



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:35 AM UTC

PDB ID : 4AKI / pdb_00004aki
Title : Dynein Motor Domain - LuAc derivative
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.70 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

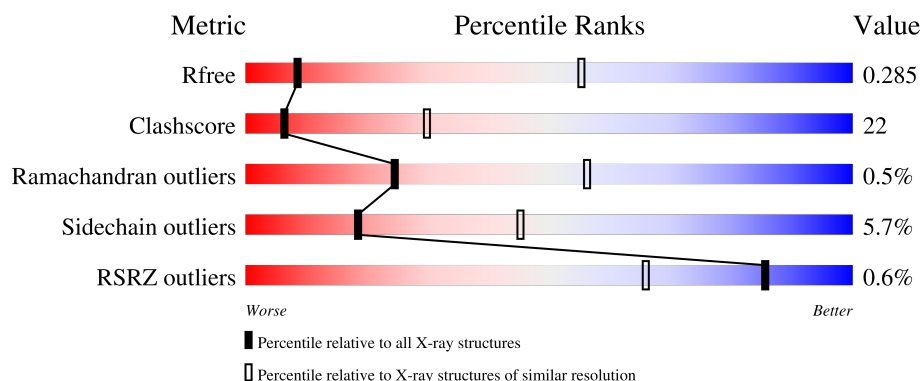
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	2695	
1	B	2695	

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
3	SO4	A	5094	-	-	X	-
3	SO4	A	5095	-	-	X	-
3	SO4	A	5096	-	-	X	-
3	SO4	B	5095	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41590 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.

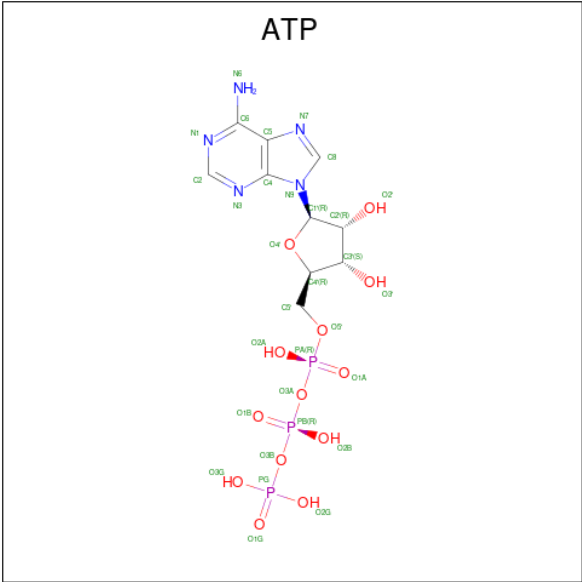
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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 8 discrepancies between the modelled and reference sequences:

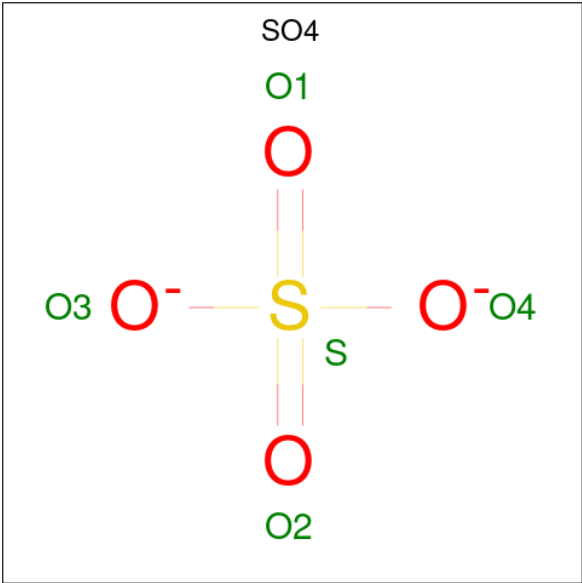
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

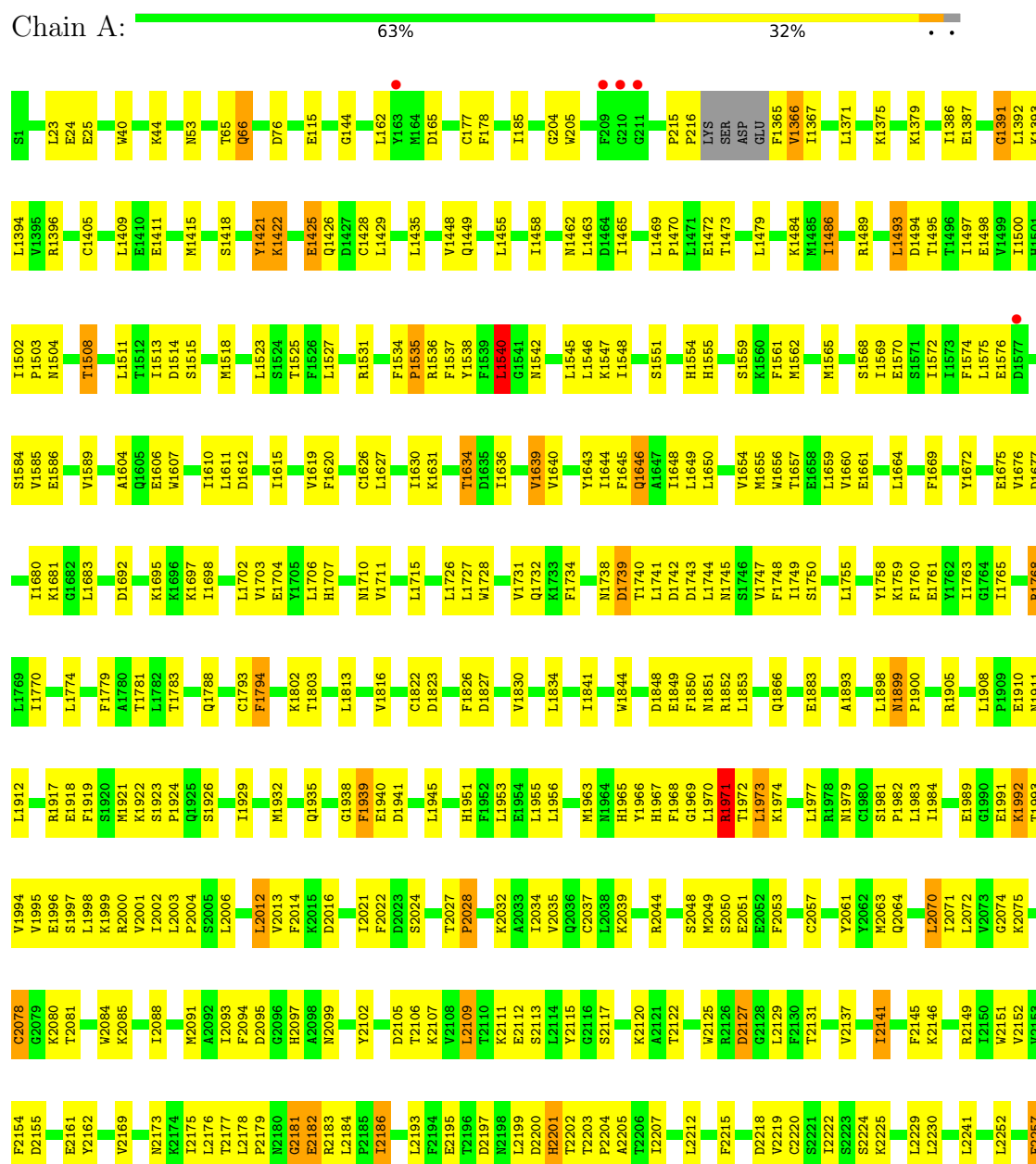
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

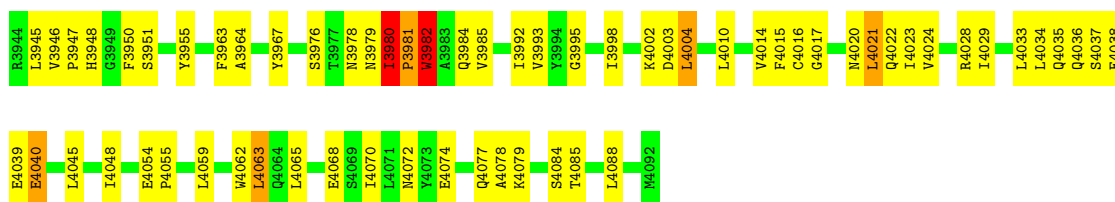
3 Residue-property plots

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.

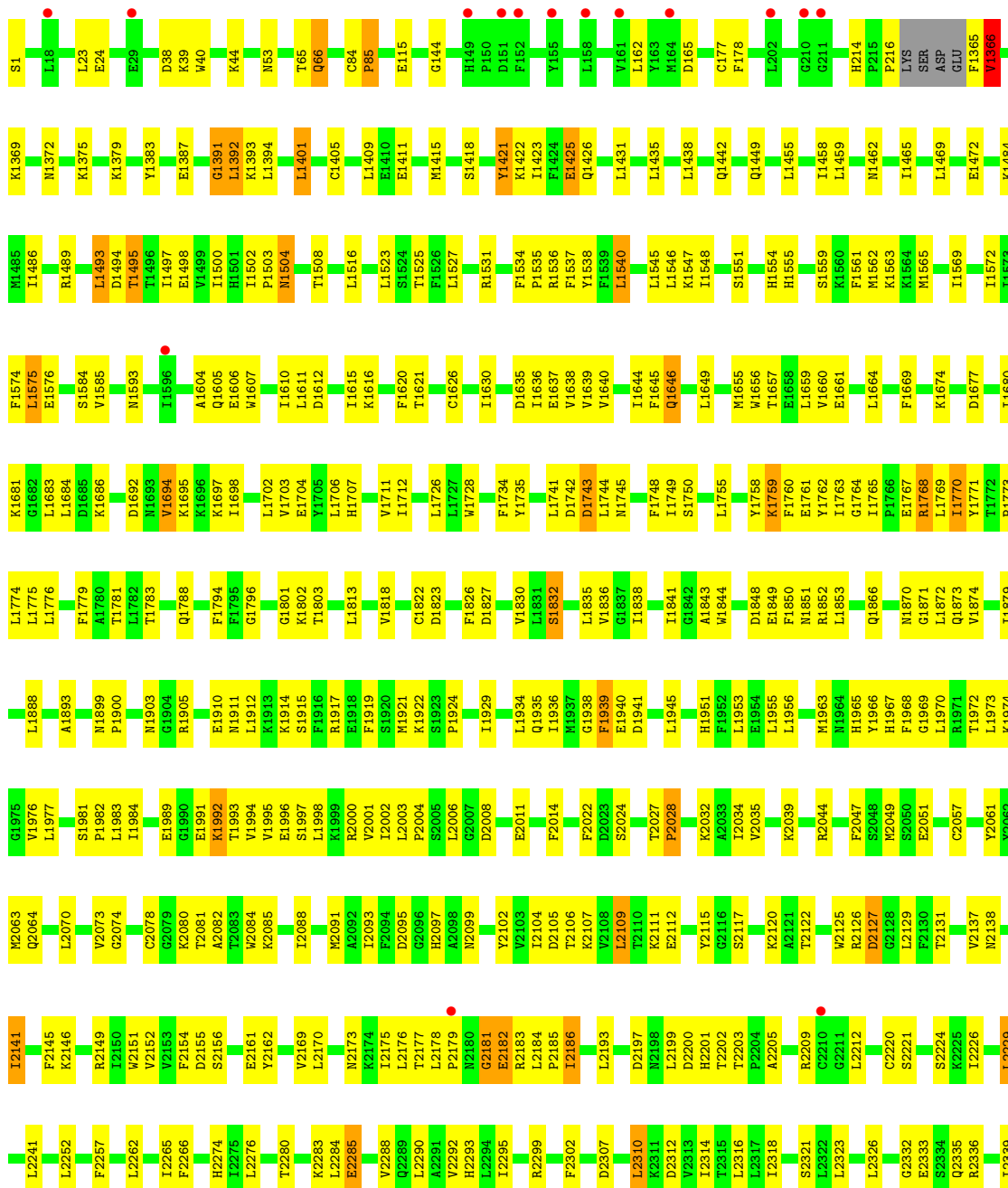
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



V3851	L3760	L3658	K3544	R3439	S3317	L2852	G2760	T2635	W2523	T2427	S2354	L2262
K3852	L3760	L3658	D3547	L3440	Q3316	L2853	A2761	G2636	W2523	H2428	D2355	L2262
T3853	L3760	L3658	D3547	L3440	S3319	L2853	R2762	P2637	I2526	L2432	Y2356	I2265
L3855	L3760	L3658	L3548	F3446	L3320	L2856	R2763	P2637	I2526	L2432	S2357	F2266
H3858	L3760	L3658	K3550	Q3453	G3322	L2856	G2765	Q2639	R2528	L2437	T2358	L2274
V3859	L3760	L3658	Y3555	E3456	N3323	T2860	K2766	T2640	H2530	V2440	I2359	H2275
T3862	L3772	L3674	L3559	D3459	I3329	R2861	L2769	S2643	H2530	V2440	N2363	L2276
A3865	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	D2364	L2276
E3869	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
K3870	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
K3872	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
K3873	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
K3874	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
K3875	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
K3876	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
C3877	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
H3878	L3772	L3674	L3559	P3460	E3330	L2865	T2770	L2644	C2535	F2445	K2365	T2280
L3884	L3799	L3690	L3587	N3475	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
F3885	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
A3886	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
P3887	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
L3888	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
L3889	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
L3890	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
R3894	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
F3895	L3803	K3692	L3590	R3476	E3341	V2878	Q2783	V2661	R2549	L2458	S2377	V2288
E3898	L3816	K3700	E3605	I3506	V3371	R2911	L2812	L2684	S2563	K2476	E2384	L2295
D3899	L3817	K3702	E3605	I3506	V3371	R2911	L2812	L2684	S2563	K2476	E2384	L2295
L3900	L3818	F3703	F3607	F3508	T3372	W2916	L2817	N2707	S2563	D2478	E2384	L2295
T3906	L3819	G3704	L3509	L3509	L3373	M2917	D2818	N2707	S2563	D2478	E2384	L2295
N3920	L3820	L3705	R3510	R3510	L3380	W2920	E2819	N2707	S2563	D2478	E2384	L2295
L3922	L3821	L3706	L3613	L3614	S3400	W2920	E2819	N2707	S2563	D2478	E2384	L2295
N3911	L3822	L3707	L3614	L3615	Q3401	M2932	L2821	N2707	S2563	D2478	E2384	L2295
G3912	L3823	E3717	V3615	V3615	D3402	M2932	L2822	N2707	S2563	D2478	E2384	L2295
F3915	L3824	E3717	Y3618	F3618	L3406	I2936	L2828	N2707	S2563	D2478	E2384	L2295
T3917	L3832	T3721	G3622	V3519	L3407	P2937	E2829	N2707	S2563	D2478	E2384	L2295
V3923	L3833	V3725	V3622	N3521	L3408	M2938	E2829	N2707	S2563	D2478	E2384	L2295
V3924	L3836	E3728	L3628	L3525	D3409	D2942	L2834	N2707	S2563	D2478	E2384	L2295
S3925	L3837	S3729	M3631	F3530	H3413	L2835	L2835	N2707	S2563	D2478	E2384	L2295
V3926	L3838	S3730	F3530	F3530	M3414	L2835	L2835	N2707	S2563	D2478	E2384	L2295
V3927	L3839	D3731	K3634	L3534	T3416	L2835	L2835	N2707	S2563	D2478	E2384	L2295
K3934	L3844	K3735	F3641	L3534	T3416	L2835	L2835	N2707	S2563	D2478	E2384	L2295
M3945	L3845	L3736	F3641	L3534	T3416	L2835	L2835	N2707	S2563	D2478	E2384	L2295
F3935	L3846	T3737	S3645	E3537	L3418	L2835	L2835	N2707	S2563	D2478	E2384	L2295
S3937	L3847	T3737	S3645	E3537	L3418	L2835	L2835	N2707	S2563	D2478	E2384	L2295
T3939	L3848	T3740	I3646	N3538	K3425	L2835	L2835	N2707	S2563	D2478	E2384	L2295
S3949	L3849	T3740	V3656	M3541	K3429	L2835	L2835	N2707	S2563	D2478	E2384	L2295
T3943	L3850	L3744	F3657	K3541	L3429	L2835	L2835	N2707	S2563	D2478	E2384	L2295



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



F3963	F3874	A3779	ALA	G3455	N3323	I2961	R2868	K2766	Q2639	T2525	S2446	Q2351
A3964	M3875	N3780	ARG	E3456	I3329	I2962	T2869	L2769	T2640	T2526	K2447	E2352
L3972	T3876	N3784	R3670	F3457	Y3330	D2963	E2870	T2770	S2643	E2527	D2448	L2353
N3978	Y3785	F3671	L3566	F3458	E3331	N2967	L2873	F2771	W2653	C2535	D2354	D2355
N3979	F3786	L3672	L3567	P3460	T3332	I2968	L2878	R2772	R2654	N2536	Y2356	S2357
L3880	L3787	E3673	L3570	I3461	Y3333	L2969	V2878	V2773	L2655	L2455	L2455	
P3981	L3883	L3674	L3576	L3462	F3334	V2982	K2883	L2779	V2663	R2543	N2463	L2361
W3982	L3884	L3677	N3576	S3463	R3342	G2983	T2890	K2780	Y2464	P2544	Y2464	A2362
A3983	A3886	Y3683	N3580	L3465	A3343	V2984	T2891	Q2783	L2681	M2546	K2365	
Q3984	P3887	L3888	L3583	A3473	L3346	N2985	C2892	P2784	L2689	R2549	T2467	
V3993	L3889	S3687	M3584	R3476	V3347	R2987	Z2893	K2785	S2690	F2550	L2471	I2375
Y3994	Q3890	A3688	L3587	R3476	K3350	P2988	P2894	I2786	S2691	T2551	T2472	
G3995	L3891	L3690	L3587	E3480	L3353	P2989	N2897	H2787	L2694	R2552	L2474	V2378
L3998	F3895	L3691	L3587	G3482	F3356	L3481	K2902	R2788	L2700	L2569	P2475	L2380
V3999	L3896	K3692	K3592	D3483	A3357	L3010	I2903	F2795	L2700	P2562	K2476	L2475
Y3997	Y3897	K3693	E3593	D3483	A3357	V3017	L2908	L2799	W2707	G2563	S2477	E2381
K4002	G3817	F3694	E3594	E3485	V3358	L3024	C2911	R2812	T2708	Q2564	I2478	V2385
D4003	S3818	N3595	N3596	E3485	K3359	L3024	R2911	T2813	W2708	K2565	K2480	W2386
L4004	L3819	N3597	E3598	K3493	D3361	N3026	C2912	L2816	L2712	S2566	L2481	
L4010	E3820	L3597	E3598	L3496	V3361	E3026	L2936	L2817	L2712	Y2571	L2482	
V4011	N3821	K3699	E3605	S3502	V3371	S3027	W2916	L2817	F2723	E2572	E2488	
F4014	L3822	T3701	E3605	S3502	T3372	V3028	M2917	L2817	C2724	L2573	L2392	
F4015	N3823	K3702	E3606	F3607	L3391	L3028	W2920	N2821	E2727	Y2574	N2489	P2393
Q4016	A3825	F3719	D3612	L3507	F3392	VAL	T2924	L2822	L2728	K2576	N2490	T2394
M4020	G3837	L3720	M3613	F3508	N3393	ASN	T2924	L2828	E2729	A2577	L2491	T2395
L4021	L3838	T3721	L3614	L3509	S3400	GLU	M2932	E2829	V2730	L2578	K2493	D2386
Q4022	G3917	V3725	V3615	R3512	Q3401	ASN	M2932	L2833	P2731	F2579	L2494	T2397
I4023	L3839	V3725	V3615	V3513	D3402	THR	I2936	L2834	S2737	K2580	D2495	L2407
V4024	L3840	I3920	O3618	F3518	F3406	THR	P2837	L2835	Y2497	K2496	K2496	L2408
V4027	I3844	Q3845	G3622	V3519	F3406	LEU	M2838	L2835	S2410	N2409	G2498	N2409
R4028	Q3845	M3846	G3622	V3519	L3407	SER	E2839	L2835	K2411	S2410	G2498	S2410
L4033	S3847	L3848	M3631	N3521	L3407	ILE	F2940	L2840	L2742	E2590	S2499	K2412
E4038	S3849	W3850	G3636	L3525	D3409	SER	T2941	L2841	R2744	K2412	G2413	G2413
L4059	W3851	V3852	G3636	L3525	H3413	LEU	D2942	L2842	I2745	T2609	V2502	L2414
S4060	K3852	K3853	F3641	F3530	H3414	VAL	F2943	L2843	R2746	Q2612	L2506	L2415
W4062	Y3854	L3855	Y3642	L3534	V3417	K3303	ILE	F2844	Z2747	S2613	R2507	P2419
L4063	L3855	Y3746	S3645	E3536	I3418	E3304	PRO	Q2845	L2749	L2616	L2508	P2420
Q4064	L3855	Y3746	S3645	E3536	L3429	R3305	ASN	G2846	V2752	L2616	L2509	P2420
L4065	H3858	V3859	I3646	E3537	S3430	W3306	ASN	Y2849	L2758	R2620	E2511	K2424
V4070	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	H2755	R2620	E2511	T2425
L4071	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	M2756	V2626	K2512	W2426
N4072	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	P2757	R2627	Q2513	L2427
V4081	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	L2758	Q2514	Q2514	K2428
S4084	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	Q2760	Y2630	K2517	L2432
T4085	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	A2761	T2631	P2518	L2437
L4088	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	S2762	T2635	E2520	
	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	R2763	G2636	W2523	W2440
	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	L2764	P2637	F2445	F2445
	V3859	T3862	L3656	N3538	F3431	L3307	LYS	L2856	G2765	R2638		

4092

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.77Å 118.19Å 202.68Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.14 – 3.70 49.14 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.14-3.70) 99.8 (49.14-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.231 , 0.289 0.226 , 0.285	Depositor DCC
R_{free} test set	4446 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	142.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 152.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: ATP, MG, SO4

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	0.77	4/21146 (0.0%)	1.16	64/28618 (0.2%)
1	B	0.64	1/21146 (0.0%)	1.07	41/28618 (0.1%)
All	All	0.71	5/42292 (0.0%)	1.12	105/57236 (0.2%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CA-CB	6.03	1.62	1.53
1	A	3980	ILE	CA-C	5.41	1.58	1.52
1	B	3980	ILE	CA-C	5.37	1.58	1.52
1	A	2867	LEU	C-N	5.33	1.40	1.33
1	A	2867	LEU	C-O	5.22	1.30	1.24

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2127	ASP	N-CA-C	11.21	123.06	111.07
1	B	144	GLY	N-CA-C	8.74	124.26	111.76
1	A	2333	GLU	N-CA-C	-8.59	102.00	111.36
1	A	2182	GLU	N-CA-C	8.06	120.37	108.60
1	A	2938	MET	N-CA-C	8.06	121.17	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	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	20207	926	0
1	B	20748	0	20206	881	0
2	A	31	0	12	4	0
2	B	31	0	12	8	0
3	A	15	0	0	9	0
3	B	15	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	41590	0	40437	1806	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 22.

The worst 5 of 1806 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:216:PRO:C	1:A:3475:ASN:HB3	1.39	1.45
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.24
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.21
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.53	1.21
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.24	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2640/2695 (98%)	2519 (95%)	107 (4%)	14 (0%)	24	56
1	B	2640/2695 (98%)	2522 (96%)	104 (4%)	14 (0%)	24	56
All	All	5280/5390 (98%)	5041 (96%)	211 (4%)	28 (0%)	24	56

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	214	HIS
1	B	1366	VAL
1	B	1391	GLY
1	A	1366	VAL

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	2218/2453 (90%)	2094 (94%)	124 (6%)	19	46
1	B	2218/2453 (90%)	2090 (94%)	128 (6%)	18	45
All	All	4436/4906 (90%)	4184 (94%)	252 (6%)	18	45

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3976	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3536	GLU
1	B	1759	LYS
1	B	3507	ILE
1	B	3839	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1622	GLN
1	B	2282	ASN
1	B	4077	GLN
1	B	3624	HIS
1	B	1646	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
2	ATP	A	5093	4	32,33,33	1.64	7 (21%)	48,52,52	1.95	9 (18%)
3	SO4	A	5095	-	4,4,4	0.55	0	6,6,6	0.70	0
3	SO4	B	5095	-	4,4,4	0.45	0	6,6,6	0.29	0
3	SO4	B	5096	-	4,4,4	0.33	0	6,6,6	0.26	0
3	SO4	B	5094	-	4,4,4	0.47	0	6,6,6	0.45	0
3	SO4	A	5096	-	4,4,4	0.37	0	6,6,6	0.28	0
3	SO4	A	5094	-	4,4,4	0.57	0	6,6,6	0.42	0
2	ATP	B	5093	4	32,33,33	1.48	7 (21%)	48,52,52	1.76	11 (22%)

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	ATP	A	5093	4	-	3/22/38/38	0/3/3/3
2	ATP	B	5093	4	-	6/22/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5093	ATP	C5-C4	4.51	1.47	1.39
2	A	5093	ATP	C5-C4	3.72	1.45	1.39
2	A	5093	ATP	C5-N7	-3.53	1.32	1.39
2	A	5093	ATP	PB-O3B	3.30	1.63	1.59
2	B	5093	ATP	PB-O3B	3.25	1.63	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5093	ATP	C5-C4-N3	-5.93	118.55	126.72
2	B	5093	ATP	C5-C4-N3	-5.33	119.38	126.72
2	B	5093	ATP	N3-C4-N9	4.51	134.84	127.17
2	A	5093	ATP	N3-C4-N9	4.50	134.81	127.17
2	A	5093	ATP	N3-C2-N1	-4.18	122.25	128.58

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

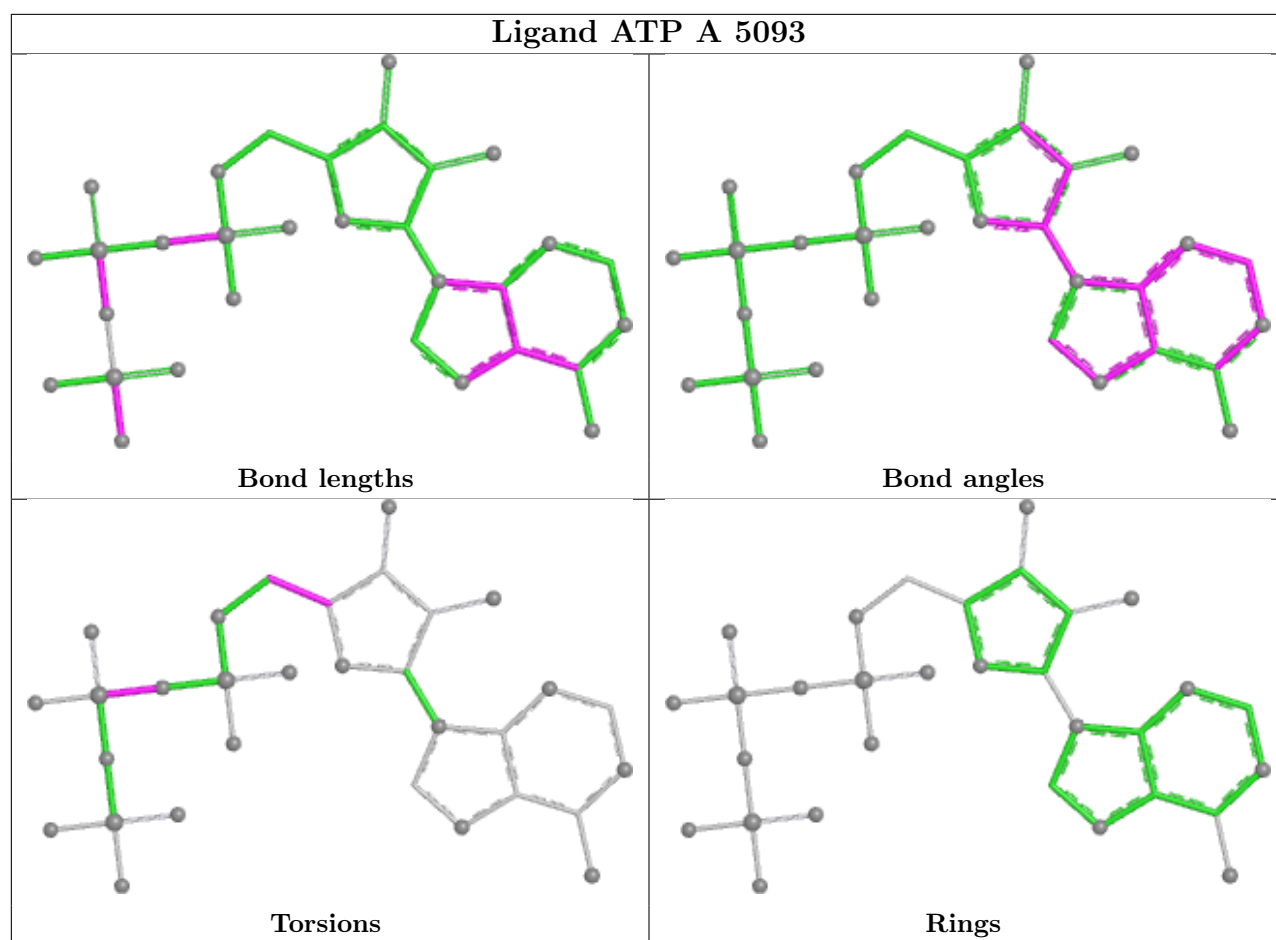
Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C3'-C4'-C5'-O5'
2	A	5093	ATP	C3'-C4'-C5'-O5'
2	A	5093	ATP	O4'-C4'-C5'-O5'

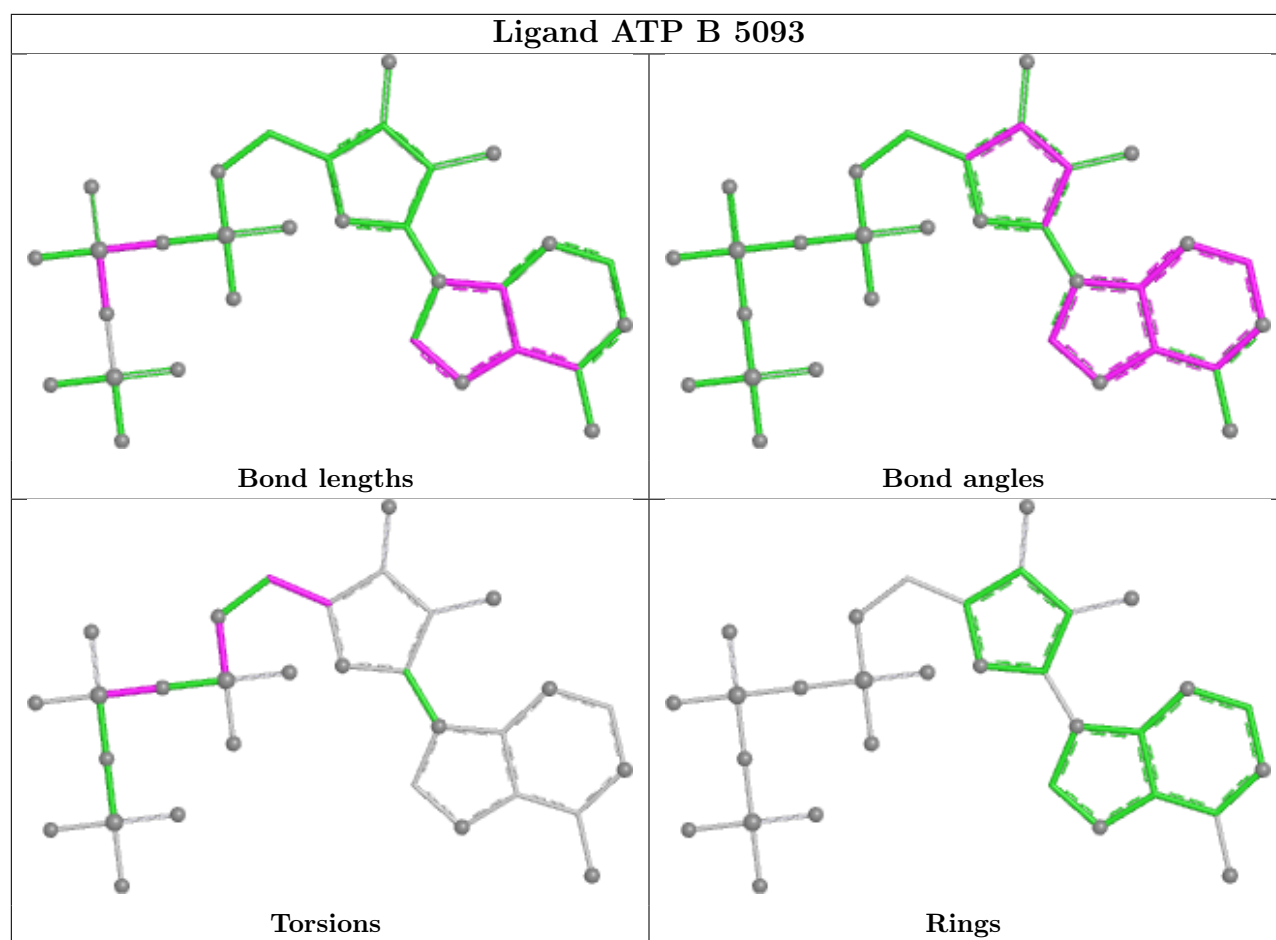
There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	4	0
3	A	5095	SO4	3	0
3	B	5095	SO4	2	0
3	B	5096	SO4	1	0
3	A	5096	SO4	2	0
3	A	5094	SO4	4	0
2	B	5093	ATP	8	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%)	-0.42	10 (0%)	88 72	80, 163, 325, 500	0
1	B	2650/2695 (98%)	-0.35	20 (0%)	82 60	117, 210, 355, 500	0
All	All	5300/5390 (98%)	-0.38	30 (0%)	85 66	80, 188, 342, 500	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2868	ASP	6.7
1	B	155	TYR	6.3
1	B	3746	TYR	4.8
1	B	152	PHE	3.8
1	B	18	LEU	3.7

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](#)

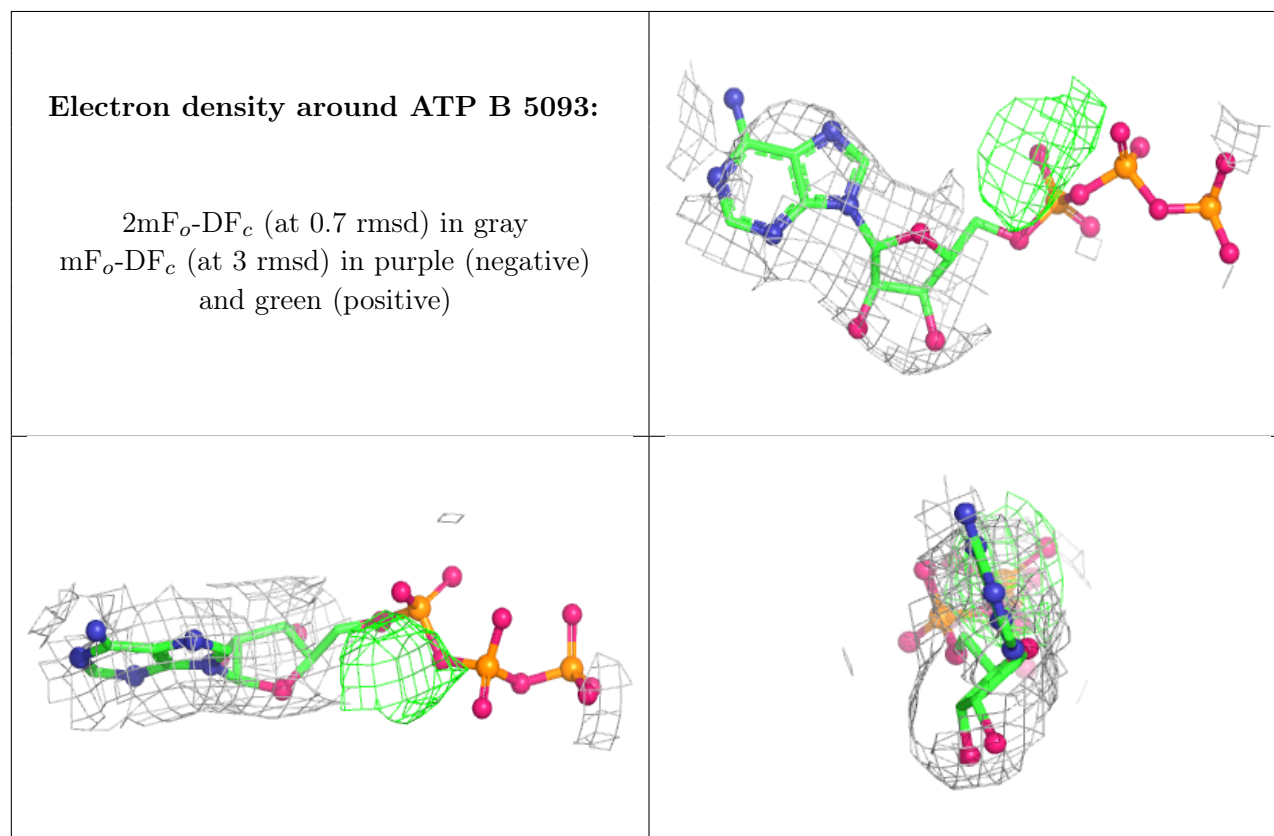
There are no oligosaccharides in this entry.

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.

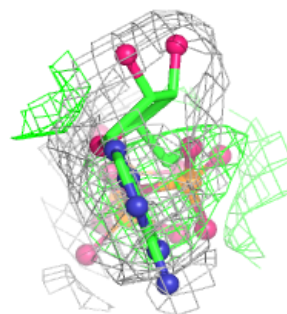
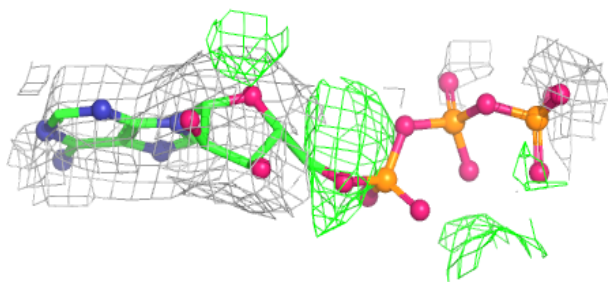
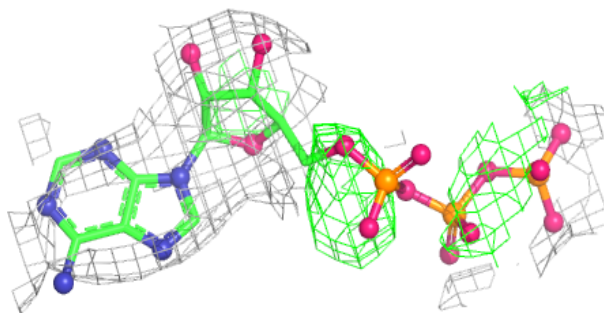
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	5096	5/5	0.88	0.08	158,193,224,235	0
3	SO4	B	5094	5/5	0.95	0.08	151,165,190,192	0
3	SO4	A	5096	5/5	0.95	0.05	128,136,144,154	0
2	ATP	B	5093	31/31	0.96	0.07	115,184,238,261	0
2	ATP	A	5093	31/31	0.97	0.08	72,125,180,196	0
3	SO4	A	5094	5/5	0.97	0.04	109,114,153,161	0
3	SO4	A	5095	5/5	0.97	0.04	108,128,132,133	0
4	MG	A	5097	1/1	0.97	0.09	59,59,59,59	0
3	SO4	B	5095	5/5	0.98	0.04	155,178,186,207	0
4	MG	B	5097	1/1	0.98	0.03	127,127,127,127	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 A 5093:

$2mF_o - DF_c$ (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.