



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:42 PM UTC

PDB ID : 4AKG / pdb_00004akg
Title : Dynein Motor Domain - ATP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.30 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

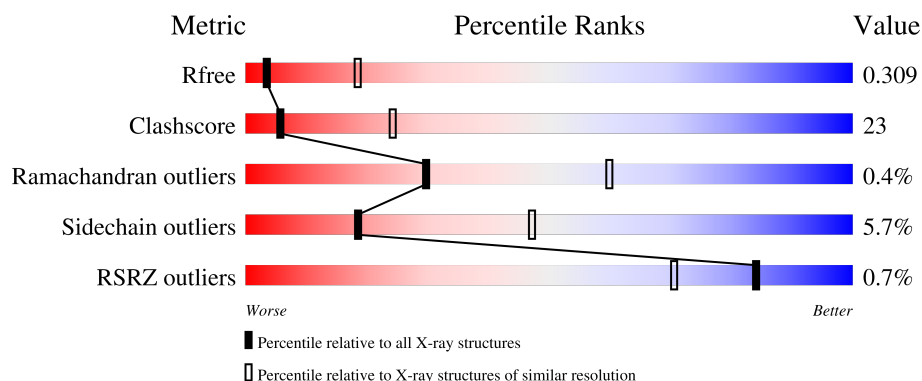
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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
2	ATP	A	5093	-	-	X	-
2	ATP	B	5093	-	-	X	-
5	SO4	A	5097	-	-	X	-
5	SO4	B	5096	-	-	X	-
5	SO4	B	5097	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41634 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.

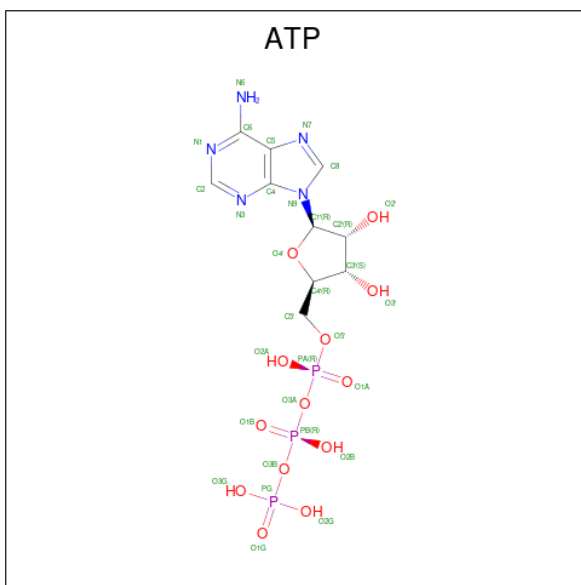
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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:

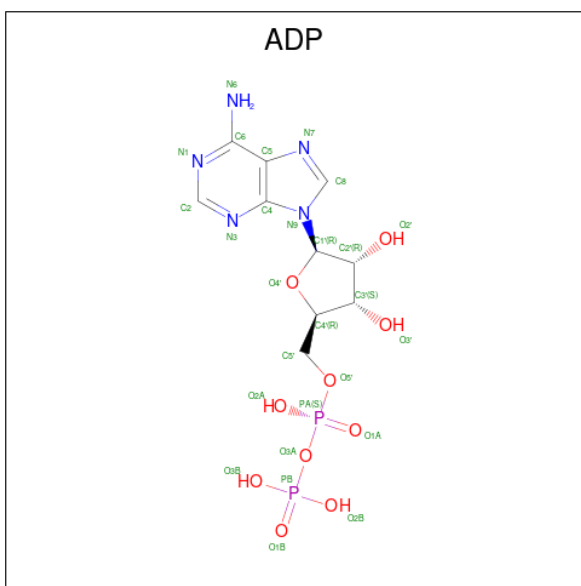
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP 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 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

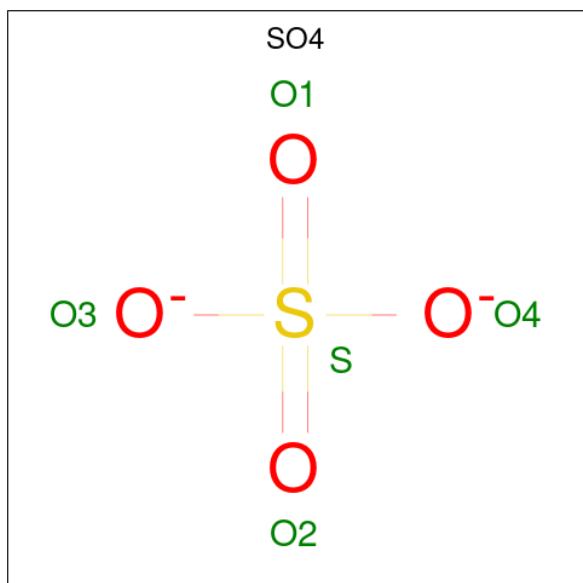


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- 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		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

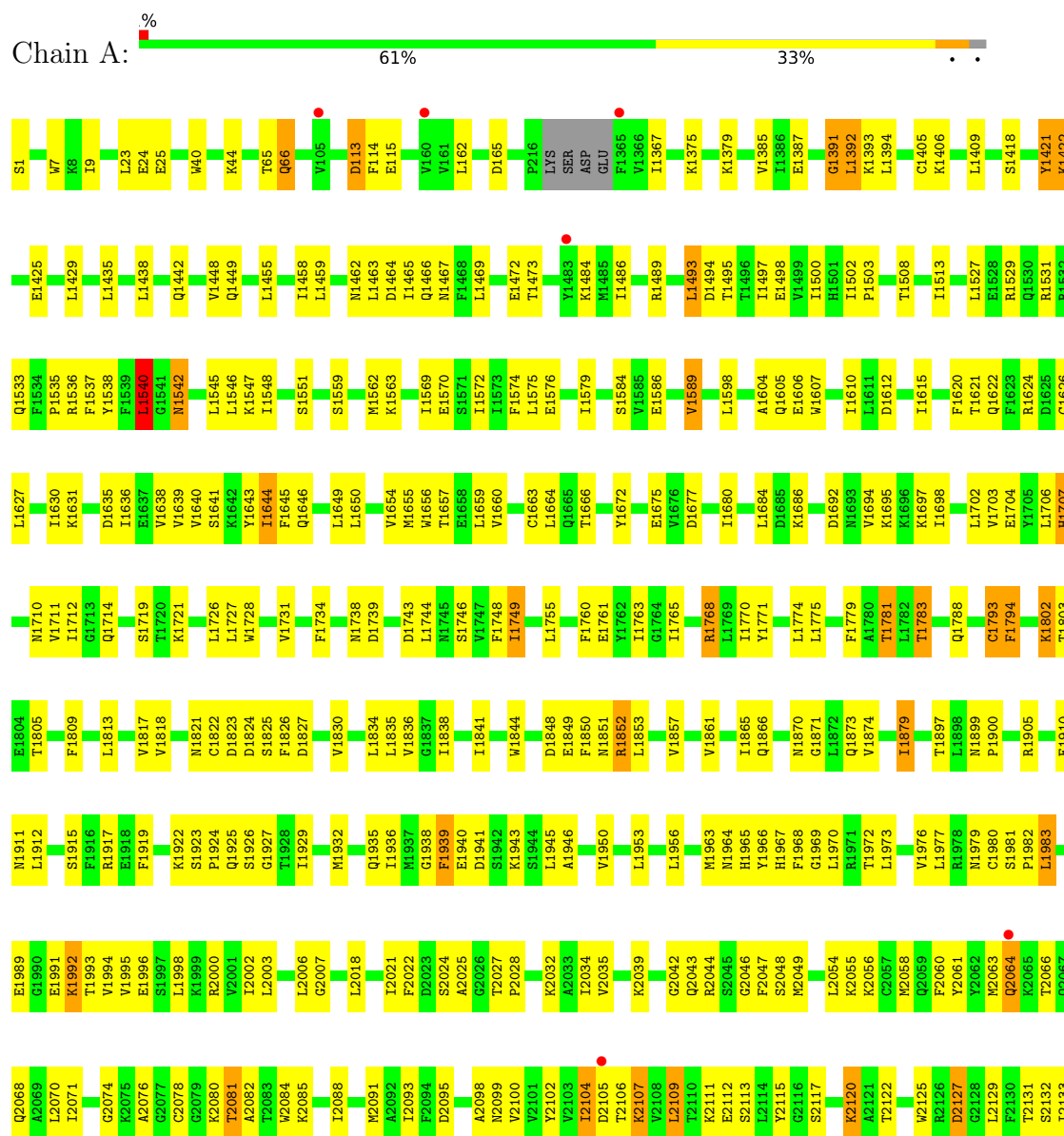


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

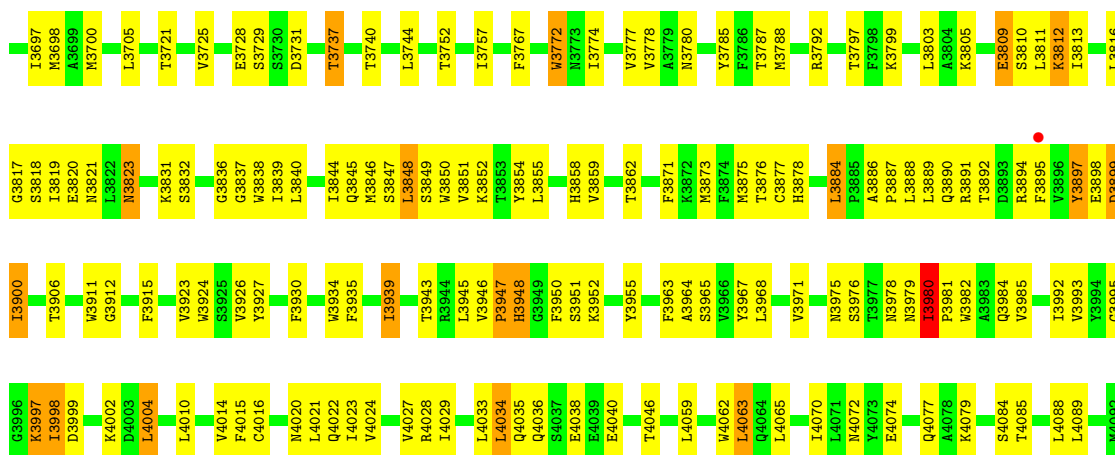
3 Residue-property plots

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.

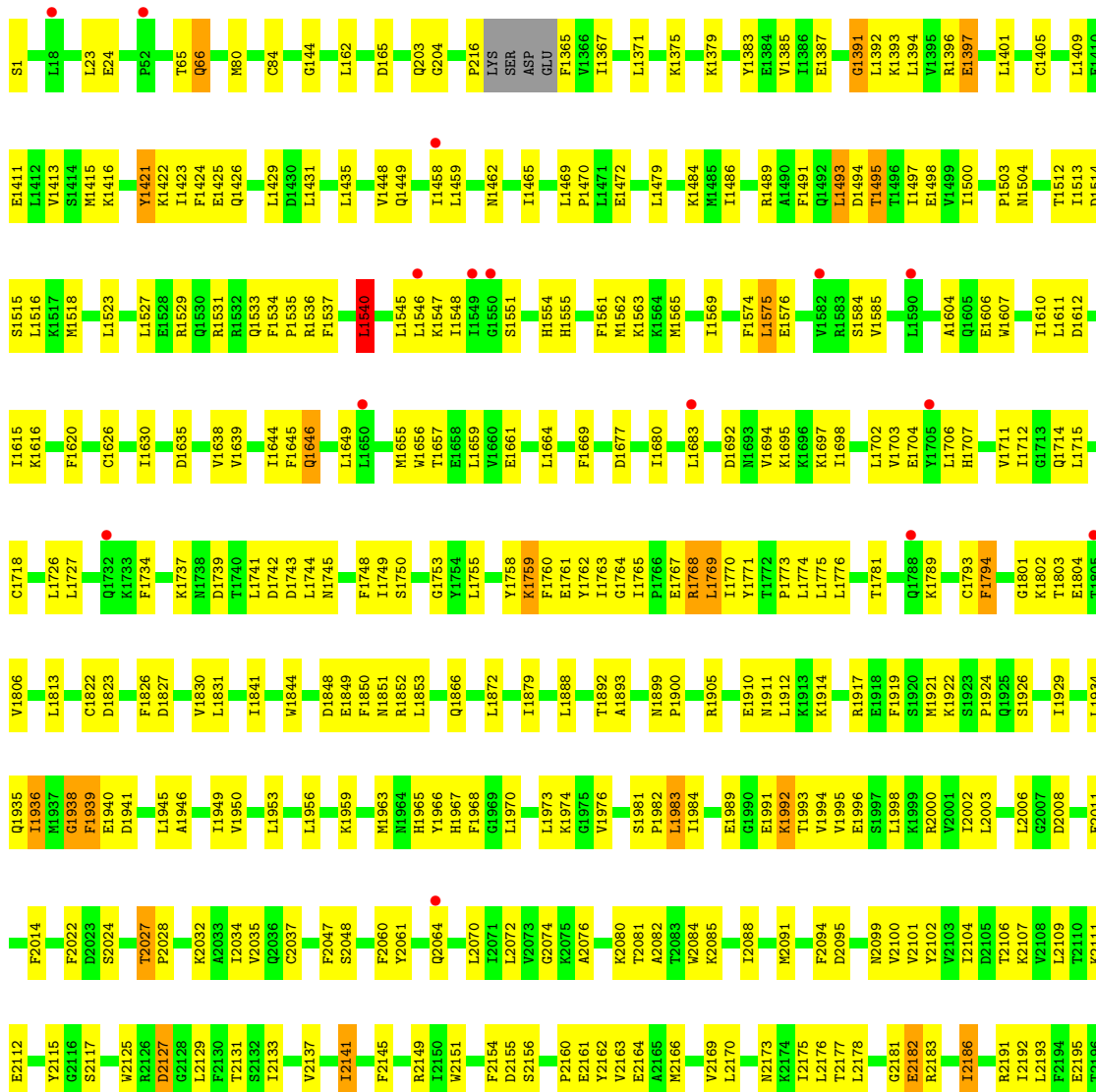
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



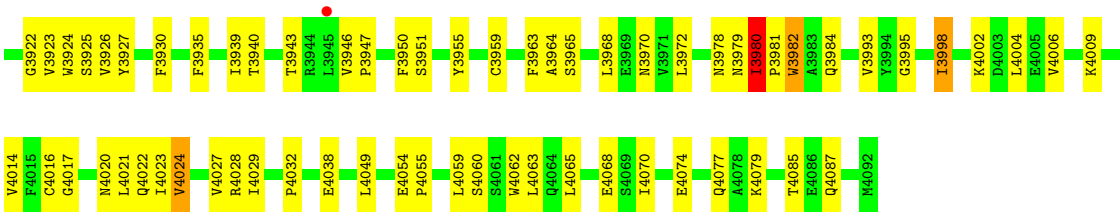
E3616	F3530	F3436	N3323	K2979	Q2783	V2677	E2488	I2403	Y2324	S2221	L2134
E3617	L3534	R3439	I3325	V2984	P2784	L2686	I2489	D2406	A2325	I2222	V2137
Y3618	T2985	L3440	C2982	N2985	I2786	P2562	N2490	L2407	L2326	S2223	N2138
G3622	P2986	P2987	I2903	S2986	R2787	S2563	L2491	G2332	G2332	K2225	S2224
V3626	S2987	S2988	S2904	S2905	H2788	G2564	P2492	N2409	E2333		I2141
K3627	P2989	P2988	P2906	P2906	R2789	K2565	K2493	S2410	S2334	H2228	F2145
F3629	G2990	G2990	L2907	A2907	D2796	S2566	L2494	K2411	Q2335	L2229	
S3630	F2991	F2991	L2908	F2991	M2797	L2567	D2496	R2412	R2336		
R3631	N2910	N2910	N2910	N2910	K2797	S2568	K2496	G2413	I2339	L2241	R2149
L3632	R2911	R2911	R2911	R2911	N2708	I2570	I2497	I2414	L2252	L2262	W2151
E3633	C2912	C2912	C2912	C2912	K2709	I2571	G2498	I2415	F2257	V2152	V2153
F3634	L2913	L2913	L2913	L2913	T2710		S2499	G2417	Q2351		V2153
D3634	I2914	I2914	I2914	I2914	D2711	Y2574	V2502	G2418	E2352		F2154
F3635	N2915	N2915	N2915	N2915	L2712	Y2575	V2503	F2419	L2353	L2262	D2155
G3636	E3012	E3012	E3012	E3012	R2812	K2576	L2504	P2420	S2354		S2156
	M2916	M2916	M2916	M2916	T2813	A2577	F2505	Y2355	D2355	I2265	
	M2917	M2917	M2917	M2917		I2578	L2506	G2421	S2357	F2266	E2161
	V2920	V2920	V2920	V2920	I2816		R2507	K2424	T2358		E2162
	T2924	T2924	T2924	T2924	I2817	L2581	Q2508	T2425	T2359	V2273	V2163
	V2928	V2928	V2928	V2928	N2821	V2582	L2509	M2426	V2360	H2274	
	V3028	V3028	V3028	V3028	I2822	T2609	M2510	I2427	I2361	I2275	M2166
LEU	V3017	V3017	V3017	V3017	L2823		K2512	N2428	A2362		V2169
LYS	V3018	V3018	V3018	V3018		Q2612	Q2513	N2430	K2365	V2278	
VAL	V3019	V3019	V3019	V3019	I2817	S2613	G2514	A2431	L2366	R2279	N2173
ASN	L3024	L3024	L3024	L3024	N2821	R2620	F2515	R2432	S2367	K2174	K2174
LEU	V3028	V3028	V3028	V3028	I2822	E2621	W2516	R2433	F2368	N2281	L2175
ASN	V3028	V3028	V3028	V3028	L2823	I2622	K2517		S2369	N2282	L2176
LYS	V3028	V3028	V3028	V3028		T2623	T2518	L2437	S2373	K2283	T2177
THR	V3028	V3028	V3028	V3028			E2520	V2440	E2374	L2284	L2178
THR	V3028	V3028	V3028	V3028		V2626	E2520	V2441	E2375	E2285	P2179
THR	V3028	V3028	V3028	V3028		R2627	K2521	V2441	P2376		N2180
THR	V3028	V3028	V3028	V3028			W2523	F2445	S2377	Q2289	G2181
THR	V3028	V3028	V3028	V3028			W2524	S2446	E2182	L2290	E2182
THR	V3028	V3028	V3028	V3028			T2525	K2447	A2291	A2291	R2183
THR	V3028	V3028	V3028	V3028			L2526	D2448	V2292	V2292	L2184
THR	V3028	V3028	V3028	V3028			E2527	T2449	H2293	H2293	F2185
THR	V3028	V3028	V3028	V3028				T2450	E2381	L2294	I2186
THR	V3028	V3028	V3028	V3028				T2451	A2382	I2295	
THR	V3028	V3028	V3028	V3028				T2451	H2383	L2295	L2193
THR	V3028	V3028	V3028	V3028				T2451	E2384	R2299	F2194
THR	V3028	V3028	V3028	V3028				T2451	V2385		E2195
THR	V3028	V3028	V3028	V3028				T2451	M2386	F2302	
THR	V3028	V3028	V3028	V3028				T2451	R2387		D2197
THR	V3028	V3028	V3028	V3028				T2451	P2388	L2310	N2198
THR	V3028	V3028	V3028	V3028				T2451	D2389	K2311	L2199
THR	V3028	V3028	V3028	V3028				T2451	D2200	D2312	D2200
THR	V3028	V3028	V3028	V3028				T2451	H2201	V2813	H2201
THR	V3028	V3028	V3028	V3028				T2451	I2392	I2314	T2202
THR	V3028	V3028	V3028	V3028				T2451	P2393	T2315	T2203
THR	V3028	V3028	V3028	V3028				T2451	T2394	L2316	P2204
THR	V3028	V3028	V3028	V3028				T2451	I2395	L2317	A2205
THR	V3028	V3028	V3028	V3028				T2451	D2397	I2318	
THR	V3028	V3028	V3028	V3028				T2451	K2319	K2319	L2212
THR	V3028	V3028	V3028	V3028				T2451	I2398	R2320	
THR	V3028	V3028	V3028	V3028				T2451	E2401	S2321	F2215
THR	V3028	V3028	V3028	V3028				T2451	L2322	L2323	C2220
THR	V3028	V3028	V3028	V3028				T2451	K2402		



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



I3844	E3728	E3605	L3509	V3371	ASN	P2937	L2728	K2577	E2488	N2409	I2318	D2197
Q3845	S3729	D3612	R3510	T3372	LYS	M2938	S2737	I2578	I2489	S2410	K2319	H2201
S3847		N3613	V3513	L3373	THR	T2941	H2741	R2579	L2490	R2411	R2320	T2202
L3848	L3736	N3614	F3518	E3375	SER	D2942		K2580	L2491	G2413	S2321	T2203
S3849	T3737	V3615	V3519	L3391	ILE	F2943		L2582	K2492	G2413	L2322	P2204
K3850	V3738		T3520	L3392	VAL	TLE	R2744	R2586	L2494	T2414	L2323	A2205
V3851	D3739		N3521	N3393	PRO	VAL	D2745		D2495	L2415		T2206
	T3740		N3521	N3393	GLU	PRO	D2746		K2496	C2417	L2326	L2207
Y3854		G3622	I3525	S3400	VAL	GLU	D2747		G2497	C2418		L2207
L3855	L3744	I3628	F3525	Q3401	ASN	ASN	A2748		G2498	P2419	G2332	R2209
R3858	R3745		F3530	D3402	LYS	LYS		S2613	S2499	G2421	S2333	
V3859	F3767	M3631		F3406	GLU	GLU	Q2751	L2616	Q2500		Q2335	L2212
S3860	F3768		L3534	F3406	LEU	LEU	V2752		V2503	T2425	F2215	
E3861	V3769	F3641	T3535	D3409	VAL	VAL	H2755	S2617	M2426	M2426	R2336	
T3862	D3770		E3536	N3309	PHE	PHE	M2756	F2618	L2427	L2427	I2339	
	E3771	S3645	E3537	T3310	THR	THR	M2757	R2620	R2506	N2428		C2220
S3869	K3772	I3646	N3538	T3311	GLU	GLU	L2758	T2623	R2507	N2429	Q2351	S2224
K3870	K3773	V3656	M3541	K3311	PRO	PRO	I2759	T2630	M2510	N2430	E2352	K2225
F3871	I3774	F3657		Q3312	ILE	ILE	G2760	T2631	E2511	A2431	L2353	
M3872		I3658	K3544	F3313	T2960	GLN	A2761	R2627	K2512	L2432	S2354	H2228
F3874	V3777	LYS		S3317	T2961		T2763	T2635	Q2513	L2437	D2355	
M3875	A3778	SER	D3547	Q3318	R2962		R2764	T2636	K2517	L2440	S2357	
T3876	N3780	ARG	L3548	E3319	D2963		G2765	A2632	T2518		I2361	
C3877	Y3785	GLU	F3549	L3320	A2964		K2766	T2635	E2519	F2445	A2362	
H3878	F3786	THR	K3550	G3322	V2965			T2636	E2520	S2446	K2365	L2262
	T3787	ALA	Y3555	N3323	N2967			G2637	V2524	K2447	K2365	L2265
R3792	K3787	ALA	K3556	G3324	N2968			T2638	T2525	D2448	L2366	F2266
	K3792	ARG	L3557	I3325	L2969			Q2639	I2526	T2449	S2367	
P3885		ARG	K3558					T2640	E2527		F2368	H2274
A3886	K3799	T3669	L3559	S3329	M2980		Q2783	S2643	R2528	E2452	S2369	L2275
P3887	L3803	R3670	L3566	Y3330	K2981		P2784		C2535	L2455	E2373	L2276
L3888		V3671	L3567	F3334	V2982		K2785	L2647	N2536		E2374	G2277
Q3890	S3807	I3674	L3570		G2983		L2786				E2375	V2278
F3895	K3808				V2984		H2787			L2458		R2279
V3896	E3809	L3677		L3337	R2985		R2788		R2543	N2463	V2378	T2280
S3897	S3810	L3678	E3579	N3338	R2986				R2654	F2464	S2379	N2282
E3898	L3811	Y3679	N3580	E3341	R2987		L2792		T2655		L2380	K2283
D3899	K3812		K3581		C2982				R2549	T2467	E2381	L2284
I3900	I3813	Y3683	E3582	L3346	L2908		F2795	L2681	T2550	S2468	A2382	E2285
P3901	I3814		L3583	V3347	F2909		L2799		R2552	K2469	H2383	
	P3815	S3687		I3348	M2910				I2556	G2470	E2384	L2290
T3906	G3817		L3587	L3349	R2911		L2808			T2472	V2385	
V3907	S3818	L3690	K3592	K3350	C2912				P2562	L2473	H2283	L2295
K3908	I3819	K3691	E3593		L2915		R2812	L2694	S2563	L2474	L2294	
	E3820	K3693	A3594	L3353	W2916		T2813		K2564	P2475	R2387	
W3911	N3821	F3694	F3595	F3356	W2920		I2816	D2703	S2566	S2476	I2390	F2302
G3912	L3822		D3500	A3357	V2924		I2817	V2707			V2391	
S3913	N3823	M3698	P3501	V3358	L3024			N2708		S2477	T2394	L2305
Q3914		A3699	S3502	K3359	V3028		N2821	K2709		L2478	L2395	L2306
F3915	K3823	M3700	S3502	Y3360	LYS		L2822		E2571	L2479	D2396	
F3916	G3837	T3701	K3505	D3361	VAL		L2823	L2712	E2572	K2480	D2397	
	W3838		F3506		ASN		E2824	V2713		N2481		L2310
G3918	L3839	M3702	E3603	I3367	LEU		T2825		Y2574		D2406	
K3919	L3840	E3717	F3508				A2826	E2727	K2576	L2484		L2314



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.33Å 117.92Å 202.76Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.30) 96.0 (50.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	REFMAC NULL	Depositor
R, R_{free}	0.239 , 0.305 0.239 , 0.309	Depositor DCC
R_{free} test set	5981 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 111.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41634	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, ADP, ATP, 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	0.85	15/21146 (0.1%)	1.22	96/28618 (0.3%)
1	B	0.70	5/21146 (0.0%)	1.10	53/28618 (0.2%)
All	All	0.77	20/42292 (0.0%)	1.16	149/57236 (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	3
1	B	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2064	GLN	CA-C	-15.98	1.31	1.52
1	A	2495	ASP	C-N	-12.19	1.17	1.34
1	A	2412	ARG	CA-C	-10.96	1.39	1.52
1	B	1759	LYS	C-O	9.26	1.35	1.23
1	A	2412	ARG	C-N	-9.18	1.25	1.33

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2138	ASN	N-CA-C	12.22	124.34	111.14
1	A	2127	ASP	N-CA-C	12.04	123.95	111.07
1	B	2127	ASP	N-CA-C	10.03	122.21	111.28
1	B	1424	PHE	N-CA-C	-9.14	101.23	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2064	GLN	O-C-N	9.04	133.39	122.27

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASP	Peptide
1	A	2007	GLY	Peptide
1	A	2521	ASN	Peptide
1	B	2727	GLU	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	988	0
1	B	20748	0	20206	923	0
2	A	31	0	12	10	0
2	B	31	0	12	23	0
3	A	27	0	12	2	0
3	B	27	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	2	0
5	B	10	0	0	4	0
All	All	41634	0	40460	1913	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 1913 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:2380:LEU:CD2	1:A:2390:ILE:HD11	1.55	1.33
1:B:1826:PHE:CE2	1:B:1831:LEU:HB2	1.66	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.55	1.24
1:B:216:PRO:O	1:B:1365:PHE:HD1	1.21	1.22
1:B:216:PRO:O	1:B:1365:PHE:CD1	1.94	1.20

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	2640/2695 (98%)	2511 (95%)	118 (4%)	11 (0%)	30	60
1	B	2640/2695 (98%)	2525 (96%)	107 (4%)	8 (0%)	36	65
All	All	5280/5390 (98%)	5036 (95%)	225 (4%)	19 (0%)	30	60

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	A	2495	ASP
1	B	1391	GLY
1	A	2476	LYS
1	A	2728	LEU

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	2218/2453 (90%)	2071 (93%)	147 (7%)	15	43
1	B	2218/2453 (90%)	2110 (95%)	108 (5%)	22	51
All	All	4436/4906 (90%)	4181 (94%)	255 (6%)	18	47

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3646	ILE
1	B	3534	LEU
1	A	4016	CYS
1	B	3502	SER
1	B	3744	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4077	GLN
1	B	3561	ASN
1	B	1951	HIS
1	B	3542	GLN
1	B	4036	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	5094	-	28,29,29	1.68	5 (17%)	43,45,45	1.75	6 (13%)
3	ADP	B	5094	-	28,29,29	1.64	6 (21%)	43,45,45	2.08	13 (30%)
5	SO4	B	5097	-	4,4,4	0.48	0	6,6,6	0.44	0
5	SO4	B	5096	-	4,4,4	0.99	0	6,6,6	1.17	1 (16%)
5	SO4	A	5096	-	4,4,4	1.05	1 (25%)	6,6,6	1.40	1 (16%)
2	ATP	A	5093	4	32,33,33	1.41	4 (12%)	48,52,52	1.78	9 (18%)
5	SO4	A	5097	-	4,4,4	0.46	0	6,6,6	0.57	0
2	ATP	B	5093	4	32,33,33	1.55	5 (15%)	48,52,52	1.75	7 (14%)

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	A	5094	-	-	6/16/32/32	0/3/3/3
3	ADP	B	5094	-	-	7/16/32/32	0/3/3/3
2	ATP	B	5093	4	-	4/22/38/38	0/3/3/3
2	ATP	A	5093	4	-	5/22/38/38	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ADP	C5-C4	5.42	1.48	1.39
3	A	5094	ADP	C5-C4	5.40	1.48	1.39
2	B	5093	ATP	C5-C4	5.11	1.48	1.39
2	A	5093	ATP	C5-C4	4.74	1.47	1.39
3	A	5094	ADP	C5-N7	-3.52	1.32	1.39

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5093	ATP	C5-C4-N3	-6.10	118.32	126.72
2	A	5093	ATP	C5-C4-N3	-5.82	118.70	126.72
3	B	5094	ADP	C5-C4-N3	-5.39	119.29	126.72
3	A	5094	ADP	N3-C2-N1	-4.91	121.14	128.58
3	B	5094	ADP	N3-C4-N9	4.89	135.49	127.17

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

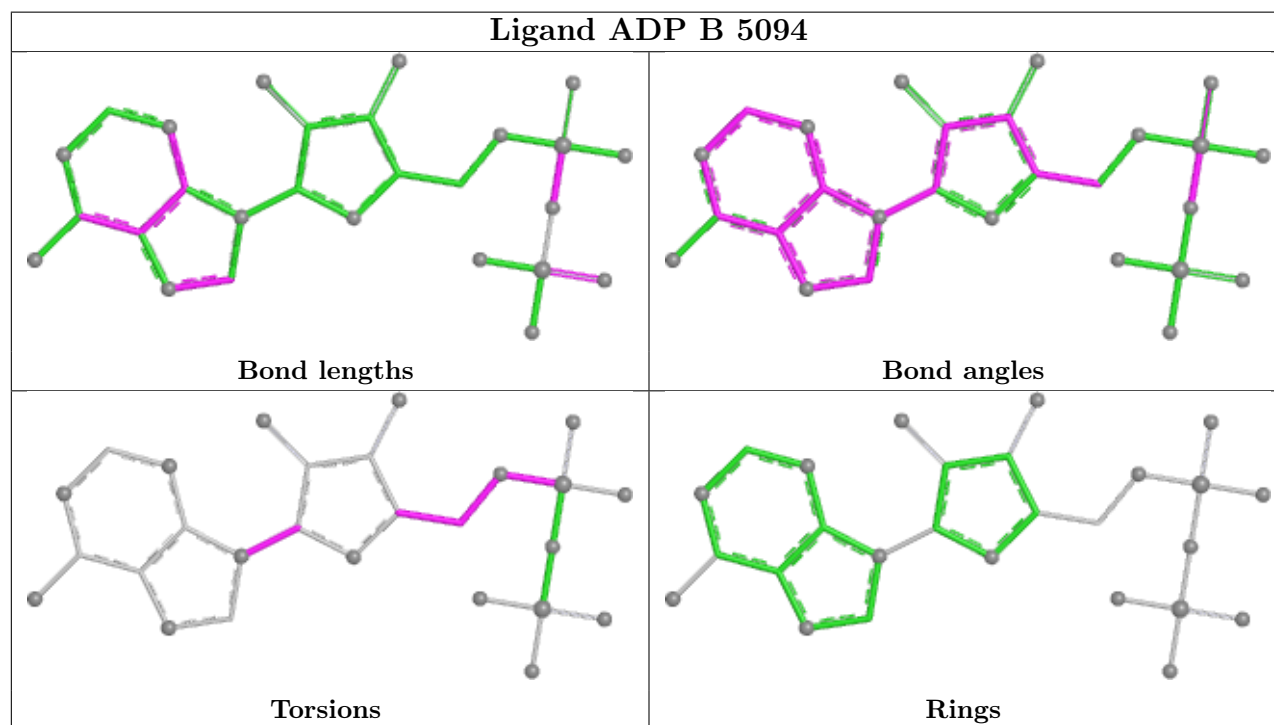
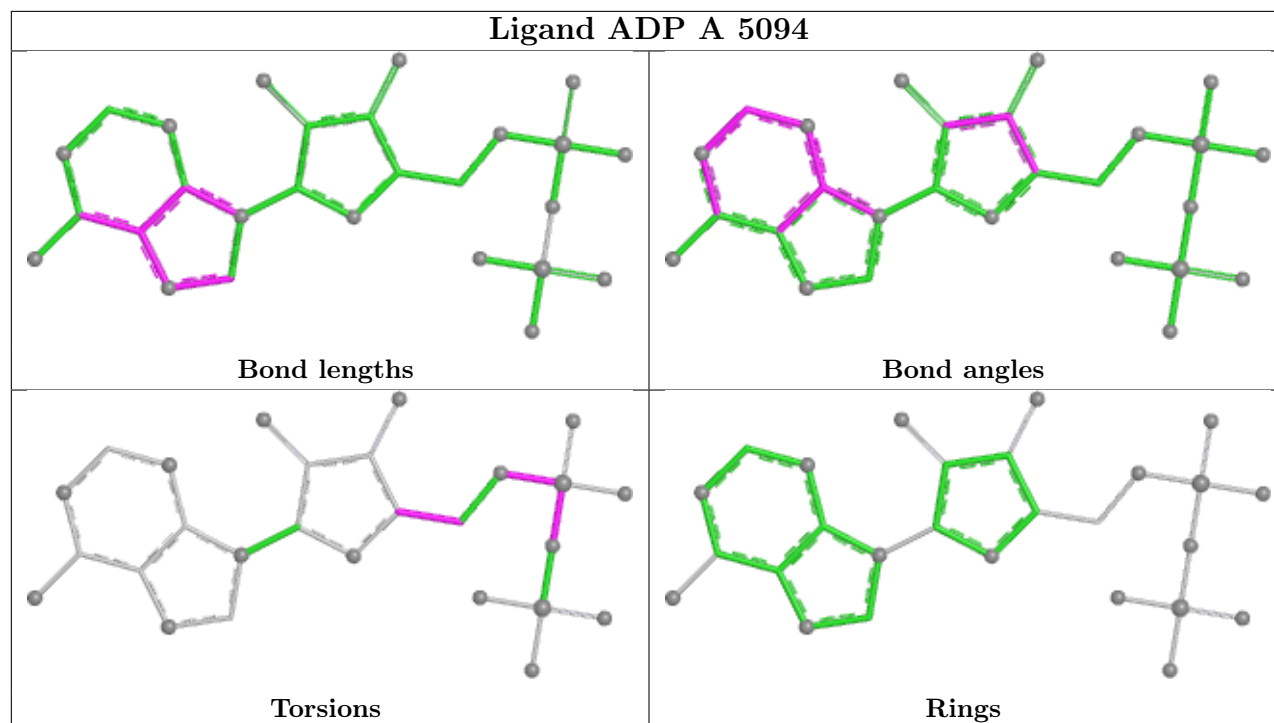
Mol	Chain	Res	Type	Atoms
2	A	5093	ATP	C5'-O5'-PA-O1A
2	B	5093	ATP	PB-O3B-PG-O2G
2	B	5093	ATP	PB-O3B-PG-O3G
3	A	5094	ADP	C5'-O5'-PA-O1A
3	B	5094	ADP	C5'-O5'-PA-O1A

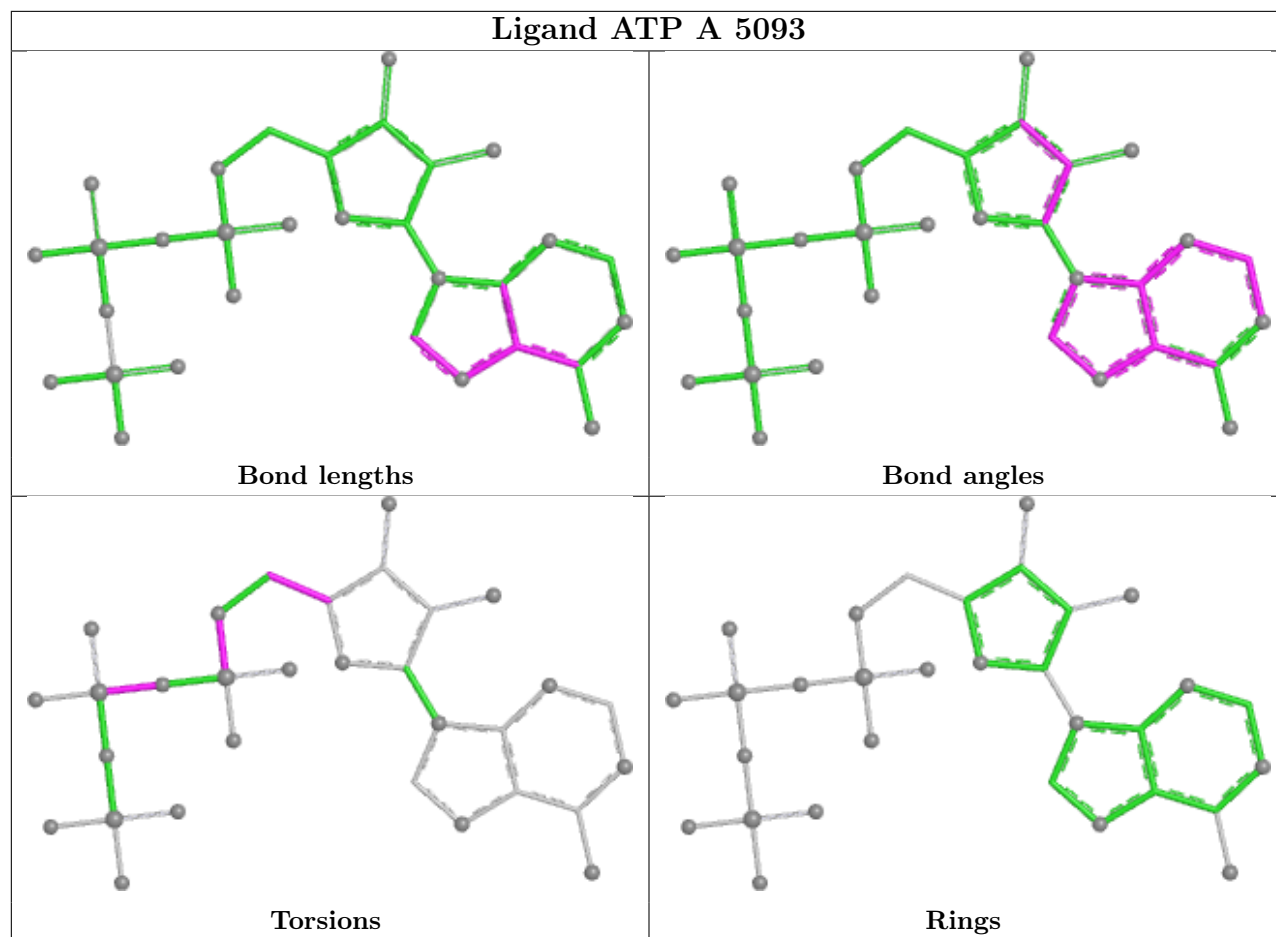
There are no ring outliers.

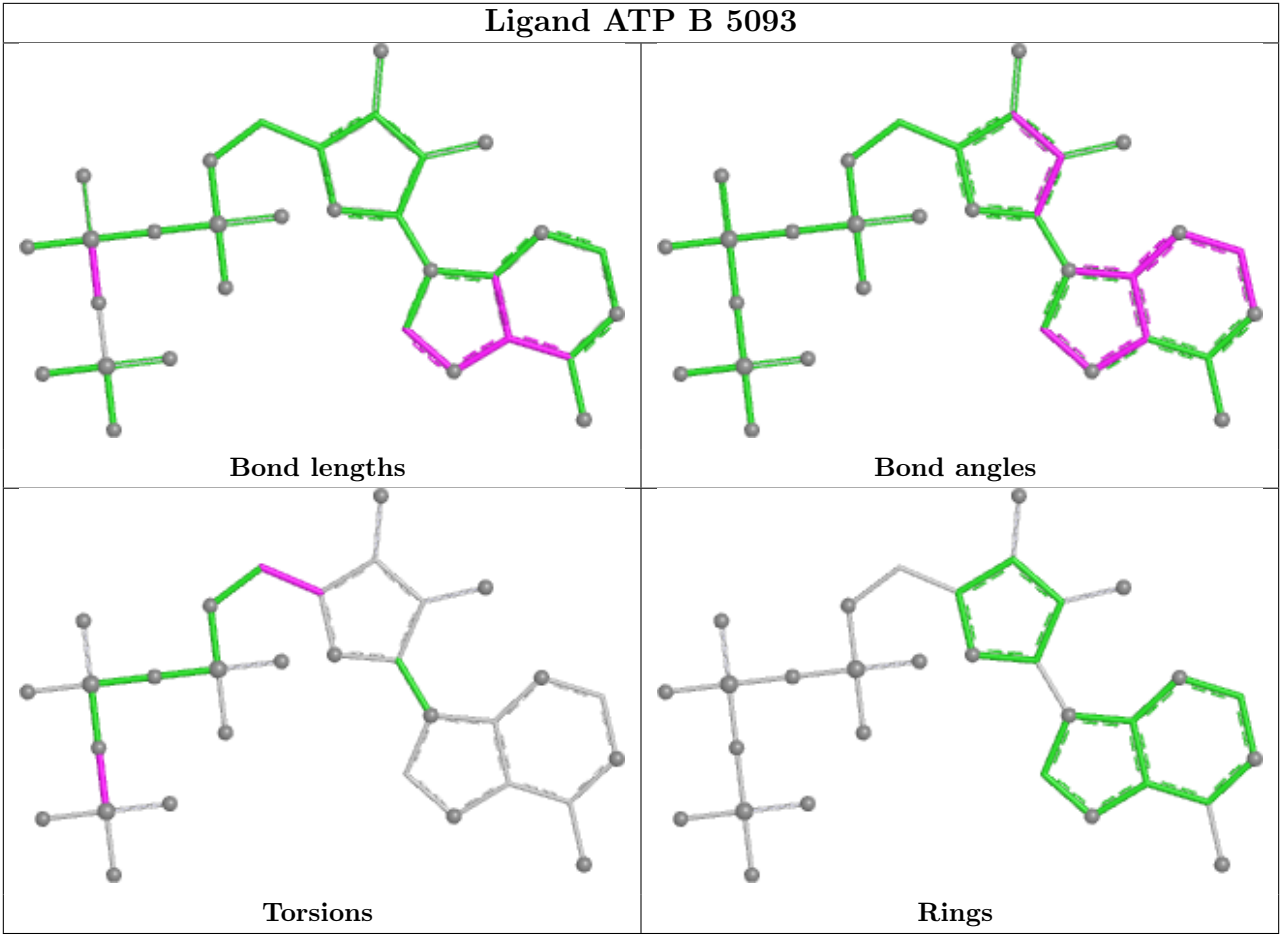
7 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5094	ADP	2	0
3	B	5094	ADP	6	0
5	B	5097	SO4	2	0
5	B	5096	SO4	2	0
2	A	5093	ATP	10	0
5	A	5097	SO4	2	0
2	B	5093	ATP	23	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2495:ASP	C	2496:LYS	N	1.17

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%)	-0.34	18 (0%)	84 70	62, 134, 265, 480	1 (0%)
1	B	2650/2695 (98%)	-0.18	20 (0%)	82 68	83, 185, 334, 500	1 (0%)
All	All	5300/5390 (98%)	-0.26	38 (0%)	84 70	62, 158, 302, 500	2 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1546	LEU	5.3
1	A	1483	TYR	5.0
1	B	18	LEU	4.4
1	A	2757	MET	4.2
1	A	3895	PHE	4.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

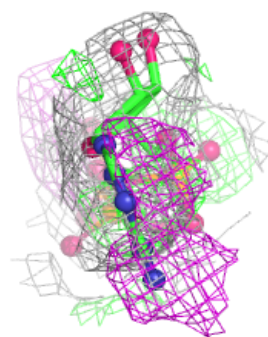
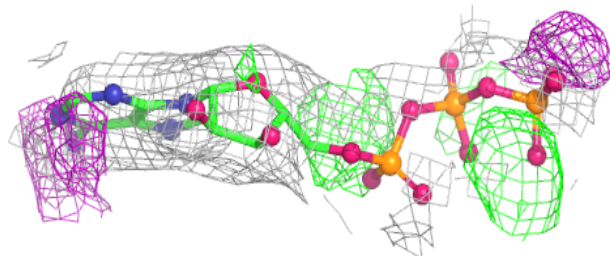
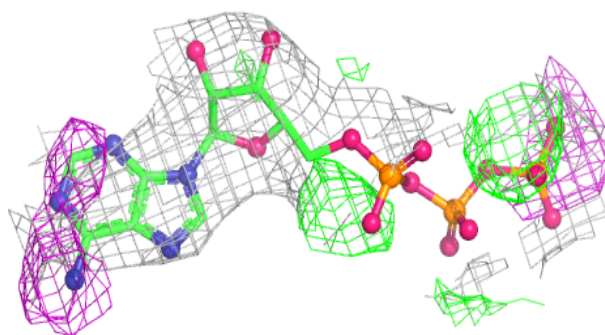
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	SO4	B	5096	5/5	0.82	0.13	86,103,146,179	0
5	SO4	A	5096	5/5	0.87	0.11	77,106,130,132	0
4	MG	A	5095	1/1	0.87	0.14	76,76,76,76	0
5	SO4	B	5097	5/5	0.90	0.05	157,162,176,183	0
4	MG	B	5095	1/1	0.94	0.10	86,86,86,86	0
2	ATP	A	5093	31/31	0.94	0.10	78,92,129,144	0
3	ADP	B	5094	27/27	0.95	0.08	81,114,155,168	0
2	ATP	B	5093	31/31	0.95	0.08	93,138,174,217	0
5	SO4	A	5097	5/5	0.96	0.05	82,93,104,115	0
3	ADP	A	5094	27/27	0.97	0.06	91,101,113,131	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.

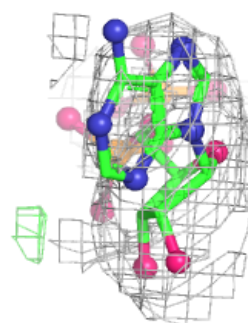
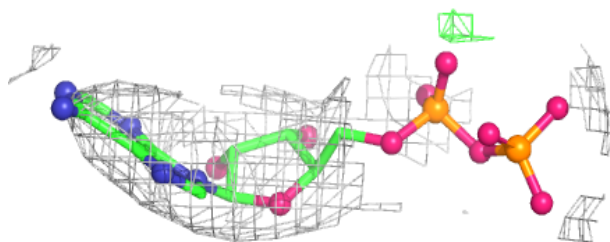
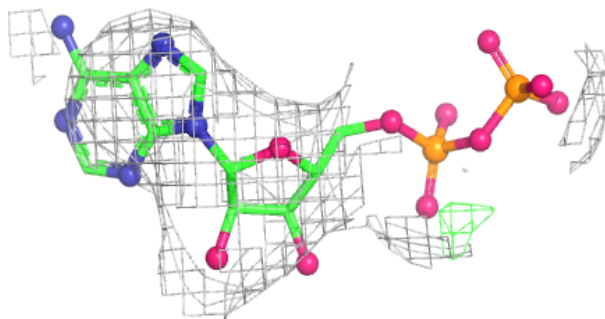
Electron density around ATP A 5093:

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

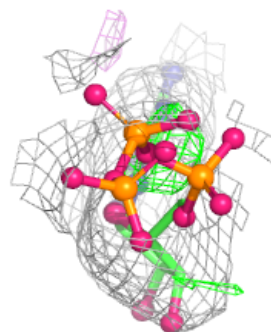
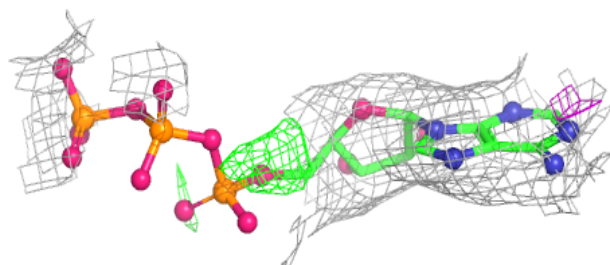
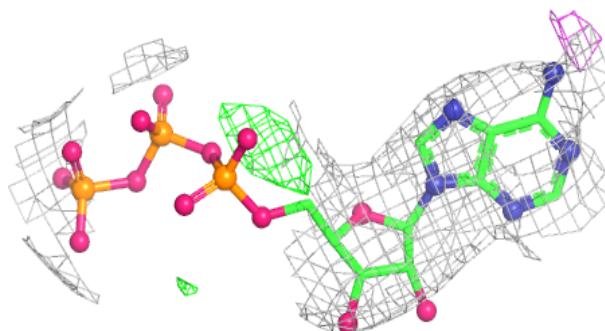


Electron density around ADP B 5094:

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

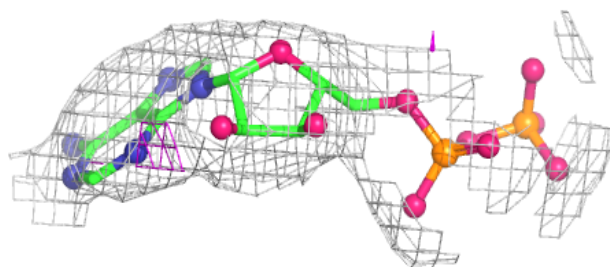
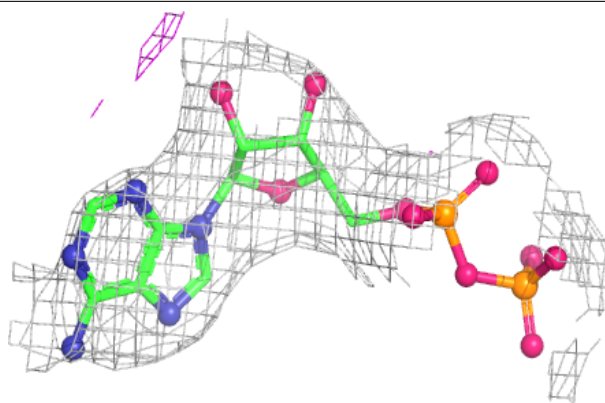
**Electron density around ATP B 5093:**

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



Electron density around ADP A 5094:

$2mF_o-DF_c$ (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.