



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 10:43 pm BST

PDB ID : 3VKH
Title : X-ray structure of a functional full-length dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

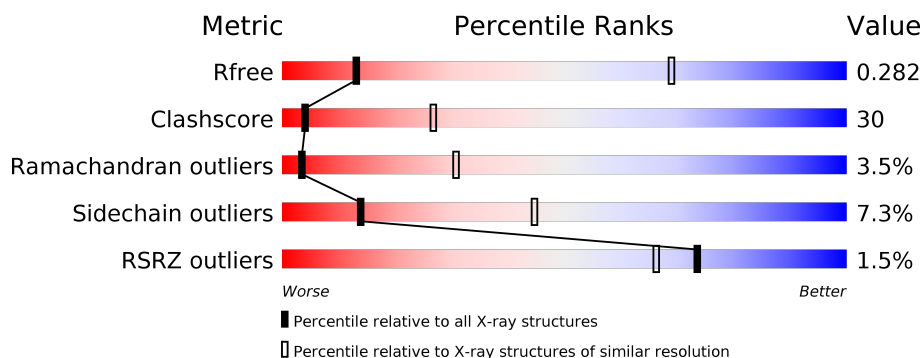
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3367	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>42%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	3367	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 45974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	3042	Total	C	N	O	S	0	0	0
			23374	14951	3955	4368	100			
1	B	2908	Total	C	N	O	S	0	0	0
			22384	14307	3792	4190	95			

There are 48 discrepancies between the modelled and reference sequences:

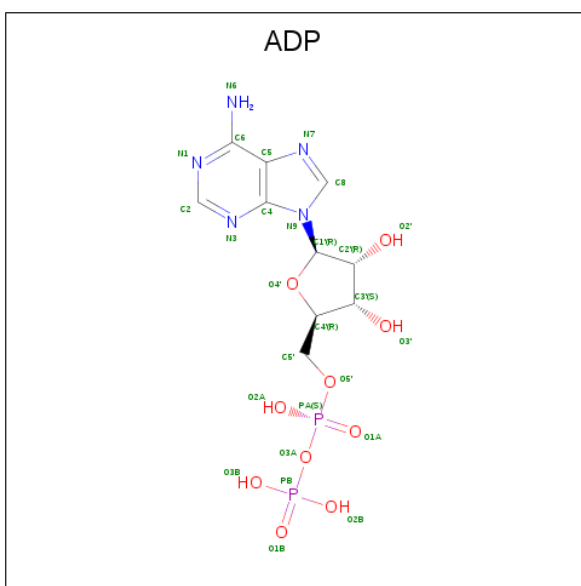
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION TAG	UNP P34036
A	1371	HIS	-	EXPRESSION TAG	UNP P34036
A	1372	HIS	-	EXPRESSION TAG	UNP P34036
A	1373	GLY	-	EXPRESSION TAG	UNP P34036
A	1374	GLY	-	EXPRESSION TAG	UNP P34036
A	1375	GLY	-	EXPRESSION TAG	UNP P34036
A	1376	ASP	-	EXPRESSION TAG	UNP P34036
A	1377	TYR	-	EXPRESSION TAG	UNP P34036
A	1378	LYS	-	EXPRESSION TAG	UNP P34036
A	1379	ASP	-	EXPRESSION TAG	UNP P34036
A	1380	ASP	-	EXPRESSION TAG	UNP P34036
A	1381	ASP	-	EXPRESSION TAG	UNP P34036
A	1382	ASP	-	EXPRESSION TAG	UNP P34036
A	1383	LYS	-	EXPRESSION TAG	UNP P34036
A	1384	GLY	-	EXPRESSION TAG	UNP P34036
A	1385	GLY	-	EXPRESSION TAG	UNP P34036
A	1386	GLY	-	EXPRESSION TAG	UNP P34036
A	1387	LYS	-	EXPRESSION TAG	UNP P34036
B	1364	MET	-	EXPRESSION TAG	UNP P34036

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1365	THR	-	EXPRESSION TAG	UNP P34036
B	1366	ARG	-	EXPRESSION TAG	UNP P34036
B	1367	HIS	-	EXPRESSION TAG	UNP P34036
B	1368	HIS	-	EXPRESSION TAG	UNP P34036
B	1369	HIS	-	EXPRESSION TAG	UNP P34036
B	1370	HIS	-	EXPRESSION TAG	UNP P34036
B	1371	HIS	-	EXPRESSION TAG	UNP P34036
B	1372	HIS	-	EXPRESSION TAG	UNP P34036
B	1373	GLY	-	EXPRESSION TAG	UNP P34036
B	1374	GLY	-	EXPRESSION TAG	UNP P34036
B	1375	GLY	-	EXPRESSION TAG	UNP P34036
B	1376	ASP	-	EXPRESSION TAG	UNP P34036
B	1377	TYR	-	EXPRESSION TAG	UNP P34036
B	1378	LYS	-	EXPRESSION TAG	UNP P34036
B	1379	ASP	-	EXPRESSION TAG	UNP P34036
B	1380	ASP	-	EXPRESSION TAG	UNP P34036
B	1381	ASP	-	EXPRESSION TAG	UNP P34036
B	1382	ASP	-	EXPRESSION TAG	UNP P34036
B	1383	LYS	-	EXPRESSION TAG	UNP P34036
B	1384	GLY	-	EXPRESSION TAG	UNP P34036
B	1385	GLY	-	EXPRESSION TAG	UNP P34036
B	1386	GLY	-	EXPRESSION TAG	UNP P34036
B	1387	LYS	-	EXPRESSION TAG	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

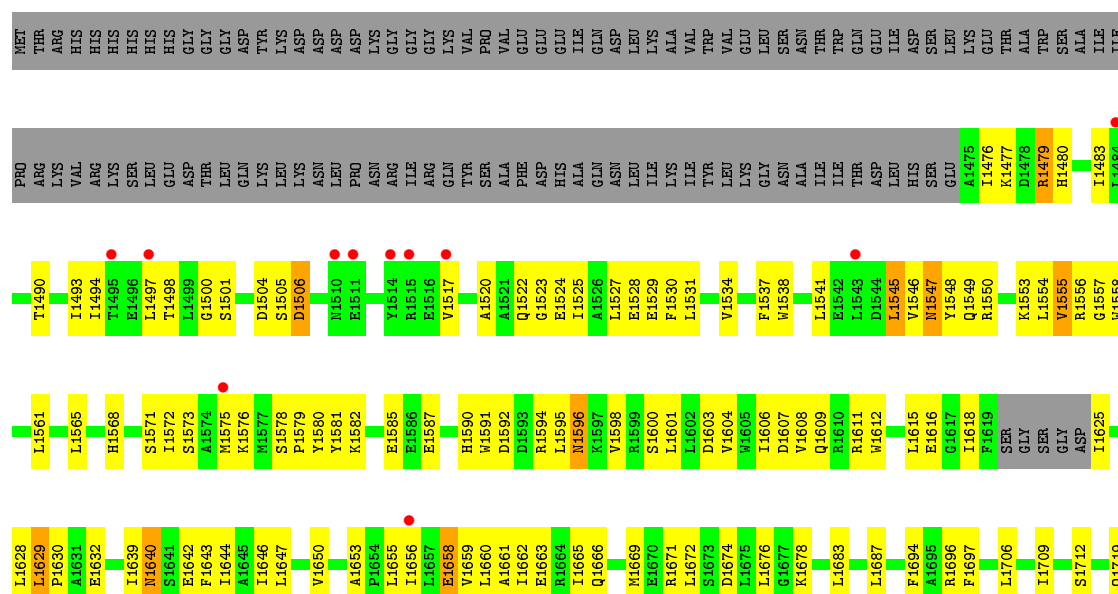
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

- Chain A: 29% 42% 42% 6% 10%

Index	Amino Acid	Chemical Structure
1	MET	
2	THR	
3	ARG	
4	HIS	
5	HIS	
6	HIS	
7	HIS	
8	GLY	
9	GLY	
10	ASP	
11	THR	
12	LEU	
13	GLN	
14	TYR	
15	LEU	
16	LYS	
17	ASP	
18	ASP	
19	ASP	
20	LYS	
21	LYS	
22	GLY	
23	GLY	
24	LYS	
25	VAL	
26	SER	
27	PRO	
28	VAL	
29	PHE	
30	GLU	
31	GLU	
32	GLU	
33	ILE	
34	GLN	
35	ASN	
36	LEU	
37	LYS	
38	ALA	
39	ILE	
40	VAL	
41	THR	
42	TRP	
43	GLN	
44	THR	
45	ASP	
46	LEU	
47	ILE	
48	ASP	
49	HIS	
50	SER	
51	ASN	
52	ALA	
53	ILE	
54	THR	
55	ALA	
56	THR	
57	ILE	
58	LYS	
59	THR	
60	ALA	
61	ASP	
62	ARG	
63	THR	
64	TRP	
65	SER	
66	LEU	
67	GLU	
68	ILE	
69	LYS	
70	THR	

L3108	R3027	R2948	H2871	V2769	L2710	K2627	N2547	M2394	T2323	V2250	P2169	K2098
K3109	F3028	P2949	Y2872	G2790	L2711	K2628	V2648	F2396	T2324	T2251	GLN	A2099
		L2950	L2873	A2791	K2712	N2629	L2549	E2396		K2252	LEU	T2101
C3112	M3032	L2951	C2792	C2792	T2713	K2630	Y2551	V2397	W2327		PRO	P2103
K3113	N3033	Y2952	R2876	N2793		VAL	Y2552	Q2398	T2328	V2255	PRO	D2102
K3114	G3034	S2953	R2877	P2794	Y2720	PRQ		L2400	D2329	E2257	ILE	D2104
T3115	L3035	N2954				SER		K2401	F2332	K2258	THR	D2105
A3116	S3036	W2955	S2880	A2798	E2727	V2634	M2560	Y2402	D2176	L2259		E2106
Q3117	L2956	G2799	R2881	G2799	T2728		S2561	A2403	A2177	L2261		E2107
K3118	W2882	R2800	W2882	V2729	L2730	A2642	P2562		E2178	Q2260		L2108
	D2883	R2806		L2731	R2731	S2643	E2563	Q2408	S2179	Q2261		
L3121	L2886	P2807	L2886	P2732		S2644	Q2564	S2409		L2262		A2109
L3122	L2887	L2808				D2645	Q2565	R2410		L2263		Q2110
L3123		L2809				D2646	T2570	C2411		Q2264		Y2190
		F2807				D2647	R2571	G2412		L2265		V2194
F3133		L2808				L2648	T2572	M2413		L2266		L2195
		L2813				T2649	R2573	W2414				L2196
Q3136	L2814	L2815				T2650	L2574	W2415		N2269		L2197
V3137	L2816	L2817				D2651	Y2575	Q2424		G2271		F2118
V3138	L2818	L2819				D2652		M2426		V2272		T2120
R3139	L2820	L2821				D2653	W2578	L2426		N2273		N2200
K3140	L2822	L2823				T2654	W2579			N2274		D2201
K3141	L2824	L2825				T2655	G2580			V2275		E2121
K3142	L2826	L2827				T2656	L2581					N2202
K3143	L2828	L2829				K2656	L2582					Q2203
V3144	L2830	L2831				V2657	G2583					L2204
F3145	L2832	L2833				D2658	Q2494					L2124
F3146	L2834	L2835				V2659	Q2495					A2125
N3147	L2836	L2837				D2660	L2501					K2206
N3148	L2838	L2839				D2661	L2502					L2207
K3149	L2840	L2841				D2662	Y2505					P2205
K3150	L2842	L2843				D2663	F2506					K2282
K3151	L2844	L2845				D2664	E2507					G2126
K3152	L2846	L2847				D2665	P2508					L2207
D3153	L2848	L2849				D2666	L2511					L2208
F3154	L2850	L2851				D2667	V2512					L2211
K3155	L2852	L2853				D2668	L2525					L2212
K3156	L2854	L2855				D2669	L2526					P2213
	L2856	L2857				D2670	D2527					L2214
	L2858	L2859				D2671	F2528					K2133
	L2860	L2861				D2672	T2529					G2135
	L2862	L2863				D2673	R2530					Q2136
	L2864	L2865				D2674	L2531					E2137
	L2866	L2867				D2675	L2532					Q2138
	L2868	L2869				D2676	L2533					L2139
	L2870	L2871				D2677	L2534					S2140
	L2872	L2873				D2678	L2535					D2221
	L2874	L2875				D2679	L2536					Q2141
	L2876	L2877				D2680	L2537					P2223
	L2878	L2879				D2681	L2538					S2143
	L2880	L2881				D2682	L2539					H2144
	L2882	L2883				D2683	L2540					Y2145
	L2884	L2885				D2684	L2541					D2146
	L2886	L2887				D2685	L2542					F2147
	L2888	L2889				D2686	L2543					G2148
	L2890	L2891				D2687	L2544					L2149
	L2892	L2893				D2688	L2545					K2150
	L2894	L2895				D2689	L2546					L2151
	L2896	L2897				D2690	L2547					K2152
	L2898	L2899				D2691	L2548					L2153
	L2900	L2901				D2692	L2549					V2154
	L2902	L2903				D2693	L2550					L2155
	L2904	L2905				D2694	L2551					V2156
	L2906	L2907				D2695	L2552					L2157
	L2908	L2909				D2696	L2553					K2163
	L2910	L2911				D2697	L2554					
	L2912	L2913				D2698	L2555					
	L2914	L2915				D2699	L2556					
	L2916	L2917				D2700	L2557					
	L2918	L2919				D2701	L2558					
	L2920	L2921				D2702	L2559					
	L2922	L2923				D2703	L2560					
	L2924	L2925				D2704	L2561					
	L2926	L2927				D2705	L2562					
	L2928	L2929				D2706	L2563					
	L2930	L2931				D2707	L2564					
	L2932	L2933				D2708	L2565					
	L2934	L2935				D2709	L2566					
	L2936	L2937				D2710	L2567					
	L2938	L2939				D2711	L2568					
	L2940	L2941				D2712	L2569					
	L2942	L2943				D2713	L2570					
	L2944	L2945				D2714	L2571					
	L2946	L2947				D2715	L2572					
	L2948	L2949				D2716	L2573					
	L2950	L2951				D2717	L2574					
	L2952	L2953				D2718	L2575					
	L2954	L2955				D2719	L2576					
	L2956	L2957				D2720	L2577					
	L2958	L2959				D2721	L2578					
	L2960	L2961				D2722	L2579					
	L2962	L2963				D2723	L2580					
	L2964	L2965				D2724	L2581					
	L2966	L2967				D2725	L2582					
	L2968	L2969				D2726	L2583					
	L2970	L2971				D2727	L2584					
	L2972	L2973				D2728	L2585					
	L2974	L2975				D2729	L2586					
	L2976	L2977				D2730	L2587					
	L2978	L2979				D2731	L2588					
	L2980	L2981				D2732	L2589					
	L2982	L2983				D2733	L2590					
	L2984	L2985				D2734	L2591					
	L2986	L2987				D2735	L2592					
	L2988	L2989				D2736	L2593					
	L2990	L2991				D2737	L2594					
	L2992	L2993				D2738	L2595					
	L2994	L2995				D2739	L2596					
	L2996	L2997				D2740	L2597					
	L2998	L2999				D2741	L2598					
	L3000	L3001				D2742	L2599					
	L3002	L3003				D2743	L2600					
	L3004	L3005				D2744	L2601					
	L3006	L3007				D2745	L2602					
	L3008	L3009				D2746	L2603					
	L3010	L3011				D2747	L2604					
	L3012	L3013				D2748	L2605					
	L3014	L3015				D2749	L2606					
	L3016	L3017				D2750	L2607					
	L3018	L3019				D2751	L2608					
	L3020	L3021				D2752	L2609					
	L3022	L3023				D2753	L2610					
	L3024	L3025				D2754	L2611					
	L3026	L3027				D2755	L2612					
	L3028	L3029				D2756	L2613					
	L3030	L3031				D2757	L2614					
	L3032	L3033				D2758	L2615					
	L3034	L3035				D2759	L2616					
	L3036	L3037				D2760	L2617					
	L3038	L3039				D2761	L2618					
	L3040	L3041				D2762	L2619					
	L3042	L3043				D2763	L2620					
	L3044	L3045				D2764	L2621					
	L3046	L3047				D2765	L2622					
	L3048	L3049				D2766	L2623					
	L3050	L3051				D2767	L2624					
	L3052	L3053				D2768	L2625					
	L3054	L3055				D2769	L2626					
	L3056	L3057				D2770	L2627					
	L3058	L3059				D2771	L2628					
	L3060	L3061				D2772	L2629					
	L3062	L3063				D2773	L2630					
	L3064	L3065				D2774	L2631					
	L3066	L3067				D2775	L2632					
	L3068	L3069				D2776	L2633					
	L3070	L3071				D2777	L2634					
	L3072	L3073				D2778	L2635					
	L3074	L3075				D2779	L2636					
	L3076	L3077				D2780	L2637					
	L3078	L3079										

G4054	E4120	L3991	F3911	N3836	R3767	F3911	F3704	F3628	S3551	T3482	E3418	R3342	H3259	E3187
E4055	I4121	L3992	S3912	A3837	D3768	S3912	F3704	A3837	K3552	A3837	K3419	R3342	Y3260	
P4056	E4122	K3993	L3913	A3841	A3771	L3913	N3707	S3630	V3553	Q3484		Q3345	D3262	R3190
I4057	E4123	G3994	R3914	A3842				V3634	K3554	T3485	T3422	V3346	L3261	
P4059	E4124	G3995	A3915	G3843	T3774	A3915	A3711	V3635	N3555	Y3486	K3424	D3349	L3264	L3192
E4060	V4126	N3997	F3916	N3844	P3775	F3916	L3712	P3635	V3557	Y3487	K3425	V3350	N3265	E3195
S4061	E4127	L3998	L3917	L3845	D3776	L3917	G3715	L3638	D3558	S3488	K3426	K3353	V3266	R3196
W4062	S4128	L3999	D3918	L3846			C3715	S3639	K3559	L3489	P3427		P3197	
W4063	S4129	F3920	L3919	D3847	S3779	S3921	C3716	E3643	S3560	ASP	E3428	V3357	V3267	
V4064	I4001	S4000	F3920	D3848	V3781	F3921	P3717	E3643	K3561	ARG	K3430	V3358	K3198	
A4065	K4002	L3922	N3922	D3849	V3782	N3922	L3719	K3647	A3562	ILE	K3431	K3359	L3270	I3200
Q4066	E4003	L3923	L3923	S3850	T3783	L3923	V3720	H3648	L3563	LYS	L3432	V3360	L3271	A3201
A4067	T4004	L3924	L3924	V3851	F3783	Q3794	Q3721		L3564		T3433	K3361		P3202
Q4068	L4005	N3925	N3925	T3854	N3784		G3715	L3652	D3565	PRD	T3433			
L4069	P4006	N3926	N3926	L3855	N3785	L3798	C3716	P3653	N3566	LEU	S3434		F3205	F3206
S4070	Q4007	N3927	N3927	L3856	F3786		E3724	S3654	K3567	ARG	K3435	D3365	K3275	
N4071	L4008	N3927	N3927	L3857	T3787		N3725	S3655	N3568	GLU	L3436	L3366	L3278	A3209
Q4072	L4011	L3930	L3930	L3858	V3788		I3726	D3655	S3569	GLU	K3437	E3367	E3281	
Q4073	L4012	K3933	K3933	K3859	T3789		D3727	C3858	R3571	GLU	T3438	K3368	E3210	
S4074	L4012	K3933	K3933	K3859	P3790		I3727	I3659	E3571	GLN	T3440	A3369	Q3282	I3211
T4075	S4013	R3939	R3939	T3862	S3791		V3729			LEU	K3441	P3371	L3283	GLY
I4076	T4014	K3939	K3939	T3863	S3792		V3729			LEU	K3441	P3371	H3284	ASN
V4077	T4015	L3943	L3943	E3864	L3793		L3730			GLU	K3442	A3372	L3285	
S4078	Q4016	L3943	L3943	E3865	Q3794		N3731			ASN	K3443	A3373		
N4079	Q4017	L3943	L3943	E3866	Q3794		P3732			ALA	K3444	I3374	L3216	
F4080	Q4018	T3947	T3947	L3867	L3798		V3733			ALA	T3445	A3375	L3217	
R4081	W4019	F3948	F3948	K3868	L3799		L3734			ASN	P3446	A3376	K3291	A3218
K4082	L4020	N3951	N3951	V3869			N3735			GLU	P3446	A3376	L3219	L3292
I4083	I4021	T3951	T3951	V3870			N3735			LEU	K3449	V3380	P3220	P3220
C4022	Q4022	F3952	F3952	V3875			K3736			LEU	K3450	S3381	P3221	P3221
L4023	L4023	N3953	N3953	V3875			GLU			K3512	K3451		E3296	
R4024	R4024	K3954	K3954	E3878			ILE			K3513	A3451		K3284	
Q4025	Q4025	V3955	V3955	E3879			ARG			K3514	T3452		D3225	
Q4026	Q4026	V3956	V3956	E3880			LVS			K3515	T3453		V3299	
H4090	V4027	L3959	L3959	V3882			GLY			D3516	K3454		K3386	A3226
P4028	P4028	L3959	L3959	V3882			GLY			E3517	K3455		H3387	
D4028	D4028	L3959	L3959	V3882			ARG			K3518	K3456		K3309	S3229
F4030	F4030	N3961	N3961	V3886			ILE			I3517	L3457		D3389	S3230
S4031	S4031	K3964	K3964	V3887			ILE			T3521	E3458		L3313	Y3233
K4032	K4032	L3965	L3965	P3888			LEU				D3459		D3314	Y3233
L4033	L4033	L3965	L3965	M3889			ILE			L3525	P3460		V3315	I3234
W4034	W4034	L3969	L3969	A3890			ARG			S3528	K3461		Q3319	T3237
D4035	D4035	L3969	L3969	A3891			LEU			L3529	F3462		T3238	T3238
H4036	H4036	L3969	L3969	S3892			GLY			A3530	D3463		G3239	G3239
Q4039	Q4039	S3975	S3975	S3893			ASP			Y3532			K3323	E3240
N4040	N4040	V3976	V3976	S3894			ASP			K3533	V3467		L3324	
D4043	D4043	K3977	K3977	S3895			VAL				R3468		V3328	A3241
W4044	W4044	T3979	T3979	V3897			ASP			K3536	K3469		K3329	R3243
F4046	F4046	N3981	N3981	F3898			PHE				A3470		D3330	R3244
F4047	F4047	N3981	N3981	F3898			SER				S3471		Q3331	L3245
F4048	F4048	E3955	E3955	E3902							K3472		A3334	Q3249
G4049	G4049	S3986	S3986	L3903							A3473		E3335	
K4050	K4050	E3987	E3987	L3904							C3474		E3335	
D4051	D4051	R3988	R3988	S3904							G3475		C3409	
Q4052	Q4052	L3989	L3989	R3905							P3476		L3337	N3254
A4119	A4119	F3990	F3990	Q3910							V3478		Q3338	V3255
											K3479		K3339	V3256
											L3700		D3340	P3257
											A3481		A3341	A3258









4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.78 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.0 (48.78-3.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.292 0.211 , 0.282	Depositor DCC
R_{free} test set	4469 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.24	0/23866	0.44	1/32482 (0.0%)
1	B	0.24	0/22846	0.43	0/31076
All	All	0.24	0/46712	0.44	1/63558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3371	PRO	N-CA-CB	5.32	109.68	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23374	0	22545	1559	0
1	B	22384	0	21550	1149	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2704	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 30.

The worst 5 of 2704 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:A:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00

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 X-ray entries followed by that with respect to entries of similar resolution.

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	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	2	24
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	6	38
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	3	31

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1836	LEU
1	A	2121	ALA
1	A	2409	SER
1	A	2560	MET
1	A	2617	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	2457/3028 (81%)	2249 (92%)	208 (8%)	10	40
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	18	50
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	14	45

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3925	ASN
1	A	4565	ILE
1	B	4258	THR
1	A	4023	LEU
1	A	4267	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4046	GLN
1	A	4715	ASN
1	B	4152	GLN
1	A	4079	ASN
1	A	4349	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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
2	ADP	B	9009	-	24,29,29	1.25	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	B	9007	-	24,29,29	1.23	3 (12%)	29,45,45	1.54	5 (17%)
2	ADP	A	9001	-	24,29,29	1.26	3 (12%)	29,45,45	1.57	5 (17%)
2	ADP	B	9010	-	24,29,29	1.24	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	B	9008	-	24,29,29	1.23	3 (12%)	29,45,45	1.55	5 (17%)
2	ADP	A	9004	-	24,29,29	1.23	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9002	-	24,29,29	1.23	2 (8%)	29,45,45	1.56	5 (17%)
2	ADP	A	9003	-	24,29,29	1.26	3 (12%)	29,45,45	1.56	5 (17%)

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
2	ADP	B	9009	-	-	5/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	4/12/32/32	0/3/3/3
2	ADP	A	9001	-	-	5/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	6/12/32/32	0/3/3/3
2	ADP	B	9008	-	-	2/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	3/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	5/12/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	2.99	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9008	ADP	C5-C4	2.95	1.48	1.40
2	B	9009	ADP	C5-C4	2.93	1.48	1.40
2	A	9003	ADP	C5-C4	2.93	1.48	1.40
2	B	9010	ADP	C5-C4	2.91	1.48	1.40

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9004	ADP	N3-C2-N1	-4.33	121.91	128.68
2	A	9003	ADP	N3-C2-N1	-4.30	121.96	128.68
2	B	9007	ADP	N3-C2-N1	-4.29	121.97	128.68
2	B	9010	ADP	N3-C2-N1	-4.27	122.00	128.68
2	A	9001	ADP	N3-C2-N1	-4.27	122.00	128.68

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9007	ADP	C5'-O5'-PA-O3A
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	B	9010	ADP	C5'-O5'-PA-O2A
2	A	9003	ADP	C5'-O5'-PA-O1A

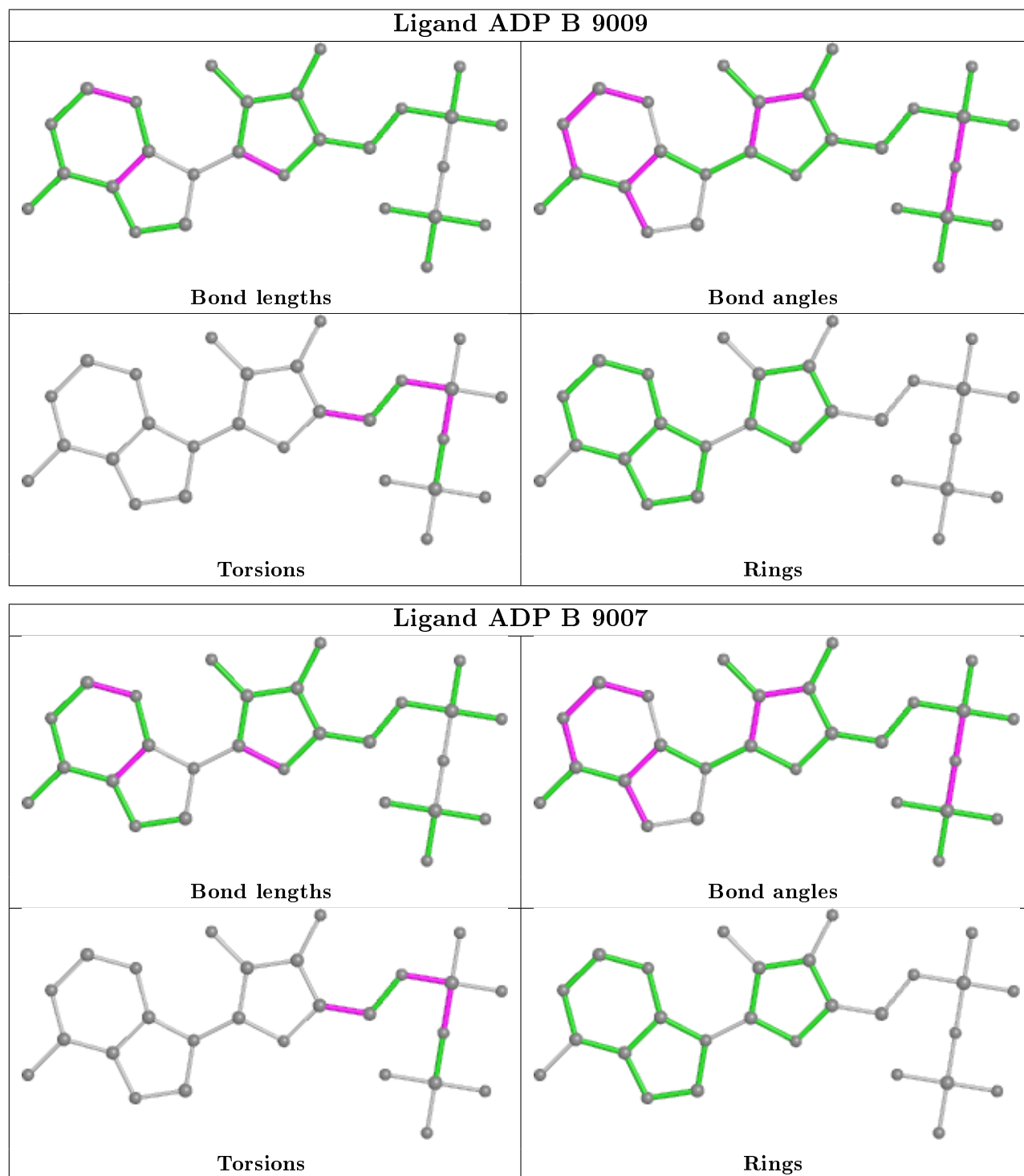
There are no ring outliers.

5 monomers are involved in 10 short contacts:

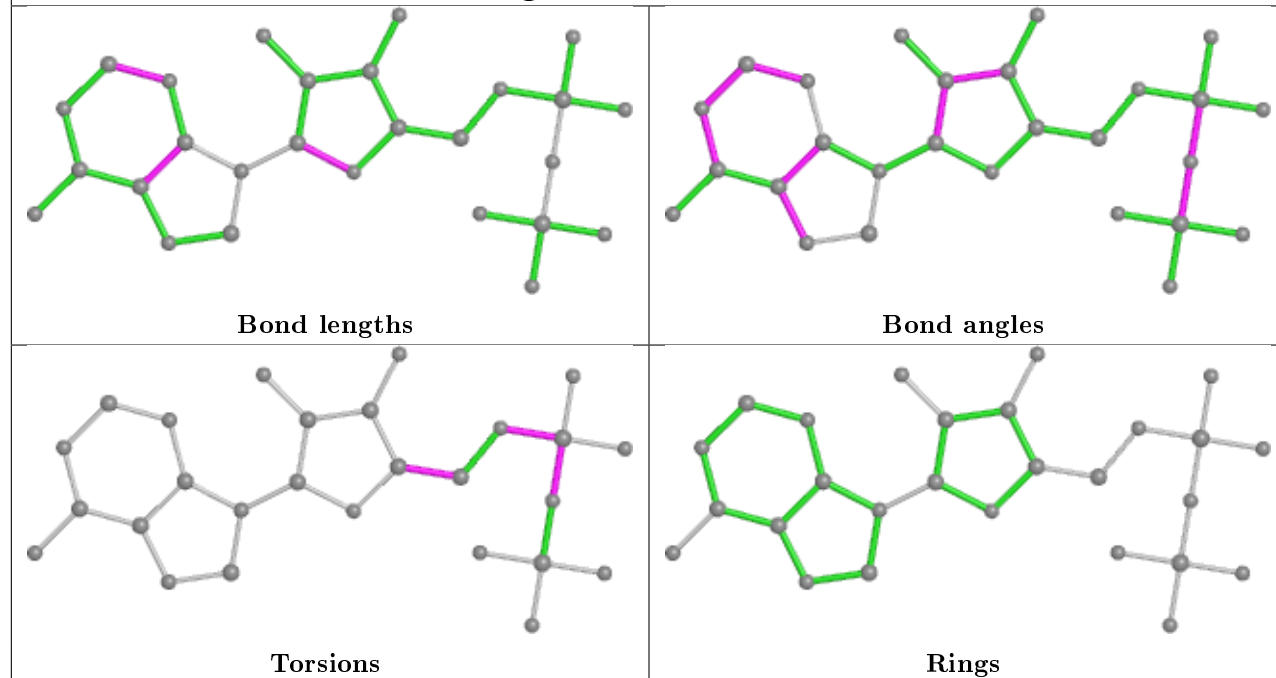
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9009	ADP	1	0
2	A	9001	ADP	1	0
2	B	9010	ADP	2	0
2	A	9004	ADP	2	0
2	A	9002	ADP	4	0

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

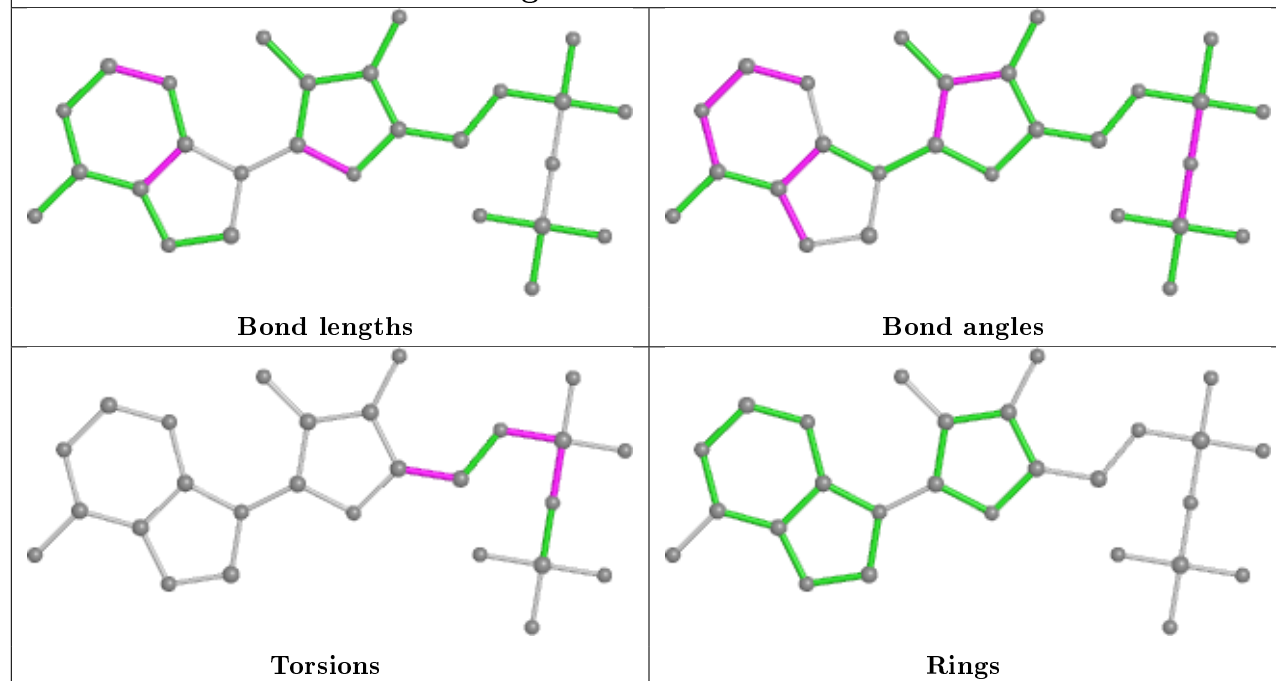
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



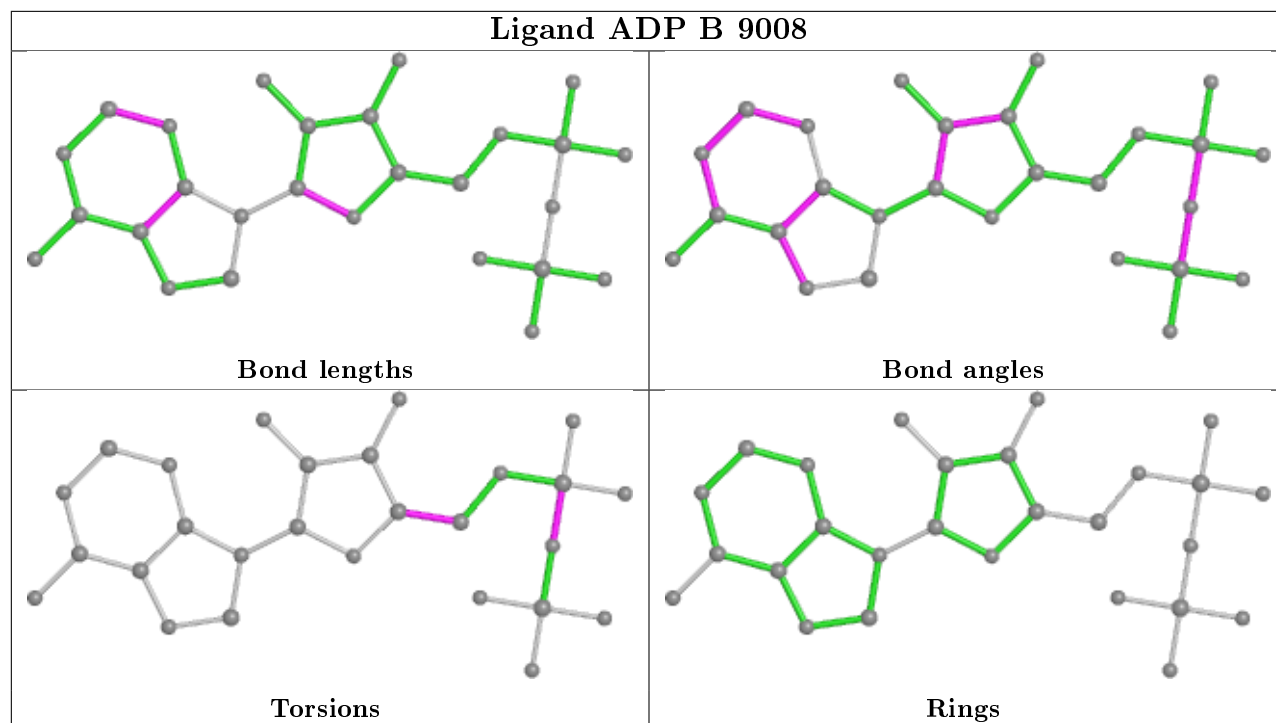
Ligand ADP A 9001



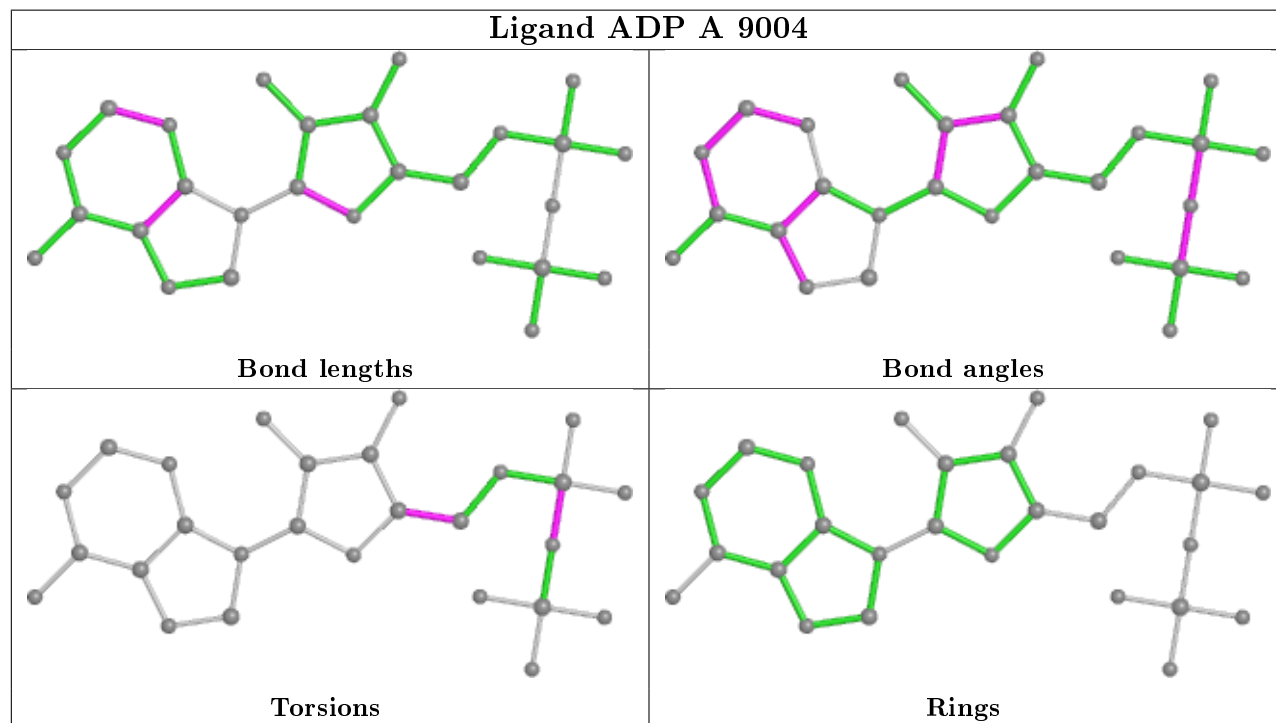
Ligand ADP B 9010

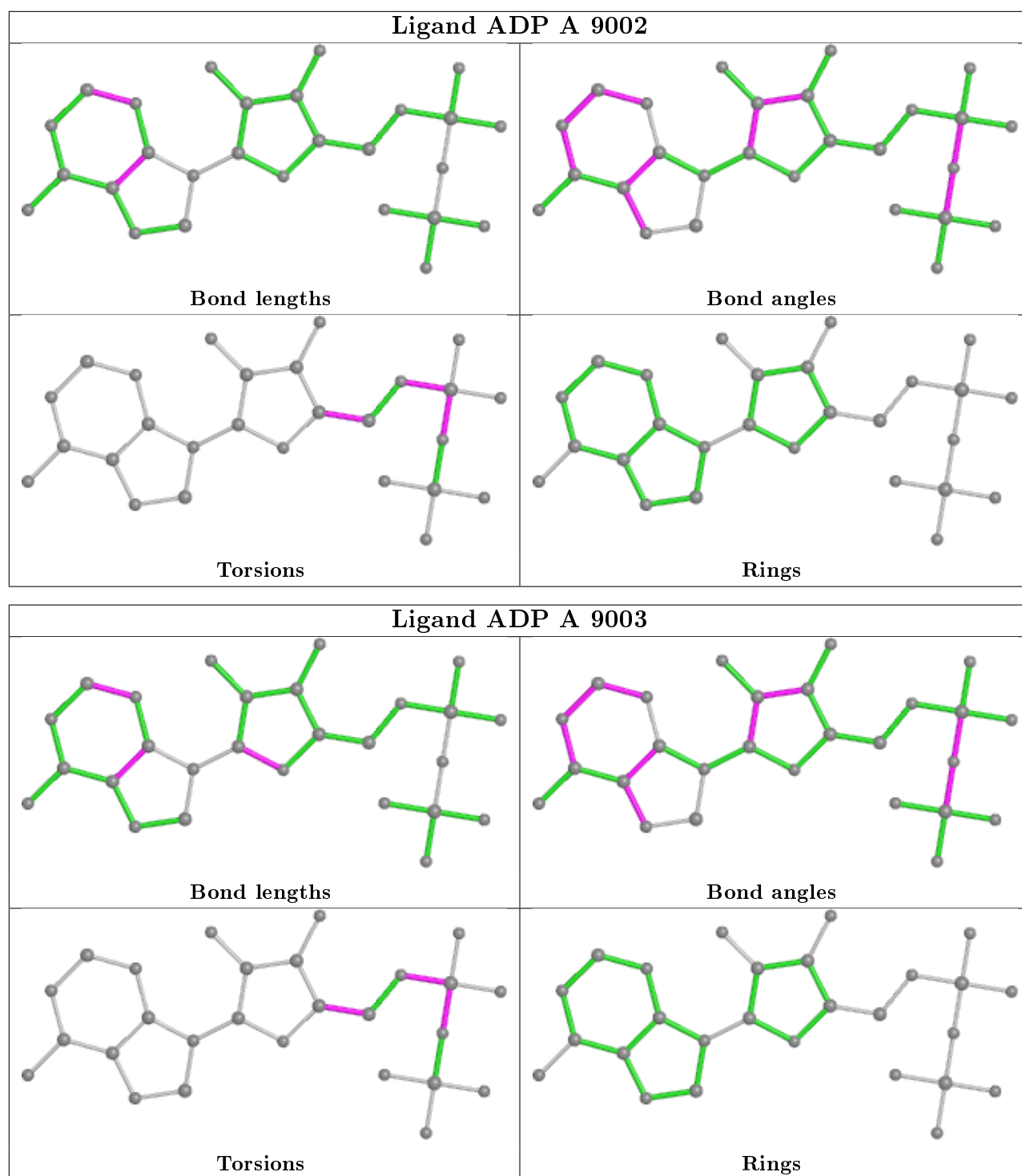


Ligand ADP B 9008



Ligand ADP A 9004





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	3042/3367 (90%)	-0.14	61 (2%) 65 58	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.18	29 (0%) 82 76	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.16	90 (1%) 73 66	64, 133, 209, 335	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.7
1	B	1517	VAL	4.8
1	A	1652	GLY	4.7
1	A	4187	LEU	4.5
1	A	1651	SER	4.1

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

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

6.3 Carbohydrates [i](#)

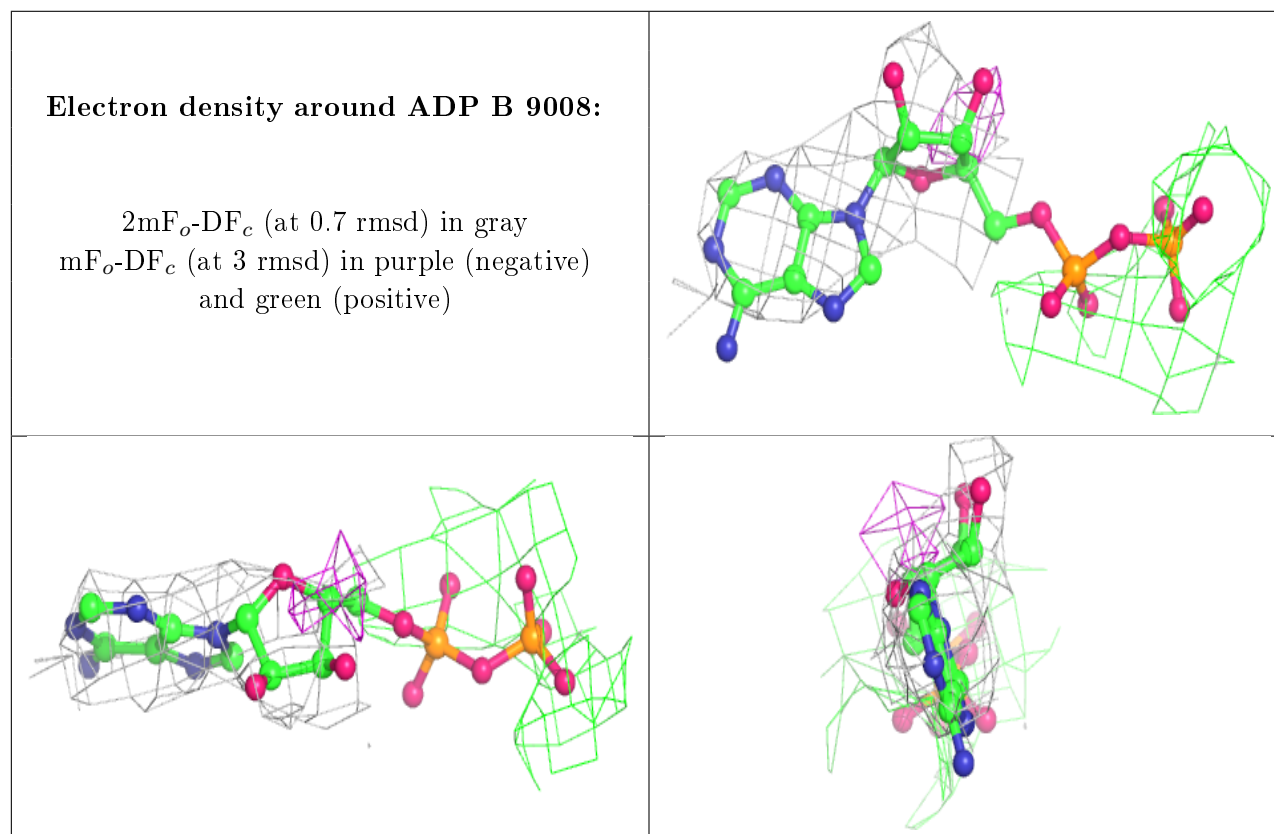
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

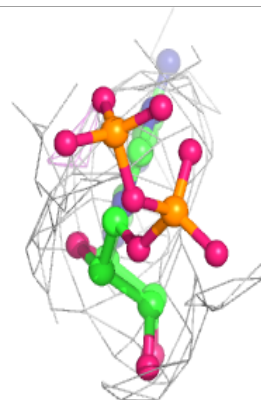
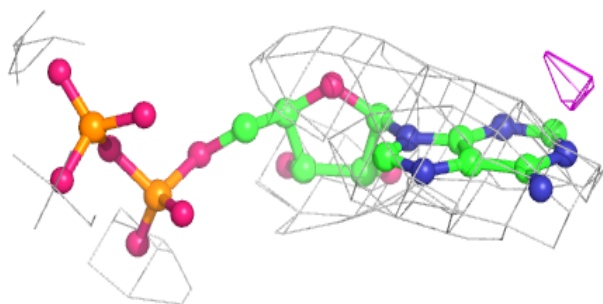
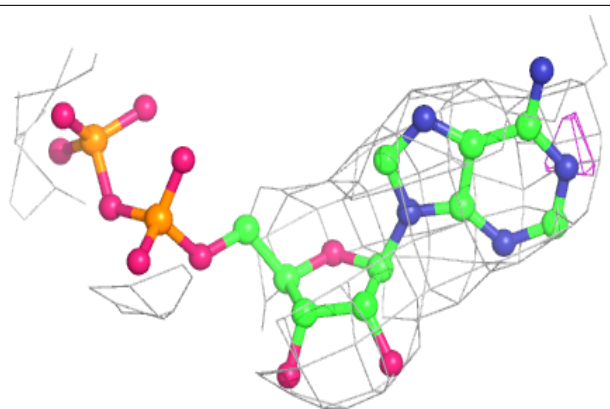
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	B	9008	27/27	0.85	0.40	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.31	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	129,129,129,129	0
2	ADP	A	9001	27/27	0.94	0.38	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	129,129,129,129	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

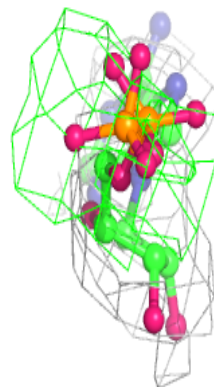
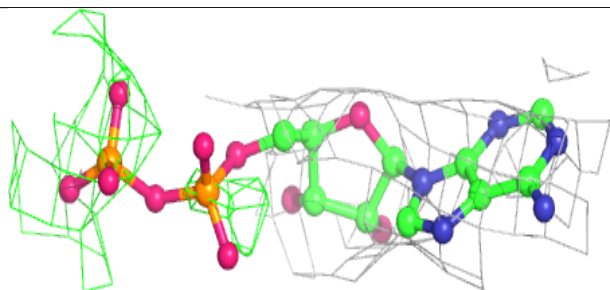
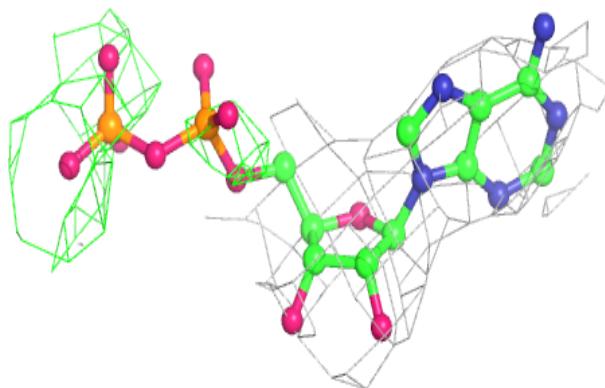


Electron density around ADP B 9010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

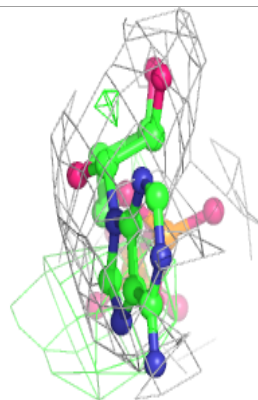
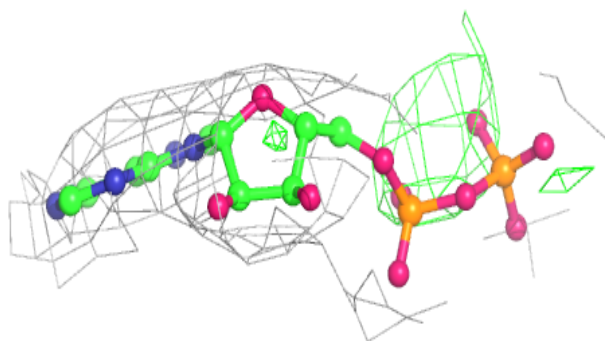
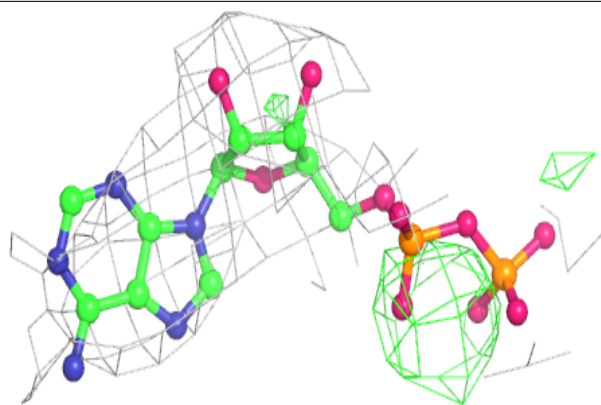
**Electron density around ADP A 9002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

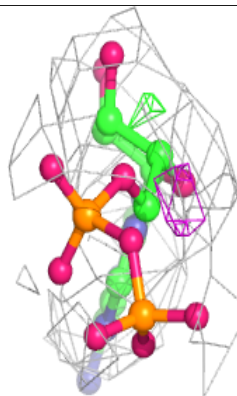
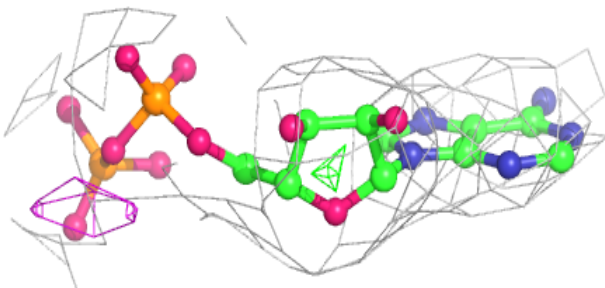
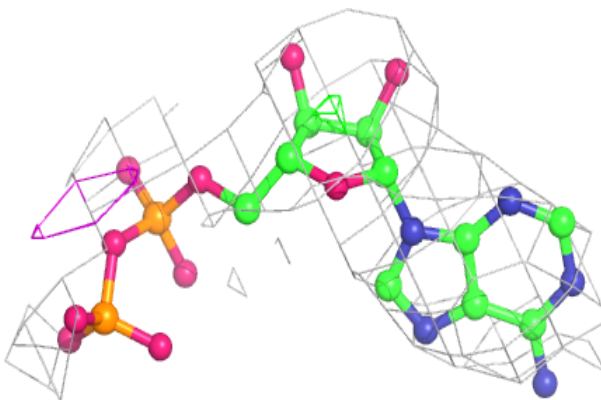


Electron density around ADP B 9007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

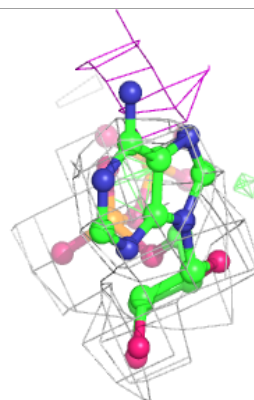
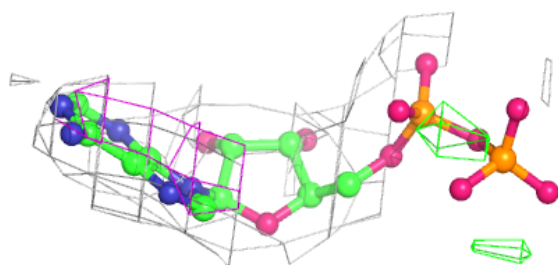
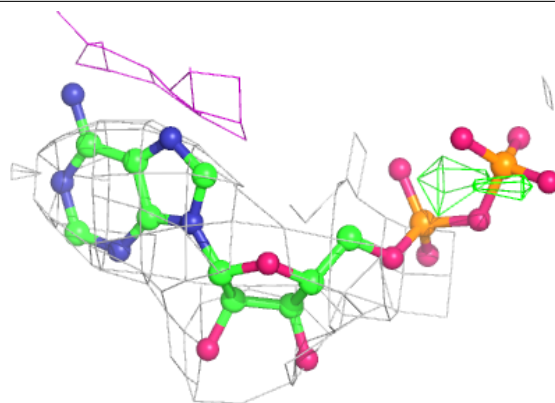
**Electron density around ADP A 9004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

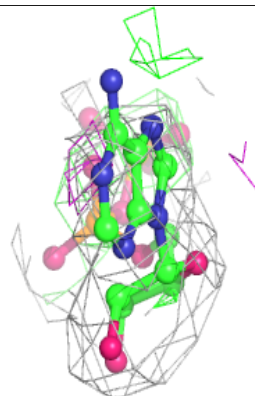
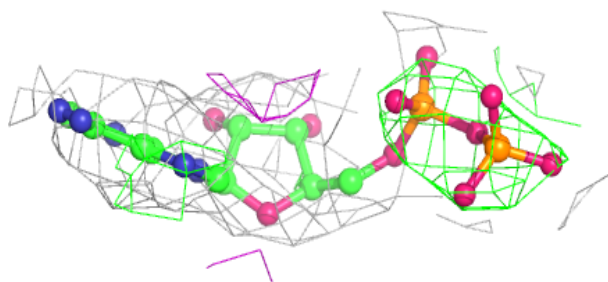
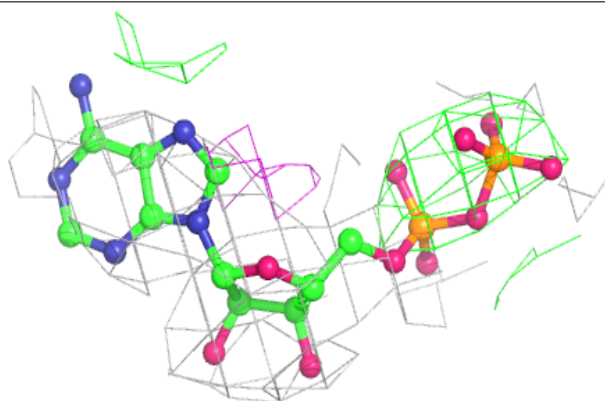


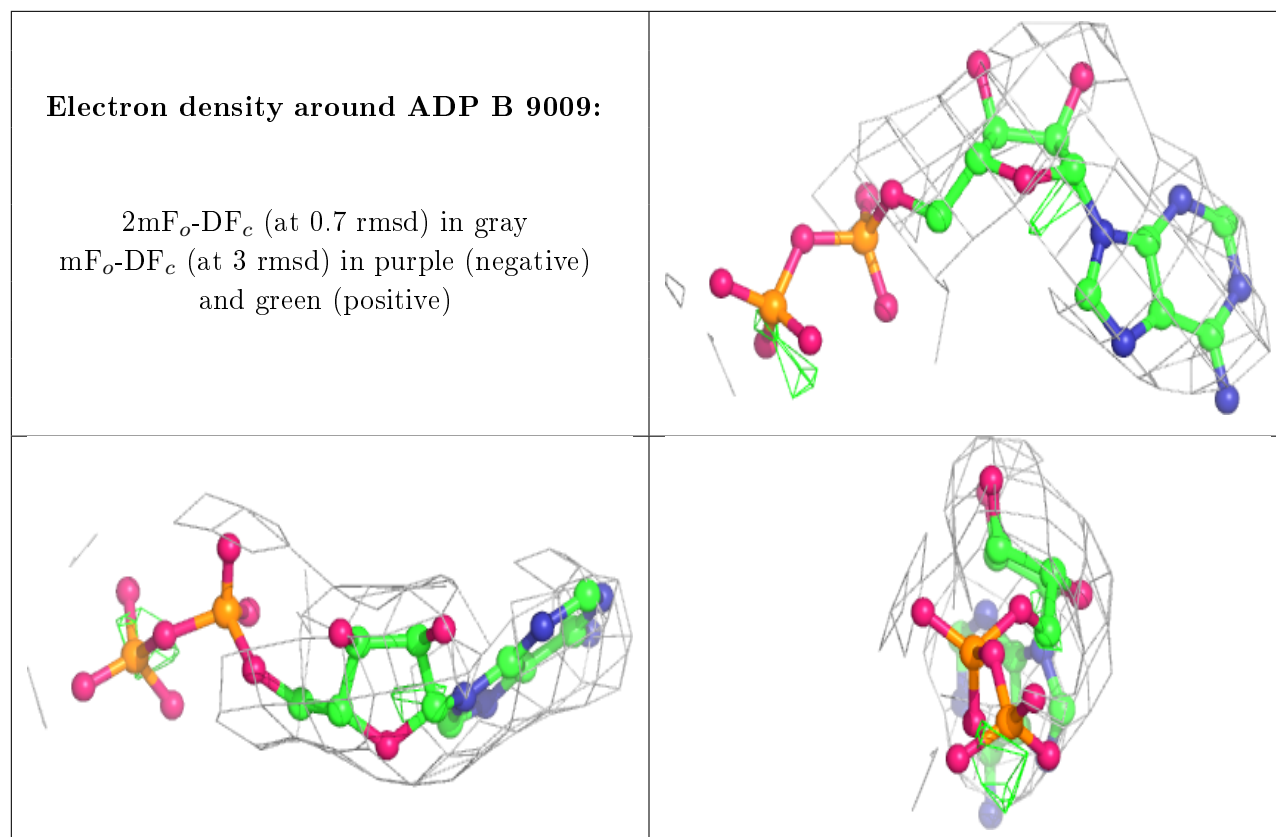
Electron density around ADP A 9003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP A 9001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.