



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2023 – 05:59 AM EDT

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 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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

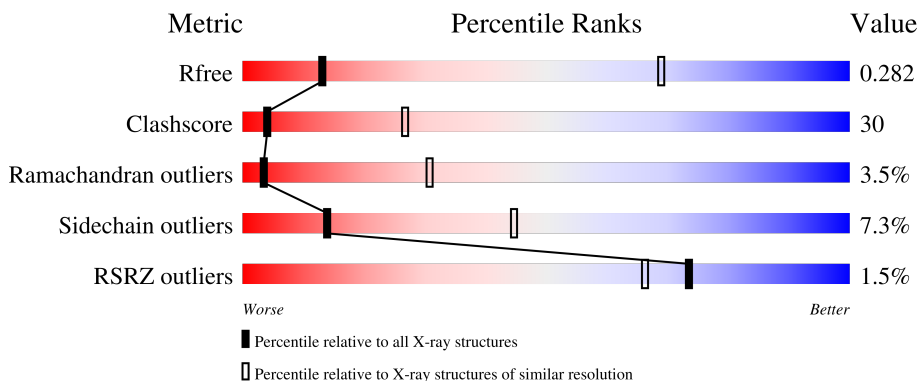
1 Overall quality at a glance

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 of 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	 2% 42% 42% 6% 10%
1	B	3367	 % 46% 37% • 14%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	3042	23374	14951	3955	4368	100	0	0	0
1	B	2908	22384	14307	3792	4190	95	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

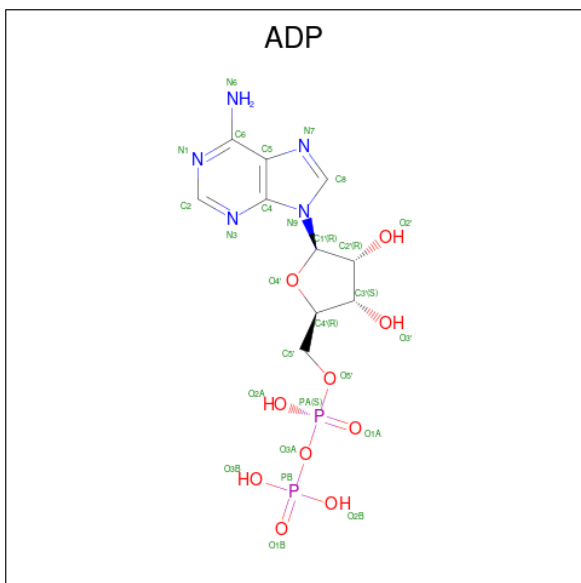
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	expression tag	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression 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

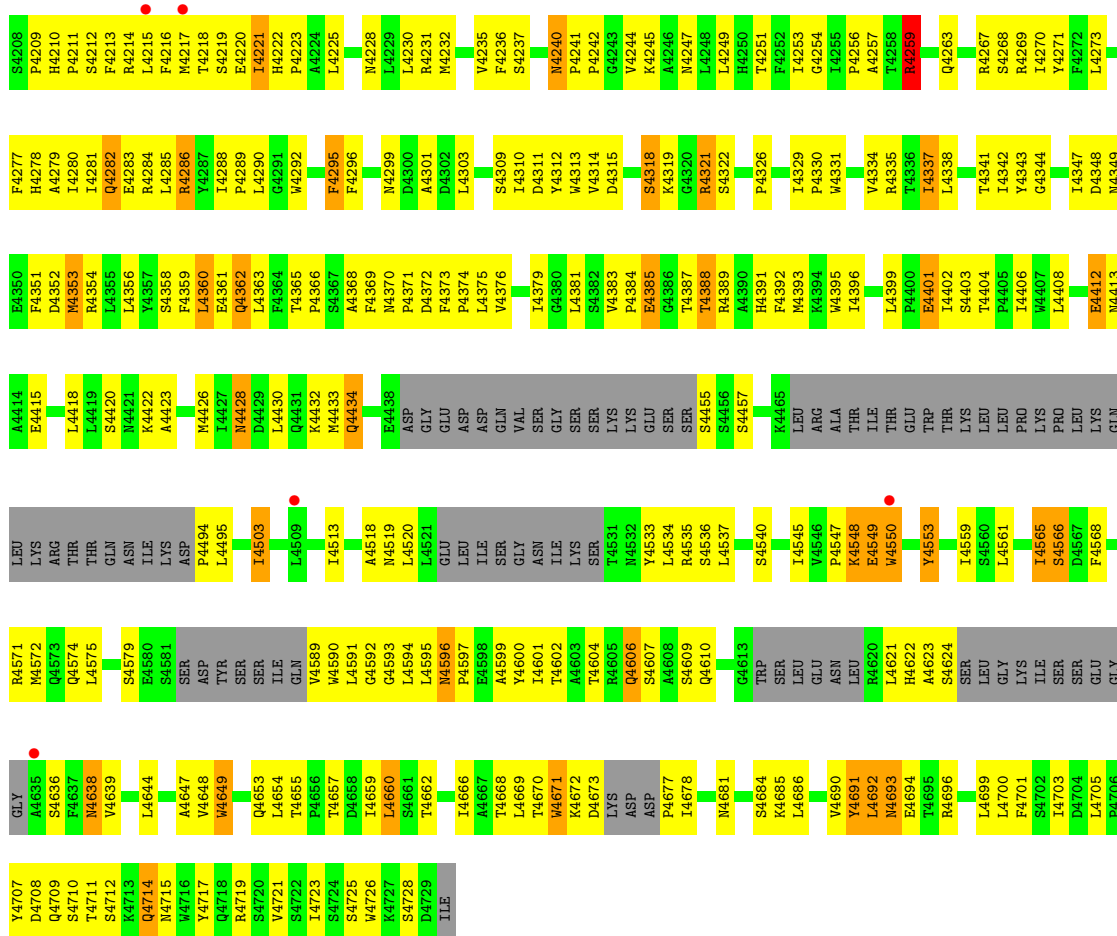
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



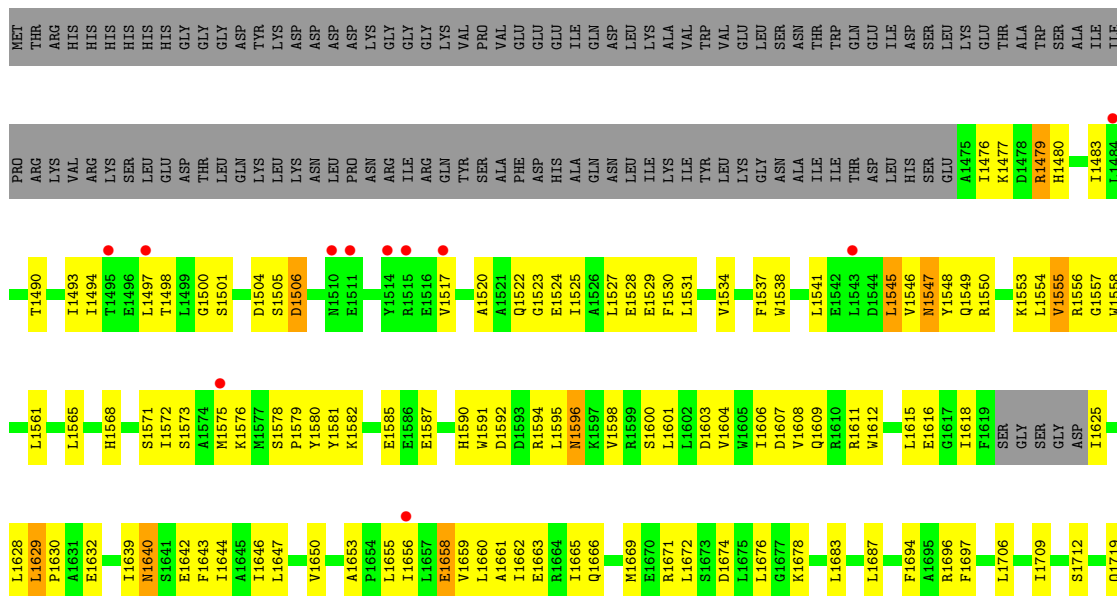
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

L3108	M3109	C5112	K3113	E3114	T3115	A3116	Q3117	R3118	F3119	L3120	L3121	L3122	L3123	F3133	Q3136	K3141	H3142	V3143	V3144	F3145	T3146	N3147	K3148	P3149	A3150	S3151	F3152	F3154	H3155	K3156	R3157	S3158	L3164	F3165	N3166	R3167	C3168	V3169	L3170	D3171	K3172	F3173	G3174	E3175	E3179	A3180	V3184	Q3185	S3186										
R2948	F2949	L2950	L2951	N2952	S2953	N2954	N2955	L2956	P2962	S2966	D2967	L2968	R2969	E2970	N2971	V2972	R2975	L2976	F2979	L2980	D2985	V2986	P2987	L2988	V2989	L2990	D2995	A3002	G3003	L2996	P2997	E3006	E3067	V2989	L2990	F2991	M2992	E2993	V2994	L2995	L2998	Q3007	P3008	L3009	Q3009	E3080	S3081	S3082	F3083	L3084	E3085	R3086	M3087	L3090	G3093	G3094	E3095	V3096	L3099
H2871	Y2872	I2873	P2876	R2877	S2880	R2881	W2882	D2883	L2886	L2887	I2890	Q2891	T2892	M2893	D2894	G2895	G2896	C2897	L2898	V2902	R2903	L2904	W2905	A2906	L2910	R2911	L2912	F2913	Q2914	L2917	V2918	E2922	K2923	Q2926	I2930	V2933	E3085	A2934	L2935	K2936	S3017	S3018	G3020	G3021	K3022	S3023	V3024	L3025	A2945										
V2789	G2790	A2791	C2792	N2793	P2794	A2798	G2799	R2800	R2806	L2808	R2809	L2813	L2814	L2815	L2816	D2817	F2818	P2819	L2824	T2825	Q2826	Y2827	Y2828	Y2829	F2831	L2832	R2833	A2834	L2835	L2838	L2839	L2842	F2845	A2846	D2847	M2848	L2849	T2850	D2851	E2855	F2856	Y2857	R2863	F2864	L2868	Q2787	A2870												
L2710	L2711	K2712	T2713	Y2720	E2727	T2728	W2729	L2730	R2731	P2732	W2738	L2739	V2740	W2741	F2742	G2743	D2744	E2745	I2746	N2747	L2748	P2749	S2750	G2751	W2752	K2753	Y2754	G2755	T2756	V2759	I2760	F2762	Q2765	M2766	R2659	A2690	F2691	F2694	E2695	T2774	T2775	S2776	T2779	W2780	I2781	K2782	L2783	D2784	K2785	Q2786	E2708	L2709							
N2547	V2648	I2649	E2650	T2651	M2660	S2661	P2662	E2663	Q2664	Q2665	T2670	N2671	I2672	L2673	L2674	Y2675	M2678	G2679	E2680	E2681	G2682	S2683	G2684	E2685	E2686	E2687	L2670	P2675	R2668	F2669	L2670	P2675	S2678	T2685	R2659	A2690	F2691	F2694	E2695	L2610	P2611	L2612	L2613	D2614	Y2615	S2616	W2617	S2618	L2619	W2624	S2625	L2626							
M2394	F2395	E2396	V2397	Q2398	Q2399	L2400	K2401	Z2402	A2403	I2408	S2409	R2410	C2411	M2412	V2413	W2415	Q2424	M2425	I2426	L2431	D2432	T2433	S2435	R2436	E2437	F2438	F2439	Q2442	E2443	Q2446	Q2447	N2450	E2451	N2452	ALA	GLN	LEU	GLN	GLN	GLN	GLN	GLN	GLN	THR	THR	THR	THR	PRO	LEU	ILE	THR								
T2323	T2324	W2327	T2328	D2329	F2332	T2335	R2338	I2339	I2340	D2341	N2342	V2343	E2346	K2349	R2350	D2351	H2352	I2353	G2357	D2358	V2359	D2360	T2361	E2362	W2363	V2364	N2366	L2367	N2368	S2369	L2370	L2371	N2374	K2375	L2376	L2377	T2378	L2379	P2380	N2381	G2382	E2383	R2384	L2385	A2386	L2387	V2391	R2392	V2393										
W2098	A2099	W2100	I2101	K2102	P2103	D2104	K2105	E2106	D2107	L2108	A2109	Q2110	V2111	M2112	L2113	W2114	S2115	F2118	K2119	T2120	A2121	E2122	M2203	L2204	P2205	A2125	K2206	L2207	T2208	V2209	D2211	L2212	P2213	L2214	C2135	Q2136	E2137	Q2138	L2139	S2140	A2141	V2222	F2223	P2224	H2144	L2228	Q2229	P2230	F2147	G2148	L2149	L2150	K2151	S2154	L2155	L2156	V2157	K2163	
P2169	GLN	LEU	PRO	PRO	ILE	THR	D2176	A2177	E2178	S2179	Y2190	V2194	L2195	L2196	N2197	S2198	I2199	N2200	D2201	E2202	M2203	L2204	P2205	K2206	L2207	T2208	V2209	D2211	L2212	P2213	L2214	C2135	Q2136	E2137	Q2138	L2218	L2219	D2221	V2222	F2223	P2224	L2228	Q2229	P2230	F2147	G2148	L2149	L2150	K2151	S2154	L2155	L2156	V2157	K2163					

E3187	H3259	R3342	E3418	T3482	S3551	F3628	F3704	R3767	X3836	F3911	L3991	G4054	N4120
E3190	Y3260	Q3346	M3419	A3483	K3552	K3629	F3704	D3768	A3837	S3912	L3992	E4055	L4121
N3191	D3262	V3346	I3422	Q3484	V3553	S3630	N3707	A3771	A3841	L3913	K3993	P4056	V4122
L3192	F3263	D3349	I3422	T3485	K3554	V3634	A3711	T3774	G3843	R3914	G3994	I4057	E4123
E3195	F3264	V3350	K3424	Y3486	N3555	P3635	A3711	P3775	F3916	A3915	I4058	P4059	K4124
N3196	N3265	V3350	I3425	Y3487	V3557	P3635	L3712	P3776	N3844	F3916	D3996	A4060	L4125
F3197	Q3266	K3353	I3426	E3489	D3558	L3638	G3715	D3776	I3845	D3918	L3998	S4061	V4126
Q3198	V3267	V3353	I3427	L3490	R3559	S3639	C3715	S3779	R3846	I3919	T3999	W4062	K4127
Y3199	Q3268	V3357	E3428	ASP	S3560	E3643	C3716	S3779	D3847	I3919	S4000	W4062	S4128
L3200	L3270	Q3358	F3429	ARG	I3561	E3643	P3717	R3780	D3848	F3920	S4000	V4064	S4129
F3202	L3271	K3359	F3431	ILE	L3563	M3647	L3718	V3781	D3849	N3922	I4001	V4064	S4130
F3205	K3274	V3360	I3432	LYS	L3564	H3648	R3720	F3783	V3850	L3923	K4002	Q4066	L4132
L3206	R3275	K3361	K3433	PRO	D3565	H3648	Q3721	V3784	V3851	N3925	T4004	Q4067	L4133
A3209	R3278	D3365	S3434	LEU	N3566	L3652	R3722	N3785	T3854	N3926	P4005	Q4068	L4134
E3210	L3278	L3366	L3435	ARG	L3567	P3653	R3723	F3786	L3855	N3927	Q4007	L4069	C4135
L3211	E3281	F3367	I3436	GLU	N3568	S3654	E3724	T3787	L3855	N3927	Q4007	S4070	S4136
GLY	Q3282	K3369	N3437	VAL	S3569	D3655	N3795	V3788	L3858	L3930	L4008	N4071	N4162
ASN	L3285	A3372	I3438	GLU	E3570	C3658	D3727	F3790	K3859	L3930	L4011	Q4072	Q4072
L3216	L3289	I3373	D3439	GLU	R3571	I3659	P3728	S3791	K3859	K3983	L4012	Q4073	Q4073
K3217	K3290	E3375	T3440	GLN	Q3578	I3659	V3729	S3791	T3862	F3947	L4012	S4074	S4074
A3218	K3291	A3376	K3441	LEU	S3578	P3659	P3729	S3792	T3863	F3948	W4019	T4075	T4075
L3219	L3292	A3377	K3442	LEU	F3581	S3654	L3730	S3792	E3864	F3948	L4020	T4076	T4076
P3220	R3293	I3373	K3443	ASN	M3582	D3655	N3731	L3793	I3865	F3948	L4020	V4077	K4158
P3221	L3296	I3374	H3444	ALA	M3582	C3658	P3732	Q3794	A3866	L3943	Q4016	W4079	W4079
R3224	E3296	V3380	R3449	ALA	Q3584	R3667	V3733	L3798	K3867	T3947	L4018	F4080	F4080
D3225	K3300	S3381	E3450	ASN	Q3584	R3667	V3733	H3799	L3867	F3948	W4019	R4081	R4081
A3226	K3309	S3381	A3451	ASN	M3585	F3668	N3735	L3794	V3869	F3948	L4020	K4082	K4082
S3229	K3309	S3381	K3451	LEU	S3587	N3669	K3736	L3802	V3875	T3951	I4021	L4084	L4084
S3230	K3309	S3381	A3452	LEU	V3588	R3670	GLU	L3803	V3875	F3952	C4022	L4086	L4086
Y3233	L3313	K3384	I3452	K3512	V3588	P3672	ILE	T3804	E3878	K3953	L4023	M4086	M4086
L3234	V3315	K3386	T3453	K3514	V3592	L3673	ARG	E3805	I3879	K3954	Q4025	K4087	K4087
T3237	K3319	H3387	T3453	D3516	S3592	V3674	LYS	P3807	V3882	R3955	Q4026	H4090	H4090
I3238	K3323	L3388	G3455	L3517	A3595	I3675	GLY	T3809	V3882	L3959	P4027	S4091	S4091
G3239	L3324	E3390	G3456	L3518	A3597	D3676	ARG	H3810	V3886	L3960	P4028	D4092	D4092
E3240	V3328	P3398	L3457	T3521	F3598	P3677	ILE	K3811	N3887	N3961	S4029	R4093	R4093
N3242	I3243	T3399	A3470	K3533	L3599	S3678	ILE	K3812	P3888	L3960	F4030	V4094	V4094
R3244	K3330	P3400	S3471	K3533	D3606	M3886	ASP	R3813	M3889	K3964	K4031	L4095	L4095
L3245	Q3331	P3400	M3405	Y3536	D3606	M3886	ASP	S3814	L3891	L3965	L4033	L4095	L4095
Q3249	E3335	P3400	V3408	L3539	D3612	M3886	ASP	L3815	S3892	L3969	D4035	S4098	S4098
E3335	C3409	P3400	G3475	I3540	D3612	M3886	ASP	L3817	C3893	L3974	H4036	H4099	H4099
N3253	I3336	L3410	L3410	E3542	R3615	M3886	ASP	K3818	V3895	S3975	Q4039	C4103	C4103
V3255	K3337	L3410	L3477	E3542	I3619	M3886	ASP	L3819	V3896	V3975	N4040	S4104	S4104
I3256	Q3338	G3414	I3478	I3646	S3620	M3886	ASP	Q3820	F3897	K3977	D4043	V4105	V4105
P3257	K3339	K3415	I3478	S3624	S3624	M3886	ASP	G3821	F3898	G3978	D4044	E4108	E4108
A3258	A3341	L3417	A3481	S3550	D3701	M3886	ASP	V3825	F3898	T3979	W4044	E4108	E4108



● Molecule 1: Dynein heavy chain, cytoplasmic



V2759	K1720
R2764	H1721
M2766	F1722
M2773	M1725
R2774	F1726
S2776	A1727
T2779	L1728
M2780	G1728
L2781	L1729
K2782	L1734
L2783	S1735
I2786	D1736
Q2787	T1739
F2788	T1740
V2789	I1741
N2793	I1742
P2794	G1743
D2797	M1744
A2798	E1748
G2799	V1752
R2800	T1753
V2801	F1754
Q2802	S1759
L2803	L1846
F2806	S1847
R2807	I1848
H2810	E1849
I2813	A1850
L2814	G1855
L2815	I1855
D2816	F1764
F2817	P1764
F2818	V1765
S2819	I1766
S2820	H1767
T2821	H1768
L2822	W1769
Y2823	L1770
L2824	V1773
T2825	A1868
Y2828	A1869
G2829	M1777
T2830	T1780
F2831	L1781
N2832	A1782
L2833	T1783
L2835	L1785
L2836	S1788
L2837	L1789
L2838	V1888
L2839	L1793
L2840	D1799
L2841	H1800
L2842	S1801
L2843	L1899
L2844	T1899
L2845	G1900
L2846	N1901
L2847	K1902
L2848	D1903
L2849	W1906
L2850	L1907
L2851	Y1908
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L2863	K1924
L2864	L1925
L2865	I1927
L2866	H1928
L2867	M1929
L2868	A1930
L2869	N1931
L2870	A1932
L2871	T1933
L2872	F1934
L2873	E1849
L2874	Q1850
L2875	Y1936
L2876	G1937
L2877	F1938
L2878	E1939
L2879	Y1940
L2880	L1941
L2881	G1942
L2882	I1943
L2883	R1946
L2884	L1947
L2885	A1869
L2886	V1948
L2887	Q1949
L2888	T1950
L2889	P1951
L2890	L1952
L2891	R1955
L2892	C1956
L2893	Y1957
L2894	L1958
L2895	L1959
L2896	A2141
L2897	L1960
L2898	L1961
L2899	Q1962
L2900	L1892
L2901	R1967
L2902	C1895
L2903	T1899
L2904	P1972
L2905	P1975
L2906	T2074
L2907	F2075
L2908	V2076
L2909	T2076
L2910	G2080
L2911	Y2081
L2912	A2082
L2913	G2083
L2914	R2084
L2915	S2085
L2916	W2086
L2917	L2091
L2918	G1992
L2919	L1999
L2920	G1999
L2921	R1993
L2922	F2095
L2923	R2096
L2924	S2097
L2925	M2098
L2926	A2099
L2927	M2100
L2928	I2101
L2929	K2102
L2930	D2104
L2931	R2105
L2932	E2106
L2933	A2109
L2934	W2112
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L2936	Y2114
L2937	S2115
L2938	Q2116
L2939	G2117
L2940	F2118
L2941	K2119
L2942	T2120
L2943	L2124
L2944	A2125
L2945	G2126
L2946	K2127
L2947	L2128
L2948	P2130
L2949	C2135
L2950	L2139
L2951	S2140
L2952	A2141
L2953	L2212
L2954	P2213
L2955	Q2143
L2956	H2144
L2957	Y2145
L2958	L2149
L2959	P2223
L2960	P2224
L2961	G2225
L2962	SER
L2963	GLN
L2964	L2228
L2965	K2153
L2966	S2154
L2967	W2155
L2968	L2156
L2969	K2163
L2970	R2164
L2971	K2165
L2972	R2166
L2973	GLN
L2974	PRO
L2975	PRO
L2976	GLN
L2977	LEU
L2978	PRO
L2979	PRO
L2980	ILE
L2981	THR
L2982	ASP
L2983	ALA
L2984	ALA
L2985	GLU
L2986	SER
L2987	LYS
L2988	THR
L2989	LYS
L2990	LYS
L2991	ALA
L2992	ALA
L2993	Q2185
L2994	Q2189
L2995	Y2190
L2996	E2191
L2997	V2194
L2998	L2195
L2999	L2196
L3000	N2197
L3001	S2198
L3002	L2124
L3003	L2124
L3004	A2125
L3005	G2126
L3006	K2127
L3007	L2128
L3008	P2130
L3009	C2135
L3010	L2139
L3011	S2140
L3012	A2141
L3013	L2212
L3014	P2213
L3015	Q2143
L3016	H2144
L3017	Y2145
L3018	L2149
L3019	P2223
L3020	P2224
L3021	G2225
L3022	SER
L3023	GLN
L3024	L2228
L3025	K2153
L3026	S2154
L3027	W2155
L3028	L2156
L3029	K2163
L3030	R2164
L3031	K2165
L3032	R2166
L3033	GLN
L3034	PRO
L3035	PRO
L3036	GLN
L3037	LEU
L3038	PRO
L3039	PRO
L3040	ILE
L3041	THR
L3042	ASP
L3043	ALA
L3044	ALA
L3045	GLU
L3046	SER
L3047	LYS
L3048	THR
L3049	LYS
L3050	LYS
L3051	ALA
L3052	ALA
L3053	Q2185
L3054	Q2189
L3055	Y2190
L3056	E2191
L3057	V2194
L3058	L2195
L3059	L2196
L3060	N2197
L3061	S2198
L3062	L2124
L3063	L2124
L3064	A2125
L3065	G2126
L3066	K2127
L3067	L2128
L3068	P2130
L3069	C2135
L3070	L2139
L3071	S2140
L3072	A2141
L3073	L2212
L3074	P2213
L3075	Q2143
L3076	H2144
L3077	Y2145
L3078	L2149
L3079	P2223
L3080	P2224
L3081	G2225
L3082	SER
L3083	GLN
L3084	L2228
L3085	K2153
L3086	S2154
L3087	W2155
L3088	L2156
L3089	K2163
L3090	R2164
L3091	K2165
L3092	R2166
L3093	GLN
L3094	PRO
L3095	PRO
L3096	GLN
L3097	LEU
L3098	PRO
L3099	ILE
L3100	THR
L3101	ASP
L3102	ALA
L3103	ALA
L3104	GLU
L3105	SER
L3106	LYS
L3107	THR
L3108	LYS
L3109	LYS
L3110	ALA
L3111	ALA
L3112	Q2185
L3113	Q2189
L3114	Y2190
L3115	E2191
L3116	V2194
L3117	L2195
L3118	L2196
L3119	N2197
L3120	S2198
L3121	L2124
L3122	L2124
L3123	A2125
L3124	G2126
L3125	K2127
L3126	L2128
L3127	P2130
L3128	C2135
L3129	L2139
L3130	S2140
L3131	A2141
L3132	L2212
L3133	P2213
L3134	Q2143
L3135	H2144
L3136	Y2145
L3137	L2149
L3138	P2223
L3139	P2224
L3140	G2225
L3141	SER
L3142	GLN
L3143	L2228
L3144	K2153
L3145	S2154
L3146	W2155
L3147	L2156
L3148	K2163
L3149	R2164
L3150	K2165
L3151	R2166
L3152	GLN
L3153	PRO
L3154	PRO
L3155	GLN
L3156	LEU
L3157	PRO
L3158	ILE
L3159	THR
L3160	ASP
L3161	ALA
L3162	ALA
L3163	GLU
L3164	SER
L3165	LYS
L3166	THR
L3167	LYS
L3168	LYS
L3169	ALA
L3170	ALA
L3171	Q2185
L3172	Q2189
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L3178	N2197
L3179	S2198
L3180	L2124
L3181	L2124
L3182	A2125
L3183	G2126
L3184	K2127
L3185	L2128
L3186	P2130
L3187	C2135
L3188	L2139
L3189	S2140
L3190	A2141
L3191	L2212
L3192	P2213
L3193	Q2143
L3194	H2144
L3195	Y2145
L3196	L2149
L3197	P2223
L3198	P2224
L3199	G2225
L3200	SER
L3201	GLN
L3202	L2228
L3203	K2153
L3204	S2154
L3205	W2155
L3206	L2156
L3207	K2163
L3208	R2164
L3209	K2165
L3210	R2166
L3211	GLN
L3212	PRO
L3213	PRO
L3214	GLN
L3215	LEU
L3216	PRO
L3217	ILE
L3218	THR
L3219	ASP
L3220	ALA
L3221	ALA
L3222	GLU
L3223	SER
L3224	LYS
L3225	THR
L3226	LYS
L3227	LYS
L3228	ALA
L3229	ALA
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L3241	A2125
L3242	G2126
L3243	K2127
L3244	L2128
L3245	P2130
L3246	C2135
L3247	L2139
L3248	S2140
L3249	A2141
L3250	L2212
L3251	P2213
L3252	Q2143
L3253	H2144
L3254	Y2145
L3255	L2149
L3256	P2223
L3257	P2224
L3258	G2225
L3259	SER
L3260	GLN
L3261	L2228
L3262	K2153
L3263	S2154
L3264	W2155
L3265	L2156
L3266	K2163
L3267	R2164
L3268	K2165
L3269	R2166
L3270	GLN
L3271	PRO
L3272	PRO
L3273	GLN
L3274	LEU
L3275	PRO
L3276	ILE
L3277	THR
L3278	ASP
L3279	ALA
L3280	ALA
L3281	GLU
L3282	SER
L3283	LYS
L3284	THR
L3285	LYS
L3286	LYS
L3287	ALA
L3288	ALA
L3289	Q2185
L3290	Q2189
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L3299	L2124
L3300	A2125
L3301	G2126
L3302	K2127
L3303	L2128
L3304	P2130
L3305	C2135
L3306	L2139
L3307	S2140
L3308	A2141
L3309	L2212
L3310	P2213
L3311	Q2143
L3312	H2144
L3313	Y2145
L3314	L2149
L3315	P2223
L3316	P2224
L3317	G2225
L3318	SER
L3319	GLN
L3320	L2228
L3321	K2153
L3322	S2154
L3323	W2155
L3324	L2156
L3325	K2163
L3326	R2164
L3327	K2165
L3328	R2166
L3329	GLN
L3330	PRO
L3331	PRO
L3332	GLN
L3333	

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)	Xtrriage
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	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.001 for l,-k,h	Xtrriage
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

Xtrriage'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	B	2029	ASN
1	B	3050	ASP
1	B	2189	GLN
1	B	2581	LEU
1	B	3620	ARG

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

Mol	Chain	Res	Type
1	B	1568	HIS
1	B	2504	GLN
1	B	1690	GLN
1	B	2029	ASN
1	B	2832	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	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	9007	-	24,29,29	1.23	3 (12%)	29,45,45	1.54	5 (17%)
2	ADP	B	9008	-	24,29,29	1.23	3 (12%)	29,45,45	1.55	5 (17%)
2	ADP	A	9003	-	24,29,29	1.26	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	B	9009	-	24,29,29	1.25	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9004	-	24,29,29	1.23	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	9007	-	-	4/12/32/32	0/3/3/3
2	ADP	B	9008	-	-	2/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	3/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/12/32/32	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	A	9004	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	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	A	9003	ADP	C5'-O5'-PA-O1A
2	A	9003	ADP	C5'-O5'-PA-O2A
2	B	9007	ADP	C5'-O5'-PA-O3A

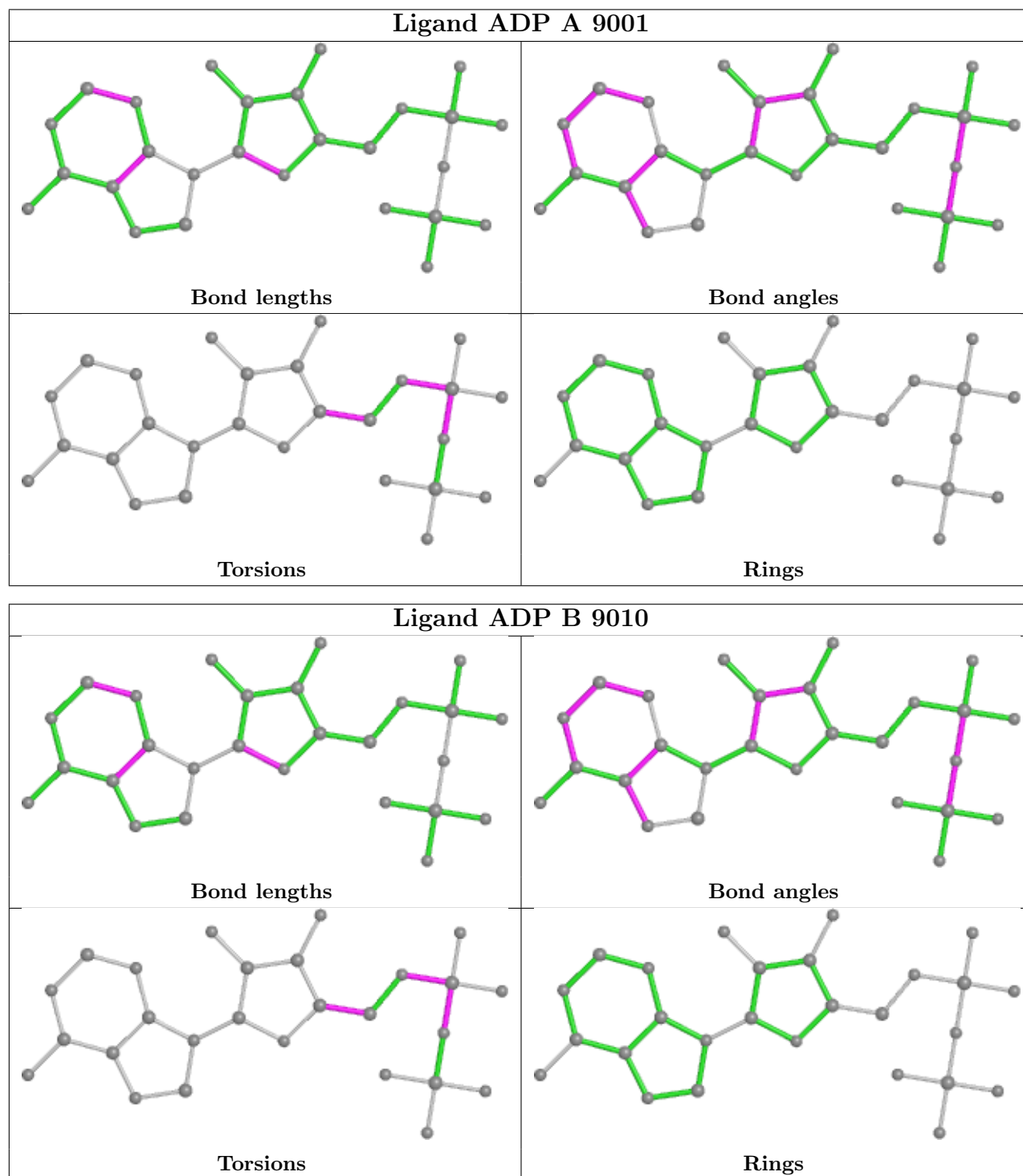
There are no ring outliers.

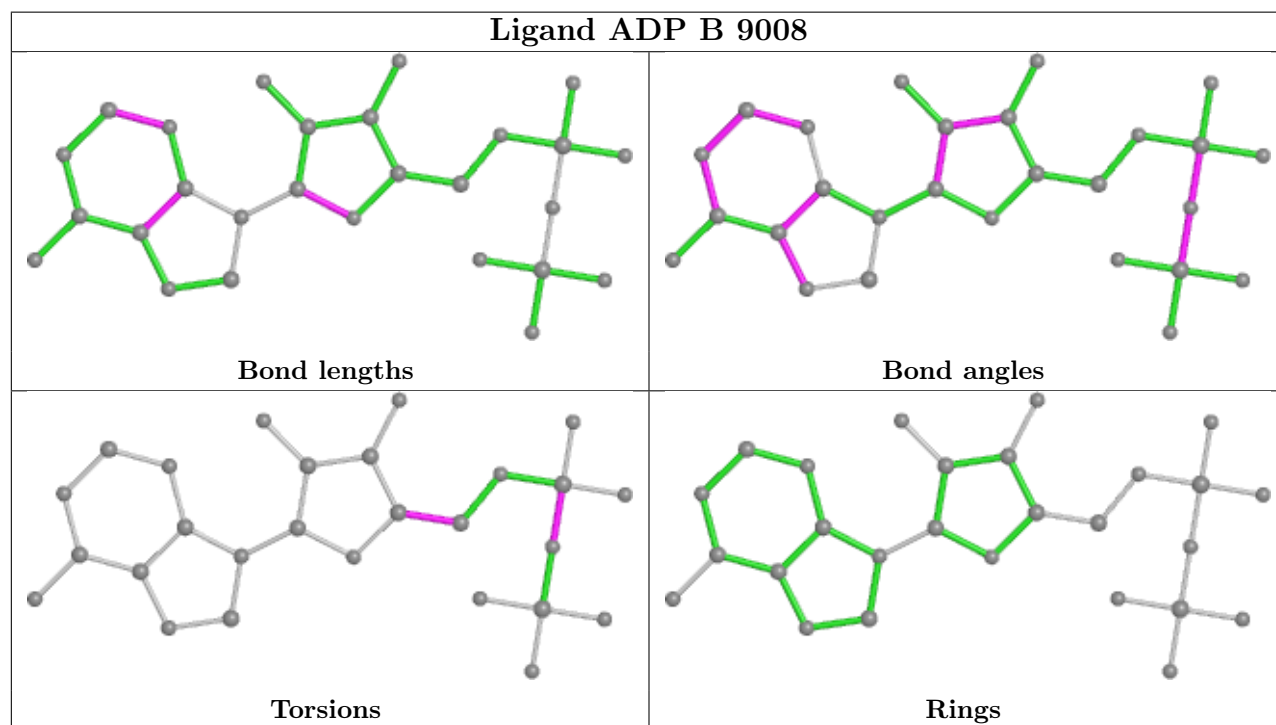
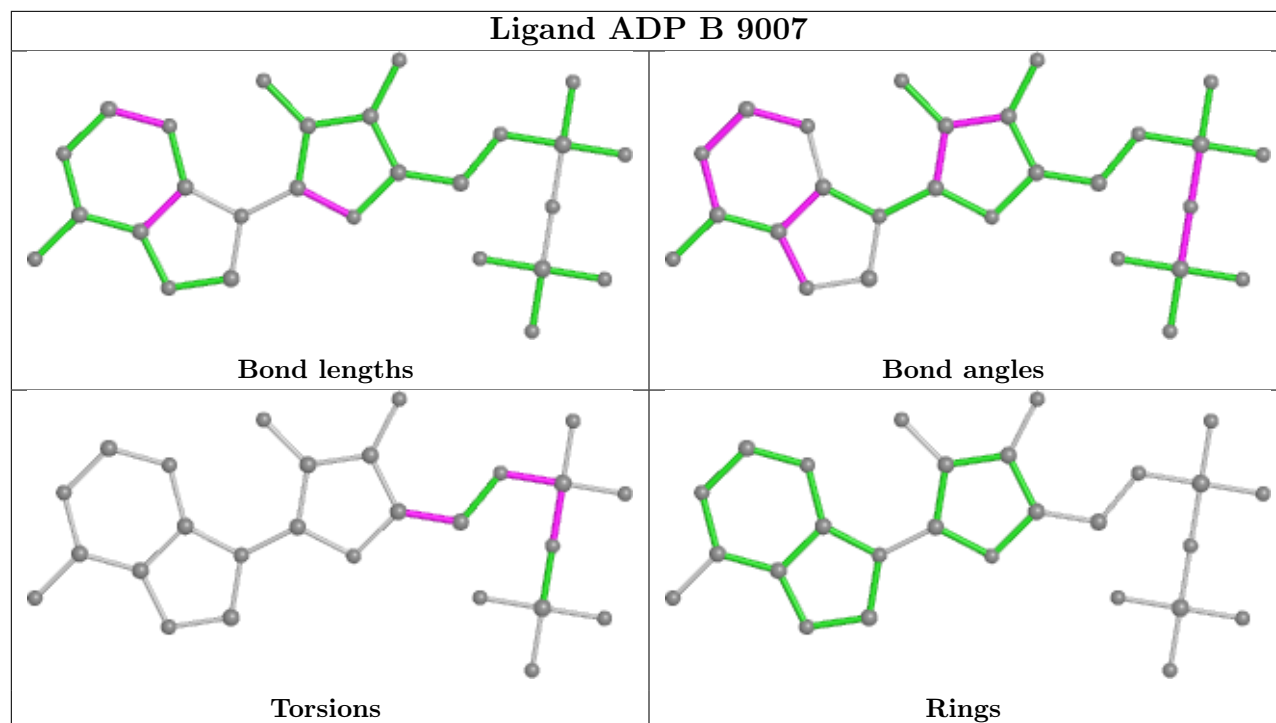
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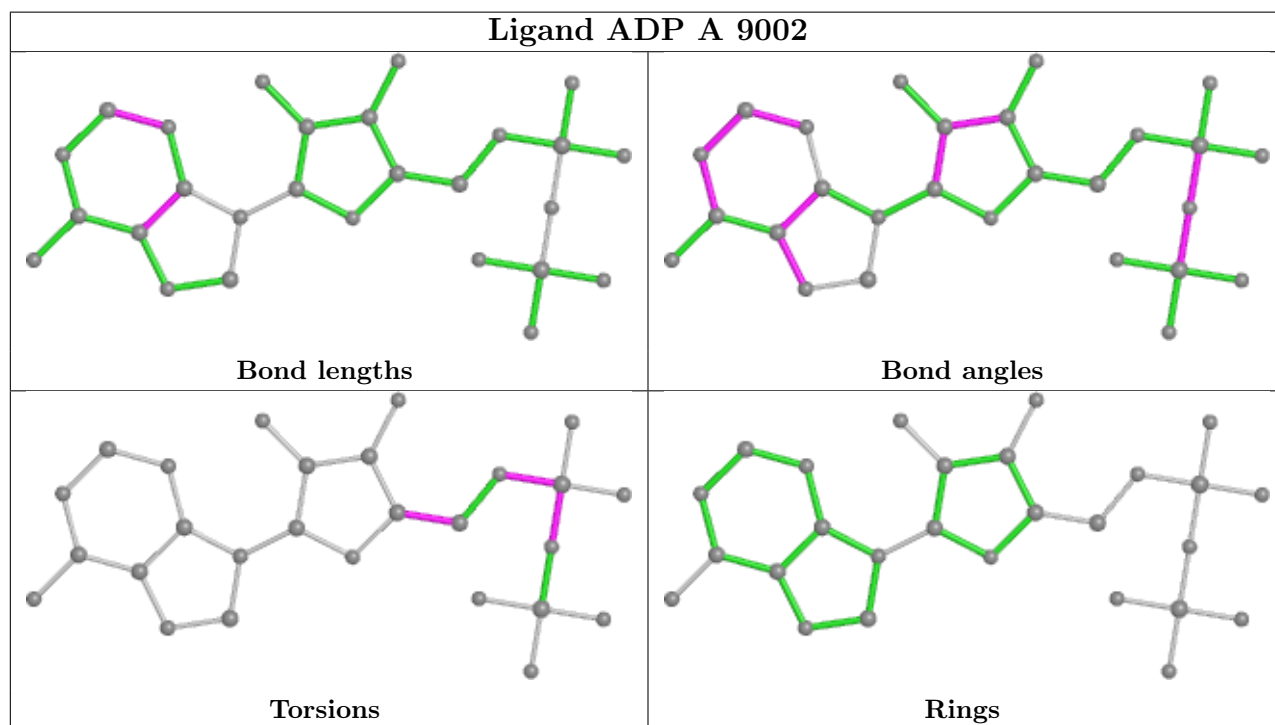
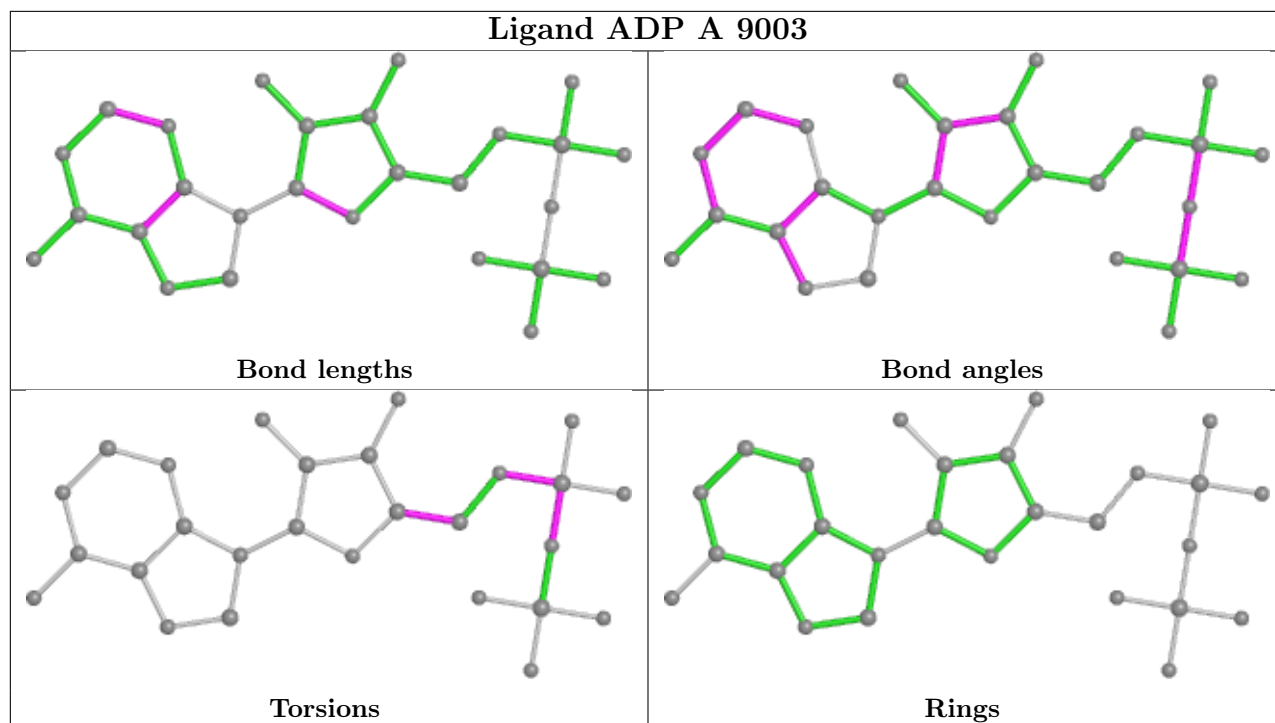
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	B	9010	ADP	2	0
2	A	9002	ADP	4	0
2	B	9009	ADP	1	0
2	A	9004	ADP	2	0

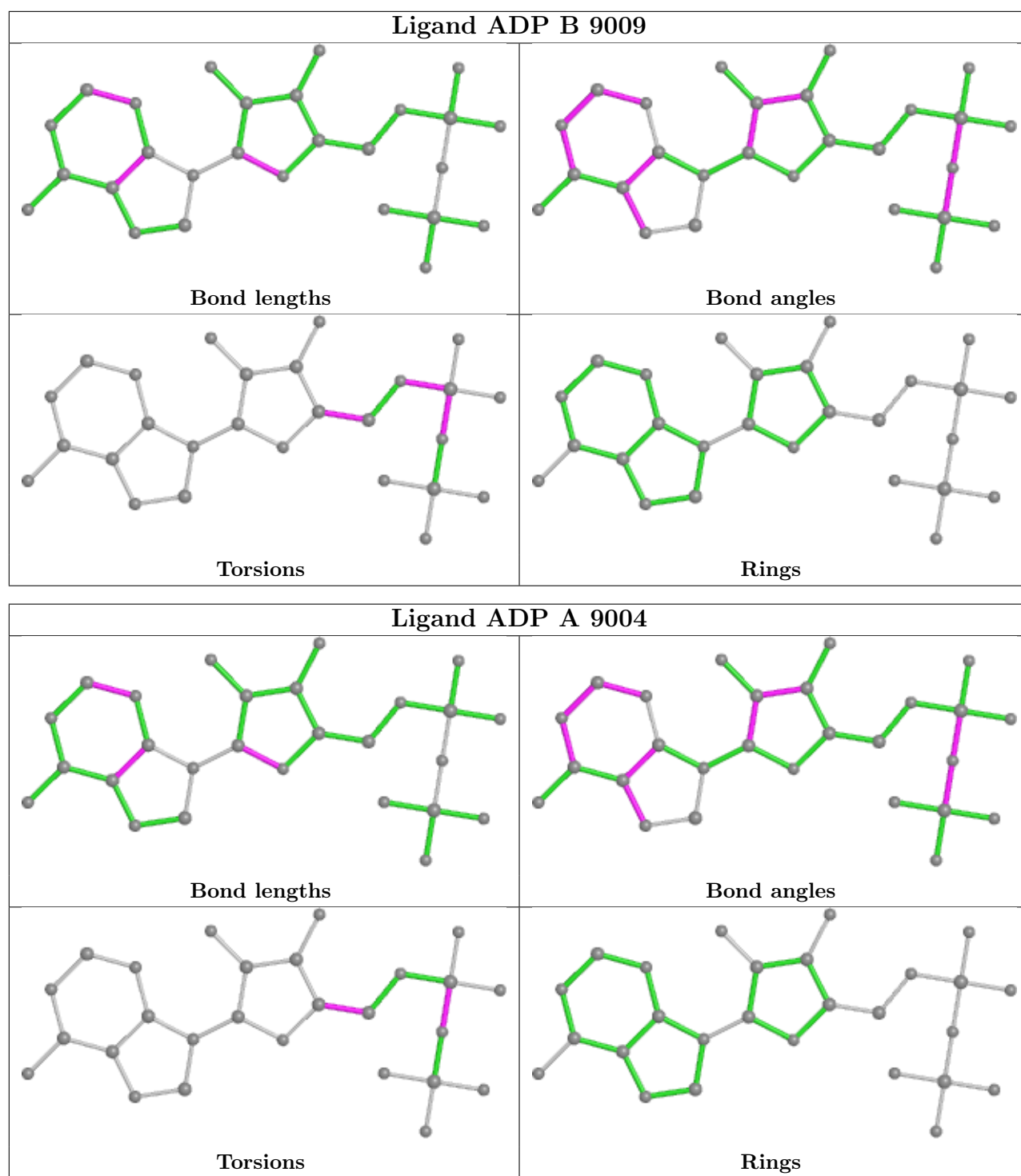
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [\(i\)](#)

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](#)

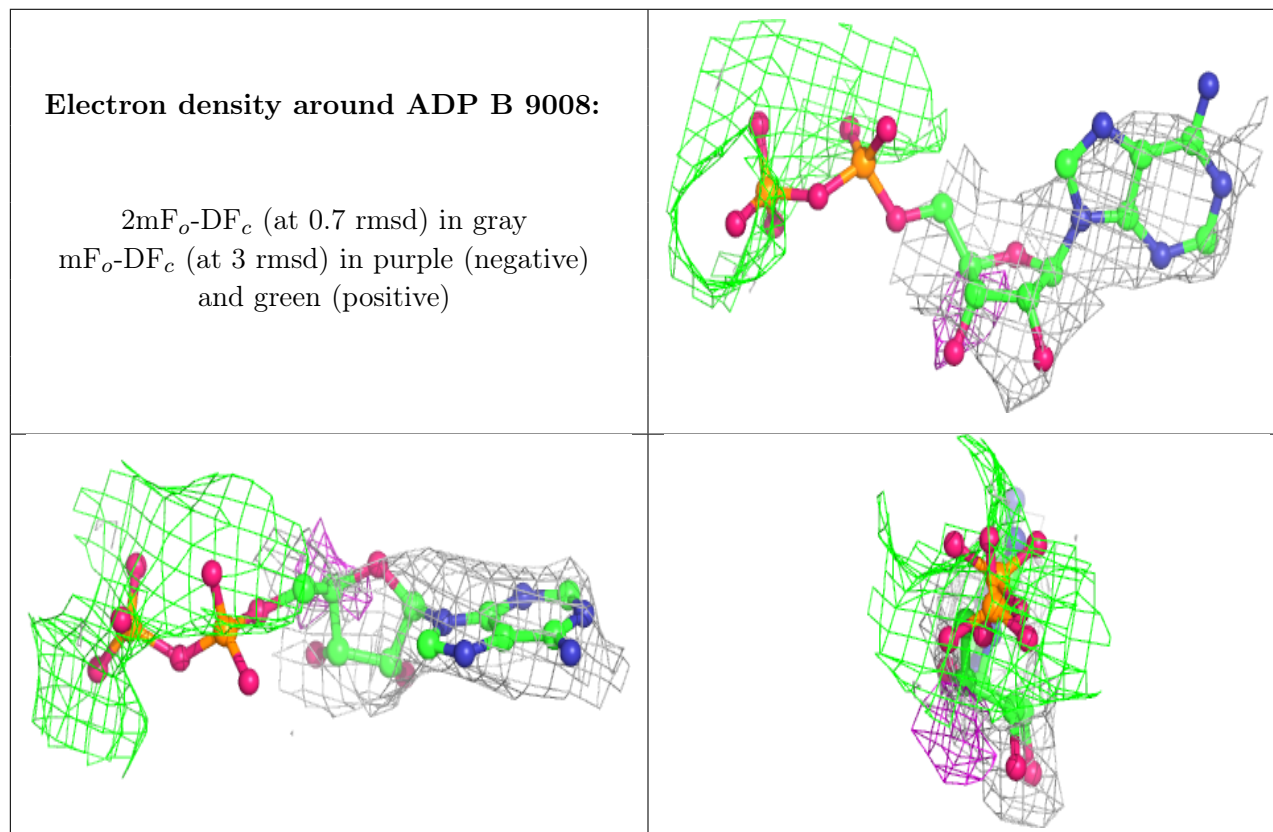
There are no monosaccharides in this entry.

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.

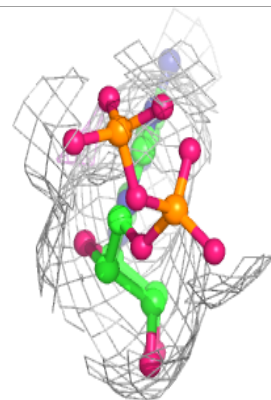
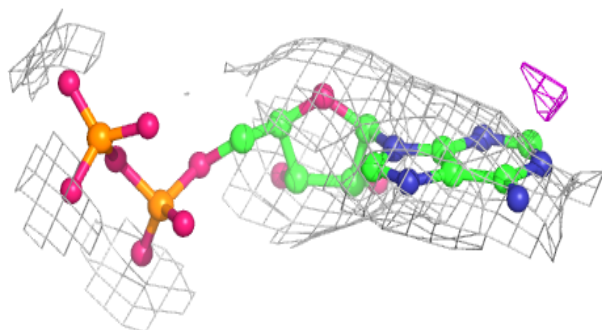
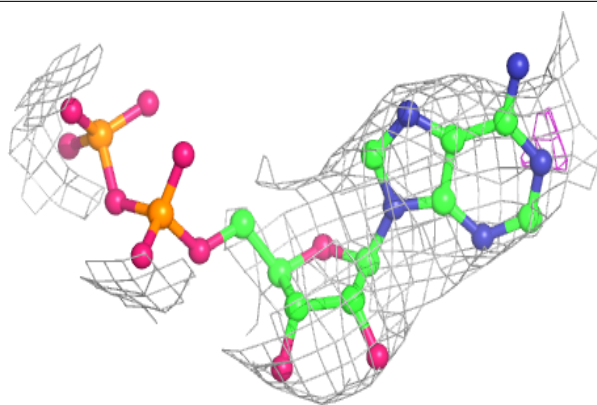
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	B	9008	27/27	0.85	0.40	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.31	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	129,129,129,129	0
2	ADP	A	9003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

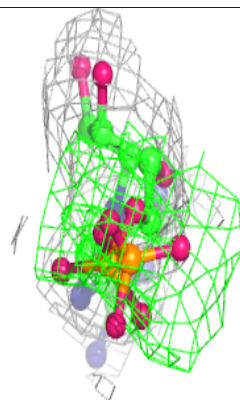
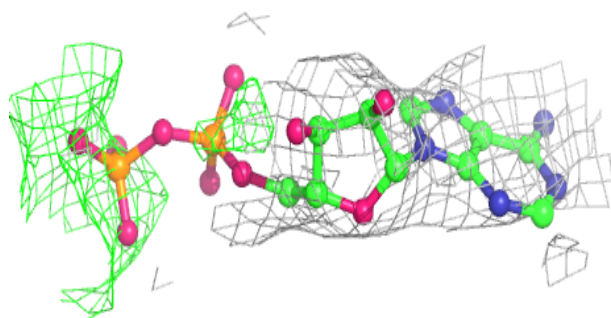
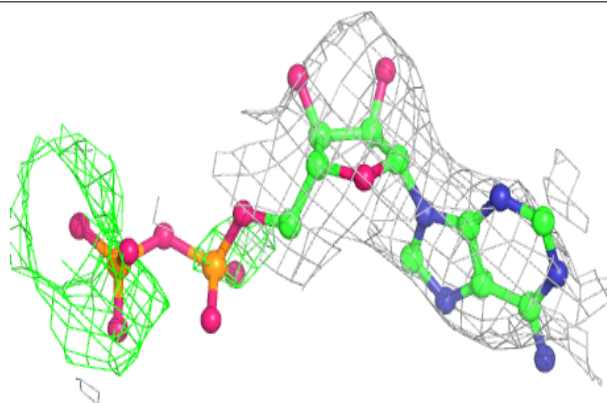


Electron density around ADP B 9010:

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

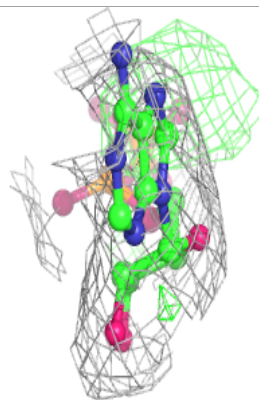
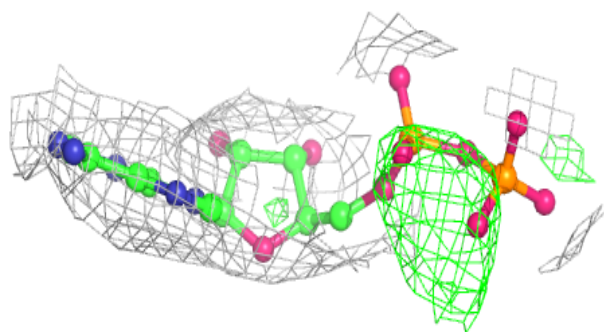
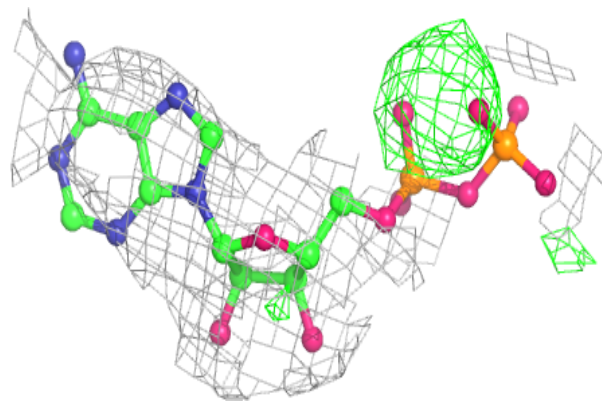
**Electron density around ADP A 9002:**

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

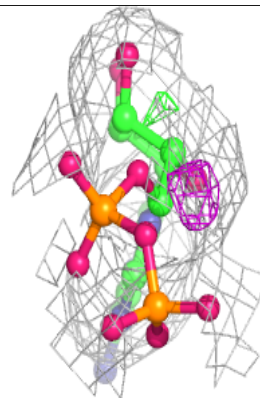
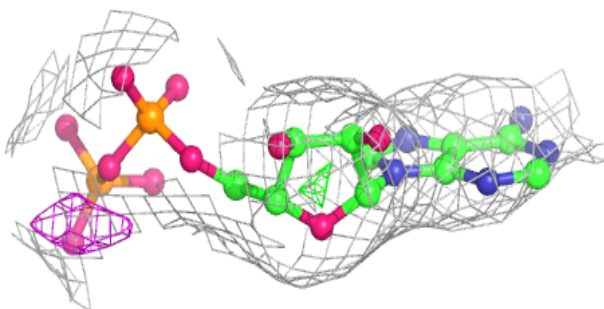
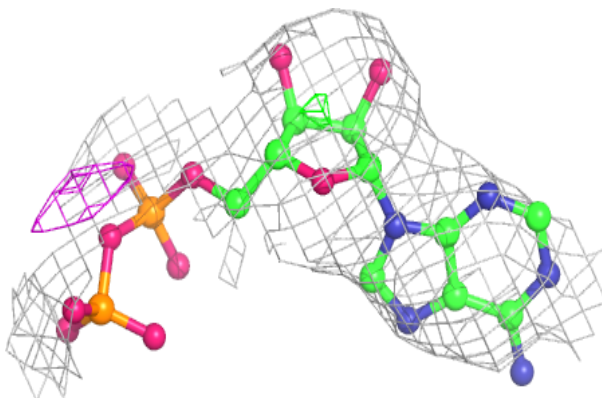


Electron density around ADP B 9007:

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

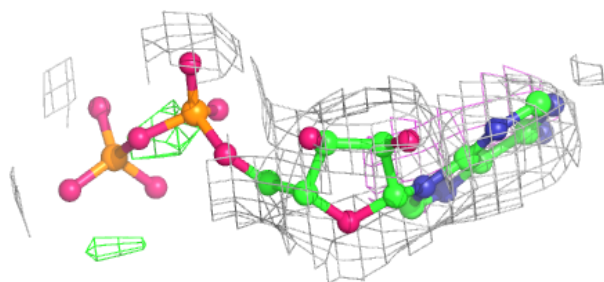
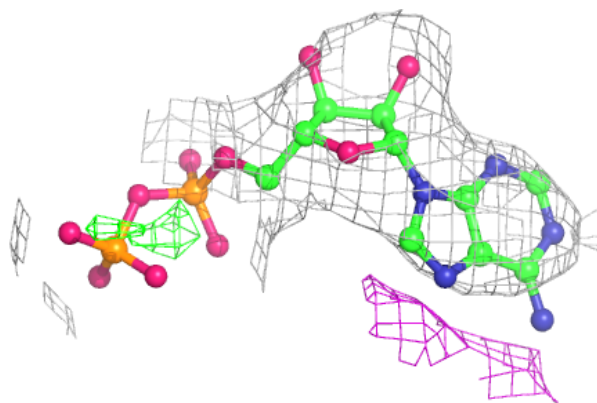
**Electron density around ADP A 9004:**

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

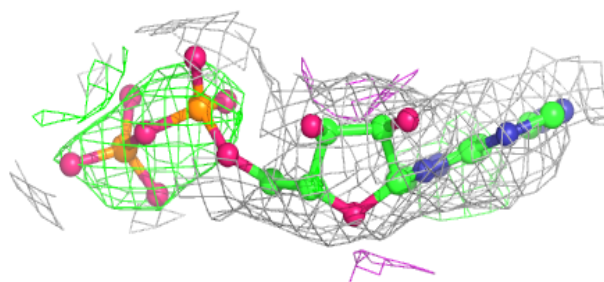
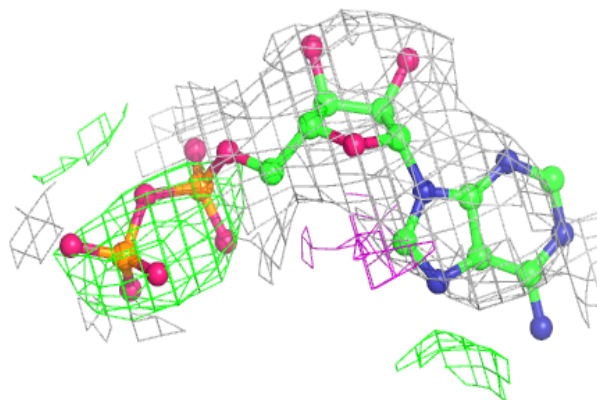


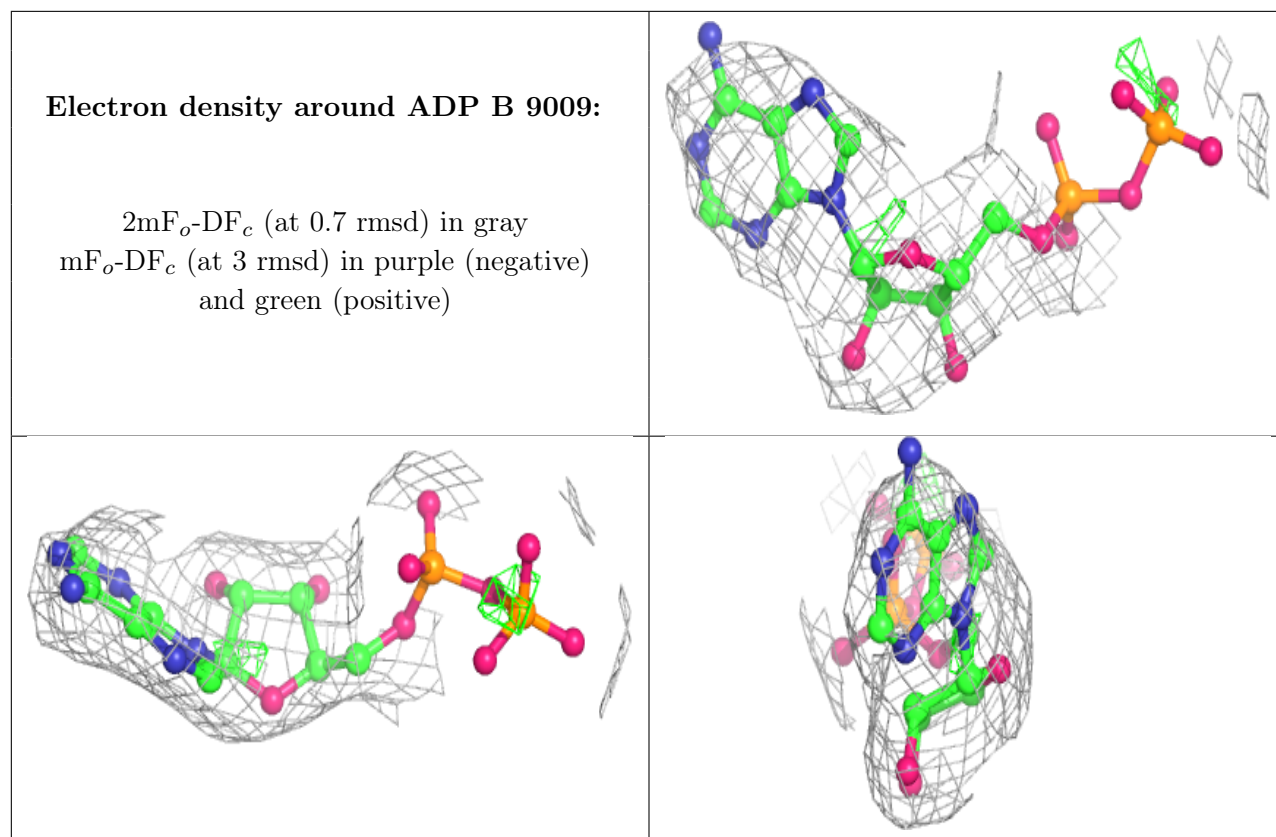
Electron density around ADP A 9003:

$2mF_o-DF_c$ (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.