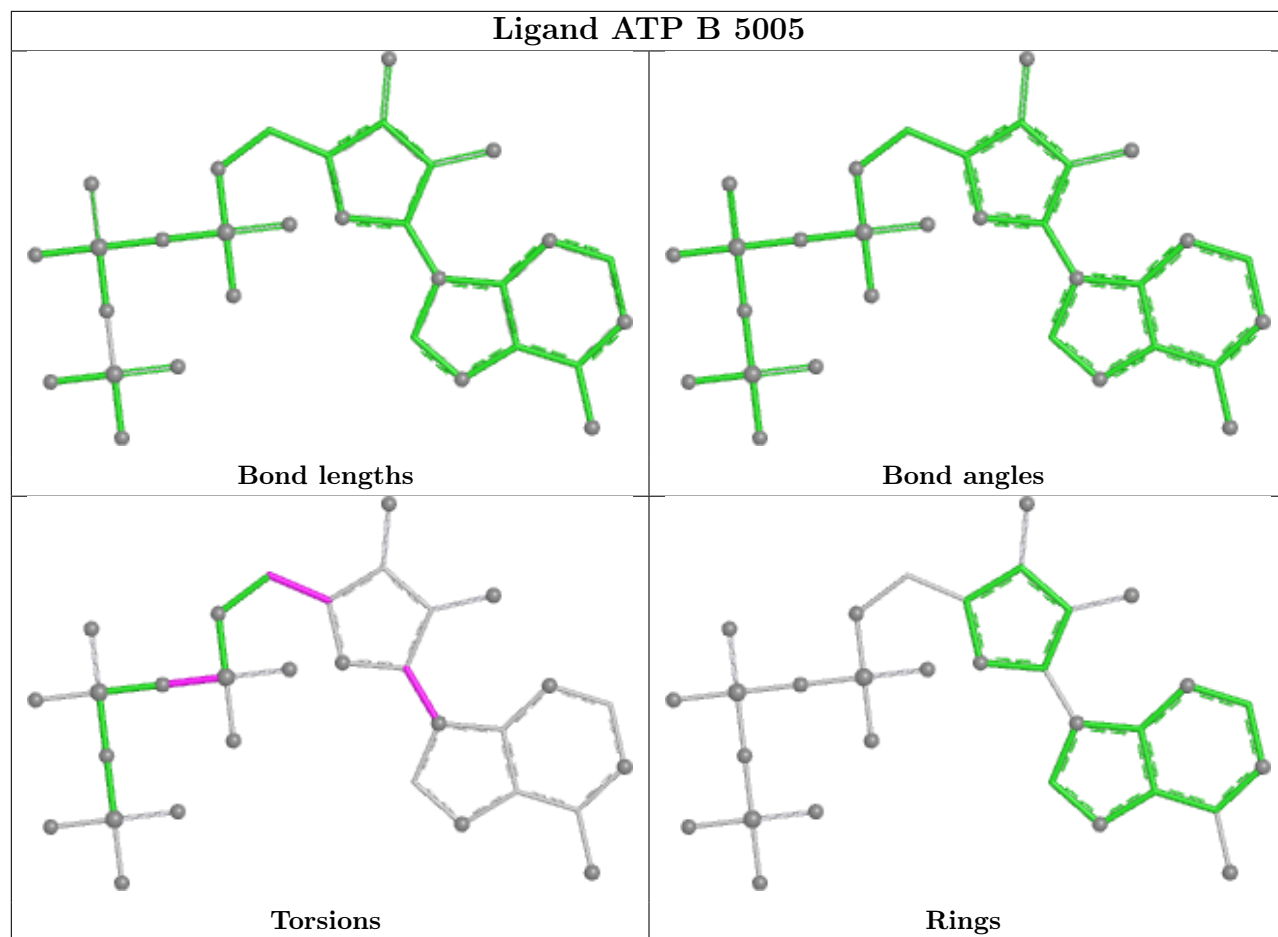
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

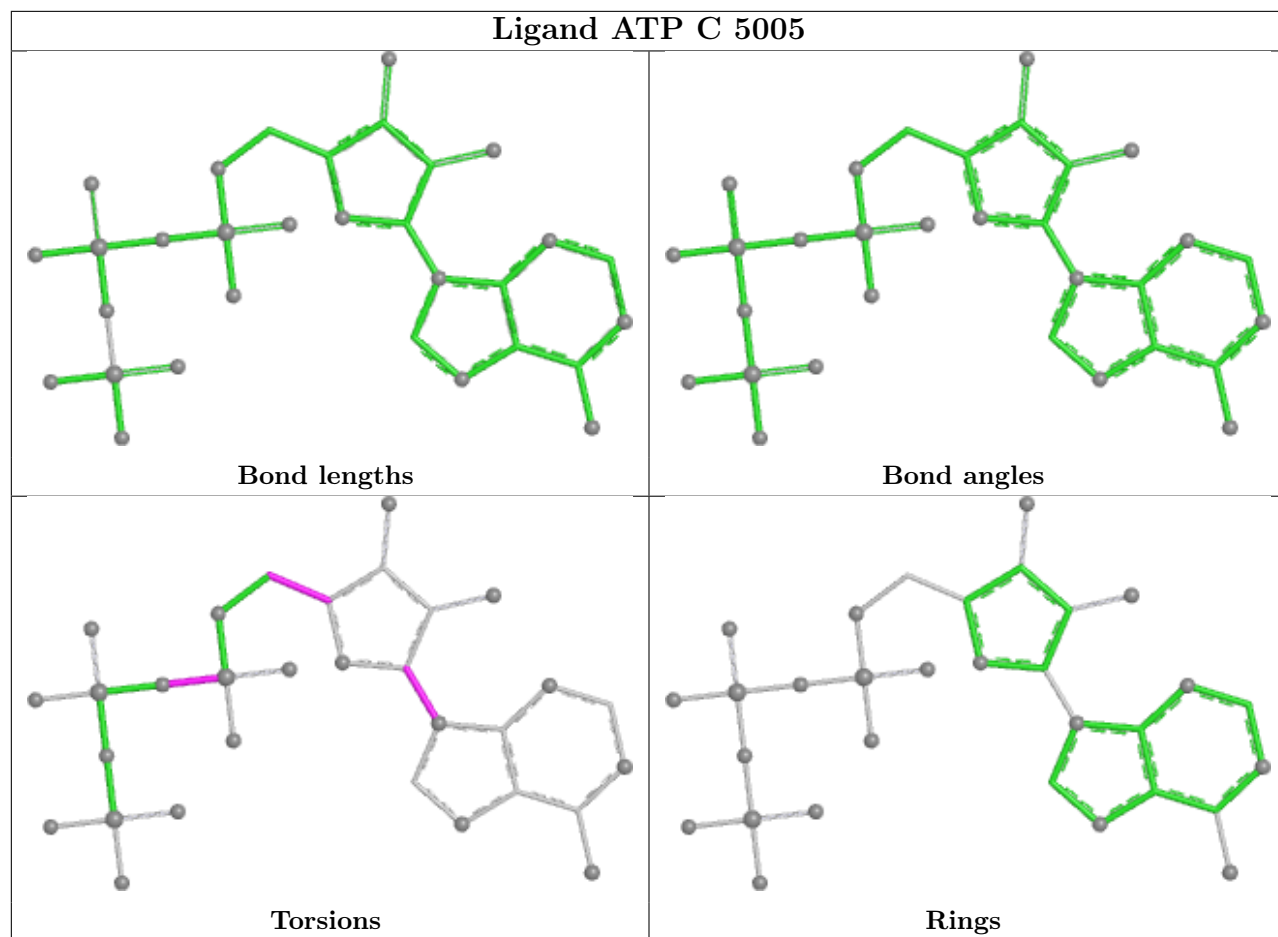


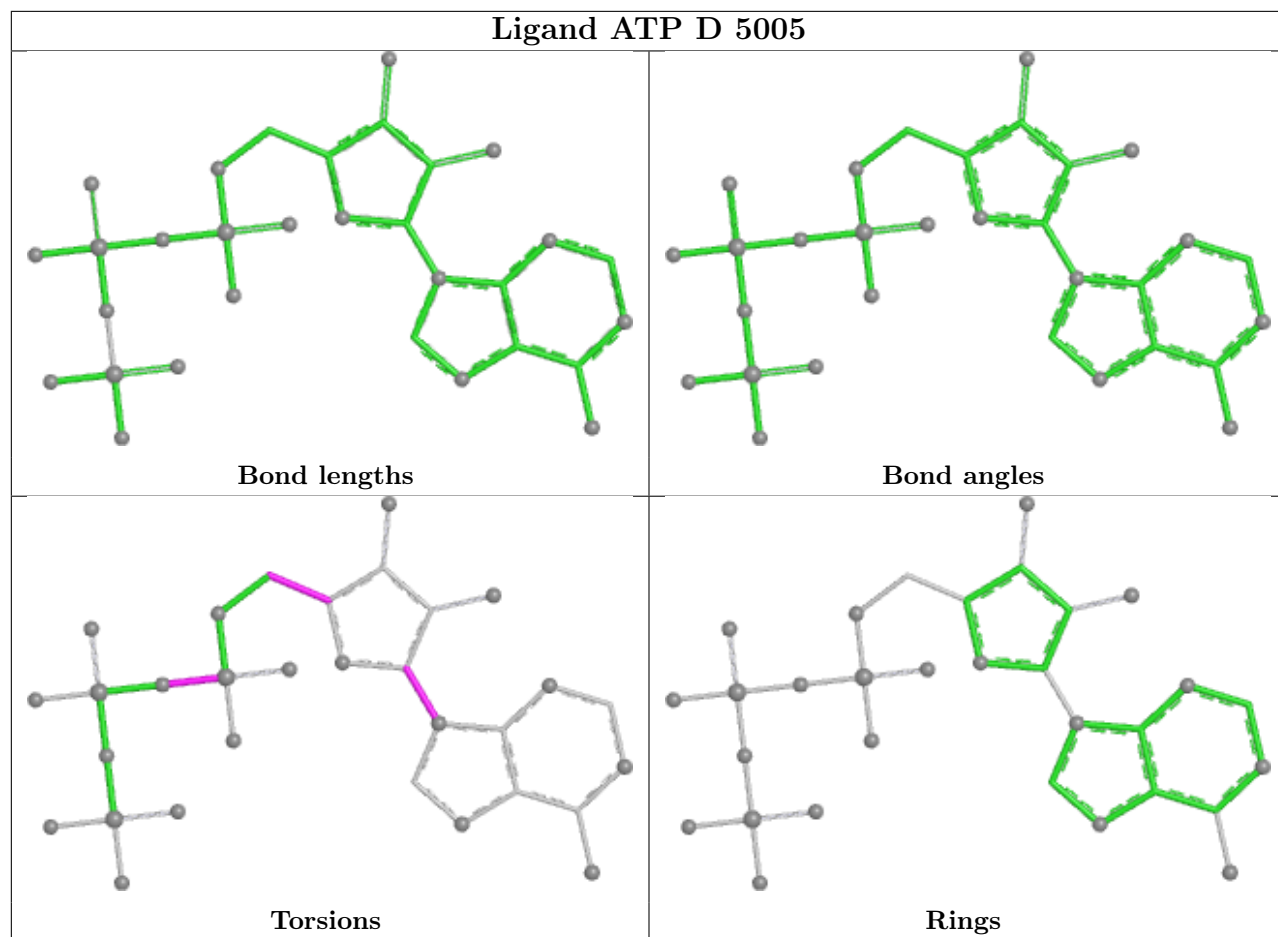




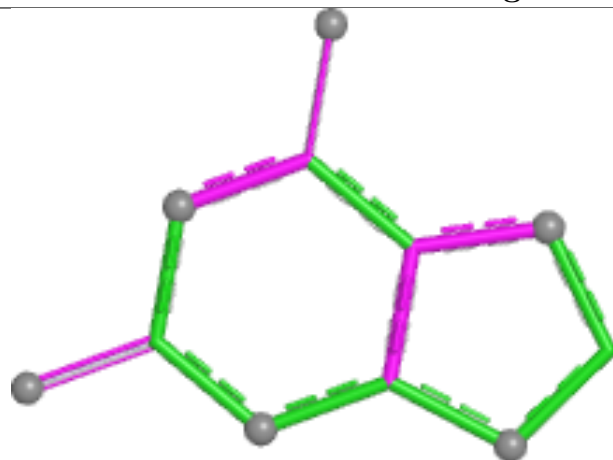




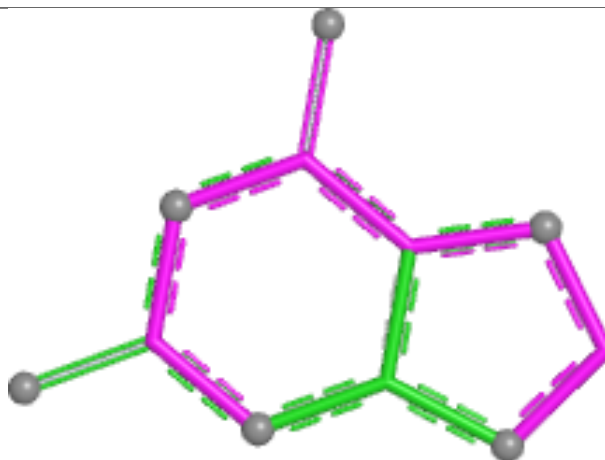




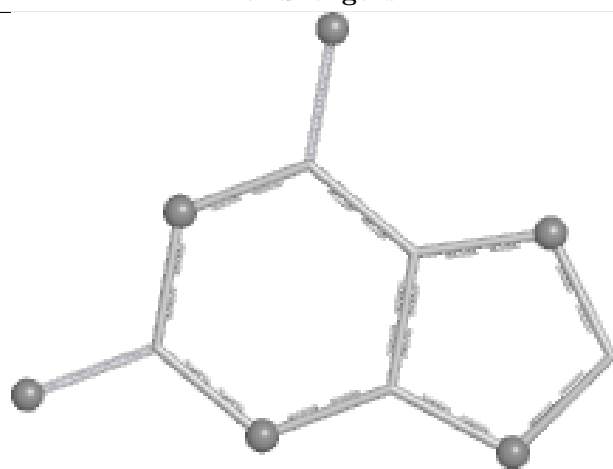
Ligand XAN C 5004



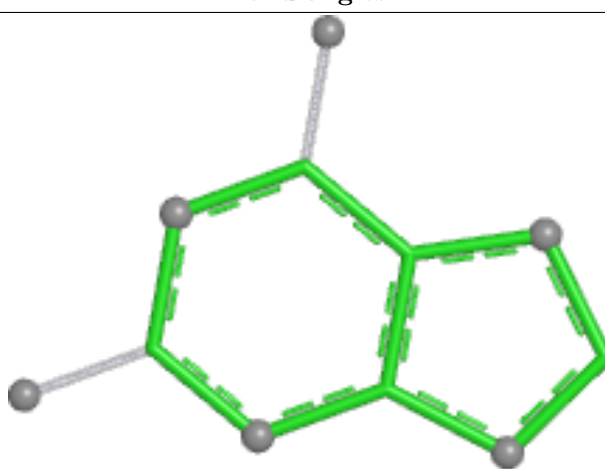
Bond lengths



Bond angles

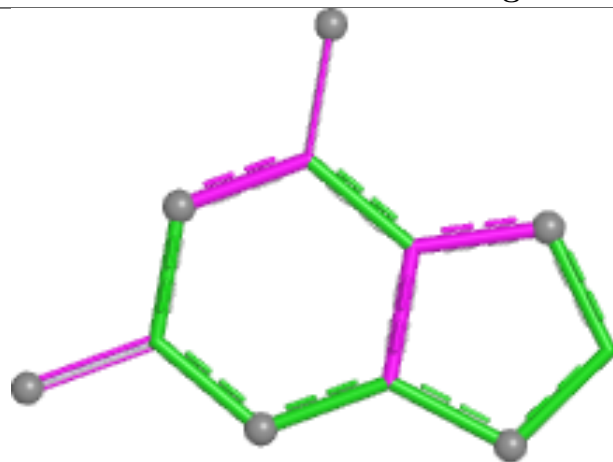


Torsions

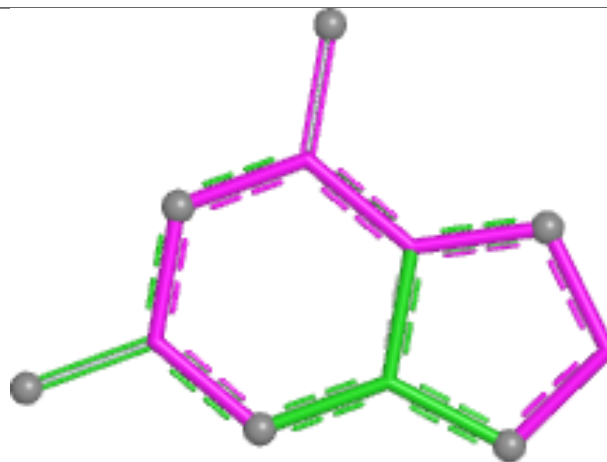


Rings

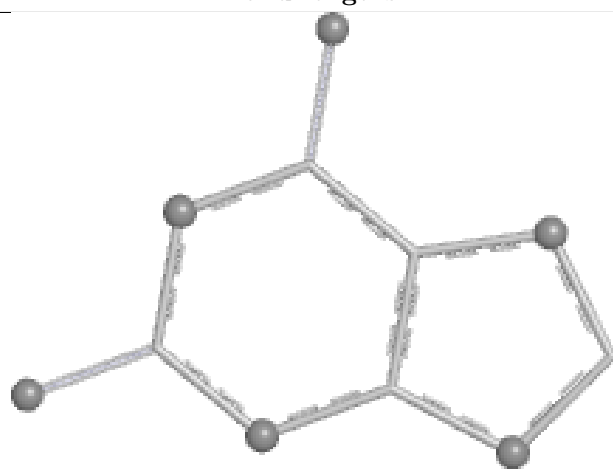
Ligand XAN D 5004



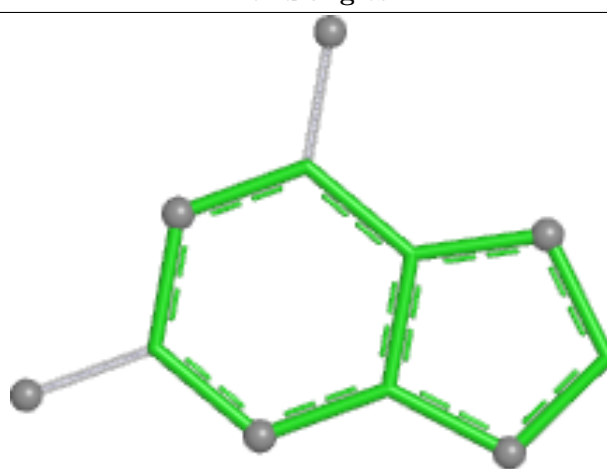
Bond lengths



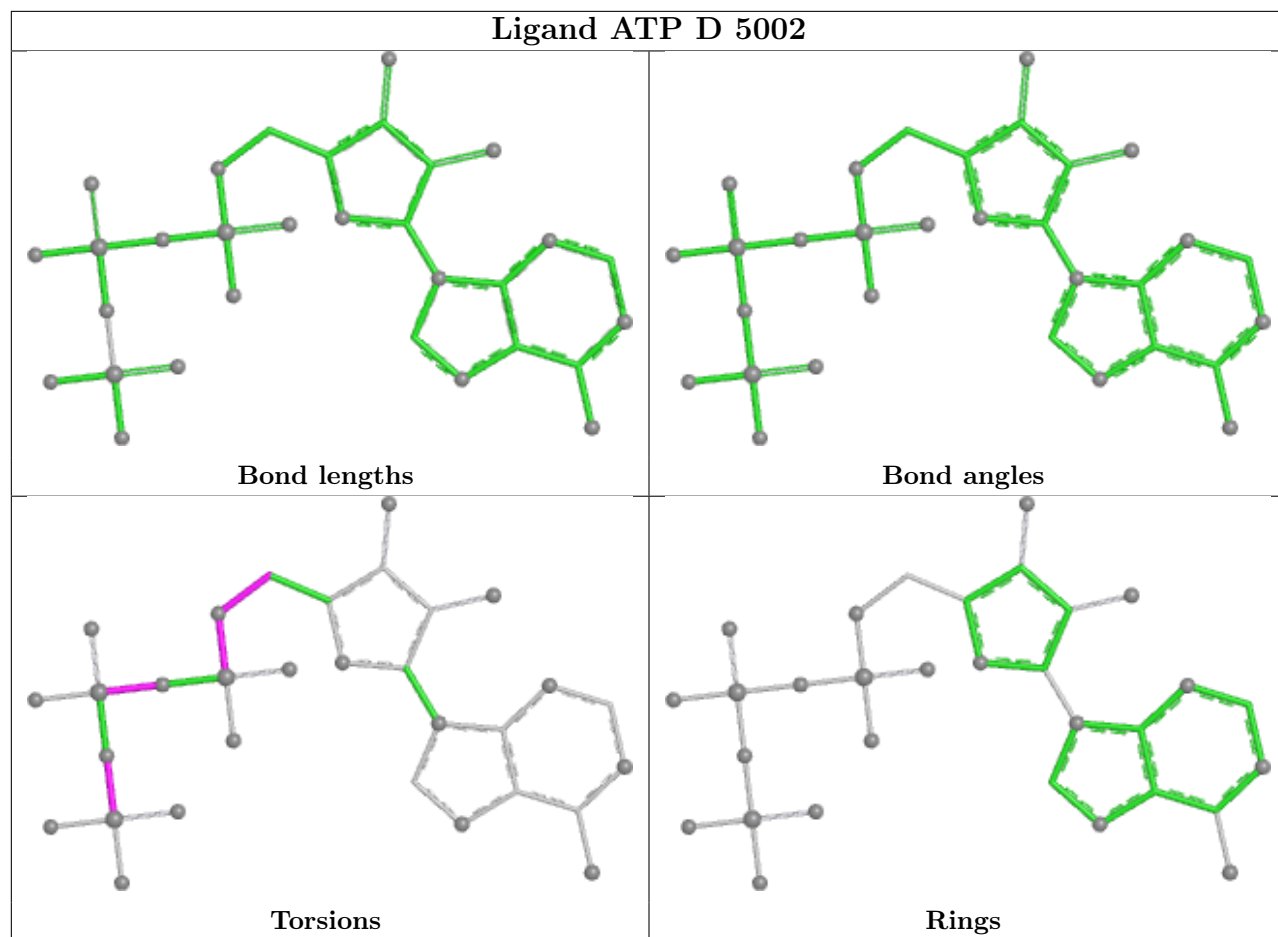
Bond angles



Torsions



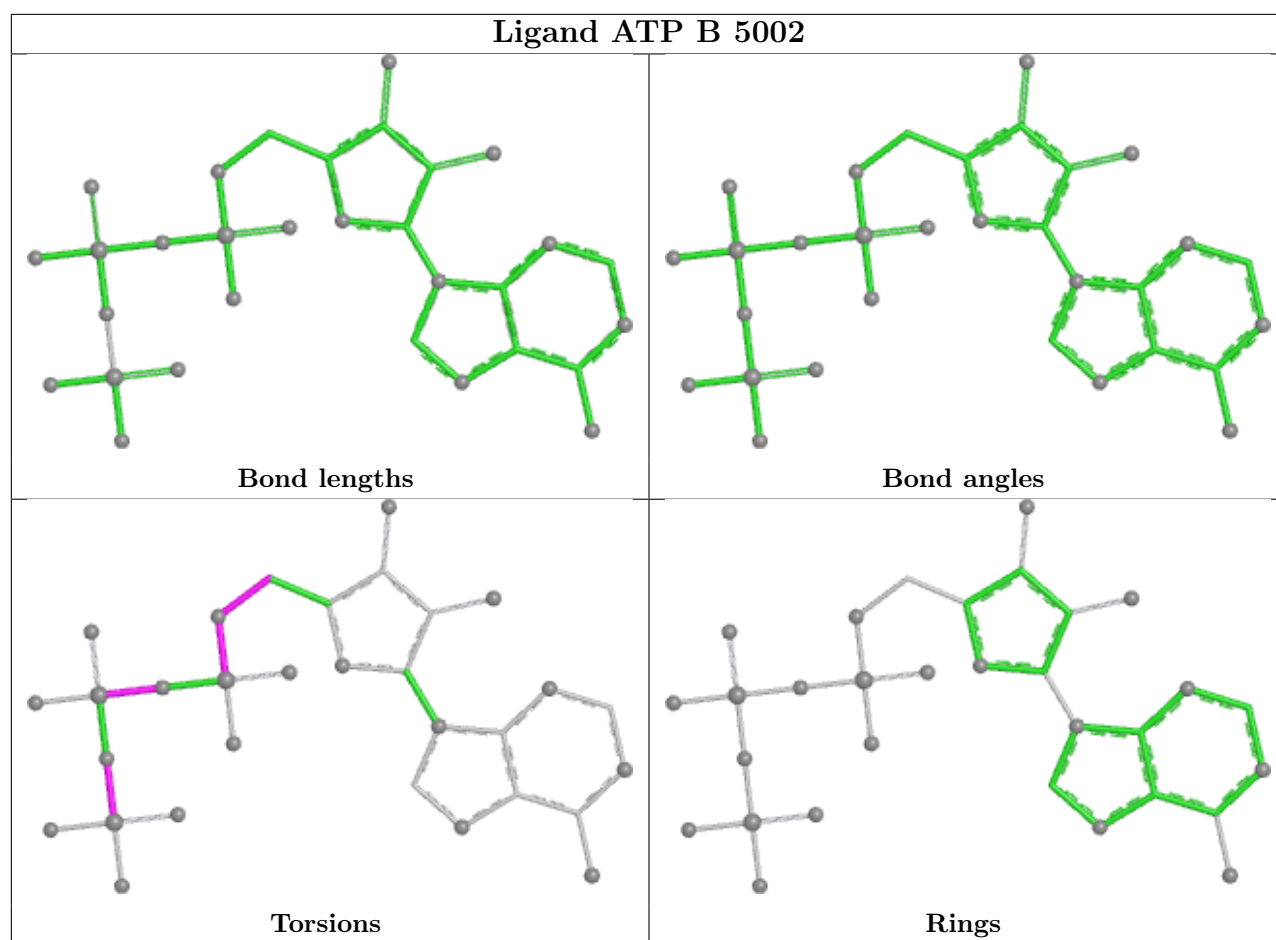
Rings



Ligand XAN B 5004

The figure displays four panels of structural analysis for Ligand XAN B 5004, which is a tricyclic molecule consisting of a benzene ring fused to a five-membered ring, which is further fused to another five-membered ring. The panels are arranged in a 2x2 grid:

- Bond lengths:** Shows the bond lengths of the molecule. The bonds are color-coded: green for the benzene ring, magenta for the five-membered ring, and grey for the other five-membered ring.
- Bond angles:** Shows the bond angles of the molecule. The bonds are color-coded: green for the benzene ring, magenta for the five-membered ring, and grey for the other five-membered ring.
- Torsions:** Shows the torsion angles of the molecule. The bonds are color-coded: green for the benzene ring, magenta for the five-membered ring, and grey for the other five-membered ring.
- Rings:** Shows the rings of the molecule. The bonds are color-coded: green for the benzene ring, magenta for the five-membered ring, and grey for the other five-membered ring.



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.

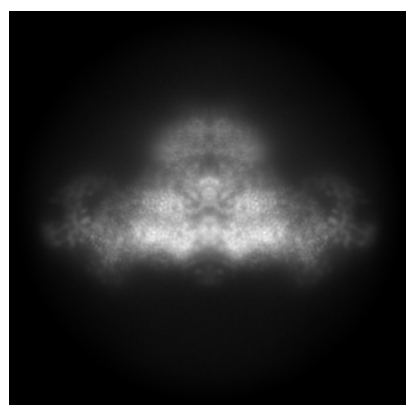
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26416. These allow visual inspection of the internal detail of the map and identification of artifacts.

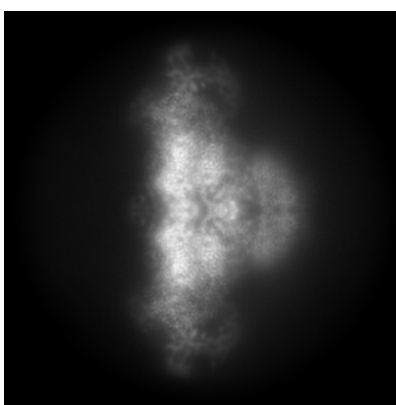
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

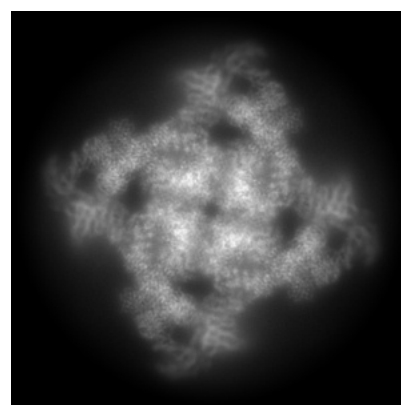
6.1.1 Primary map



X



Y

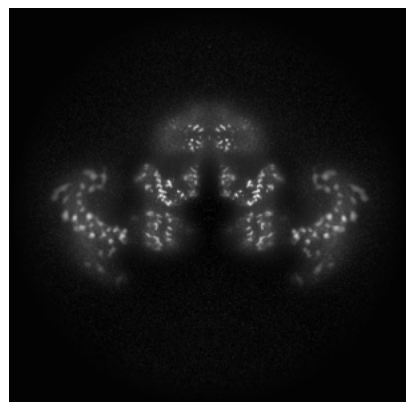


Z

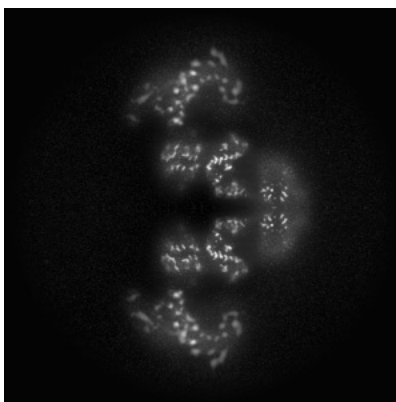
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

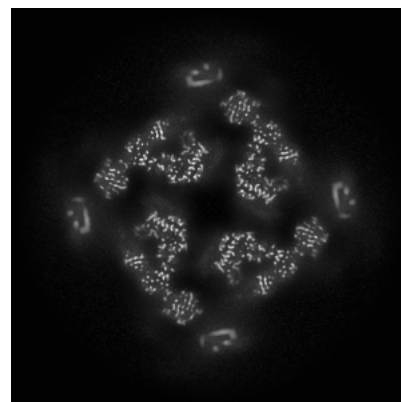
6.2.1 Primary map



X Index: 256



Y Index: 256

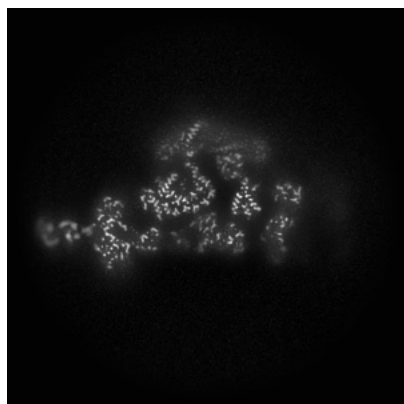


Z Index: 256

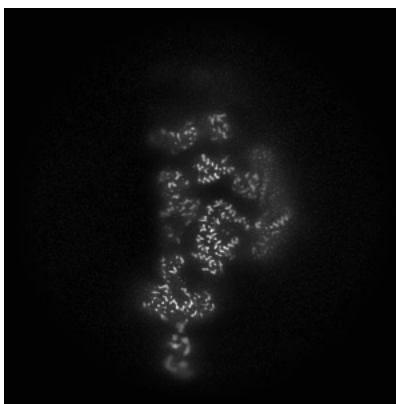
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

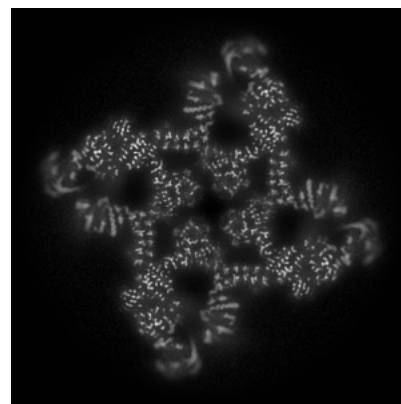
6.3.1 Primary map



X Index: 206



Y Index: 306

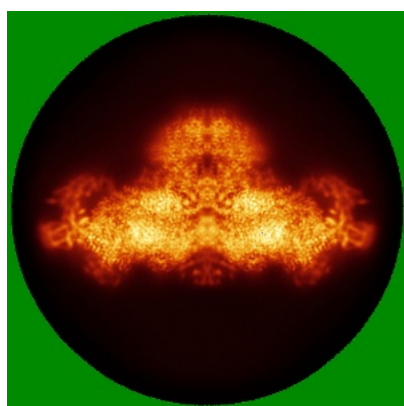


Z Index: 227

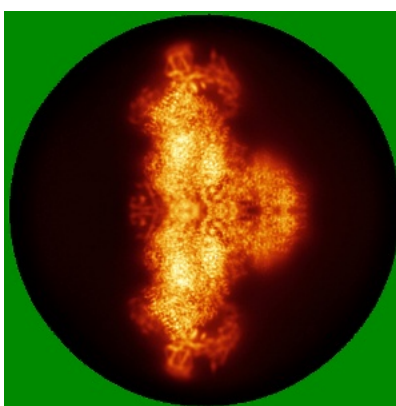
The images above show the largest variance slices of the map in three orthogonal directions.

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

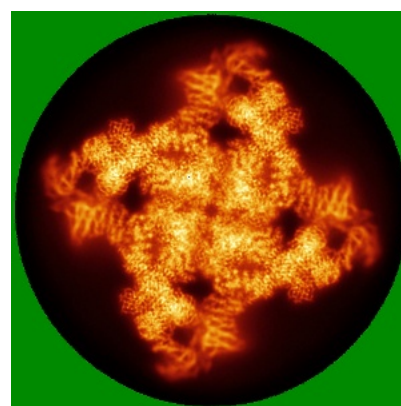
6.4.1 Primary map



X



Y

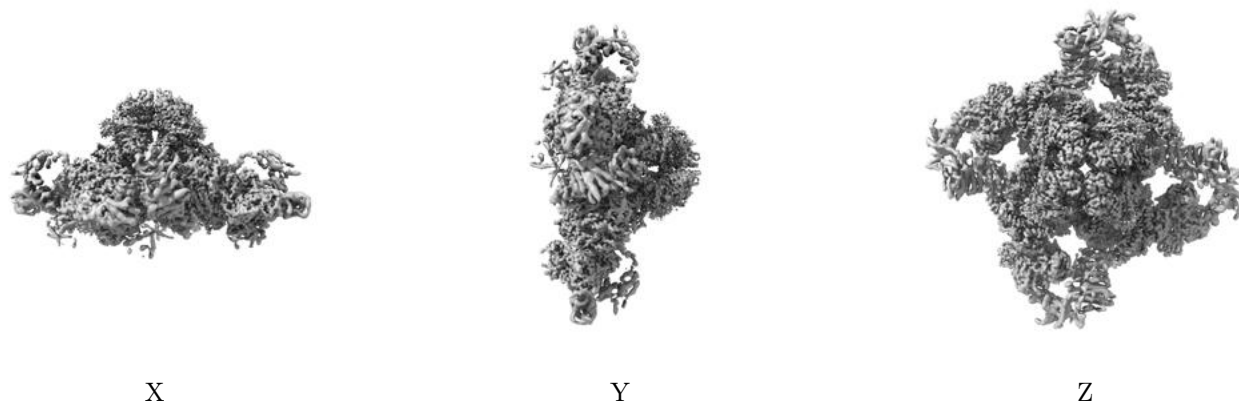


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

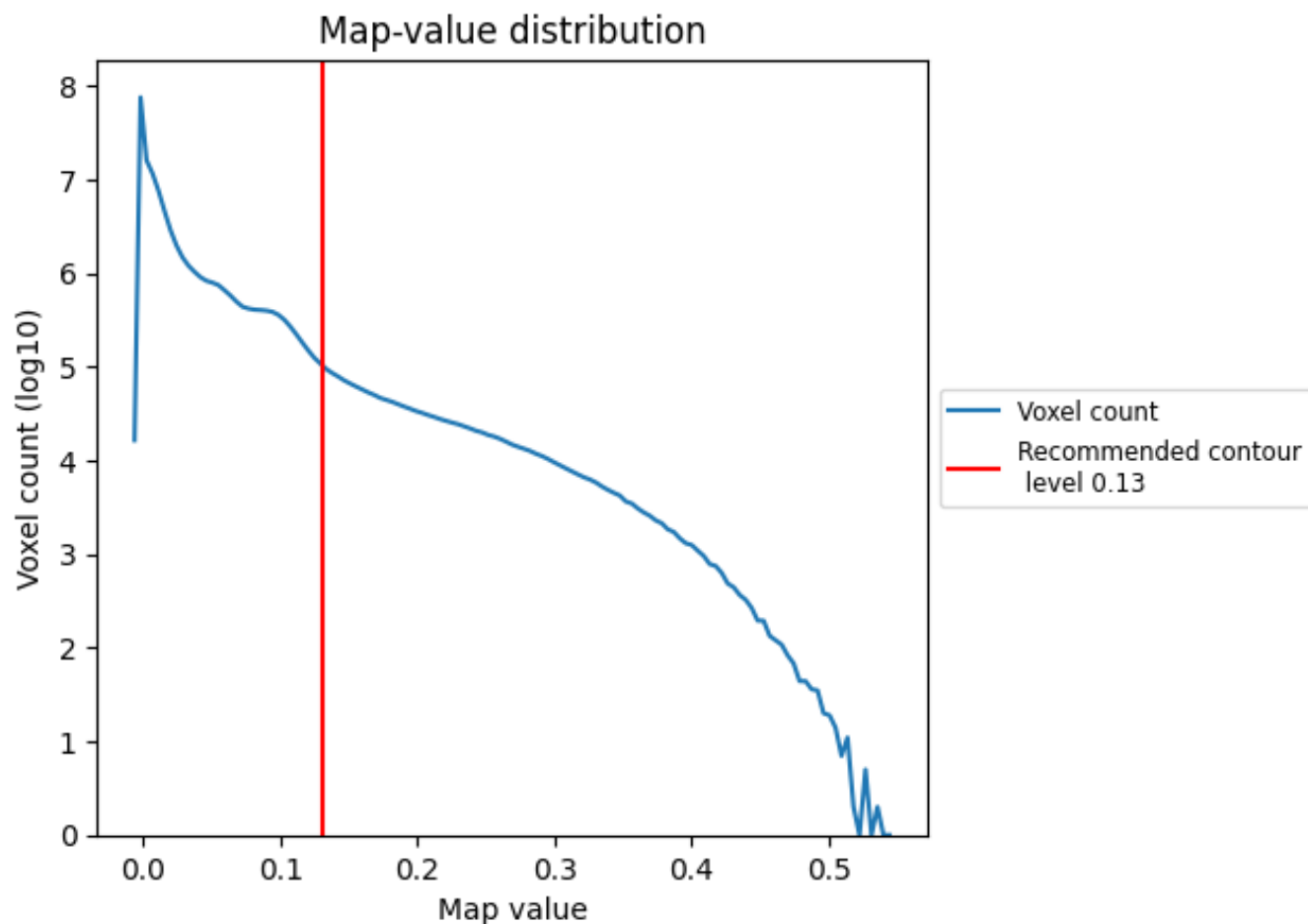
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

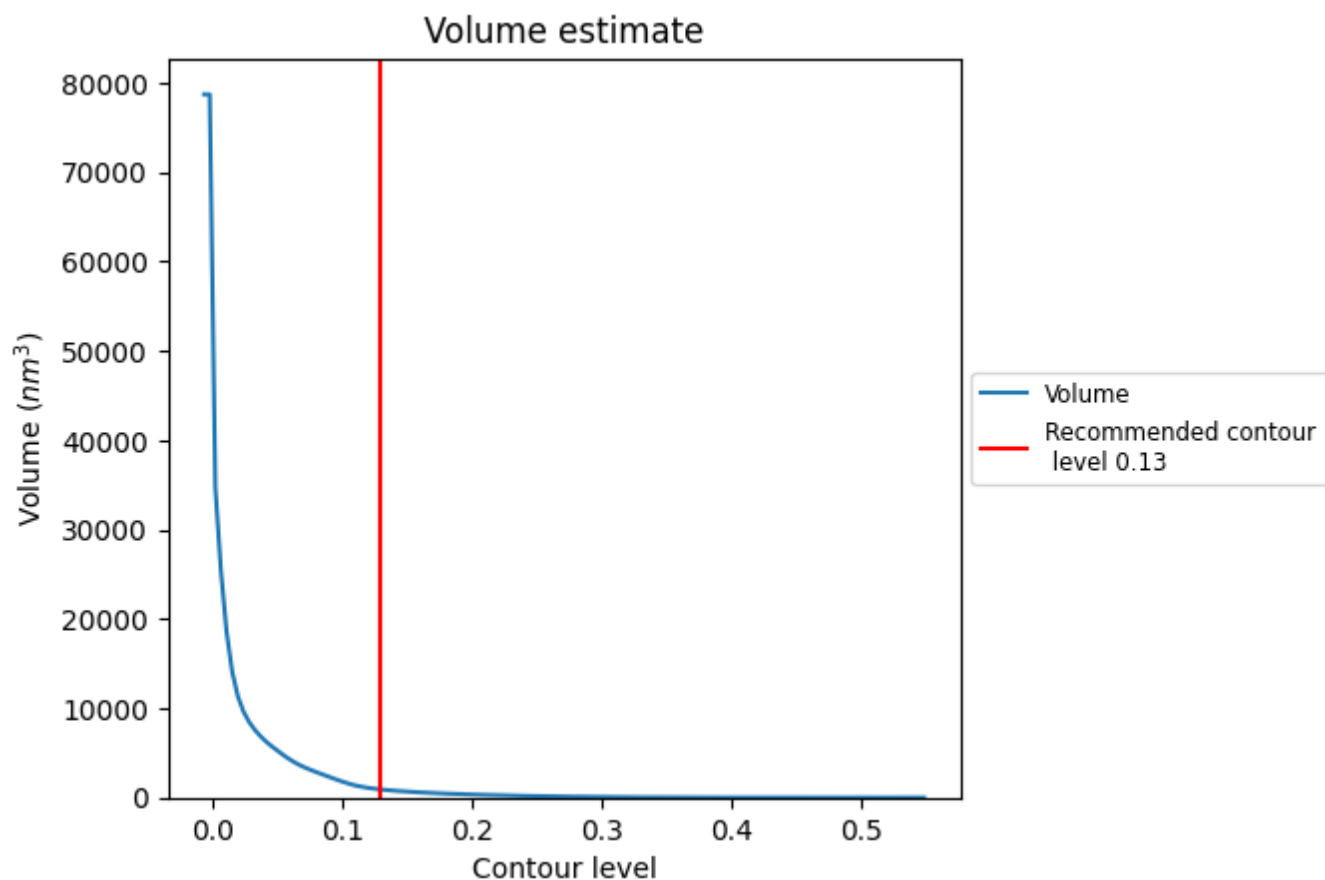
This section contains the results of statistical analysis of the map.

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.

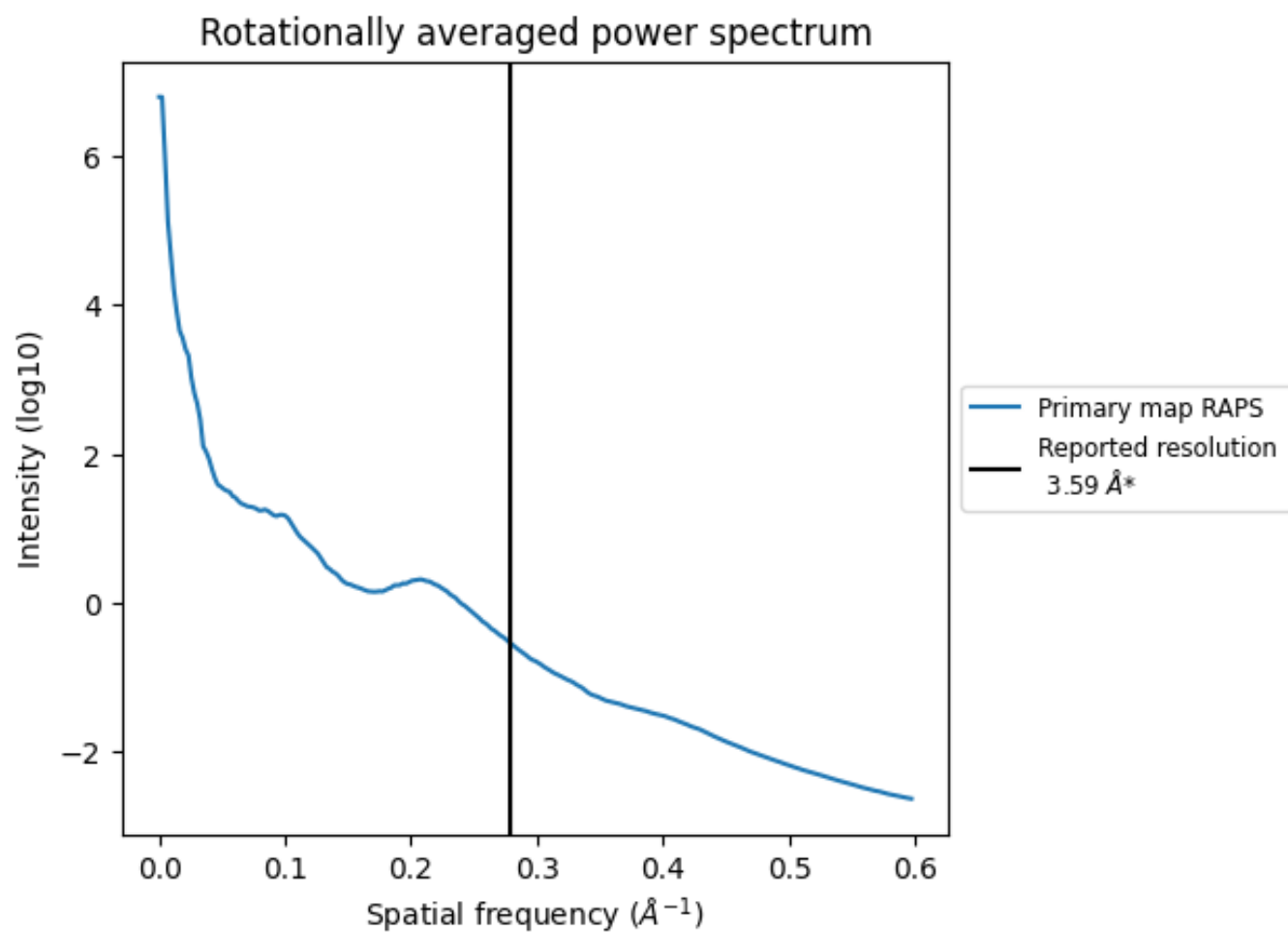
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 901 nm^3 ; this corresponds to an approximate mass of 814 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 0.279 Å⁻¹

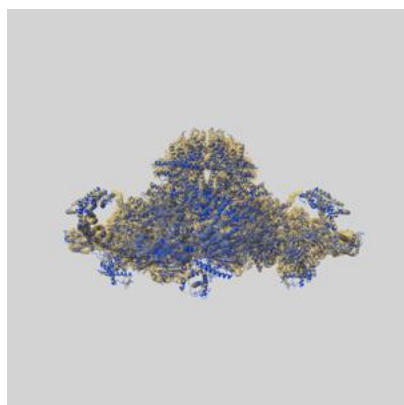
8 Fourier-Shell correlation ⓘ

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

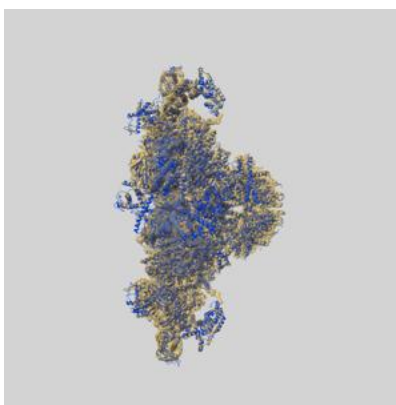
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26416 and PDB model 7UA9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

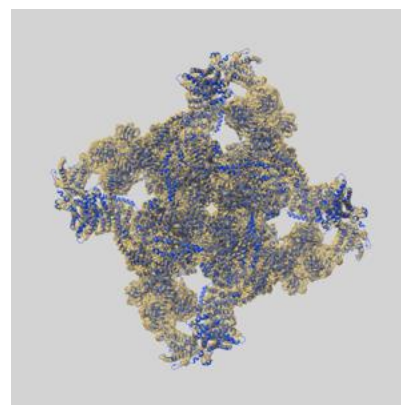
9.1 Map-model overlay [i](#)



X



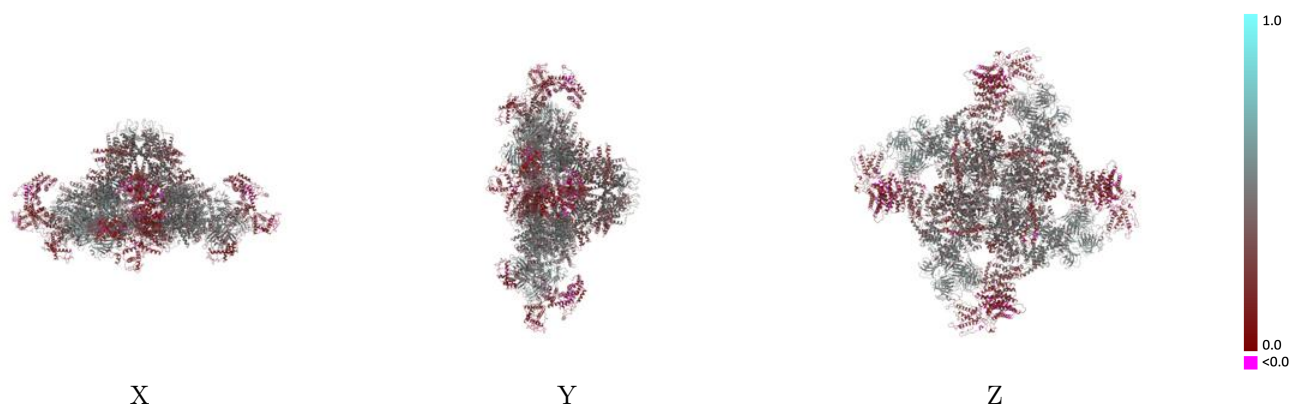
Y



Z

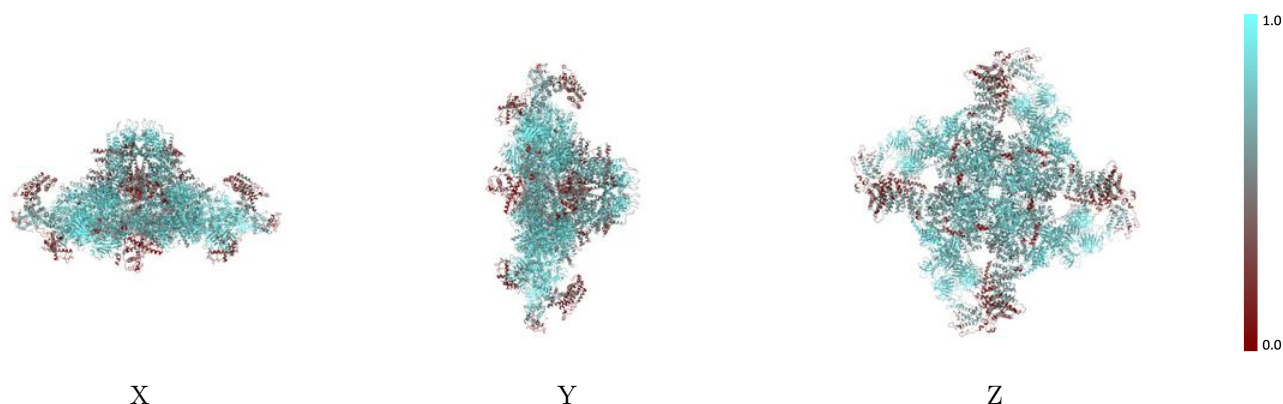
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



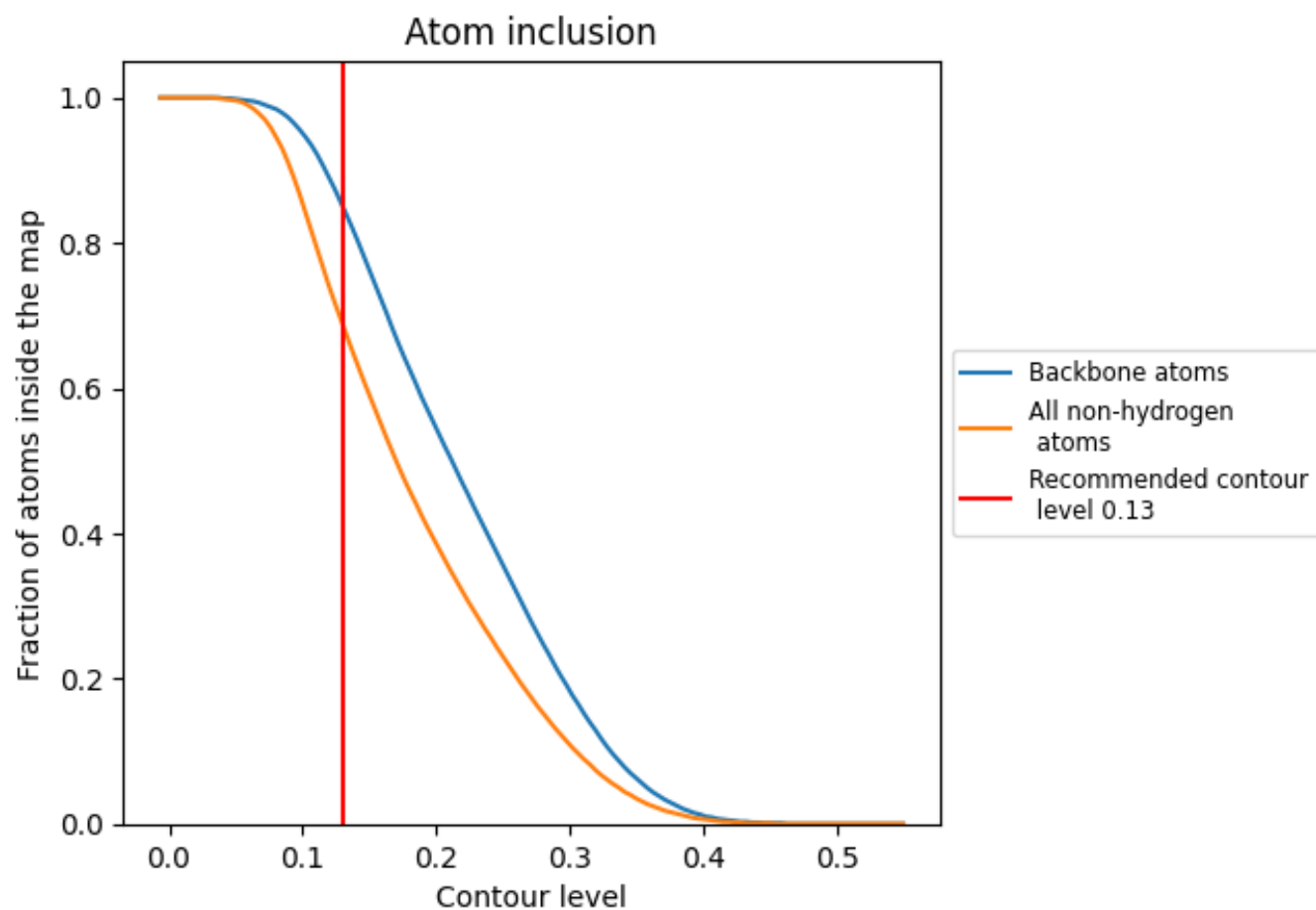
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 69% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.3670
A	0.6900	0.3740
B	0.6770	0.3560
C	0.6860	0.3720
D	0.6770	0.3530
E	0.8610	0.5070
F	0.8620	0.4990
G	0.8470	0.5000
H	0.8510	0.5010

1.0

0.0

<0.0