



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 4AI6 / pdb_00004ai6
Title : Dynein Motor Domain - ADP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-08
Resolution : 3.40 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

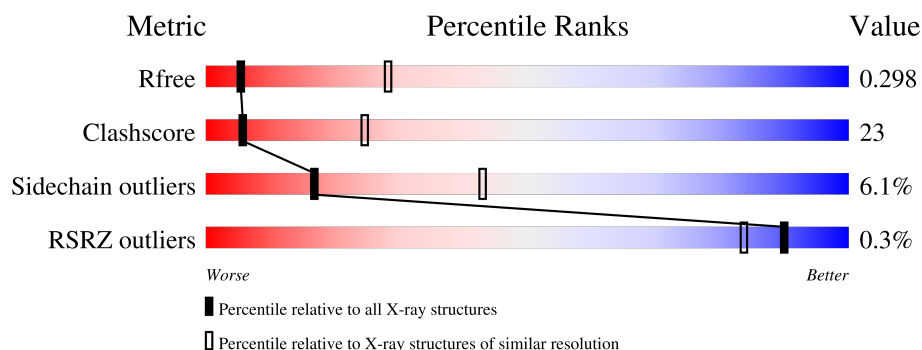
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	2695	 65% 31% . .
1	B	2695	 65% 31% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5400	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	B	5403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41678 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 GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 10 discrepancies between the modelled and reference sequences:

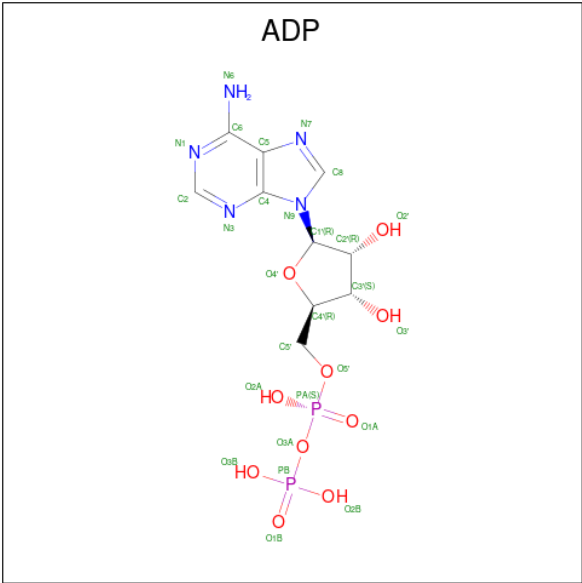
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	linker	UNP P36022
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	217	LYS	-	linker	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

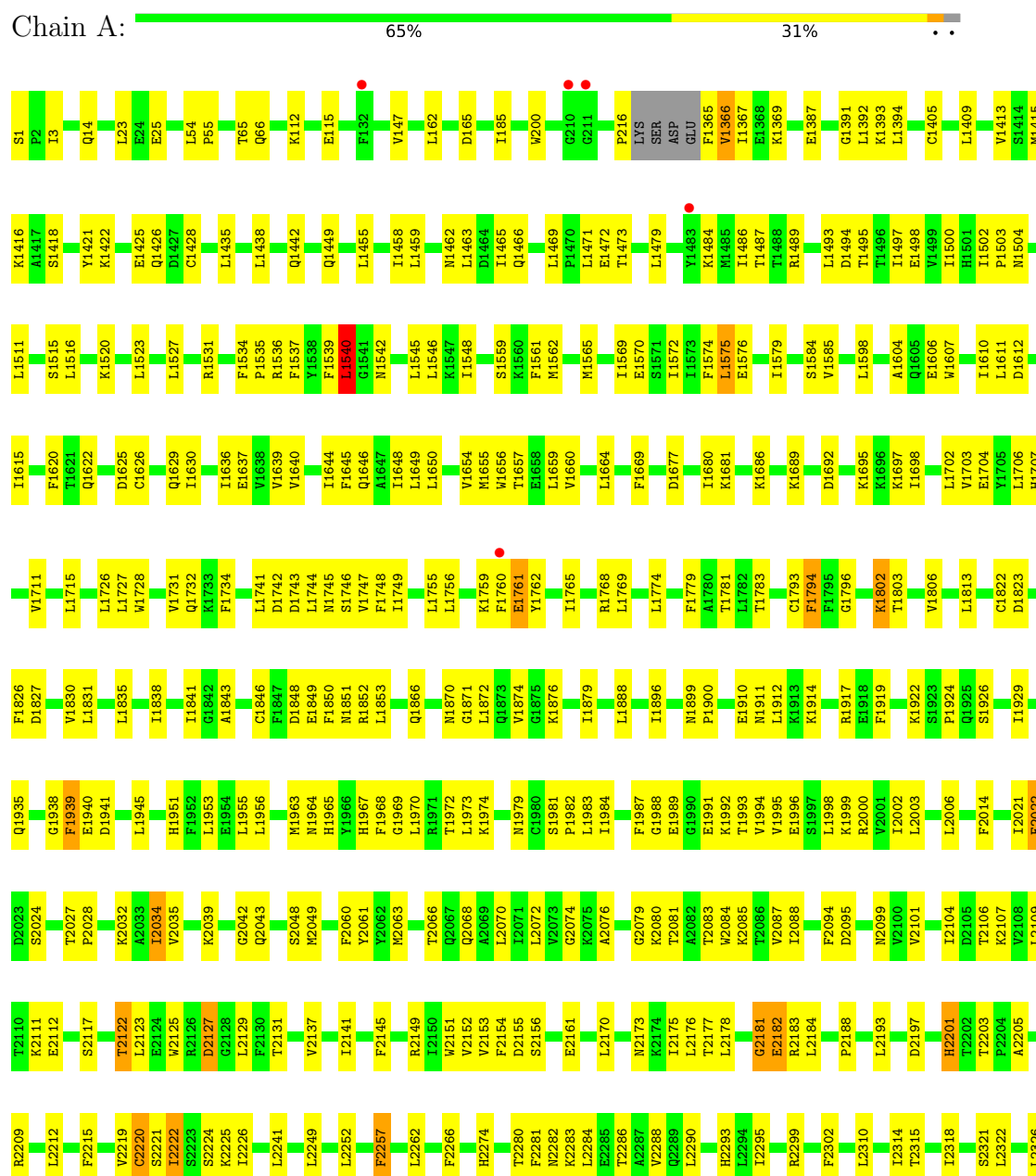
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots

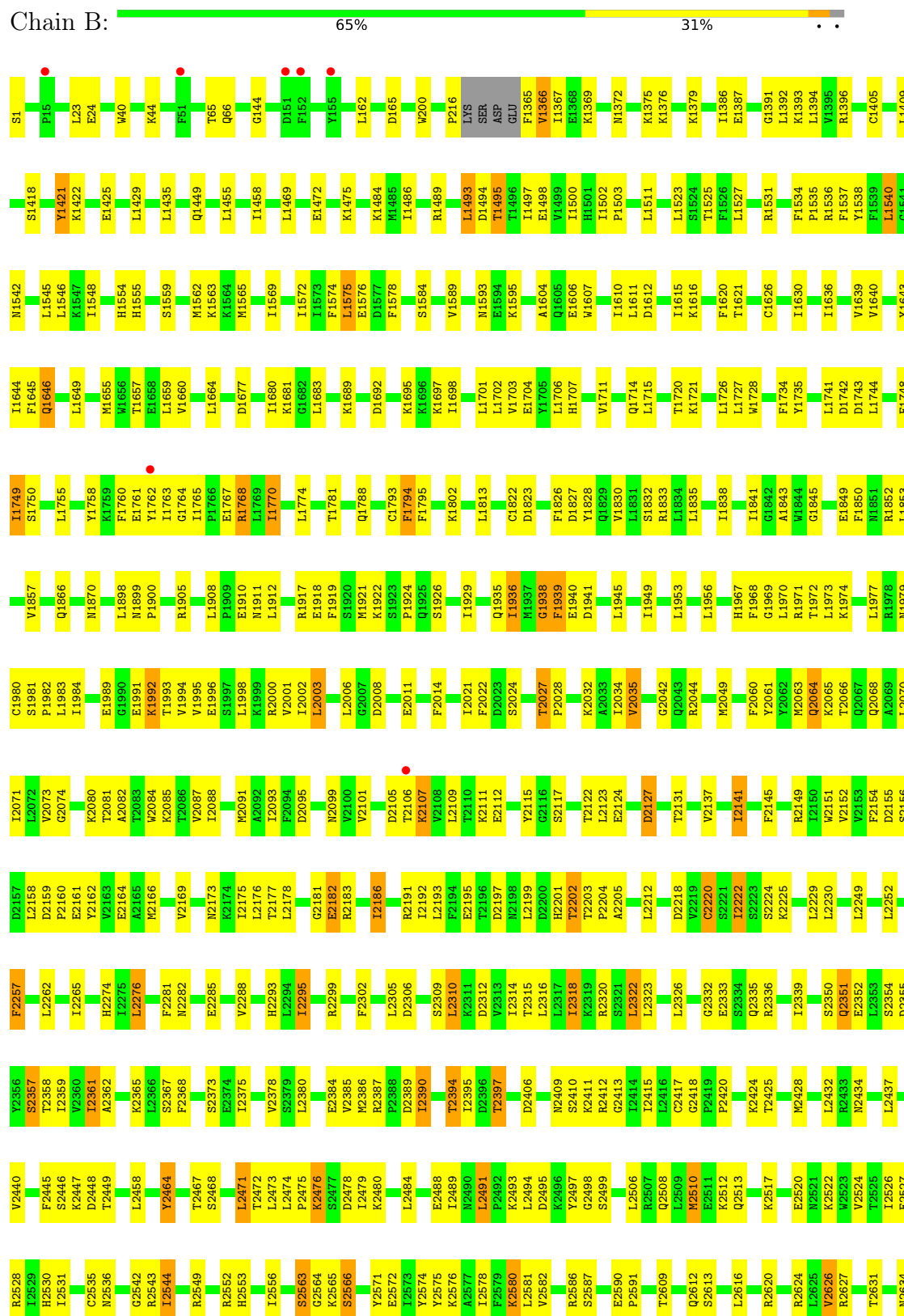
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



I3998	F3915	S3830	S3645	D3547	R3439	L3320	N2987	H2886	L2779	N2634	K2512	R2412	G2332
K4002	K3919	K3833	I3646	L3548	L3440	I3321	M2980	F2889	K2760	T2635	Q2514	G2413	S2332
L4003	V3923	G3837	F3649	K3550	F3446	G3324	G2982	G2981	P2420	P2637	K2517	G2421	S2334
L4004	K3924	K3838	L3650	Y3555	L3452	I3325	G2984	L2891	T2518	Q2639	T2518	Q2421	Q2335
C4011	S3925	I3839	V3656	L3556	L3452	I3326	V2984	C2892	K2424	T2640	N2521	K2424	R2336
V4014	F3926	I3844	F3657	L3557	E3456	S3328	N2986	D2893	T2425	T2643	N2521	T2425	T2339
F4015	Y3927	M3846	L3658	L3559	F3457	I3329	R2987	P2894	M2426	L2644	Y2524	M2426	S2330
D4019	K3934	S3847	LVS	L3566	D3459	Y3330	S2988	M2902	T2525	W2653	L2526	M2428	L2333
N4020	F3935	L3848	SER	L3567	P3461	Y3331	P2989	S2904	R2527	R2654	R2527	A2431	L2353
N4021	T3939	S3849	ARG	L3570	I3461	E3331	P2989	S2905	L2432	L2655	R2528	L2432	D2355
L4022	V3926	M3850	THR	L3578	S3463	F3334	T2989	L2908	L2437	D2658	A2534	L2437	S2357
I4023	K3852	K3852	ALA	L3579	R3464	E3341	L3002	F2909	F2445	V2677	C2535	F2445	V2360
V4024	T3943	T3853	ALA	M3580	S3457	R3342	L3010	R2911	S2446	K2447	N2536	K2447	T2361
V4027	L3945	L3855	ARG	L3583	N3471	L3346	V3017	W2916	R2448	T2449	R2549	T2449	K2362
R4028	V3946	H3858	T3669	L3587	H3472	K3350	L3024	M2917	R2448	N2463	F2550	N2463	K2365
I4029	P3947	V3778	R3670	L3592	A3473	K3353	V3028	P2937	L2471	L2472	T2551	L2471	F2368
P4030	K3948	N3780	V3671	E3593	V3476	G3354	L3028	M2938	T2472	L2473	R2552	L2473	S2369
Q4031	G3949	N3780	L3674	E3594	Y3477	K3355	LEU	A2929	L2474	L2474	R2555	L2474	C2372
L4033	S3950	N3780	L3675	M3595	T3478	V3358	LYS	M2932	L2475	L2475	A2555	L2475	S2373
L4034	K3952	N3780	W3676	K3596	G3482	V3360	ASN	V2933	L2476	L2476	R2563	L2476	S2374
Q4035	Q4035	F3786	L3677	K3597	D3483	Y3360	GLU	V2933	L2477	L2477	K2565	L2477	P2475
Q4036	F3955	T3787	V3678	E3598	G3483	D3361	LEU	V2936	L2478	L2478	S2566	L2478	K2476
S4037	F3956	R3792	Y3679	L3601	I3505	D3361	ASN	I2936	L2479	L2479	T2566	L2479	T2378
E4038	C3959	D3793	Y3683	F3607	P3506	I3367	LYS	M2938	L2480	L2480	Q2569	L2480	S2379
E4040	F3963	V3794	S3687	F3607	L3509	I3370	THR	P2937	L2481	L2481	Y2571	L2481	A2381
W4062	A3964	T3797	K3692	D3612	R3510	V3371	LEU	D2942	L2482	L2482	Y2574	L2482	A2382
L4063	S3965	F3798	K3692	M3613	V3513	T3372	SER	F2943	L2483	L2483	Y2574	L2483	V2385
Q4064	V3966	L3800	M3696	L3614	F3518	L3373	ILE	ILE	L2484	L2484	Y2575	L2484	M2396
L4065	Y3967	L3800	L3697	V3615	V3519	M3377	VAL	VAL	Q2845	Q2845	K2576	Q2845	V2391
E4068	L3968	I3801	M3698	E3616	V3519	I3377	VAL	PRO	L2485	L2485	A2577	L2485	L2490
S4069	V3971	E3802	M3698	E3617	N3521	K3386	LEU	GLY	L2486	L2486	L2578	L2491	T2392
I4070	T3974	L3803	A3699	Y3618	F3520	K3386	LEU	VAL	L2487	L2487	L2578	L2491	T2392
L4071	T3974	K3805	M3700	L3621	N3521	K3386	LEU	VAL	E2847	E2847	L2578	L2491	T2392
N4072	N3975	A3806	T3702	L3622	L3525	K3386	LEU	ASN	E2848	E2848	L2578	L2491	T2392
Y4073	N3975	S3807	F3703	L3622	L3525	K3386	LEU	ASN	Y2849	Y2849	L2578	L2491	T2392
E4074	N3978	K3808	F3703	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
Q4077	N3979	E3809	E3717	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
A4078	S3980	S3810	A3718	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
A4078	P3981	L3803	A3718	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
K4079	K3982	L3803	A3718	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
T4085	K3982	L3803	A3718	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
M4092	L3989	L3816	L3721	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
	A3990	G3817	M3722	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
	T3991	L3818	V3725	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
	L3992	L3818	V3725	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
	V3993	L3818	V3725	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
	Y3994	L3818	V3725	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392
	G3995	L3818	V3725	L3622	L3525	K3386	LEU	ASN	L2581	L2581	L2578	L2491	T2392

● Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



L4088	P3981	L3884	S3807	S3687	K3471	L3353	V3028	I2936	V2837	M2756	T2635
M4092	W3962	P3885	K3808	A3688	H3472	K3359	LEU	I2937	A2838	M2757	G2636
	A3886	A3689	L3583	T3688	A3473	Y3360	VAL	M2938	D2839	L2758	P2637
	P3887	L3690	M3684	L3690	R3476	D3361	ASN	T2941	L2840	L2759	L2638
	L3888	K3812	L3691	D3691	V3477	V3477	GLU	D2942	D2842	A2761	Q2639
	L3889	L3813	K3692	K3692	T3478	I3367	LEU	F2943	L2843	S2762	T2640
	Q3890	F3814	F3693	F3694	T3481	V3371	ASN	I2944	F2844	L2641	L2641
	R3894	F3815	K3694	K3694	D3483	T3372	THR	VAL	G2846	R2763	R2642
	F3895	L3816	M3698	M3698	D3483	L3380	THR	PRO	G2846	G2765	S2643
	V3896	G3817	A3594	A3594	D3483	L3391	THR	LEU	Y2849	K2766	R2646
	V3897	S3818	M3595	M3595	V3488	L3392	THR	VAL	Y2849	T2767	R2646
	E3898	M3700	N3596	N3596	V3488	L3393	THR	VAL	L2852	T2768	Y2653
	D3899	T3701	N3596	N3596	V3488	L3394	THR	VAL	L2853	L2769	R2654
	E4005	M3702	E3605	E3605	S3502	N3392	THR	VAL	L2853	T2770	K2664
	V4006	F3708	D3612	D3612	S3502	N3393	THR	VAL	L2856	R2771	K2664
	V4014	F3708	N3613	N3613	T3506	S3400	THR	VAL	L2856	L2779	L2673
	G4017	L3720	L3614	L3614	P3506	Q3401	THR	PHE	T2860	K2780	L2673
	S4018	V3725	V3615	V3615	F3508	D3402	THR	THR	T2860	L2781	Y2677
	D4019	S3730	Y3618	Y3618	F3508	A3403	THR	THR	L2865	V2782	Y2677
	N4020	S3729	S3510	S3510	R3510	F3406	THR	PRO	L2866	Q2783	L2686
	L4021	S3730	S3512	S3512	R3512	L3407	THR	PRO	L2867	Q2784	L2686
	Q4022	D3731	V3513	V3513	V3513	L3408	THR	GLN	Y2870	K2785	L2689
	K3919	G3836	G3837	G3837	F3629	D3409	THR	LEU	E2870	L2786	S2690
	I3920	F3838	F3838	F3838	S3630	D3409	THR	LEU	L2873	S2691	S2691
	V3923	T3839	T3839	T3839	M3631	H3413	THR	LEU	L2873	L2694	L2694
	W3924	N3843	N3843	N3843	N3631	M3414	THR	LEU	F2877	L2792	L2695
	S3925	L3844	L3844	L3844	N3632	F3313	THR	LEU	V2878	L2795	L2702
	V3926	Q3845	Q3845	Q3845	E3633	V3417	THR	LEU	H2886	D2796	L2702
	Y3927	K3846	K3846	K3846	K3634	L3429	THR	LEU	F2889	M2797	V2707
	L4034	S3847	S3847	S3847	F3641	L3429	THR	LEU	F2889	L2798	K2709
	S4037	L3760	L3760	L3760	F3530	V3437	THR	LEU	L2891	L2799	K2709
	F4038	F3767	F3767	F3767	L3634	K3438	THR	LEU	C2892	S2611	L2712
	E4039	F3768	F3768	F3768	T3535	R3439	THR	LEU	D2893	R2611	L2713
	E4040	V3769	V3769	V3769	E3536	L3440	THR	LEU	P2894	T2613	L2713
	S4060	V3856	V3856	V3856	N3538	A3443	THR	LEU	L2903	C2814	L2728
	P3947	F3657	F3657	F3657	K3541	F3446	THR	LEU	S2904	L2815	K2732
	H3948	L3658	L3658	L3658	M3541	F3446	THR	LEU	S2905	L2816	V2733
	G3949	LYS	LYS	LYS	K3544	V3450	THR	LEU	S2906	L2817	L2734
	F3950	ARG	ARG	ARG	K3544	V3450	THR	LEU	A2907	D2818	L2734
	S3951	THR	THR	THR	D3547	D3454	THR	LEU	N2910	S2737	S2737
	Y3955	ALA	ALA	ALA	L3548	G3455	THR	LEU	R2911	L2822	K2738
	F3956	ALA	ALA	ALA	L3549	E3456	THR	LEU	C2912	L2823	V2739
	F3963	ALA	ALA	ALA	K3550	E3456	THR	LEU	C2912	E2824	D2740
	A3964	ALA	ALA	ALA	L3551	D3459	THR	LEU	L2913	T2825	H2741
	S3965	ARG	ARG	ARG	E3554	P3460	THR	LEU	L2914	A2826	L2742
	L3968	F3785	F3785	F3785	Y3555	L3461	THR	LEU	N2915	E2829	L2743
	N3978	T3787	T3787	T3787	V3555	L3462	THR	LEU	W2916	R2830	L2743
	T4077	R3792	R3792	R3792	V3671	S3463	THR	LEU	M2917	M2831	L2745
	A4078	K3799	K3799	K3799	L3674	R3464	THR	LEU	W2920	N2832	Q2761
	T4085	L3800	L3800	L3800	L3677	L3465	THR	LEU	T2924	L2833	V2752
		H3803	H3803	H3803	Y3683	L3466	THR	LEU	K2924	L2834	G2754
						S3467	THR	LEU	M2932	L2835	H2755
						F3470	THR	LEU		A2836	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	174.89Å 119.17Å 193.97Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	49.29 – 3.40 49.29 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.29-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.303 (Not available) , 0.298	Depositor DCC
R_{free} test set	5512 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	133.4	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 149.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	41678	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: ADP, SO4, MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.72	3/21146 (0.0%)	1.15	76/28618 (0.3%)
1	B	0.71	3/21146 (0.0%)	1.13	68/28618 (0.2%)
All	All	0.72	6/42292 (0.0%)	1.14	144/57236 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLU	N-CA	6.86	1.55	1.46
1	B	2765	GLY	C-N	-6.46	1.25	1.33
1	A	3980	ILE	CA-C	5.60	1.58	1.52
1	B	2755	HIS	CA-C	-5.59	1.46	1.52
1	B	2464	TYR	N-CA	5.21	1.52	1.46

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	SER	CA-C-N	10.93	133.50	119.84
1	A	1	SER	C-N-CA	10.93	133.50	119.84
1	B	2479	ILE	N-CA-C	10.34	121.17	110.62
1	B	1422	LYS	N-CA-C	9.36	121.09	111.07
1	B	3920	ILE	N-CA-C	-8.72	105.43	113.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3308	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	966	0
1	B	20748	0	20207	946	0
2	A	31	0	12	6	0
2	B	31	0	12	22	0
3	A	54	0	24	31	0
3	B	54	0	24	29	0
4	A	5	0	0	1	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41678	0	40485	1915	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 23.

The worst 5 of 1915 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:B:2732:MET:HB2	3:B:5402:ADP:C6	1.40	1.57
1:B:1365:PHE:CD1	1:B:1366:VAL:HG23	1.34	1.57
1:B:2732:MET:HE1	1:B:2768:ILE:CG2	1.41	1.46
1:A:1365:PHE:CE2	1:A:1366:VAL:HG23	1.55	1.39
1:A:1365:PHE:CD2	1:A:1366:VAL:HG23	1.68	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1197/2453 (49%)	1117 (93%)	80 (7%)	15	41
1	B	2218/2453 (90%)	2089 (94%)	129 (6%)	18	45
All	All	3415/4906 (70%)	3206 (94%)	209 (6%)	17	43

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2295	ILE
1	B	2797	MET
1	B	3943	THR
1	B	2323	LEU
1	B	2566	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2927	GLN
1	B	3890	GLN
1	B	3025	ASN
1	B	3521	ASN
1	A	4077	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
3	ADP	B	5401	-	28,29,29	1.77	6 (21%)	43,45,45	1.75	9 (20%)
2	ATP	A	5400	-	32,33,33	1.49	7 (21%)	48,52,52	1.73	10 (20%)
3	ADP	A	5401	-	28,29,29	1.64	6 (21%)	43,45,45	1.77	10 (23%)
4	SO4	B	5403	-	4,4,4	0.43	0	6,6,6	0.44	0
3	ADP	B	5402	-	28,29,29	1.48	5 (17%)	43,45,45	1.83	10 (23%)
4	SO4	A	5403	-	4,4,4	0.42	0	6,6,6	0.70	0
2	ATP	B	5400	-	32,33,33	1.42	5 (15%)	48,52,52	1.73	10 (20%)
3	ADP	A	5402	-	28,29,29	1.49	5 (17%)	43,45,45	1.94	11 (25%)

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
3	ADP	B	5401	-	-	7/16/32/32	0/3/3/3
2	ATP	A	5400	-	-	4/22/38/38	0/3/3/3
3	ADP	A	5401	-	-	8/16/32/32	0/3/3/3
3	ADP	B	5402	-	-	0/16/32/32	0/3/3/3
2	ATP	B	5400	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	5402	-	-	6/16/32/32	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5401	ADP	C5-C4	5.35	1.48	1.39
3	B	5401	ADP	C5-C4	4.93	1.47	1.39
3	B	5402	ADP	C5-C4	4.88	1.47	1.39
2	B	5400	ATP	C5-C4	4.67	1.47	1.39
3	A	5402	ADP	C5-C4	4.62	1.47	1.39

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5402	ADP	C5-C4-N3	-5.82	118.71	126.72
3	B	5402	ADP	C5-C4-N3	-5.71	118.86	126.72
3	A	5401	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	5400	ATP	C5-C4-N3	-5.63	118.97	126.72
2	B	5400	ATP	C5-C4-N3	-5.50	119.14	126.72

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5400	ATP	C5'-O5'-PA-O2A
2	B	5400	ATP	C5'-O5'-PA-O2A
3	A	5401	ADP	PA-O3A-PB-O2B
3	A	5401	ADP	C5'-O5'-PA-O1A
3	A	5401	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

8 monomers are involved in 91 short contacts:

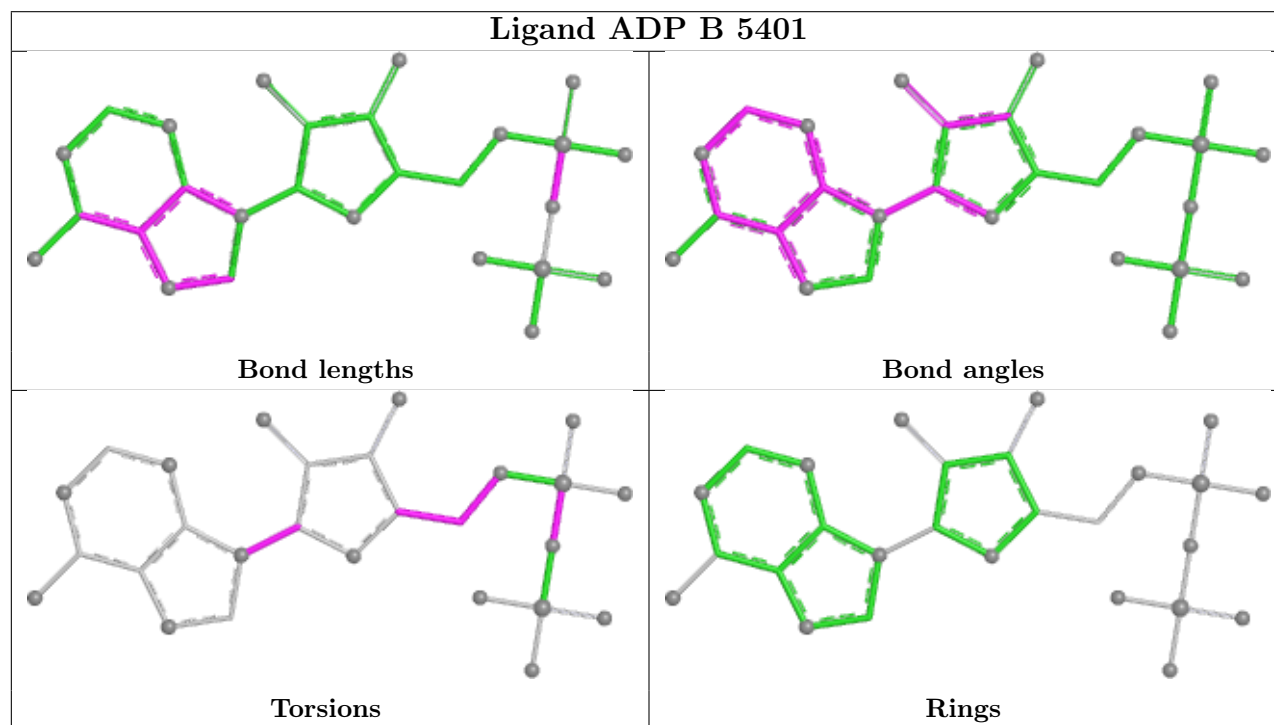
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5401	ADP	6	0
2	A	5400	ATP	6	0
3	A	5401	ADP	13	0
4	B	5403	SO4	2	0
3	B	5402	ADP	23	0
4	A	5403	SO4	1	0
2	B	5400	ATP	22	0

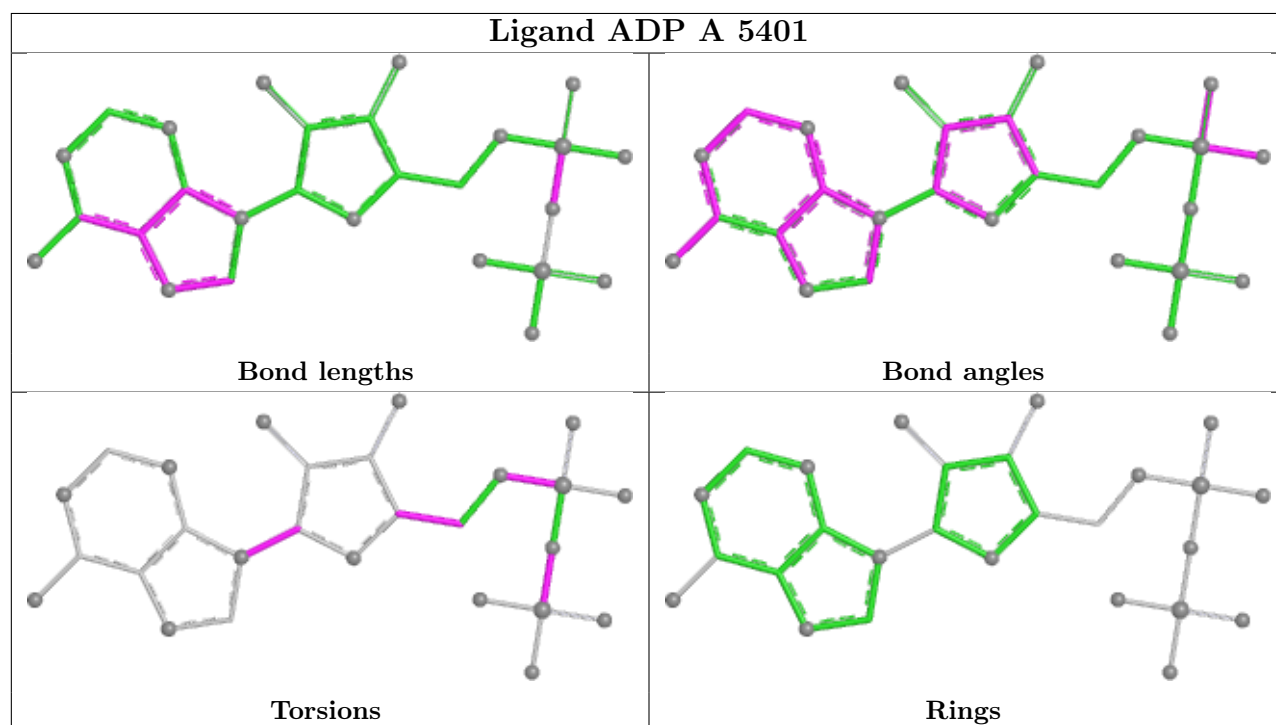
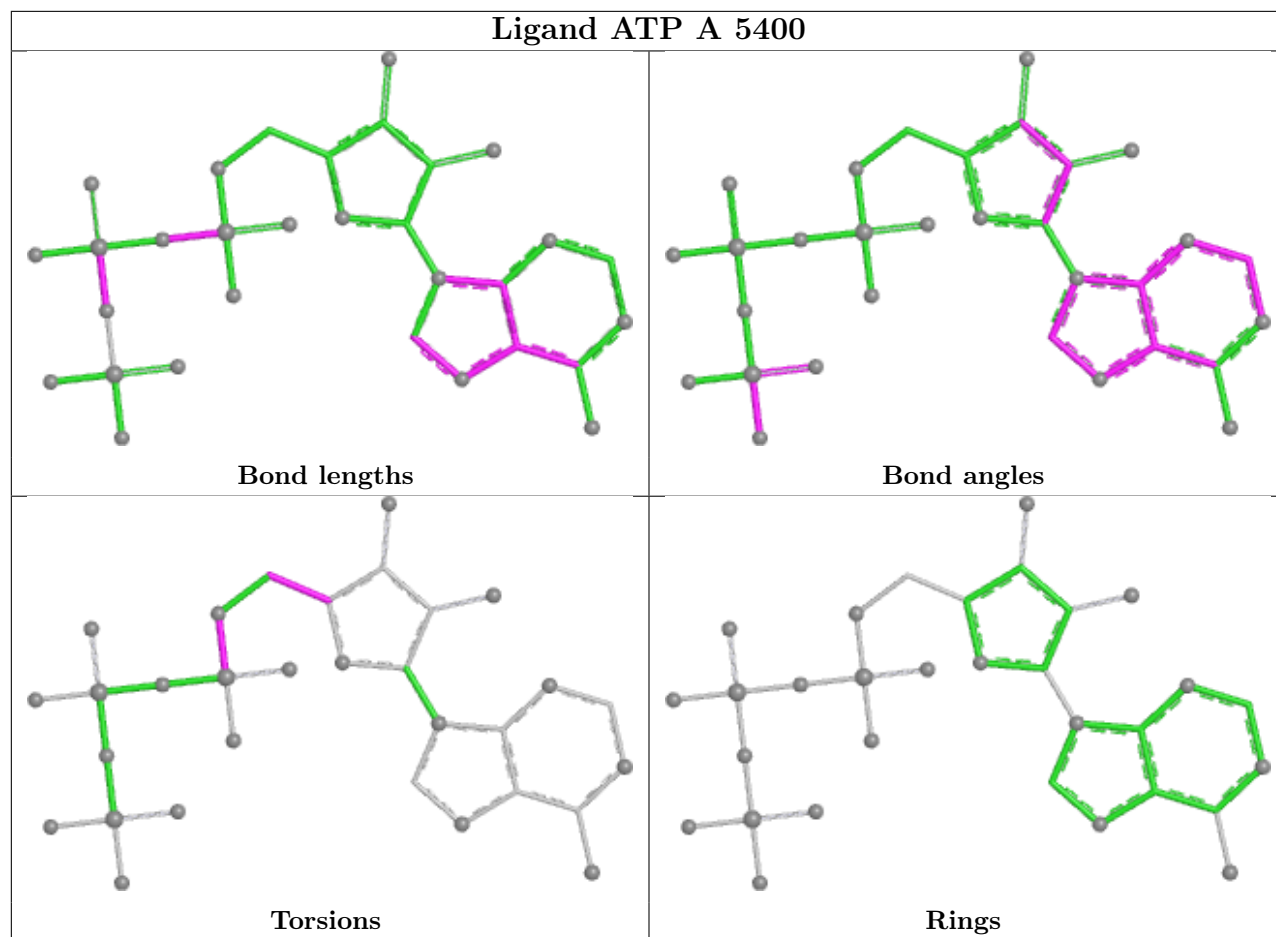
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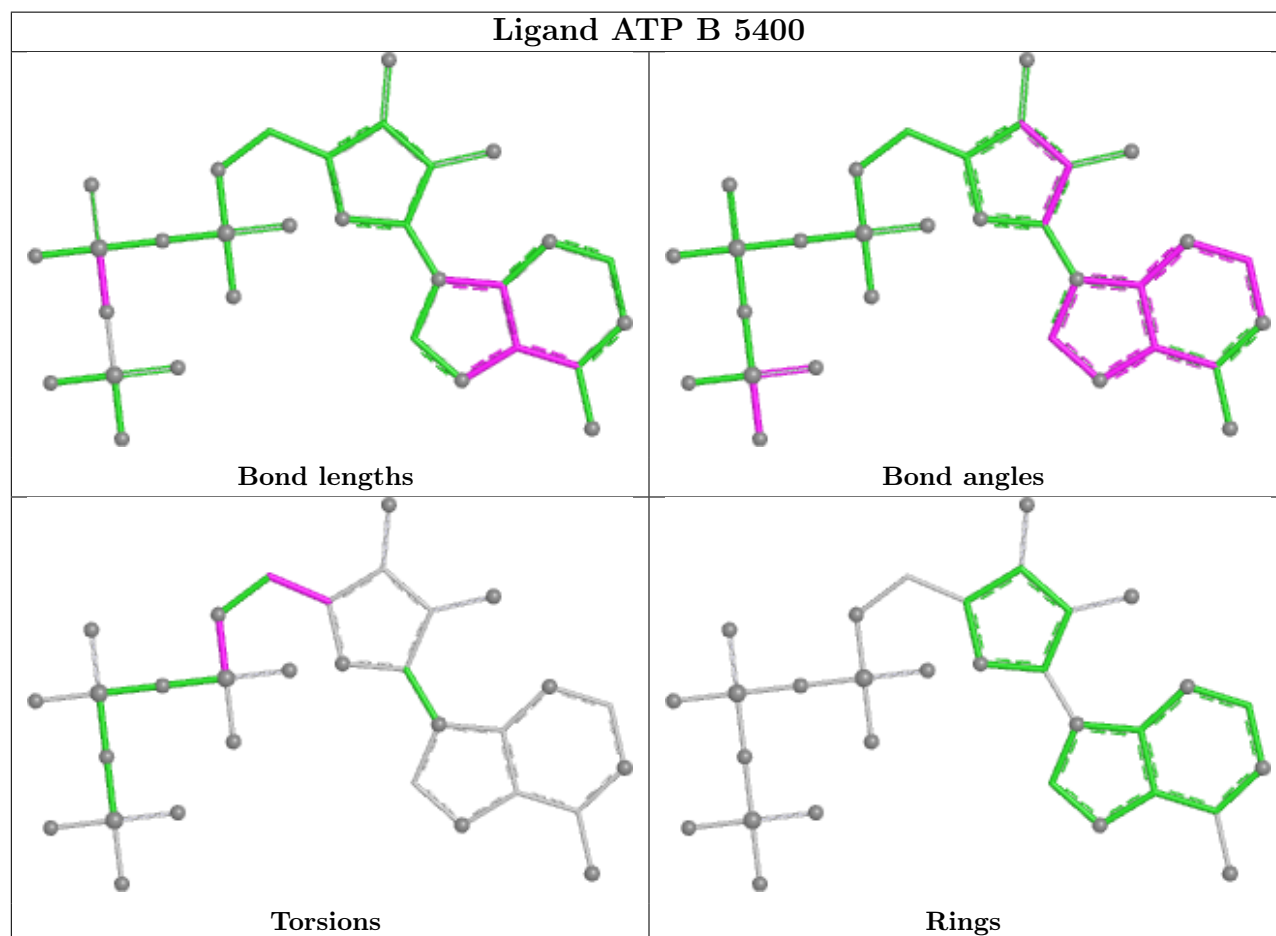
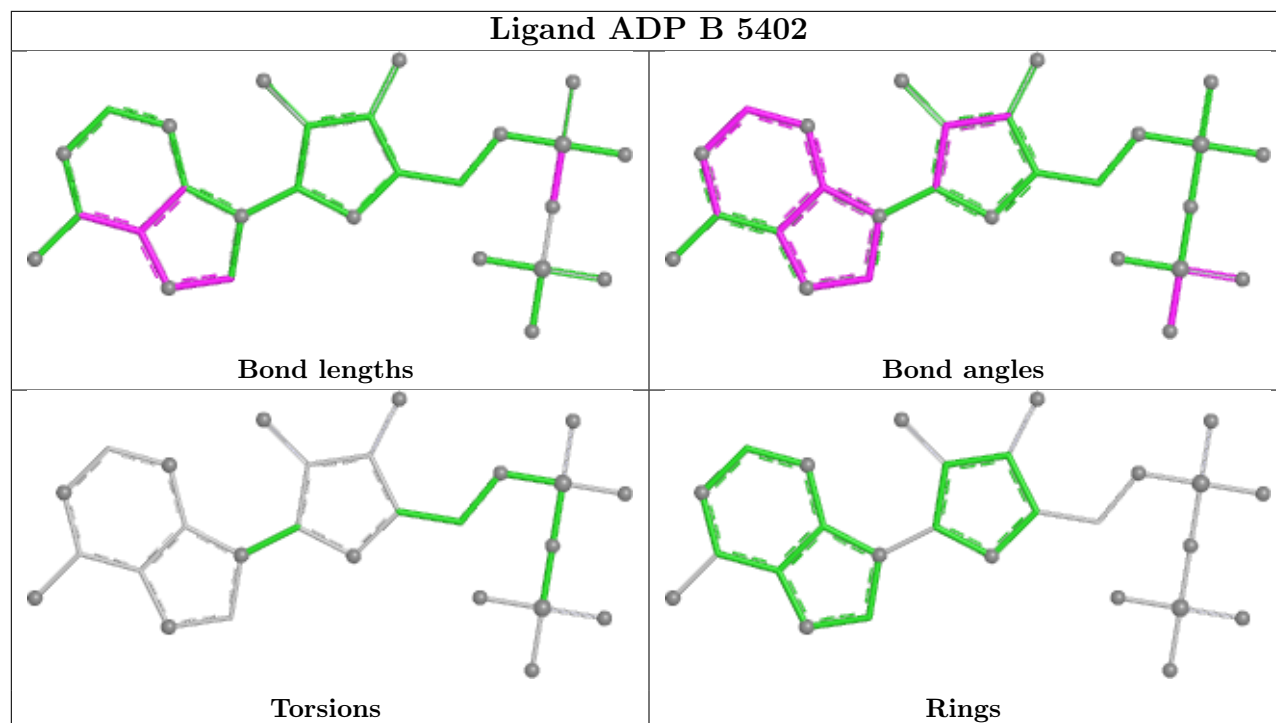
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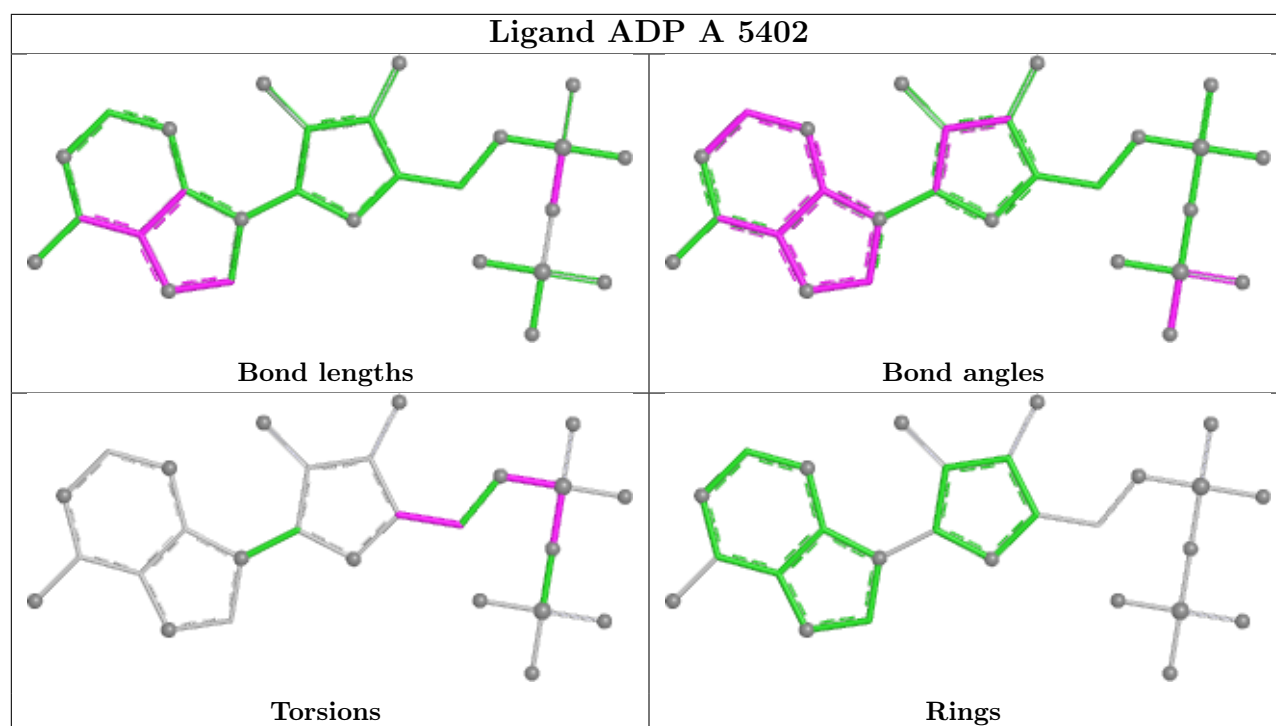
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5402	ADP	18	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	2650/2695 (98%)	-0.48	6 (0%) 91 87	88, 185, 310, 500	1 (0%)
1	B	2650/2695 (98%)	-0.50	8 (0%) 90 84	96, 180, 317, 500	1 (0%)
All	All	5300/5390 (98%)	-0.49	14 (0%) 90 84	88, 183, 311, 500	2 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	3.5
1	B	152	PHE	3.3
1	B	2106	THR	2.9
1	A	132	PHE	2.9
1	A	1483	TYR	2.9

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](#)

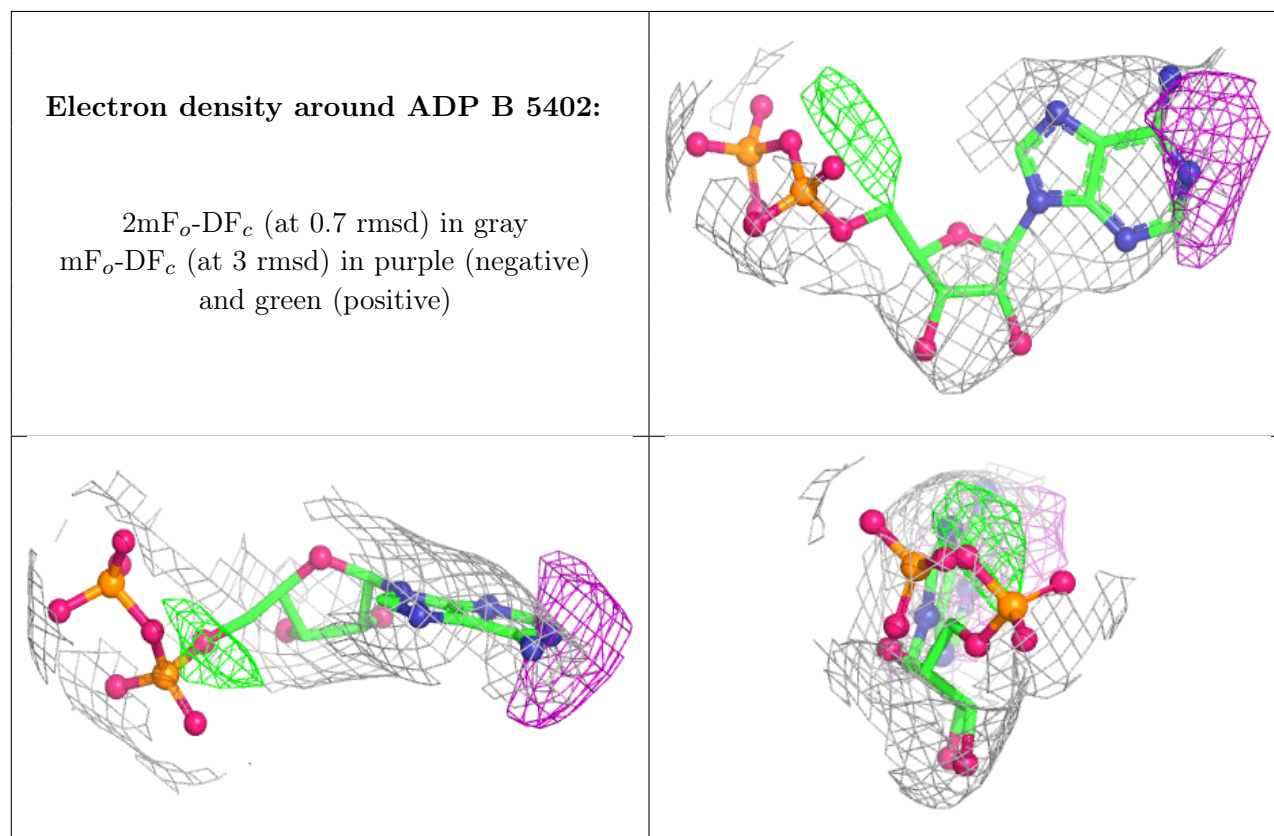
There are no oligosaccharides in this entry.

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.

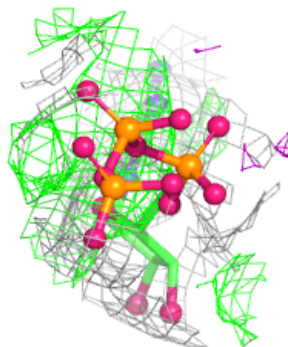
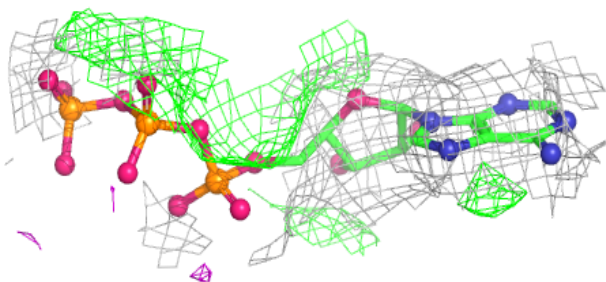
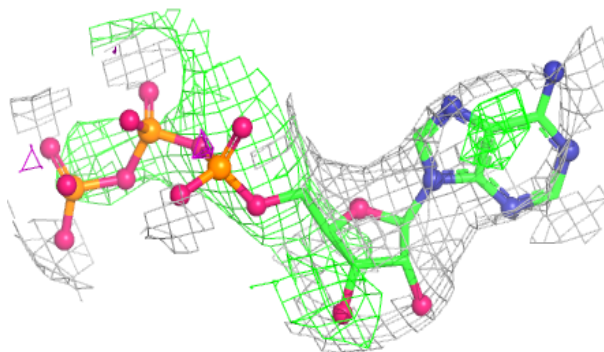
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	5404	1/1	0.86	0.09	97,97,97,97	0
3	ADP	B	5402	27/27	0.93	0.08	108,145,183,194	0
2	ATP	B	5400	31/31	0.93	0.10	124,160,195,221	0
5	MG	B	5404	1/1	0.93	0.06	107,107,107,107	0
3	ADP	A	5401	27/27	0.95	0.06	126,146,191,198	0
3	ADP	A	5402	27/27	0.96	0.05	134,176,208,218	0
4	SO4	B	5403	5/5	0.96	0.06	139,143,171,171	0
3	ADP	B	5401	27/27	0.97	0.06	98,121,138,153	0
2	ATP	A	5400	31/31	0.97	0.08	122,147,224,246	0
4	SO4	A	5403	5/5	0.97	0.04	101,136,142,145	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.

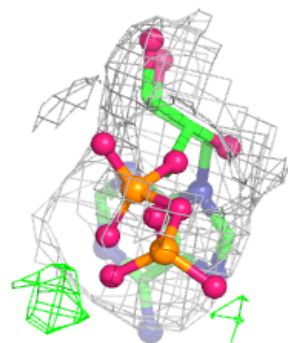
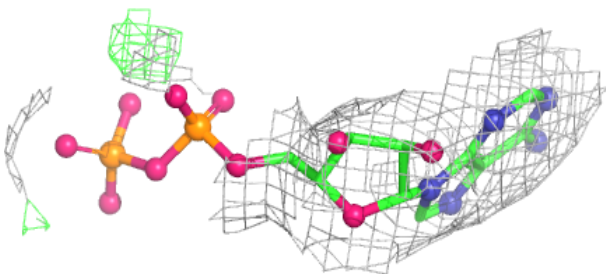
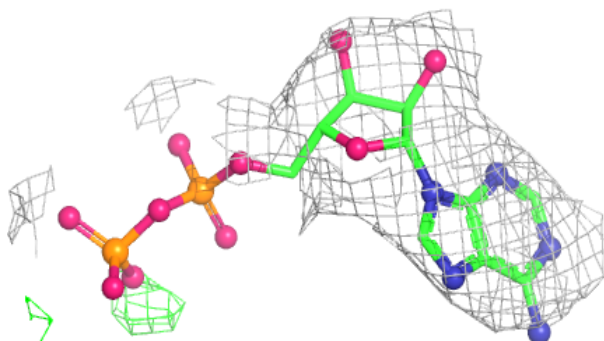


Electron density around ATP B 5400:

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

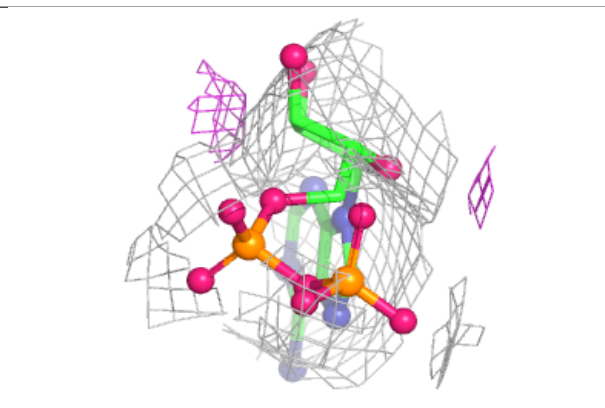
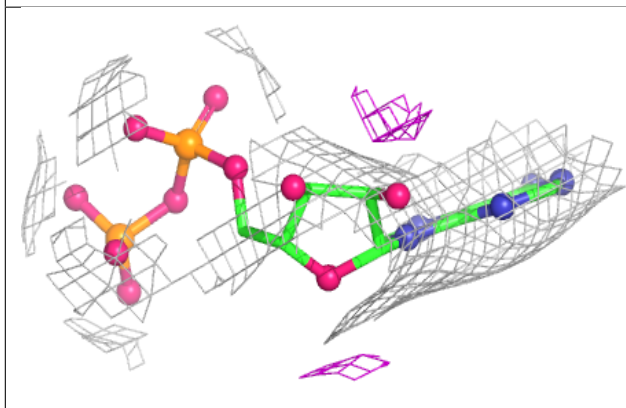
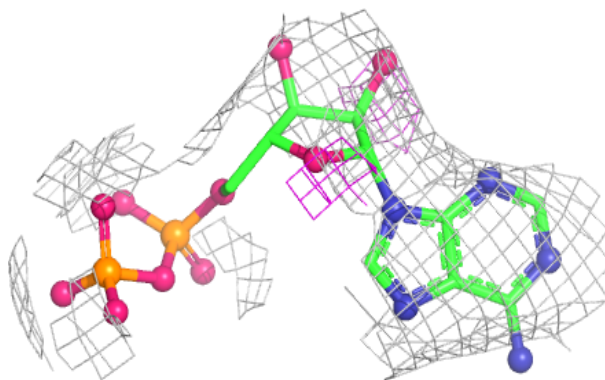
**Electron density around ADP A 5401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

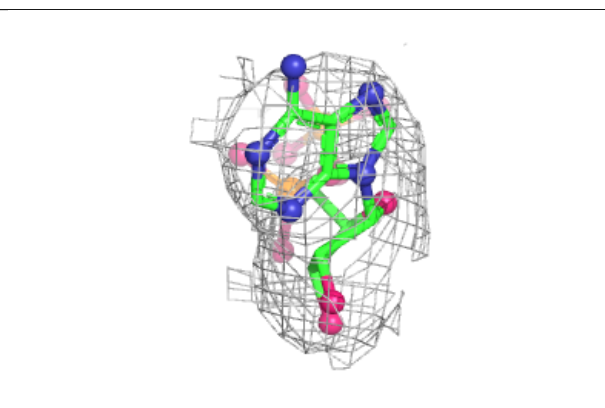
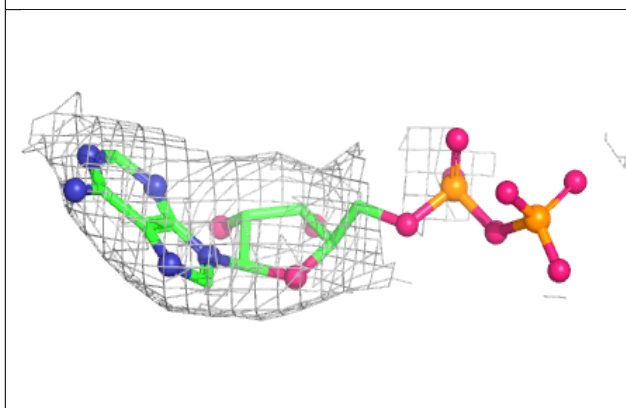
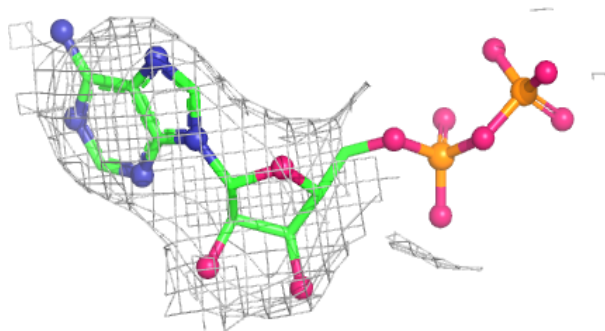


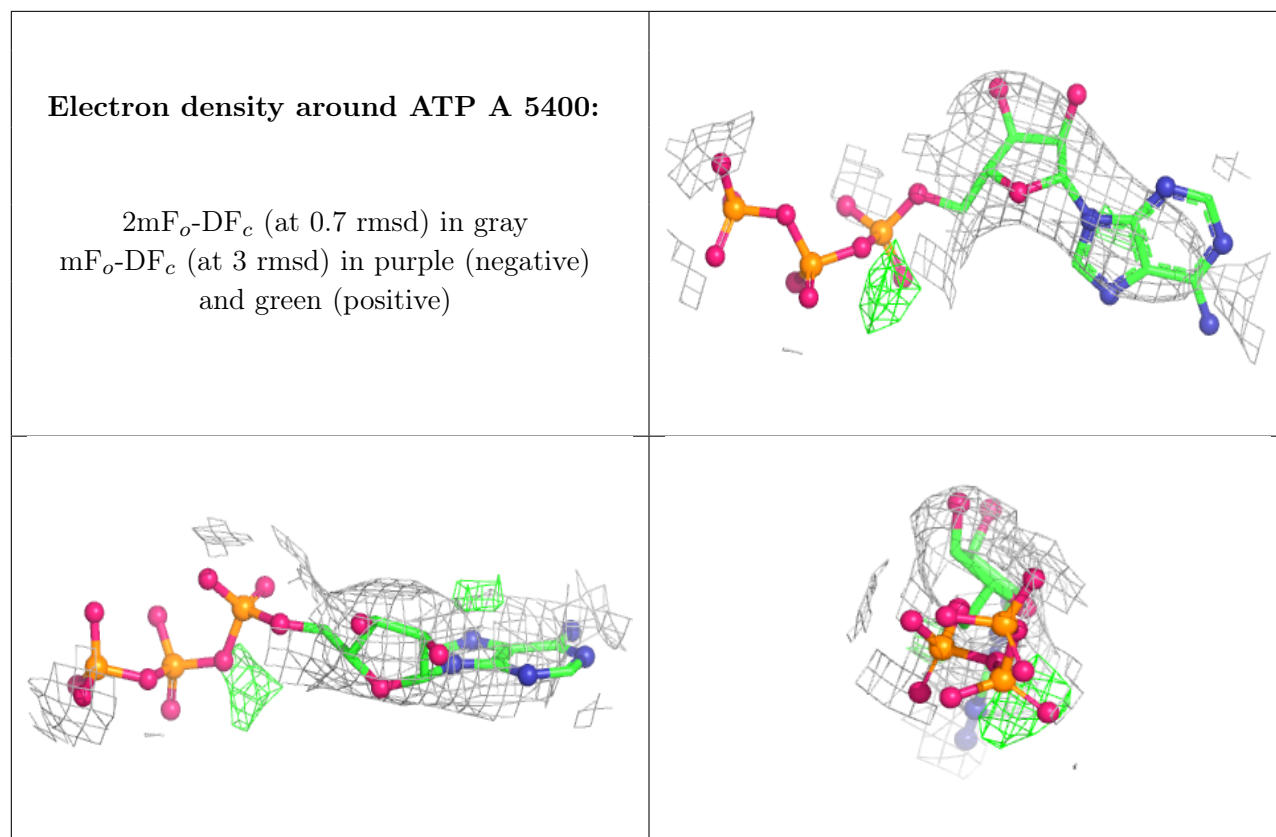
Electron density around ADP A 5402:

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

**Electron density around ADP B 5401:**

$2mF_o-DF_c$ (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.