



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 02:28 PM BST

PDB ID : 3VKG
Title : X-ray structure of an MTBD truncation mutant of dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 2.81 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 : 2.13
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) : 2.13

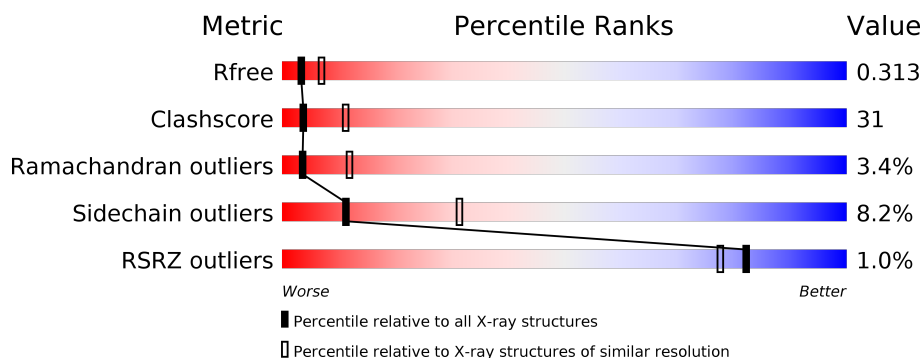
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	3245	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>41%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	3245	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>38%</div> <div>6%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 45284 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	2954	Total	C	N	O	S	0	0	0
			22821	14585	3870	4270	96			
1	B	2853	Total	C	N	O	S	0	0	0
			22146	14131	3745	4174	96			

There are 52 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
A	3494	THR	-	LINKER	UNP P34036

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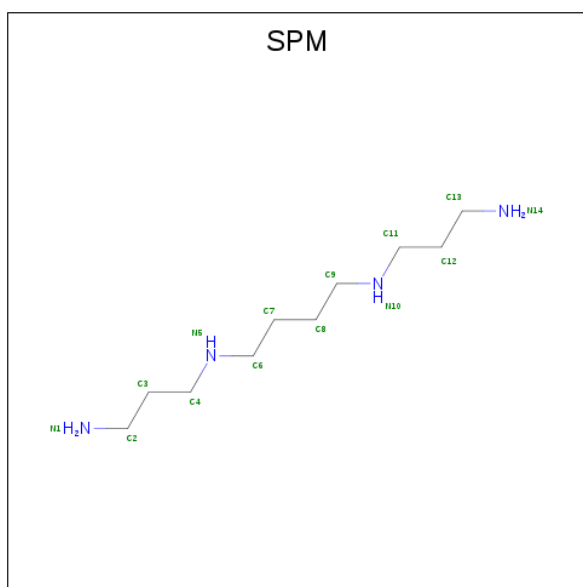
Chain	Residue	Modelled	Actual	Comment	Reference
A	3495	GLY	-	LINKER	UNP P34036
B	1364	MET	-	EXPRESSION TAG	UNP P34036
B	1365	THR	-	EXPRESSION TAG	UNP P34036
B	1366	ARG	-	EXPRESSION TAG	UNP P34036
B	1367	HIS	-	EXPRESSION TAG	UNP P34036
B	1368	HIS	-	EXPRESSION TAG	UNP P34036
B	1369	HIS	-	EXPRESSION TAG	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
B	3494	THR	-	LINKER	UNP P34036
B	3495	GLY	-	LINKER	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		

- Molecule 3 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	10	4		
3	A	1	Total	C	N	0	0
			14	10	4		
3	B	1	Total	C	N	0	0
			14	10	4		
3	B	1	Total	C	N	0	0
			14	10	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	1	Total	Mg	0	0
			1	1		

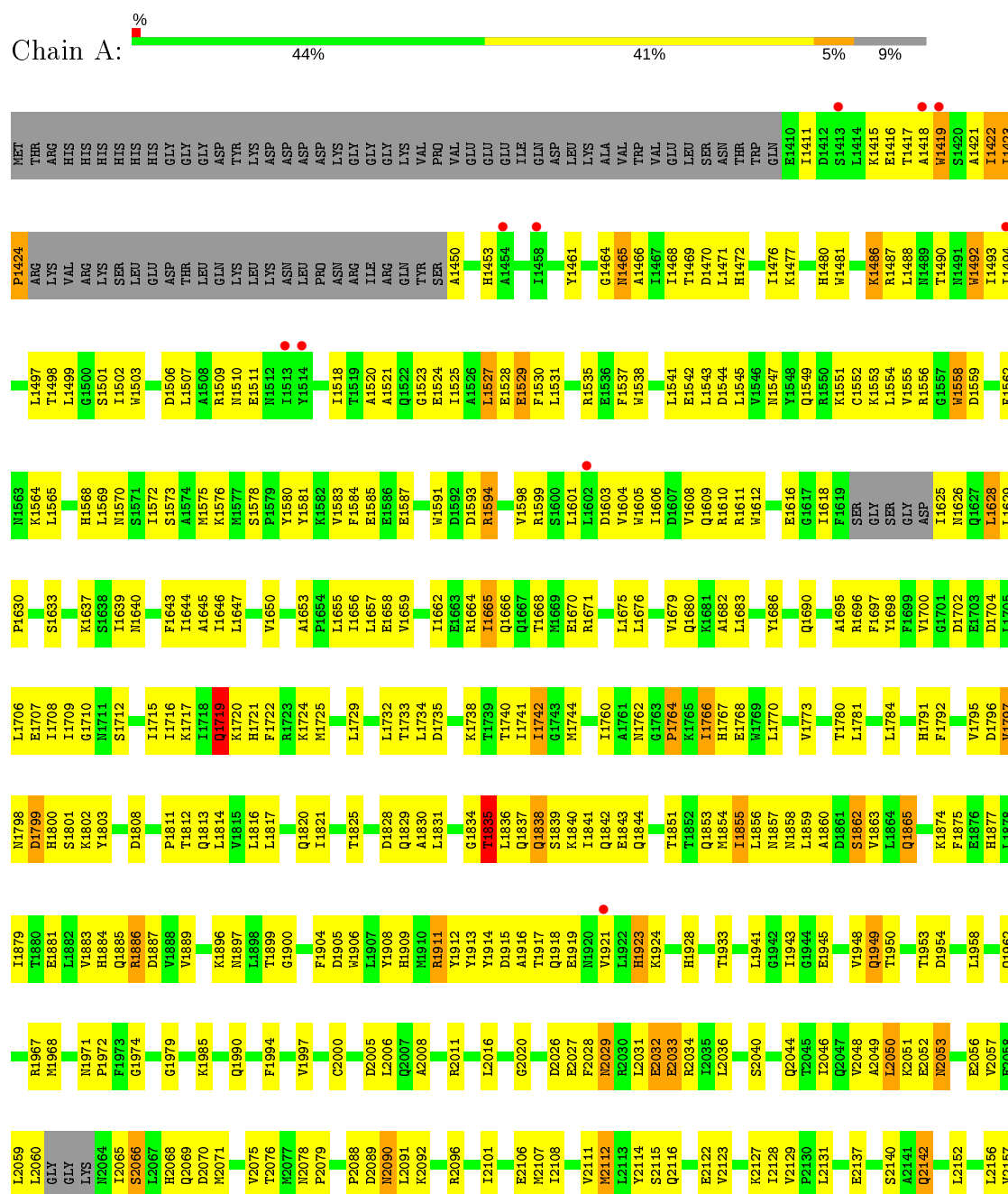
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	19	Total	O	0	0
			19	19		

3 Residue-property plots

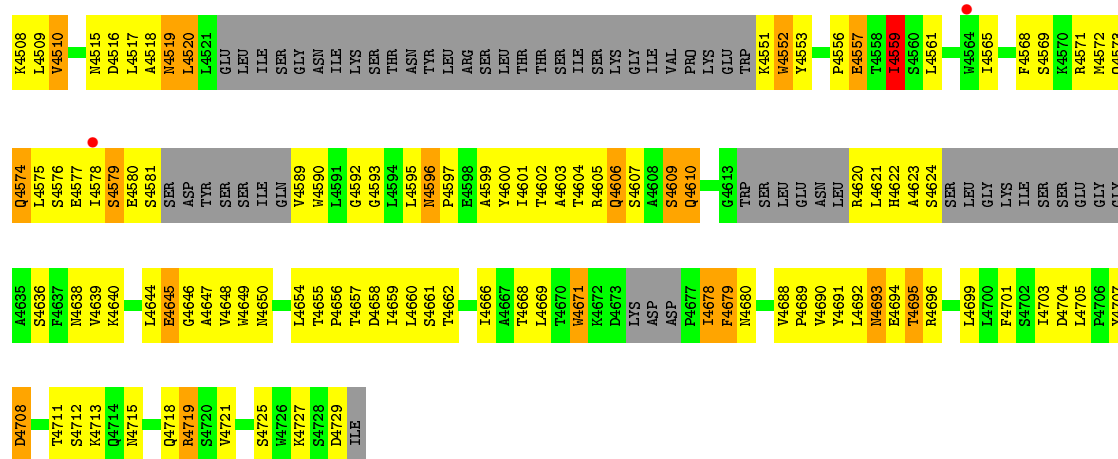
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ($RSRZ > 2$). 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.

- Molecule 1: Dynein heavy chain, cytoplasmic

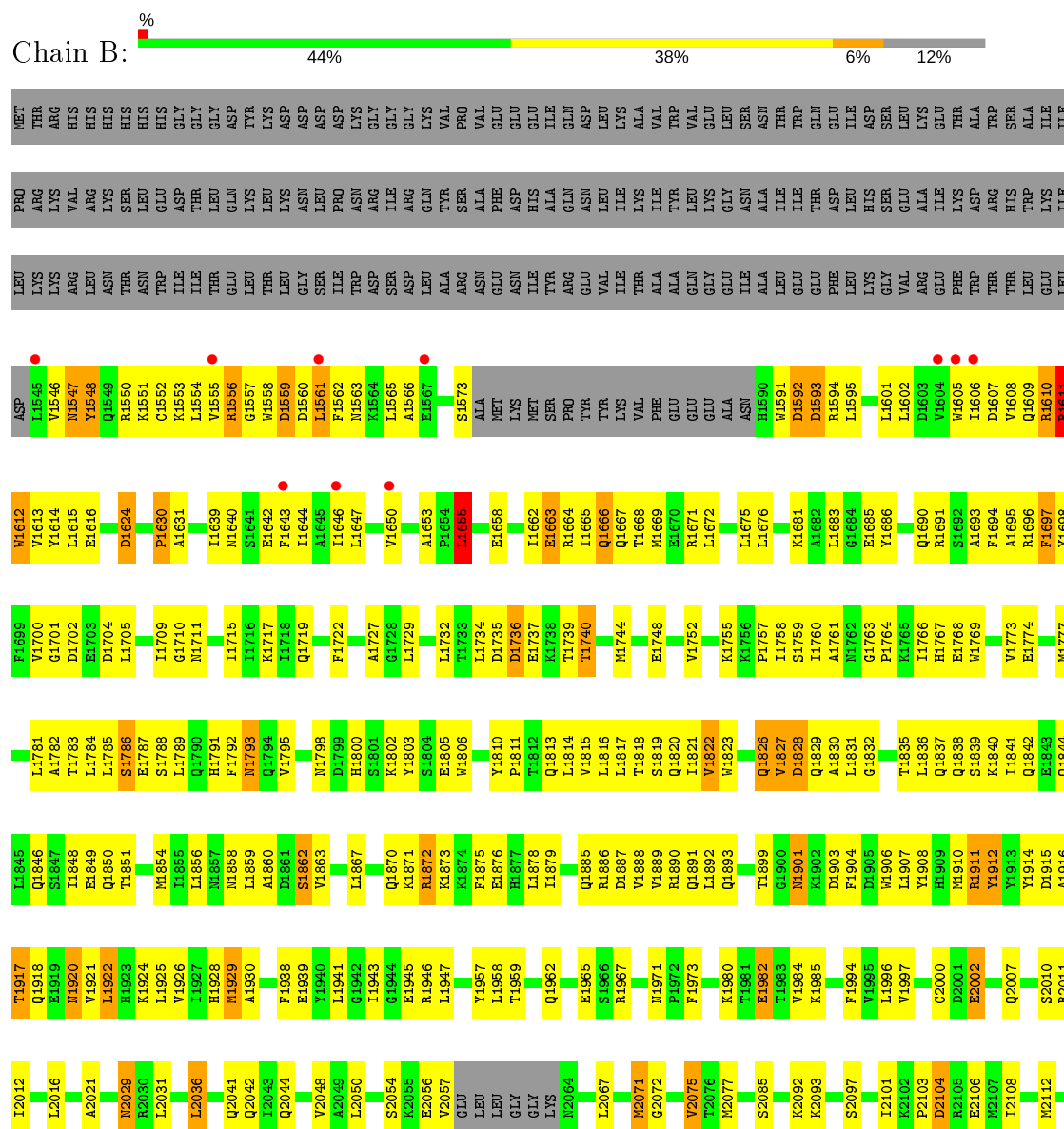




D4439	GLY	T4341	N4247	Y4176	Y4105	P4006	N3929	D3848	S3759	K3696	F3605	L3513	N3327	Q3249
GLU	T4342	A4177	N4247	A4177	D4109	Q4007	L3930	D3849	F3760	T3697	F3609	K3514	D3330	Q3250
ASP	Q4344	A4178	T4251	A4179	D4111	L4011	D3932	S3850	K3762	S3698	R3610	Q3515	Q3331	R3251
GLN	ASP	T4183	R4259	T4183	N4112	L4012	K3934	V3851	F3763	PHE	V3624	E3517	Q3332	Q3252
VAL	GLN	Y4184	Q4263	Y4184	T4113	Q4017	D3935	K3852	L3764	LEU	ASP	T3521	Q3333	N3253
GLY	GLU	Y4185	Q4263	Y4185	GLU	K4018	P3936	S3853	F3765	SER	ASP	T3522	A3334	Y3954
SER	F4351	L4186	Q4267	L4186	L4116	W4019	N3937	T3857	K3767	F3704	F3628	T3523	E3335	V3255
SER	D4352	L4187	R4267	L4187	L4117	L4020	E3938	L3858	R3768	K3705	K3629	T3524	I3336	T3256
LYS	SER	K4188	Y4271	K4188	N4118	L4021	R3939	K3705	S3630	K3706	S3630	A3524	Q3337	P3257
LYS	LYS	L4189	Y4271	L4189	A4119	L4021	R3939	K3706	F3769	K3707	S3631	L3525	Q3338	R3258
GLU	LYS	L4190	F4277	L4190	L4120	L4033	L3941	K3859	T3770	L3708	L3632	E3526	H3259	H3259
SER	GLU	L4191	H4278	L4191	K3860	Y4034	Y3942	K3860	F3773	K3527	S3633	K3527	A3341	Y3260
SER	SER	L4192	H4278	L4192	E3861	Y4034	Y3942	E3861	T3774	A3711	V3634	S3528	R3342	F3263
S4455	SER	A4193	H4278	L4193	T3862	H4036	I3947	T3862	T3775	GLY	P3635	S3529	Q3345	F3264
LEU	SER	P4194	Q4282	P4194	R3863	Q4037	F3948	R3863	D3776	ASP	S3636	A3530	V3346	N3285
ARG	LEU	Q4195	Q4282	Q4195	E4125	L4038	Y3951	E3864	L3777	G3715	P3641	T3531	Q3347	Q3347
ALA	LEU	L4196	R4284	L4196	Y4126	Q4039	T3951	E3865	C3778	C3716	E3642	Y3532	L3348	V3268
THR	GLU	L4197	L4285	L4197	S4128	W4040	R3954	A3866	S3779	L3718	E3644	Y3536	D3349	V3269
ILE	THR	Y4198	R4286	Y4198	Y4127	Q4040	V3955	Q3873	R3780	L3719	R3644	Y3539	V3350	L3270
THR	THR	L4200	Y4287	L4200	S4130	K4045	V3955	T3872	T3781	V3720	W3647	L3540	R3351	Q3279
THR	THR	E4201	P4289	E4201	P4131	K4046	V3955	E3873	T3782	D3722	H3648	Y3546	N3352	Q3279
THR	THR	L4204	G4291	L4204	L4134	Q4047	R3954	T3873	F3783	D3723	S3651	Y3546	E3353	E3280
THR	THR	H4205	W4292	H4205	C4135	F4047	V3955	E3874	V3788	V3723	S3651	Y3546	E3354	E3281
LYS	THR	L4213	Y4293	L4213	S4136	Q4048	V3955	E3875	T3789	G3716	E3656	Y3555	E3355	E3282
LYS	LYS	R4214	K4294	R4214	Y4137	Q4049	V3955	E3876	F3790	ASP	E3656	Y3555	A3356	L3283
LYS	LYS	P4216	K4294	P4216	P4138	Q4050	V3955	E3877	S3791	ASP	E3656	Y3555	A3356	L3284
LEU	LEU	Q4217	L4303	Q4217	Y4140	Q4051	V3955	E3878	S3792	PRO	E3660	Y3559	K3358	L3285
PRO	PRO	S4218	L4303	S4218	Y4140	Q4052	V3955	E3879	S3792	VAL	N3661	Y3559	K3359	N3286
LYS	LYS	F4219	A4306	F4219	S4143	Q4053	T3972	E3880	R3806	LEU	N3661	Y3559	V3360	L3287
LYS	LYS	R4219	S4309	R4219	S4144	Q4054	T3973	E3881	F3807	ASN	N3664	L3563	K3361	G3288
LYS	LYS	L4215	S4309	L4215	K4145	Q4055	T3973	E3882	R3808	ASN	L3665	L3564	K3362	G3288
GLN	GLN	F4216	I4310	F4216	K4146	Q4056	V3976	E3883	T3809	VAL	K3666	L3567	Y3363	L3289
LEU	LEU	W4217	D4311	W4217	Y4147	I4057	V3976	E3884	S3809	LEU	K3667	L3567	A3364	K3291
LYS	LYS	T4218	Y4312	T4218	P4148	Q4059	K3977	E3885	T3809	LEU	N3667	R3571	D3365	K3291
LYS	LYS	S4219	W4313	S4219	P4149	Q4060	N3981	E3886	S3814	ASN	F3668	R3571	L3366	T3295
ARG	ARG	E4220	Y4314	E4220	L4149	Q4061	E3982	E3887	D3815	LYS	N3669	R3574	GLU	Q3298
THR	THR	L4221	D4315	L4221	L4153	W4062	E3982	E3888	L3816	GLU	R3670	E3574	ALA	V3299
THR	THR	H4222	D4316	H4222	H4154	Q4063	E3985	E3889	L3817	ILE	Y3671	E3575	GLU	K3300
GLN	GLN	P4223	Y4317	P4223	Y4157	Q4064	E3987	E3890	K3818	ARG	P3672	S3578	PRO	K3301
ASN	ASN	L4224	S4318	L4224	Y4157	Q4065	E3988	E3891	L3819	LYS	V3674	S3578	THR	L3302
LYS	LYS	G4320	G4319	G4320	K4158	Q4066	E3989	E3892	Q3820	GLY	L3675	P3581	GLY	Q3303
ASP	ASP	R4321	R4321	R4321	S4159	Q4067	F3990	E3901	F3823	GLY	D3676	N3582	P3496	Q3308
L4495	L4495	I4324	I4324	I4324	F4160	A4067	L3991	E3902	I3824	ARG	P3677	T3583	L3497	K3309
C4498	C4498	I4329	I4329	I4329	S4164	Q4070	L3992	E3903	V3825	ILE	S3678	Q3584	E3500	K3310
F4499	F4499	P4330	P4330	P4330	P4165	Q4072	K3993	E3904	K3826	LEU	M3682	Q3585	V3501	R3311
E4500	E4500	W4331	W4331	W4331	E4166	Q4073	G3994	E3905	L3834	ARG	L3685	Q3586	F3502	E3312
E4501	E4501	L4332	L4332	L4332	G4167	S4074	G3995	E3906	L3835	LEU	L3686	Q3587	Q3503	V3315
E4502	E4502	Q4432	Q4432	Q4432	E4168	Q4081	D3996	E3907	L3836	GLY	M3687	T3587	E3504	K3316
I4503	I4503	O4434	R4336	O4434	E4169	K4082	G3997	E3908	N3837	ASP	L3688	V3592	E3505	N3317
S4504	S4504	F4237	F4237	F4237	E4170	K4082	L3998	E3909	L3837	GLN	Q3688	V3592	N3506	R3318
T4505	T4505	Y4238	Y4238	Y4238	A4171	L4085	T3999	E3910	L3838	ASP	A3690	F3598	A3507	E3319
G4506	G4506	L4239	L4239	L4239	E4172	L4085	K4002	E3911	S3839	VAL	D3691	Y3601	A3508	Q3319
G4507	G4507	S4340	S4340	S4340	K4173	L4085	E4003	E3912	Q3840	ASP	L3694	T3602	N3509	R3322
					S4174	L4085	T4004	E3913	A3841	PHE	L3694	G3603	E3510	K3512
					I4175	L4085	I4005	P3928	I3845	PRO	T3695	F3604		



• Molecule 1: Dynein heavy chain, cytoplasmic



F3152	R3086	G3019	V2941	L2839	E2745	A2662	E2589	V2514	ASN	L2379	D2297	L2215	S2115
R3157	M3087	K3022	N2942	P2840	I2746	S2665	R2590	V2515	GLU	P2380	N2298	V2222	Q2116
S3158	N3088	S3023	L2943	N2841	N2747	S2665	E2591	R2552	ASN	N2381	I2299	V2222	T2120
A3159	T3089	F3024	A2944	R2842	L2748	E2666	E2592	R2552	ALA	F2223	K2300	P2224	T2120
T3160	L3090	L3025	L2946	R2843	P2749	R2667	F2593	L2525	LEU	E2383	D2307	G2225	K2127
S3161	A3092	L3025	V2947	F2845	A2751	P2669	I2597	F2528	GLN	R2384	P2308	SER	I2128
F3162	G3093	F3028	R2948	N2848	T2756	L2670	Q2598	F2528	GLN	L2385	K2309	GLN	V2129
E3163	E3094	V3029	L2950	Q2861	Q2757	P2676	I2599	R2532	GLN	L2387	A2310	L2228	P2130
A3164	E3095	A3030	L2951	Q2862	Q2758	G2677	A2601	R2533	GLN	P2388	T2311	P2229	L2131
F3165	P3032	M3032	Y2952	R2863	V2759	G2677	L2602	R2534	GLN	P2389	T2312	P2230	P2230
R3166	N3033	N3033	Y2952	F2864	T2760	T2687	T2603	N2536	THR	I2390	K2313	I2231	Q2142
I3170	G3034	G3034	Y2960	F2864	T2761	L2688	P2604	S2536	THR	P2395	D2314	I2232	S2143
D3171	E3101	L3035	Q2961	T2865	F2762	L2688	V2605	S2536	ILE	E2396	Q2815	N2233	H2144
F3172	G3102	S3036	P2962	P2866	I2763	E2689	P2606	L2540	THR	E2397	L2316	N2236	Y2145
F3173	E3103	Y3038	V2963	P2866	I2763	A2690	A2607	N2541	PRO	Q2398	F2317	L2236	Y2145
G3174	E3104	Y3038	N2964	Q2869	N2766	P2692	T2608	R2542	ILE	K2340	L2320	K2237	L2149
E3175	F3105	V3042	R2965	H2871	E2767	D2693	T2609	R2543	LEU	V2401	D2321	K2238	K2153
Q3183	T3106	N3043	S2966	A2870	E2768	F2694	I2610	S2544	THR	Y2402	L2322	I2240	K2153
V3184	A3107	N3044	L2967	H2872	E2768	F2694	T2611	R2545	SER	L2403	L2321	E2242	K2163
G3185	N3109	N3045	L2968	I2873	E2768	V2696	L2612	N2547	PRO	T2404	L2322	E2242	K2164
S3186	Y3046	Y3046	E2970	Y2874	N2773	V2696	L2613	N2547	PRO	T2404	L2331	I2243	K2165
K3187	K3047	K3047	E2971	S2875	T2775	L2699	D2614	V2548	THR	T2407	P2332	A2244	C2166
F3188	A3111	S3043	V2972	R2876	T2775	L2699	V2615	L2549	THR	K2440	P2332	V2250	GLN
S3189	S3049	S3049	K2973	R2877	I2781	A2704	S2616	E2550	SER	R2440	I2340	T2251	PRO
F3190	D3050	D3050	A2974	D2883	L2782	T2705	E2617	Y2551	SER	M2413	D2341	T2252	PRO
N3191	F3051	F3051	L2975	R2884	L2783	T2706	S2618	R2552	SER	V2414	N2342	Q2253	LEU
L3192	D3052	D3052	L2976	K2785	R2784	P2707	I2619	Q2553	SER	N2415	P2343	Q2254	PRO
R3193	K3053	K3053	K2977	L2887	L2786	R2711	D2621	H2555	SER	F2416	R2344	V2255	PRO
L3194	D3054	D3054	E2982	E2888	Q2787	K2712	A2622	S2556	THR	T2420	G2345	V2256	T2174
E3195	L3055	L3055	E2983	A2889	F2788	T2713	M2623	R2556	THR	L2421	E2346	E2257	S2178
F3205	M3057	M3057	L2984	Q2891	A2791	D2714	V2624	P2560	SER	T2422	S2347	K2258	S2179
L3206	L3058	L3058	L2985	Q2891	C2792	H2716	L2626	R2566	THR	T2423	L2259	L2260	K2190
Q3207	K3060	K3060	Y2986	L2904	P2794	C2718	V2627	Q2564	MET	Q2424	K2349	Q2261	K2190
E3210	R3061	R3061	L2990	H2907	P2795	E2719	K2628	N2564	THR	N2425	L2353	L2262	Q2185
T3211	A3062	A3062	F2991	E2908	T2796	Y2720	M2629	Q2566	ILE	I2426	L2354	R2263	I2186
M3212	G3063	G3063	L2995	E2909	D2797	K2721	E2630	N2566	PRO	P2427	F2355	Q2264	I2187
E3218	K3064	K3064	L2996	L2910	A2798	R2722	V2631	Y2568	GLN	Q2428	D2358	L2265	C2188
ASN	K3065	K3065	D2997	R2911	E2799	T2723	PRO	R2572	G2492	N2429	D2359	L2266	Q2189
E3219	E3066	E3066	L2998	R2912	R2800	P2724	VAL	L2574	K2493	Y2430	D2360	N2267	Y2190
LEU	E3067	E3067	R3000	F2913	V2801	S2725	E2635	L2575	K2493	L2431	P2361	V2273	E2191
F3217	K3068	K3068	R3000	R2916	H2810	G2726	E2636	S2576	K2493	T2432	L2364	V2274	I2192
A3218	C3070	C3070	R3000	L2917	A2811	E2727	V2637	L2577	G2492	Q2433	V2364	G2276	L2196
T3219	F3073	F3073	R3003	V2918	P2812	L2730	T2638	N2578	C2498	L2434	V2364	P2277	N2197
P3220	D3074	D3074	V3004	E2921	S2823	R2731	V2641	Q2579	C2498	P2438	L2367	S2278	N2197
R3223	Q3009	Q3009	Q3009	E2921	S2823	R2731	A2642	V2579	I2501	F2439	N2368	S2278	N2200
R3224	G3010	G3010	G3010	V2925	L2827	T2732	A2642	L2580	I2502	D2440	S2369	K2282	D2201
R3225	H3011	H3011	L3011	V2925	L2827	T2732	V2651	L2581	I2502	D2440	S2369	K2282	D2201
A3226	L3012	L3012	A3012	K2928	F2831	Q2734	Q2734	G2582	Q2504	Q2442	D2372	Y2289	L2204
V3232	E3080	E3080	L3013	F2831	F2831	Q2734	R2655	S2583	LYS	E2443	D2372	Y2289	P2205
T3233	F3083	F3083	L3014	L2835	L2835	L2738	R2656	S2584	GLU	GLU	N2374	E2291	K2206
L3234	L3084	L3084	V3017	R2836	R2836	L2739	V2657	N2585	GLN	GLN	K2375	E2291	K2206
H3235	E3085	E3085	S3018	K2837	K2837	V2741	L2660	G2586	LYS	LYS	L2376	E2294	Y2212
				L2838	L2838		H2661	V2588	H2511	ARG	T2378	Q2295	Y2212
									H2513			V2296	L2214





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	204.26Å 221.81Å 192.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.45 – 2.81 96.45 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (96.45-2.81) 98.1 (96.45-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.82Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.262 , 0.319 0.255 , 0.313	Depositor DCC
R_{free} test set	10425 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	45284	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: MG, SPM, 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	0.50	0/23297	0.67	0/31692
1	B	0.47	0/22599	0.67	3/30724 (0.0%)
All	All	0.48	0/45896	0.67	3/62416 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2376	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	4054	GLY	N-CA-C	-5.92	98.30	113.10
1	B	3219	ILE	C-N-CD	-5.09	109.41	120.60

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	22821	0	21998	1375	0
1	B	22146	0	21438	1397	0
2	A	108	0	48	14	0
2	B	108	0	48	9	0
3	A	28	0	52	2	0
3	B	28	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	0	1	0
5	B	19	0	0	1	0
All	All	45284	0	43636	2766	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 31.

The worst 5 of 2766 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:3330:ASP:HB3	1:A:3532:TYR:HE2	1.12	1.12
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.31	1.12
1:A:3766:THR:HG22	1:A:3768:ASP:H	1.14	1.09
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.20	1.06
1:B:1655:LEU:HD22	1:B:1655:LEU:H	1.20	1.05

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	2908/3245 (90%)	2474 (85%)	332 (11%)	102 (4%)	3	11
1	B	2813/3245 (87%)	2376 (84%)	347 (12%)	90 (3%)	4	13
All	All	5721/6490 (88%)	4850 (85%)	679 (12%)	192 (3%)	3	12

5 of 192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1465	ASN
1	A	1583	VAL
1	A	1797	VAL
1	A	1835	THR
1	A	1839	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	2408/2921 (82%)	2220 (92%)	188 (8%)	12	33
1	B	2369/2921 (81%)	2163 (91%)	206 (9%)	10	28
All	All	4777/5842 (82%)	4383 (92%)	394 (8%)	11	31

5 of 394 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4606	GLN
1	B	2029	ASN
1	B	4209	PRO
1	A	4655	THR
1	B	1736	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 210 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4278	HIS
1	B	1842	GLN
1	B	4199	GLN
1	A	4349	ASN
1	A	4718	GLN

5.3.3 RNA ⓘ

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](#)

Of 15 ligands modelled in this entry, 3 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$
2	ADP	A	9002	4	24,29,29	1.39	3 (12%)	29,45,45	1.58	5 (17%)
2	ADP	B	9007	4	24,29,29	1.07	3 (12%)	29,45,45	1.60	5 (17%)
2	ADP	B	9009	-	24,29,29	1.34	2 (8%)	29,45,45	1.47	6 (20%)
2	ADP	A	9003	-	24,29,29	1.36	3 (12%)	29,45,45	1.58	6 (20%)
2	ADP	B	9008	4	24,29,29	1.43	3 (12%)	29,45,45	1.51	6 (20%)
3	SPM	A	9016	-	13,13,13	0.53	0	12,12,12	0.89	0
3	SPM	A	9012	-	13,13,13	0.60	0	12,12,12	0.82	0
3	SPM	B	9018	-	13,13,13	0.57	0	12,12,12	0.86	0
2	ADP	B	9010	-	24,29,29	1.08	1 (4%)	29,45,45	1.52	3 (10%)
3	SPM	B	9022	-	13,13,13	0.41	0	12,12,12	0.96	0
2	ADP	A	9001	-	24,29,29	1.25	3 (12%)	29,45,45	1.57	6 (20%)
2	ADP	A	9004	-	24,29,29	1.16	2 (8%)	29,45,45	1.55	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	A	9002	4	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9007	4	-	5/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	6/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	6/12/32/32	0/3/3/3
2	ADP	B	9008	4	-	4/12/32/32	0/3/3/3
3	SPM	A	9016	-	-	11/11/11/11	-
3	SPM	A	9012	-	-	6/11/11/11	-
3	SPM	B	9018	-	-	8/11/11/11	-
2	ADP	B	9010	-	-	6/12/32/32	0/3/3/3
3	SPM	B	9022	-	-	7/11/11/11	-
2	ADP	A	9001	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/12/32/32	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)
2	B	9009	ADP	C5-C4	3.11	1.49	1.40
2	B	9008	ADP	C2-N3	3.02	1.37	1.32
2	B	9008	ADP	C5-C4	2.94	1.48	1.40
2	A	9002	ADP	C2-N3	2.91	1.36	1.32
2	A	9004	ADP	C5-C4	2.88	1.48	1.40

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9007	ADP	N3-C2-N1	-4.83	121.13	128.68
2	A	9003	ADP	N3-C2-N1	-4.49	121.67	128.68
2	A	9001	ADP	N3-C2-N1	-4.36	121.86	128.68
2	A	9002	ADP	N3-C2-N1	-4.25	122.03	128.68
2	B	9008	ADP	N3-C2-N1	-4.16	122.17	128.68

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9002	ADP	C5'-O5'-PA-O3A
2	B	9007	ADP	C5'-O5'-PA-O1A
2	B	9007	ADP	C5'-O5'-PA-O2A
2	B	9009	ADP	C5'-O5'-PA-O1A
2	B	9009	ADP	C5'-O5'-PA-O2A

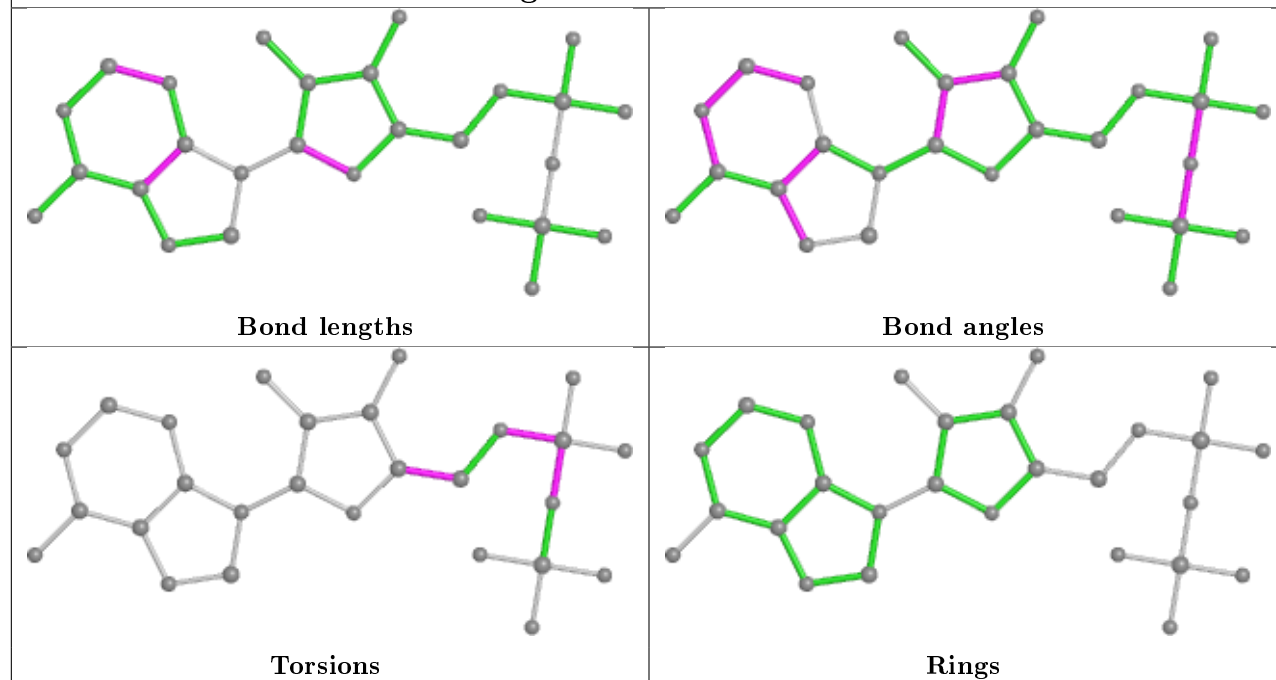
There are no ring outliers.

12 monomers are involved in 30 short contacts:

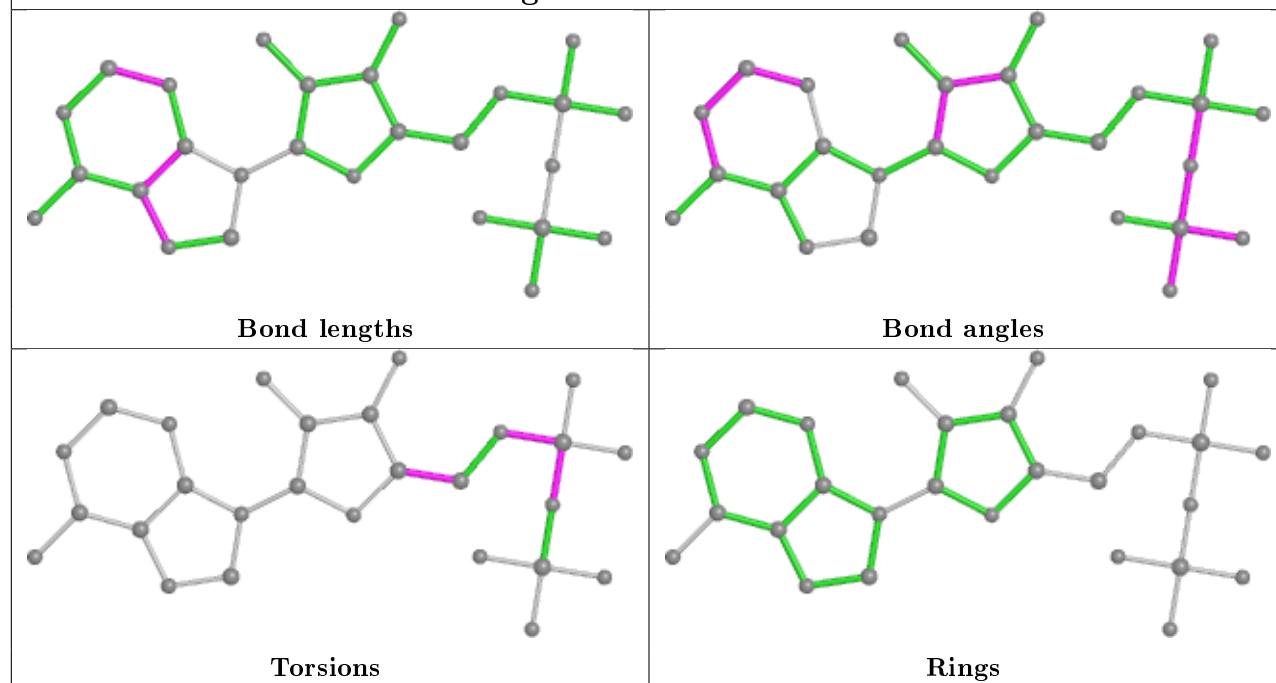
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9002	ADP	3	0
2	B	9007	ADP	2	0
2	B	9009	ADP	2	0
2	A	9003	ADP	4	0
2	B	9008	ADP	2	0
3	A	9016	SPM	1	0
3	A	9012	SPM	1	0
3	B	9018	SPM	2	0
2	B	9010	ADP	3	0
3	B	9022	SPM	3	0
2	A	9001	ADP	1	0
2	A	9004	ADP	6	0

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.

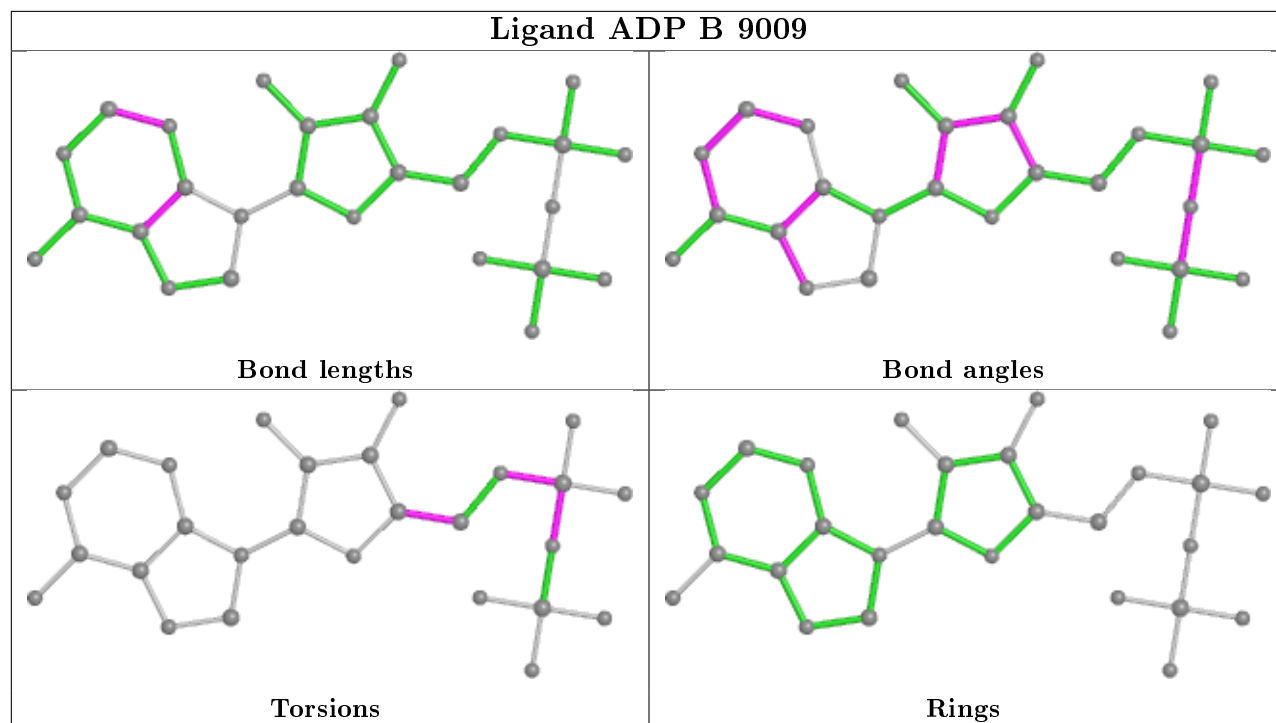
Ligand ADP A 9002



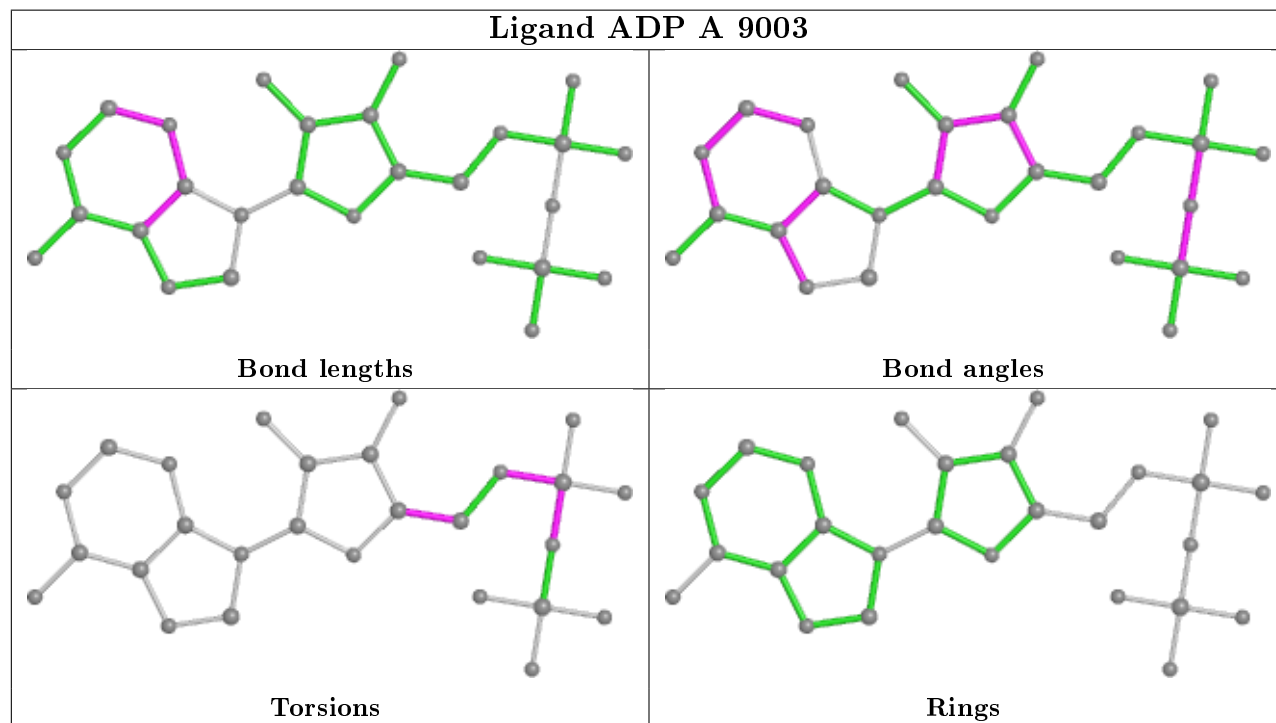
Ligand ADP B 9007

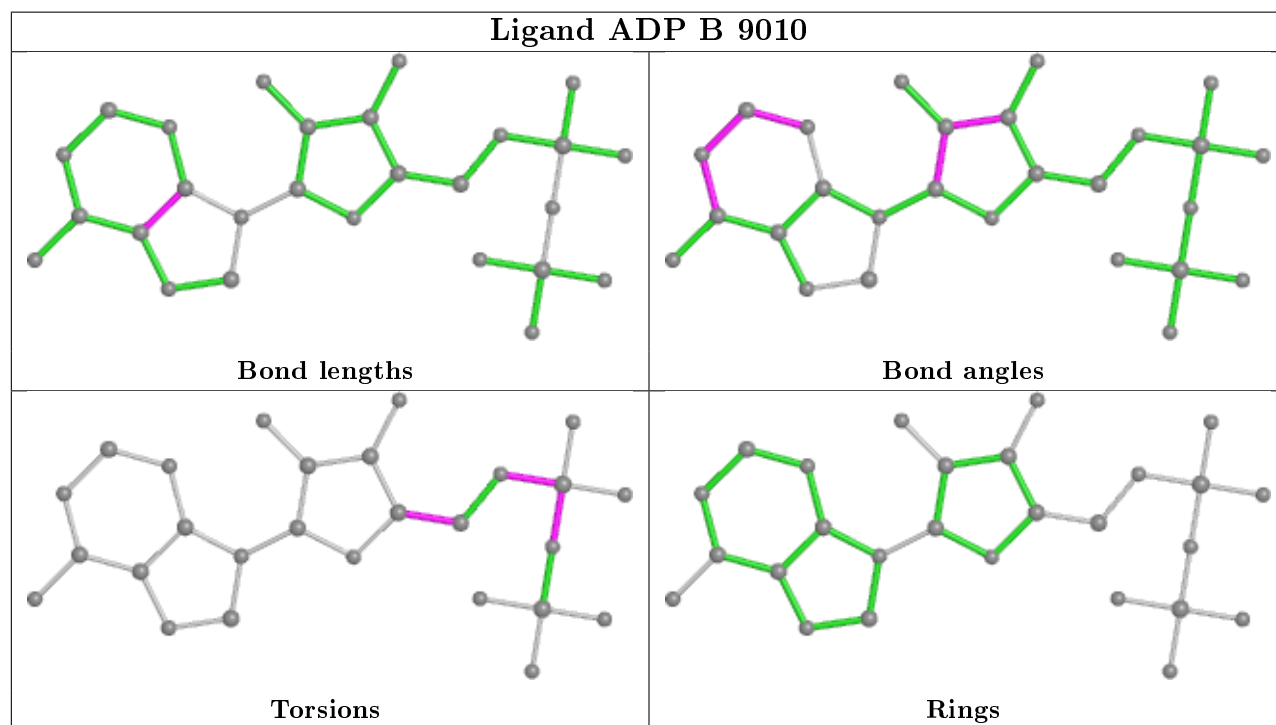
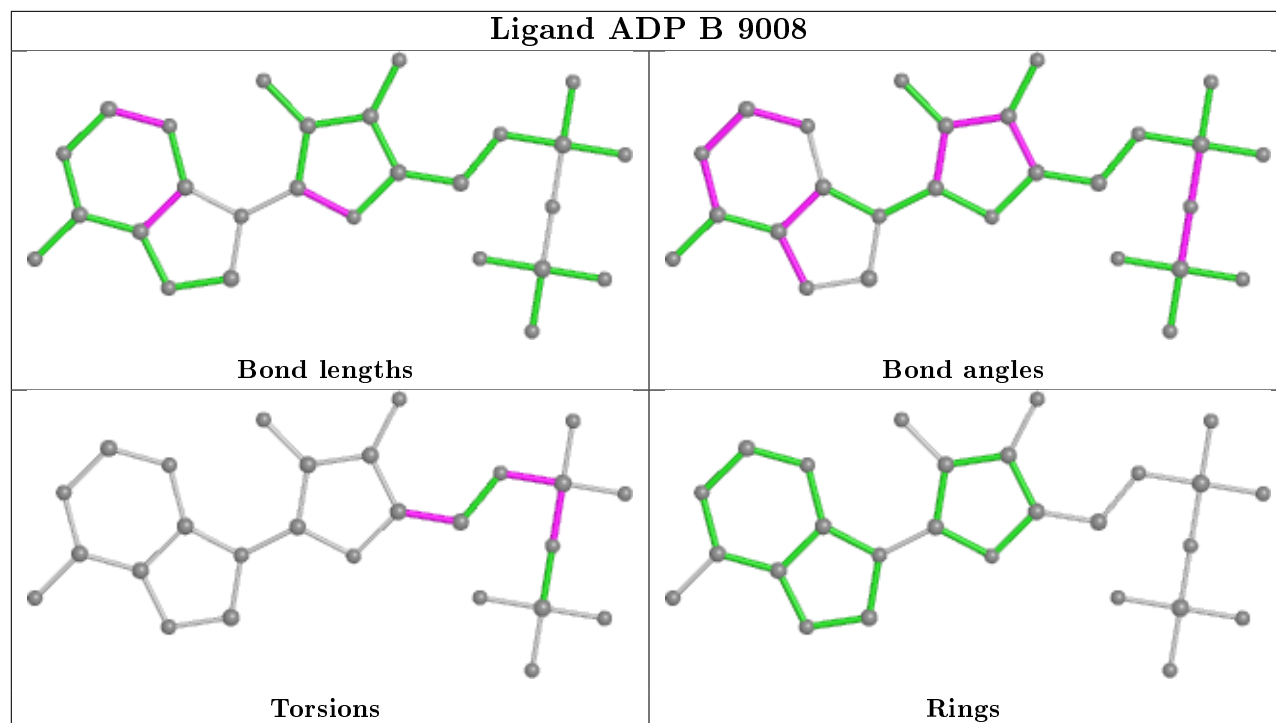


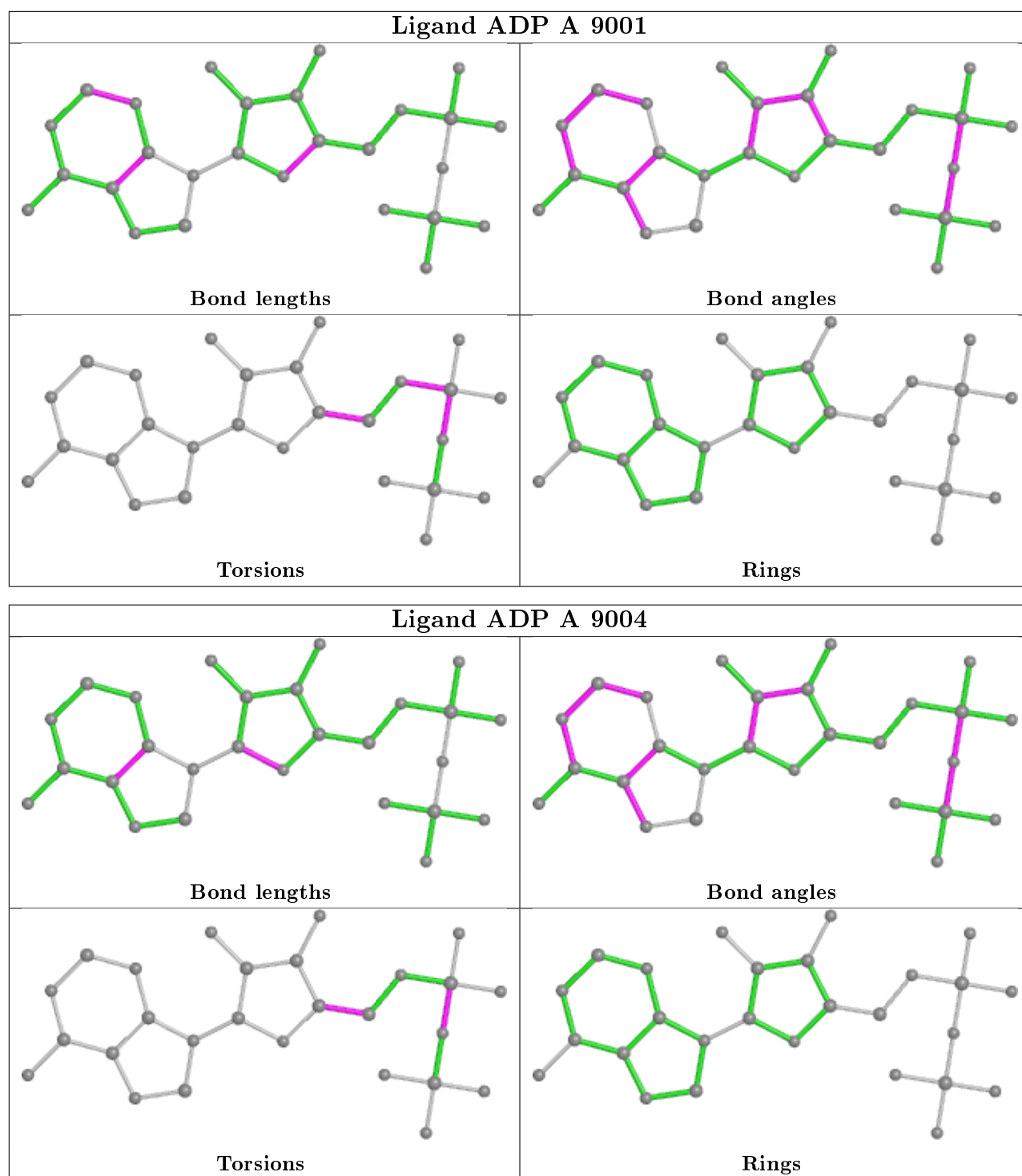
Ligand ADP B 9009



Ligand ADP A 9003







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	2954/3245 (91%)	-0.03	32 (1%) 80 75	17, 53, 78, 102	0
1	B	2853/3245 (87%)	-0.08	25 (0%) 84 80	24, 52, 75, 100	0
All	All	5807/6490 (89%)	-0.05	57 (0%) 82 77	17, 52, 77, 102	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1494	ILE	4.2
1	B	1643	PHE	3.8
1	B	1605	TRP	3.5
1	A	4191	HIS	3.2
1	B	1555	VAL	3.0

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](#)

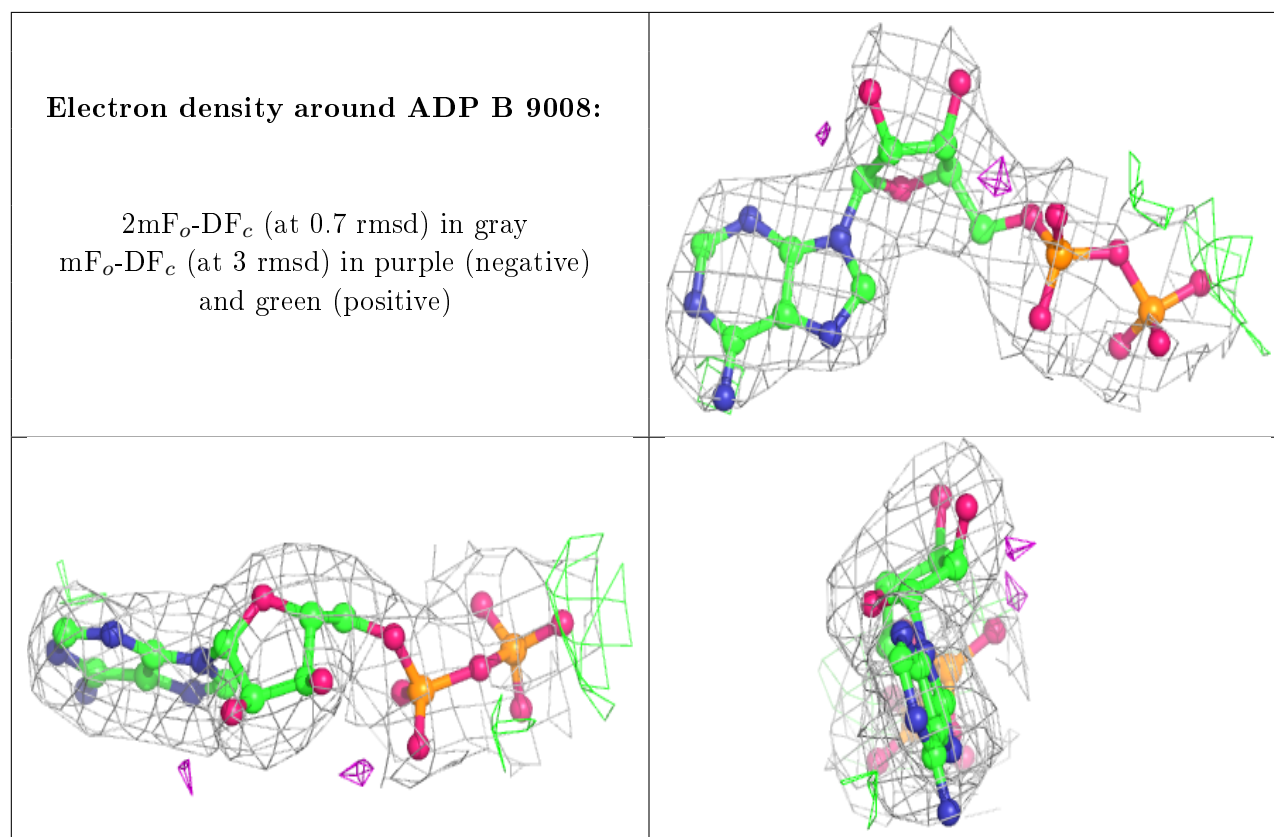
There are no monosaccharides in this entry.

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.

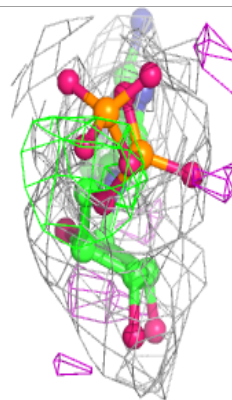
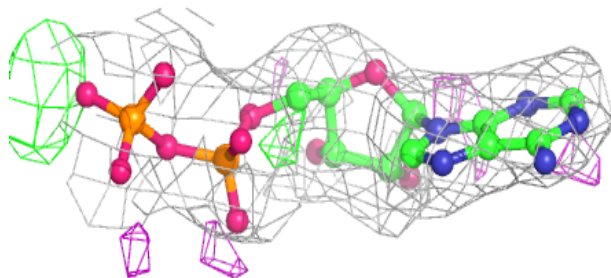
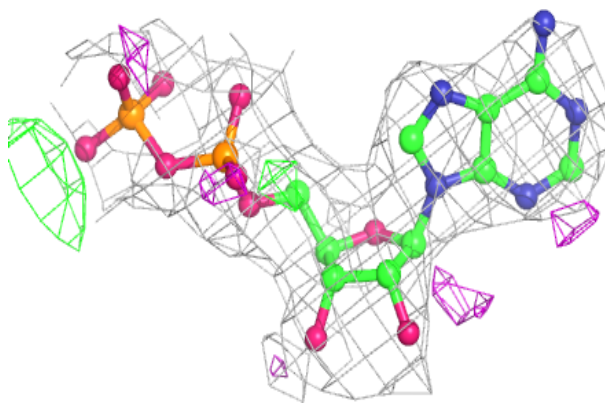
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SPM	A	9016	14/14	0.83	0.25	43,50,54,55	0
3	SPM	A	9012	14/14	0.87	0.22	37,41,45,47	0
4	MG	B	2	1/1	0.87	0.14	50,50,50,50	0
3	SPM	B	9018	14/14	0.89	0.21	57,57,59,59	0
4	MG	B	3	1/1	0.91	0.22	28,28,28,28	0
3	SPM	B	9022	14/14	0.91	0.20	37,43,49,49	0
2	ADP	B	9008	27/27	0.93	0.23	41,51,53,54	0
2	ADP	A	9002	27/27	0.93	0.23	47,49,52,54	0
2	ADP	A	9003	27/27	0.95	0.21	41,45,50,52	0
2	ADP	B	9009	27/27	0.96	0.20	39,45,48,51	0
2	ADP	B	9007	27/27	0.96	0.20	38,47,50,52	0
2	ADP	A	9001	27/27	0.96	0.21	32,38,42,44	0
2	ADP	A	9004	27/27	0.96	0.15	44,49,54,56	0
2	ADP	B	9010	27/27	0.97	0.18	31,37,46,48	0
4	MG	A	1	1/1	0.98	0.22	44,44,44,44	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.

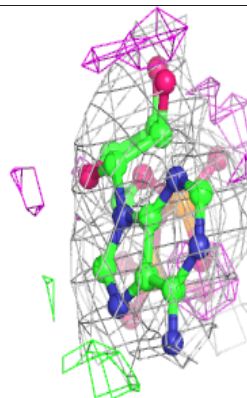
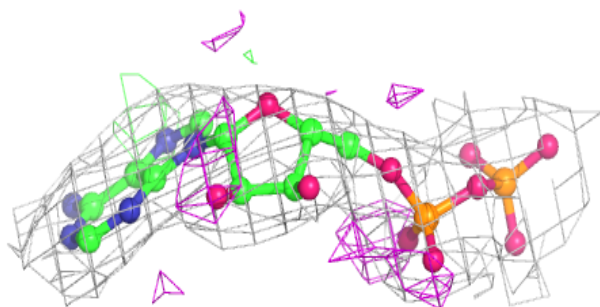
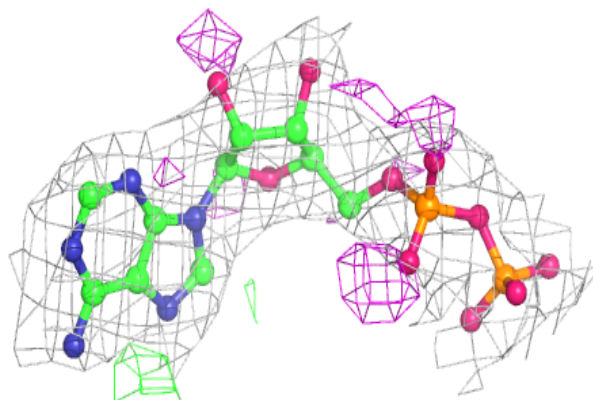


Electron density around ADP A 9002:

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

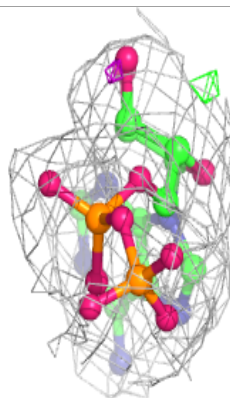
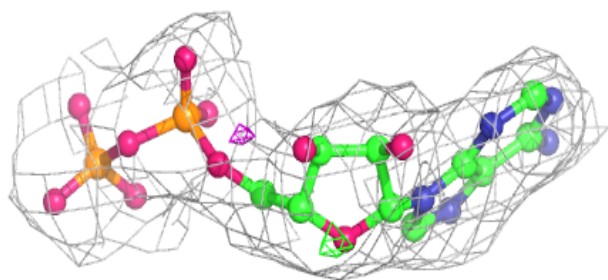
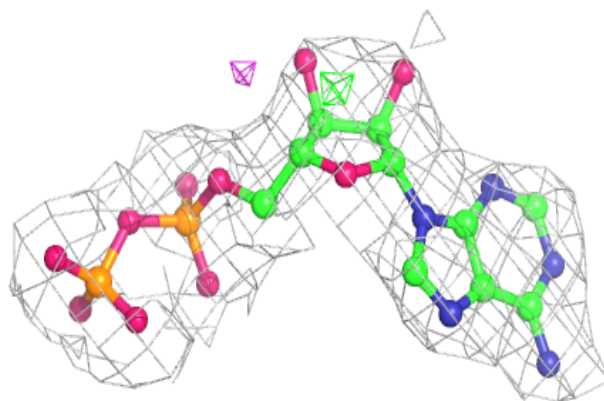
**Electron density around ADP A 9003:**

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

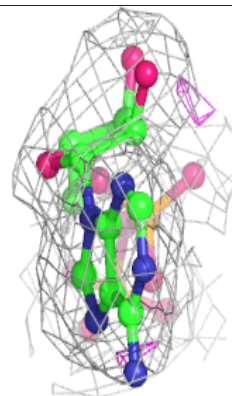
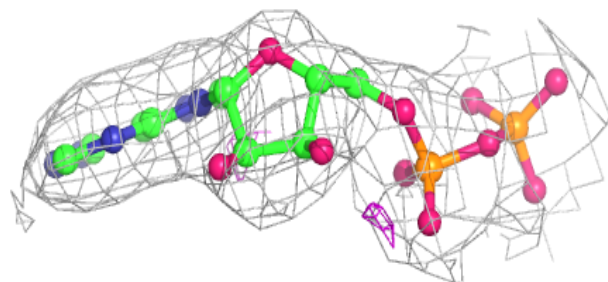
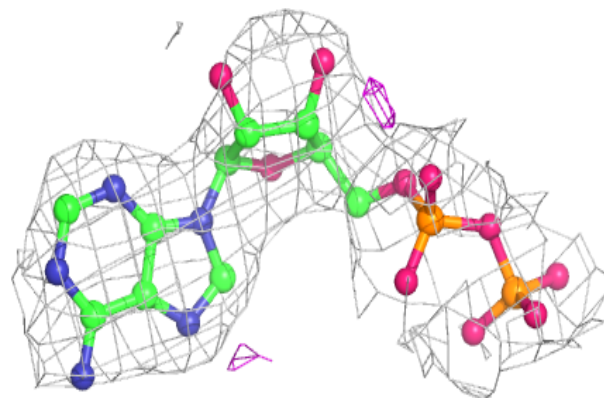


Electron density around ADP B 9009:

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

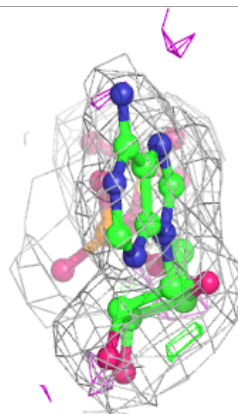
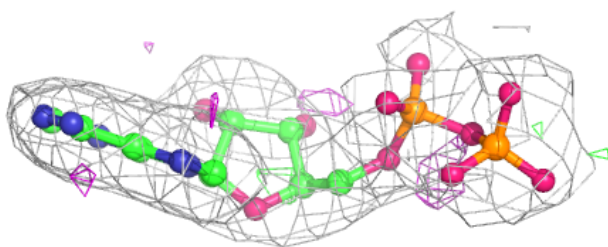
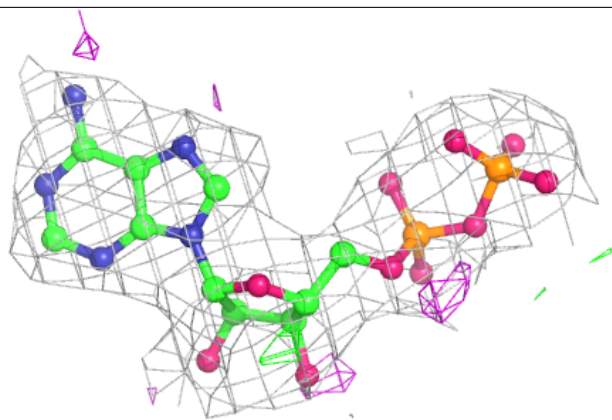
**Electron density around ADP B 9007:**

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

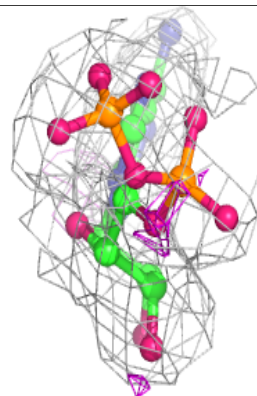
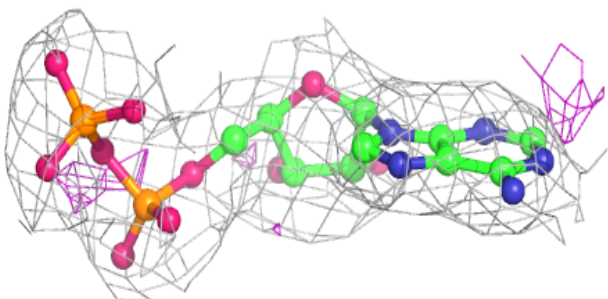
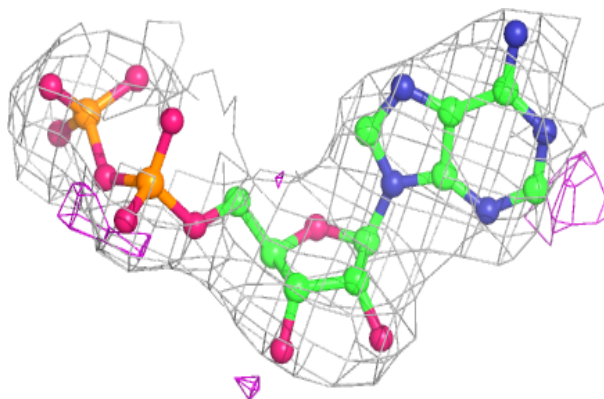


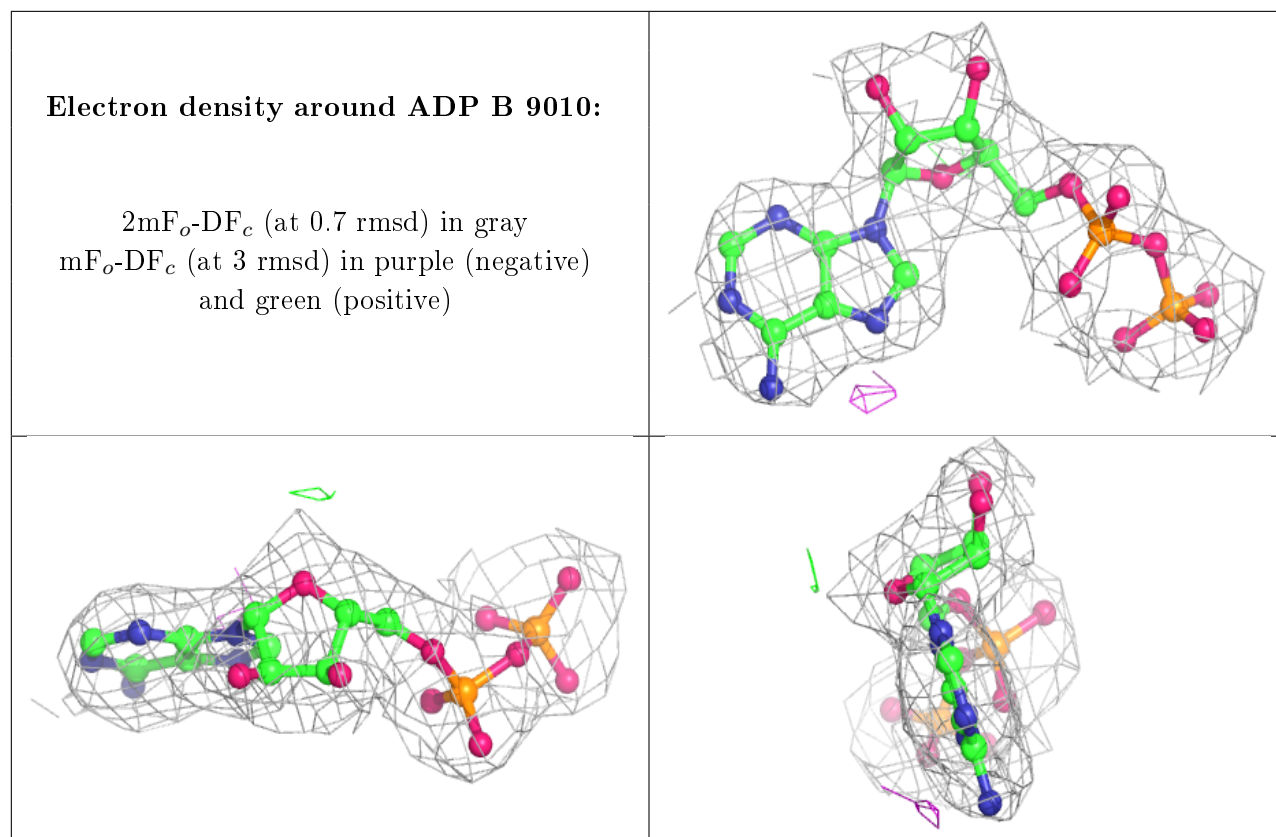
Electron density around ADP A 9001:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.