



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:52 am BST

PDB ID : 4AKG
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 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 : 2.11
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) : 2.11

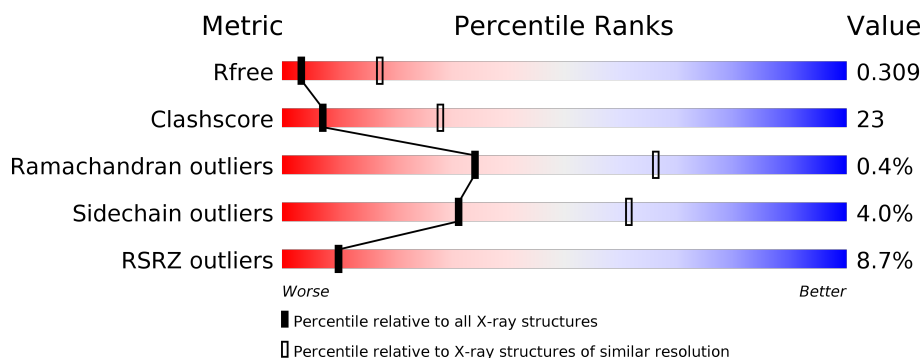
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	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.

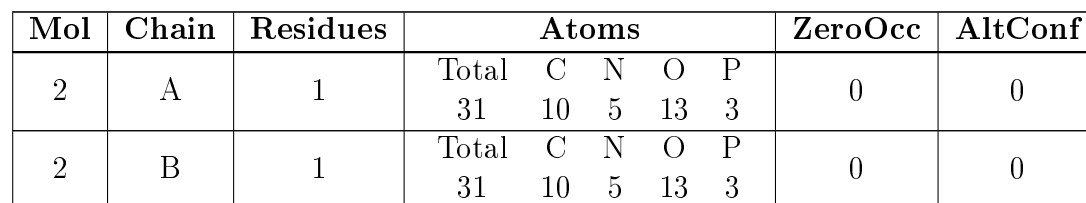
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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 (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



- # ADP

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



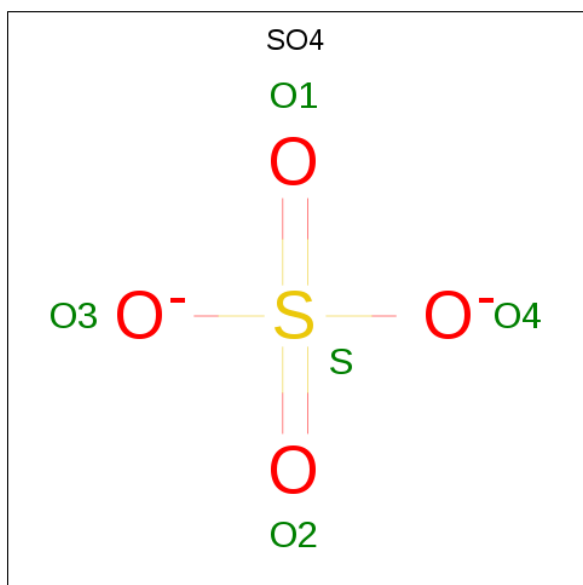
Continued from previous page...

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

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

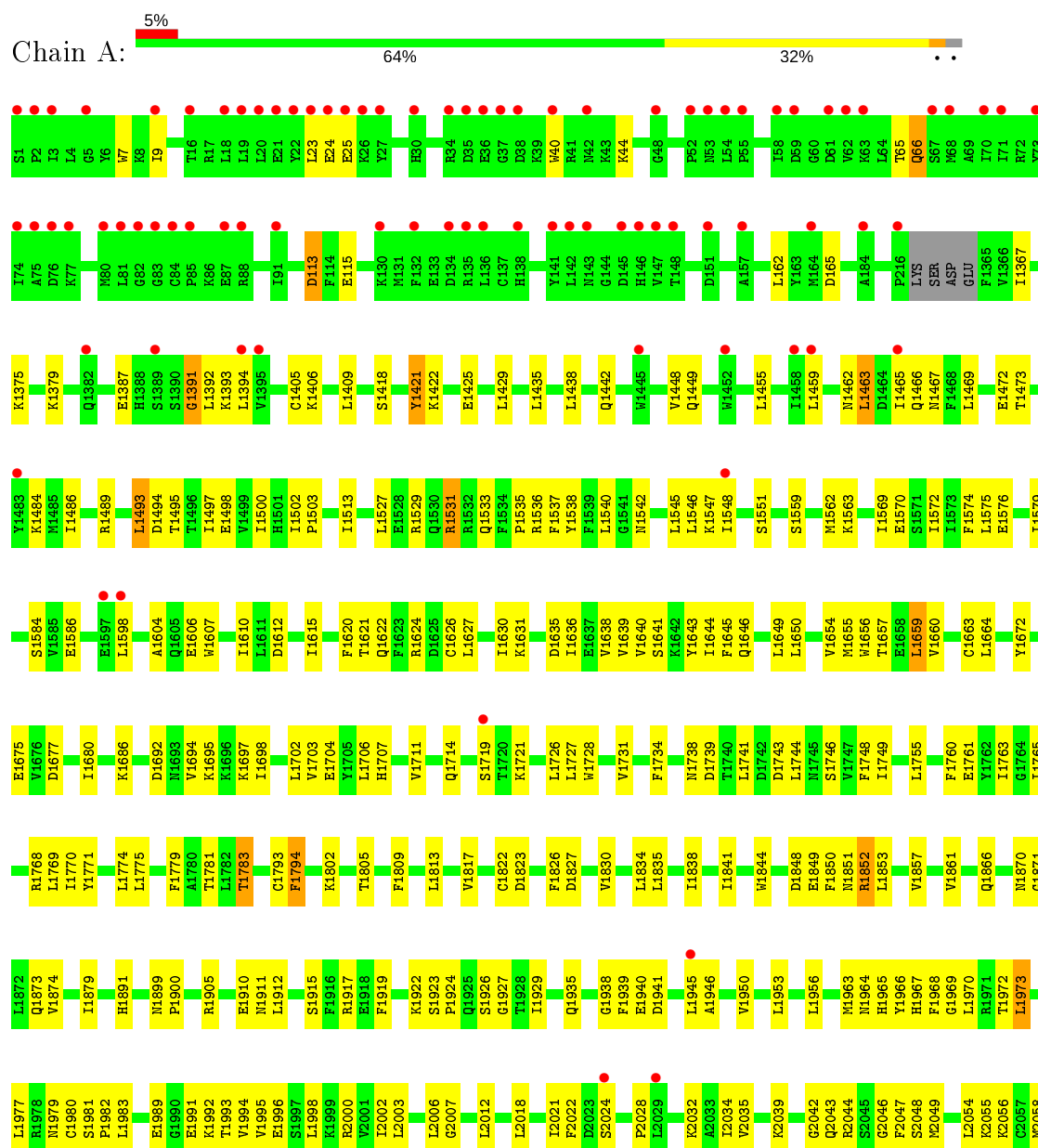


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

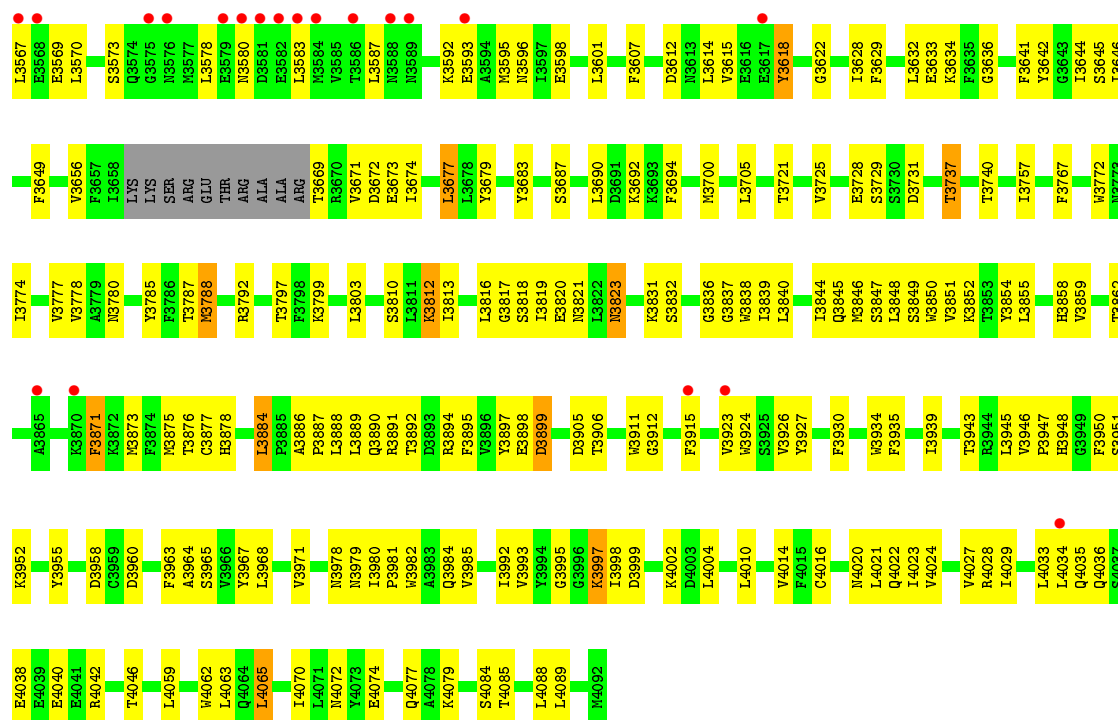
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

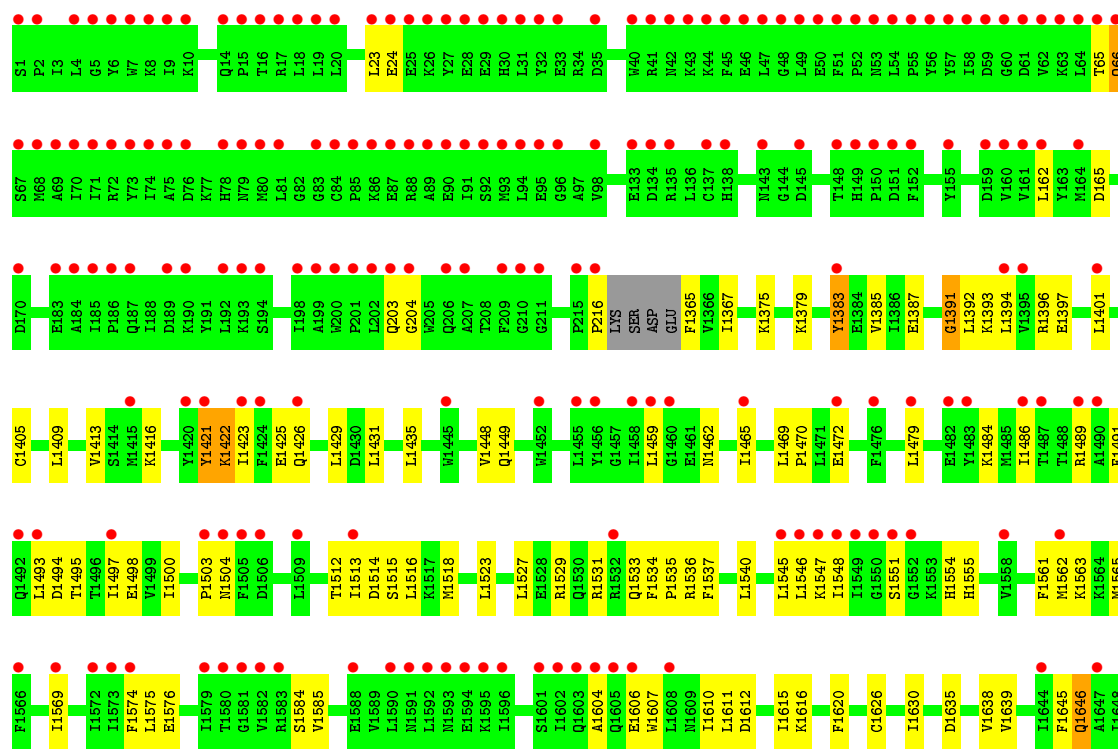
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC







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



L2843	Q2751	S2613	D2495	K2411	E2195	L2109	Z2023	M1937	L1831	T1740	L1649
F2844	V2752	L2616	K2496	I2415	T2196	T2110	S2024	G1938	L1835	L1741	L1650
G2846	G2497	G2498	G2497	I2416	D2197	E2112	A2025	F1939	L1841	D1742	M1655
Y2849	S2499	R2620	S2499	C2417	H2201	S2117	T2027	D1941	L1844	M1745	M1656
L2853	V2503	T2623	V2503	P2420	T2203	G2127	P2027	L1945	M1844	F1748	L1664
L2856	L2506	R2627	L2506	G2421	A2205	A2121	L2029	A1946	G1846	I1749	F1669
T2860	R2507	Y2630	R2507	T2425	T2207	W2125	K2032	V1949	D1848	G1753	Y1672
T2863	K2510	T2631	K2510	I2427	I2207	D2127	L2034	F1850	F1850	Y1754	Y1673
L2865	R2511	A2632	R2511	M2428	T2208	G2128	V2035	L1953	M1851	L1755	K1674
L2867	K2512	G2635	K2512	N2429	R2209	L2129	G2036	L1956	R1852	E1675	E1675
Q2870	Q2513	T2635	Q2513	N2430	I2212	T2130	C2037	L1970	L1853	Y1758	Y1676
Q2871	K2517	G2637	K2517	L2437	F2215	T2131	F2047	M1963	M1864	F1759	D1677
L2873	T2518	R2638	T2518	F2445	C2220	L2133	S2048	N1964	L1865	F1760	M1678
Y2878	P2519	Q2639	P2519	S2446	S2224	V2137	Q2058	H1965	Q1866	E1761	K1679
K2883	E2520	T2640	E2520	K2447	K2225	I2141	Q2059	Y1966	L1872	Y1762	L1680
V2888	V2524	S2643	V2524	D2448	D2228	F2145	Y2061	F1968	I1879	I1763	K1681
V2889	T2525	L2647	T2525	T2449	E2228	F2145	Y2061	F1968	T1880	I1765	G1682
T2890	K2526	R2653	K2526	E2452	H2228	F2145	Q2064	L1970	L1881	E1767	L1683
L2891	F2527	L2654	F2527	E2452	L2241	R2149	L2068	L1973	L1882	R1768	L1684
L2892	R2528	T2655	R2528	L2455	L2252	L2150	Q2068	K1974	L1888	L1769	D1692
L2908	C2535	L2655	C2535	L2458	L2252	W2151	G1975	V1976	L1893	I1770	M1693
F2909	N2536	F2669	N2536	H2459	L2262	F2154	L2071	S1981	A1893	T1772	V1694
R2911	R2543	L2681	R2543	R2460	L2265	D2155	L2072	P1982	V1894	P1773	K1695
C2912	R2549	Q2684	R2549	N2463	F2266	S2156	L2073	L1983	M1899	L1774	K1696
N2915	F2550	Q2684	F2550	Y2464	H2274	P2160	G2074	P1984	P1900	L1775	K1697
N2920	T2551	L2689	T2551	T2467	H2274	E2161	A2076	I1984	R1905	L1776	L1698
T2924	R2552	S2690	R2552	S2468	L2275	Y2162	K2080	E1989	T1781	L1702	L1703
V2935	L2556	S2691	L2556	G2470	L2276	E2164	T2081	E1990	E1910	E1704	E1704
L2936	P2562	D2703	P2562	T2471	G2277	V2169	A2082	E1991	M1911	Y1705	Y1705
T2937	S2563	N2707	S2563	L2472	V2278	L2170	T2083	T1993	L1912	G1792	L1706
N2938	Q2564	K2709	Q2564	L2473	F2281	L2170	W2084	V1994	K1913	C1793	H1707
T2941	K2565	L2712	K2565	L2474	F2282	N2173	K2085	E1996	K1914	F1794	V1711
D2942	S2566	N2713	S2566	P2475	K2283	G2174	L2088	S1997	R1917	G1801	L1712
V2943	Y2571	E2727	Y2571	K2476	L2284	L2175	I2091	L1998	E1916	K1802	G1713
V2936	E2572	L2728	E2572	S2477	E2285	L2176	D2094	K1999	F1919	T1803	L1714
L2937	L2573	E2727	L2573	L2478	L2290	T2177	F2095	R2000	S1920	E1804	L1715
N2938	Y2574	L2728	Y2574	K2480	L2293	L2178	D2095	V2001	M1921	T1805	L1726
T2941	L2578	S2737	L2578	N2481	H2293	N2180	L2099	I2002	K1922	V1806	L1727
D2942	F2579	S2737	F2579	L2484	L2294	G2181	V2100	L2003	S1923	L1813	L1727
F2943	K2580	H2741	K2580	L2488	L2295	E2182	G2007	L2006	Q1925	K1730	K1730
V2943	L2581	R2744	L2581	E2488	L2302	R2183	D2008	C1822	S1926	V1731	V1731
V2943	V2582	R2744	V2582	I2489	F2302	L2186	Y2102	D1823	I1929	Q1732	Q1732
P2943	Y2690	L2745	Y2690	T2491	L2305	R2191	V2103	E2011	L1933	F1734	K1733
V2943	L2491	L2745	L2491	D2406	D2306	L2192	G2105	F2014	L1934	D1826	F1734
V2943	P2492	R2746	P2492	N2409	D2307	L2192	T2106	F2014	Q1829	D1827	K1737
V2943	E2590	A2748	E2590	L2494	L2310	F2194	V2108	F2022	I1936	Q1829	H1738
V2943										V1830	D1739

V4014	K3924	K3850	T3740	K3631	K3544	H3413	E3304	LYS
F4015	S3925	V3851	R3745	F3641	D3547	V3417	R3305	GLU
G4017	V3926	Y3854	L3855	F3641	L3548	L3549	W3306	LEU
		H3856	F3767	S3645	K3550	S3429	N3307	VAL
M4020	F3930	K3857	F3768	I3646	Y3555	S3430	N3308	PHE
L4021	V3934	H3858	V3769	K3854	K3556	F3431	T3310	THR
Q4022	F3935	V3859	W3772	R3855	L3557	R3439	K3311	GLU
I4023	F3935	E3860	N3773	V3856	K3558	L3440	Q3312	PRO
V4024	I3939	A3865	I3774	F3657	L3559	R3439	F3313	ILE
		E3866	V3777	L3658		L3453	T2960	GLN
V4027	T3943	K3869	A3778	LYS	R3565	F3458	I2961	I2961
R4028	K3944	K3870	V3778	LYS	L3566	D3459	R2962	R2962
I4029	L3945	S3879	N3780	SER	L3567	P3460	D2963	D2963
E4038	P3947	F3871	N3780	ARG	L3570	I3461	A2964	A2964
L4049		K3872	Y3785	GLU	N3571	N3323	V2965	V2965
		F3873	F3786	THR	N3572	I3462	N2967	N2967
E4054	F3950	F3874	T3787	ARG	S3573	S3463	L2968	L2968
P4055	S3951	M3875	T3787	ALA		L3465	L2969	L2969
		T3876	R3792	ARG	E3579	A3473	V2982	V2982
L4059	Y3955	C3877	K3799	T3669	N3580	R3476	G2983	G2983
S4060	D3958	H3878	L3803	R3670	D3581	F3334	S2988	S2988
S4061	C3959	D3882	L3803	V3671	E3582	N3338	P2989	P2989
W4062	F3883	K3884	S3807	I3674	L3583	E3341	G2990	G2990
L4063	P3885	P3885	K3808	L3677	M3584	I3481	L2999	L2999
L4065	A3964	A3886	F3809	L3678	T3585	G3482	L3010	L3010
	S3965	P3887	S3810	V3679	T3586	L3494	V3017	V3017
L4070	L3968	L3888	L3811	Y3683	L3587	D3500	G3020	G3020
E4074	E3969	L3889	I3812	Y3683	N3588	P3501	L3024	L3024
A4078	N3970	Q3890	I3813	S3687	N3589	S3502	V3028	V3028
K4079	L3972	F3895	I3814	K3687	K3591	I3505	LYS	LYS
		V3896	P3815	L3690	E3592	L3509	VAL	VAL
N3978	N3979	Y3897	L3816	D3691	E3593	R3510	ASN	ASN
I3980	E3898	E3897	G3817	D3691	A3594	V3513	GLU	GLU
P3981	D3899	S3818	S3817	K3692	N3595	F3518	LEU	LEU
N3982	I3900	I3819	I3819	K3692	N3596	V3519	ASN	ASN
A3983	P3901	E3820	N3821	F3694	I3597	N3521	THR	THR
Q3984	D3905	N3822	L3822	K3698	E3598	I3525	SER	SER
V3985	T3906	N3823	N3823	A3699	K3600	F3530	ILE	ILE
V3993	V3907	I3834	I3834	T3701	E3603	T3533	SER	SER
G3995	K3908	G3837	W3838	R3702	E3605	L3534	LEU	LEU
		I3838	I3839	V3706	D3612	F3400	VAL	VAL
I3998	G3912	L3840	L3840	L3726	N3613	F3406	T3300	T3300
K4002	S3913	L3841	L3841	S3727	L3614	N3538	F3301	F3301
D4003	F3916	F3915	F3915	E3728	V3615	E3375	E3302	E3302
L4004	T3917	F3916	I3844	S3729	Y3618	L3391	K3297	K3297
E4005	G3918	K3919	Q3845		G3622	S3400	T3300	T3300
W4006	I3920	L3948	S3847	F3734	I3628	F3406	F3301	F3301
K4009	V3923	S3849	S3849	L3736		D3409	E3302	E3302
				T3737			K3303	K3303

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 48.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.30) 96.1 (48.81-3.30)	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	5980 reflections (4.99%)	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)	0.27 , 102.5	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: ATP, MG, SO4, 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	0.62	7/21146 (0.0%)	0.85	21/28618 (0.1%)
1	B	0.51	2/21146 (0.0%)	0.72	4/28618 (0.0%)
All	All	0.57	9/42292 (0.0%)	0.79	25/57236 (0.0%)

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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2064	GLN	CA-C	-8.38	1.31	1.52
1	B	2841	PRO	N-CD	-7.95	1.36	1.47
1	A	2495	ASP	C-N	-7.35	1.17	1.34
1	B	1759	LYS	C-O	6.47	1.35	1.23
1	A	2488	GLU	CD-OE1	5.63	1.31	1.25

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2412	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	B	2471	LEU	CA-CB-CG	8.90	135.76	115.30
1	A	3459	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	2012	LEU	CA-CB-CG	7.53	132.62	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2212	LEU	CB-CG-CD1	-7.18	98.80	111.00

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	20205	957	0
1	B	20748	0	20206	896	0
2	A	31	0	12	10	0
2	B	31	0	12	24	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	40459	1855	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 1855 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

Continued on next page...

Continued from previous page...

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%)	34	66
1	B	2640/2695 (98%)	2525 (96%)	107 (4%)	8 (0%)	41	71
All	All	5280/5390 (98%)	5036 (95%)	225 (4%)	19 (0%)	34	66

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%)	2115 (95%)	103 (5%)	27	58
1	B	2218/2453 (90%)	2145 (97%)	73 (3%)	38	66
All	All	4436/4906 (90%)	4260 (96%)	176 (4%)	31	61

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3729	SER
1	A	3997	LYS
1	B	3737	THR
1	A	3788	MET
1	A	3899	ASP

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

Mol	Chain	Res	Type
1	A	4020	ASN
1	B	1851	ASN
1	B	3890	GLN
1	A	4077	GLN
1	B	1707	HIS

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 carbohydrates 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$
5	SO4	B	5096	-	4,4,4	0.93	0	6,6,6	1.19	0
5	SO4	A	5096	-	4,4,4	1.03	1 (25%)	6,6,6	1.46	1 (16%)
2	ATP	B	5093	4	26,33,33	1.05	2 (7%)	31,52,52	1.64	5 (16%)
5	SO4	B	5097	-	4,4,4	0.38	0	6,6,6	0.43	0
5	SO4	A	5097	-	4,4,4	0.37	0	6,6,6	0.59	0
2	ATP	A	5093	4	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
3	ADP	B	5094	-	24,29,29	1.26	2 (8%)	29,45,45	1.67	5 (17%)
3	ADP	A	5094	-	24,29,29	1.15	1 (4%)	29,45,45	1.62	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	ATP	A	5093	4	-	6/18/38/38	0/3/3/3
2	ATP	B	5093	4	-	4/18/38/38	0/3/3/3
3	ADP	B	5094	-	-	5/12/32/32	0/3/3/3
3	ADP	A	5094	-	-	7/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ADP	C5-C4	2.96	1.48	1.40
3	A	5094	ADP	C5-C4	2.95	1.48	1.40
2	B	5093	ATP	C5-C4	2.75	1.48	1.40
3	B	5094	ADP	C4-N3	2.70	1.39	1.35
2	A	5093	ATP	C5-C4	2.50	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5094	ADP	N3-C2-N1	-4.82	121.14	128.68
3	B	5094	ADP	N3-C2-N1	-4.44	121.73	128.68
3	B	5094	ADP	C3'-C2'-C1'	4.05	107.07	100.98
2	B	5093	ATP	C3'-C2'-C1'	3.77	106.65	100.98
2	B	5093	ATP	PA-O3A-PB	-3.61	120.43	132.83

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

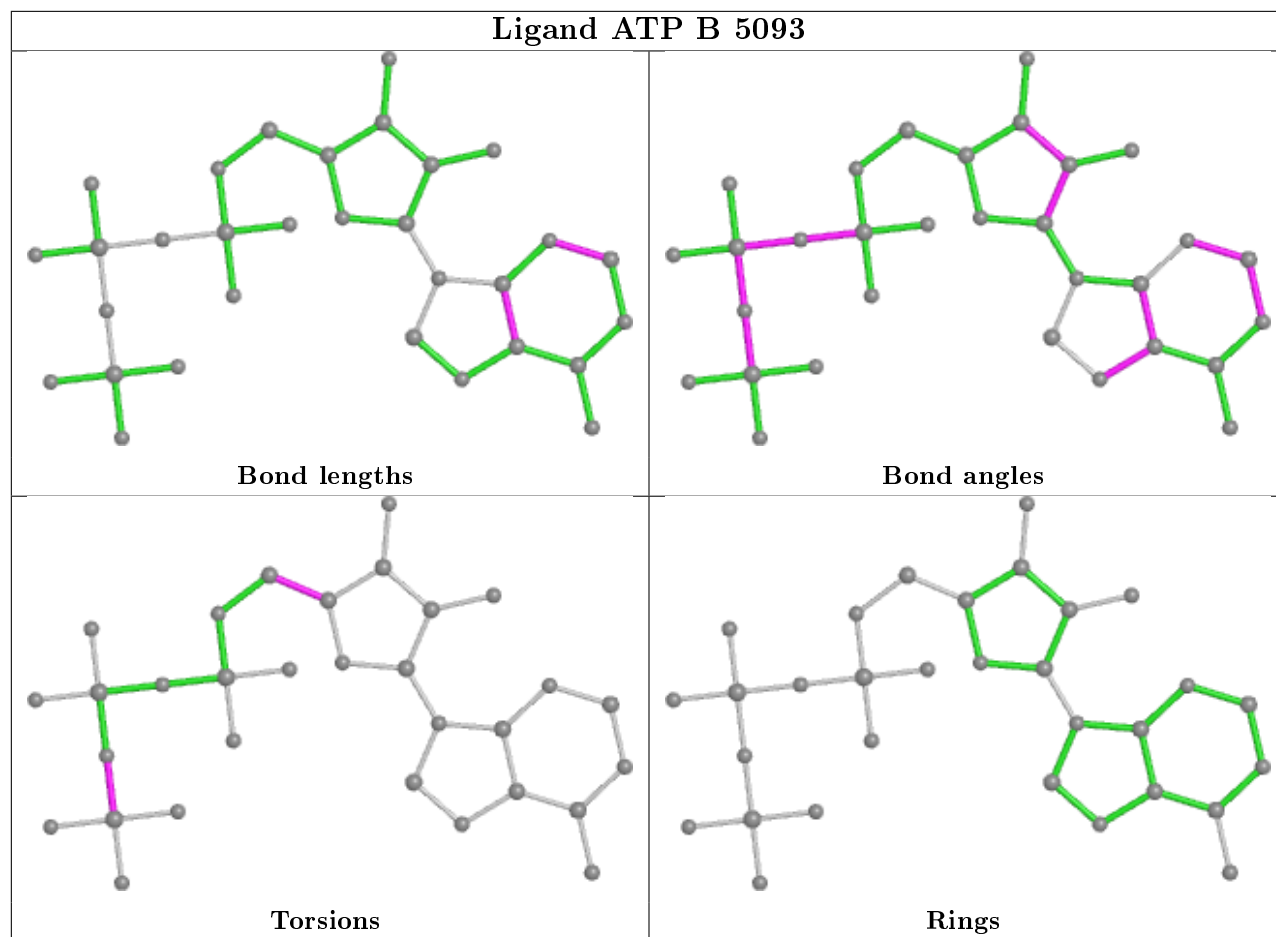
Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	PB-O3B-PG-O2G
2	B	5093	ATP	PB-O3B-PG-O3G
2	A	5093	ATP	C5'-O5'-PA-O1A
3	B	5094	ADP	C5'-O5'-PA-O1A
3	B	5094	ADP	C3'-C4'-C5'-O5'

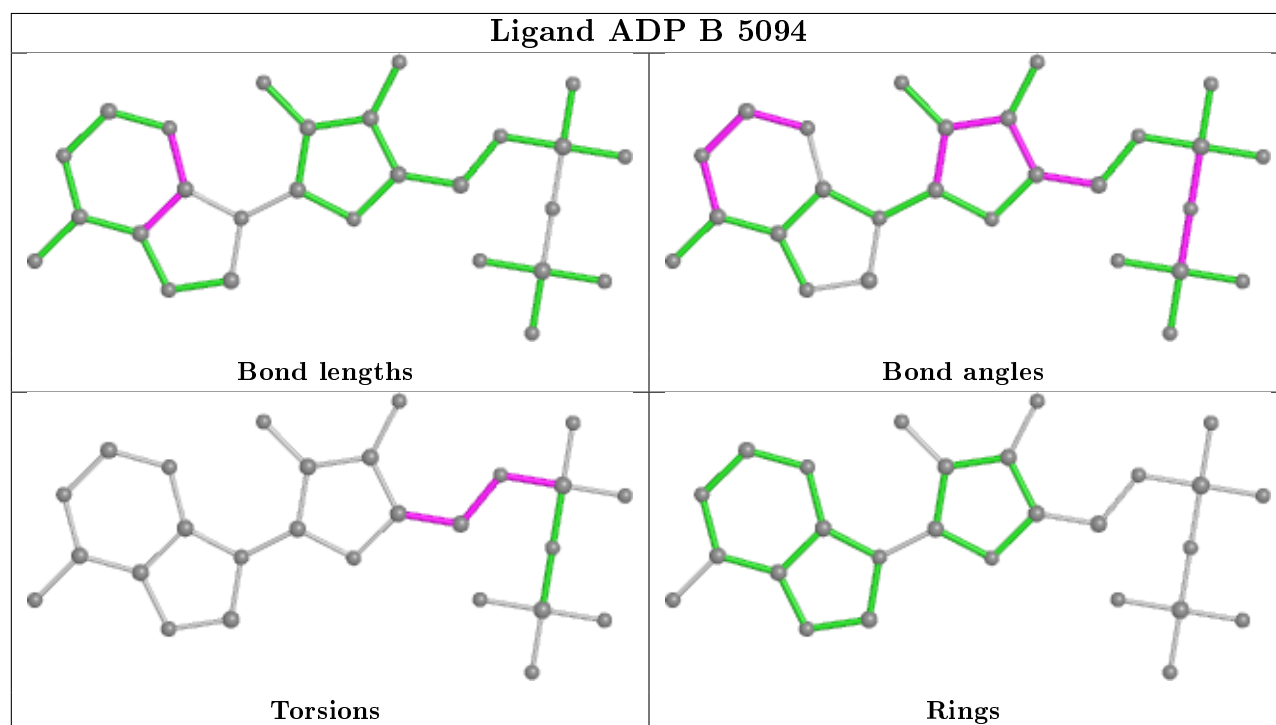
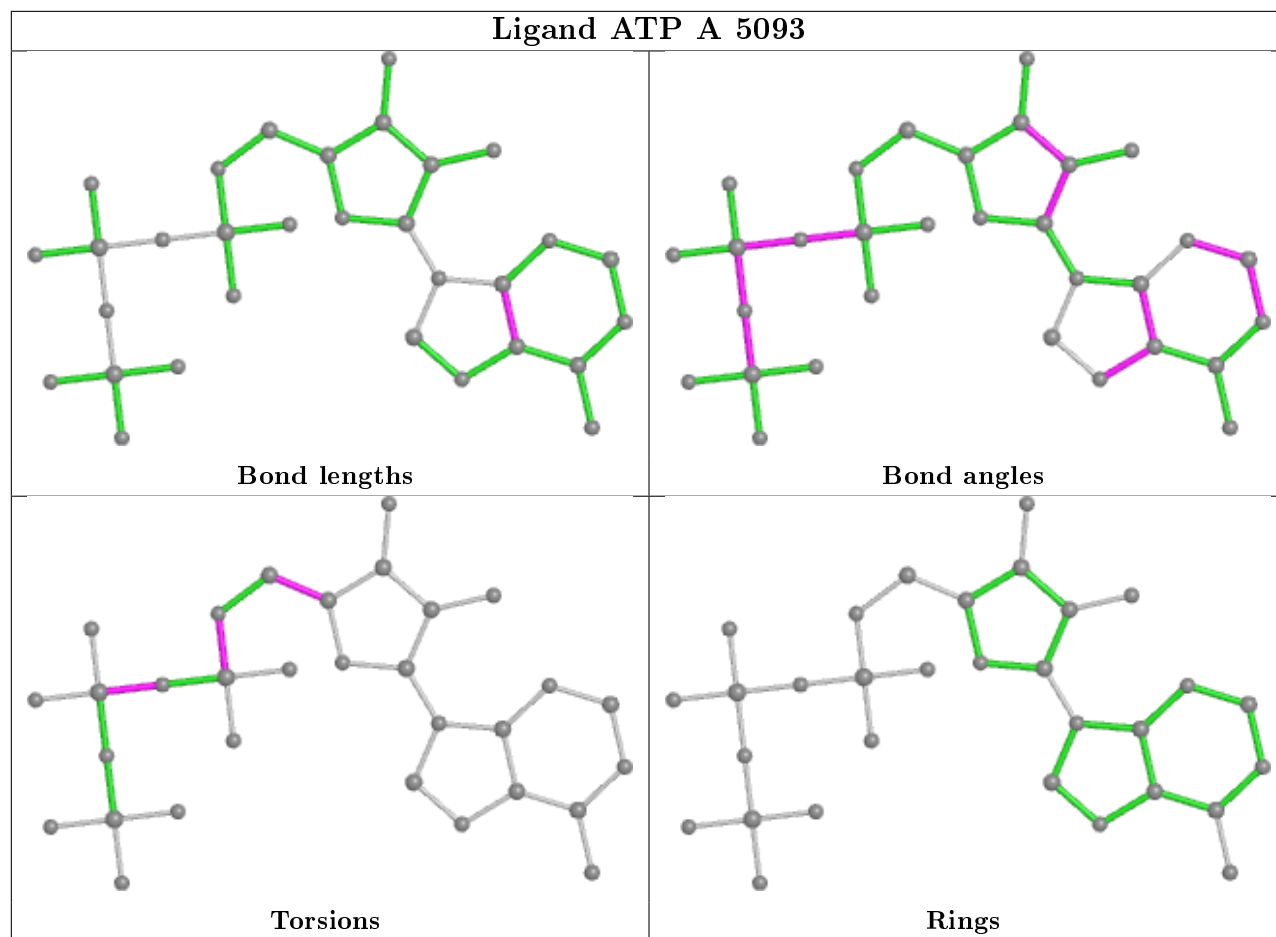
There are no ring outliers.

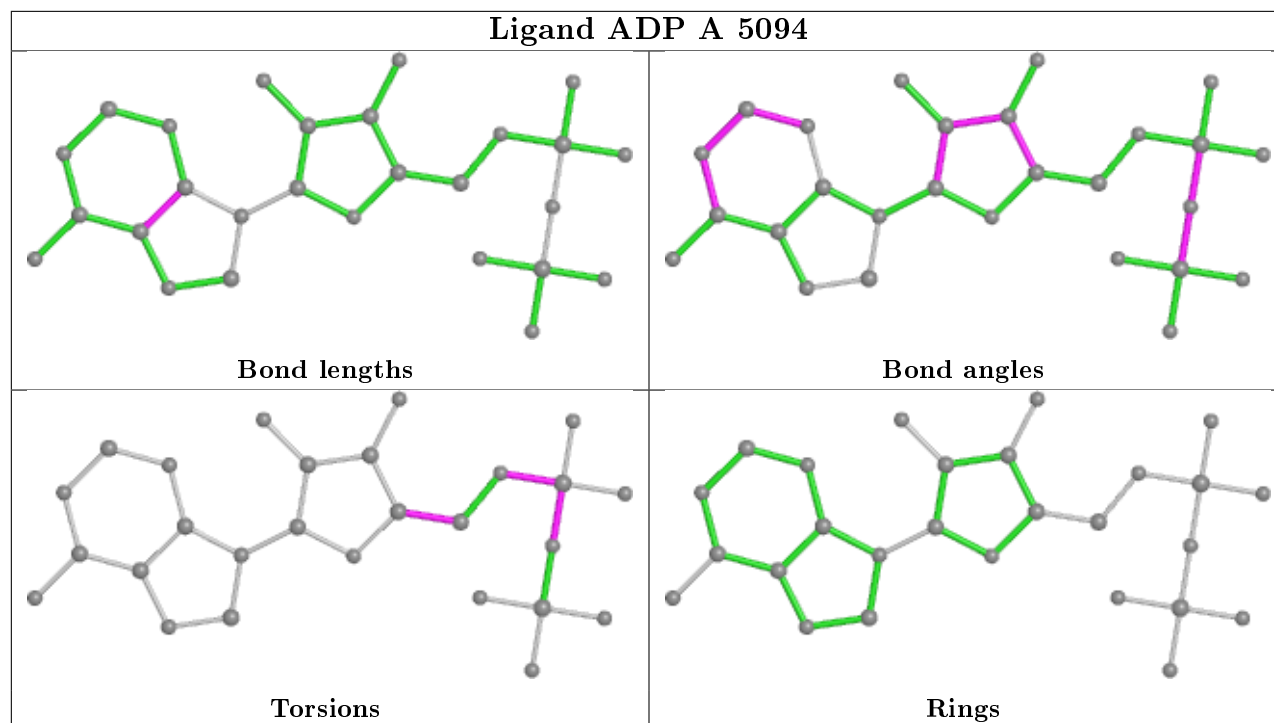
7 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5096	SO4	2	0
2	B	5093	ATP	24	0
5	B	5097	SO4	2	0
5	A	5097	SO4	2	0
2	A	5093	ATP	10	0
3	B	5094	ADP	6	0
3	A	5094	ADP	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.18	139 (5%)	27 25	62, 134, 265, 480	1 (0%)
1	B	2650/2695 (98%)	0.66	323 (12%)	4 3	83, 185, 334, 500	1 (0%)
All	All	5300/5390 (98%)	0.42	462 (8%)	10 10	62, 158, 303, 500	2 (0%)

The worst 5 of 462 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	20.3
1	B	69	ALA	17.4
1	B	59	ASP	17.2
1	B	31	LEU	16.8
1	B	60	GLY	15.0

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](#)

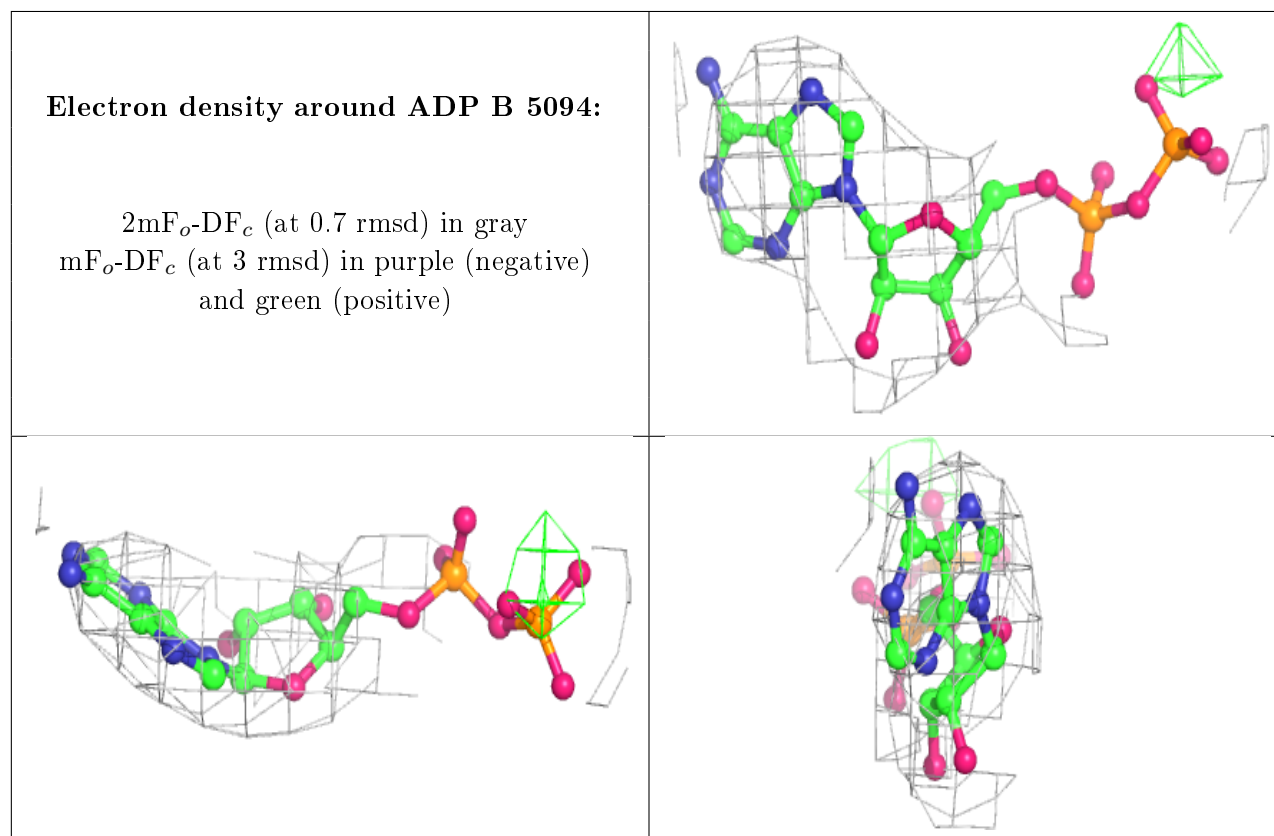
There are no carbohydrates in this entry.

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.

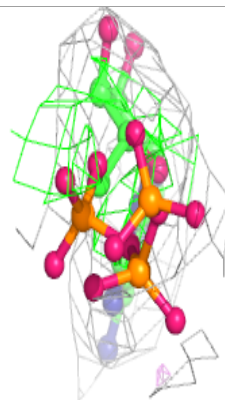
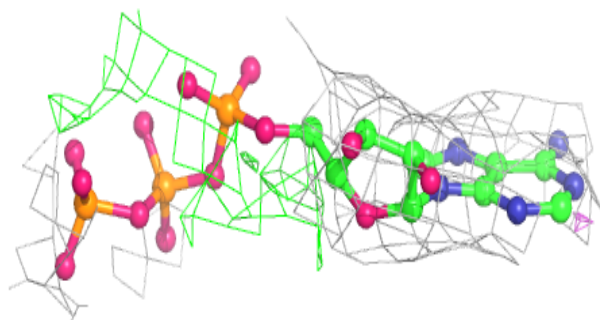
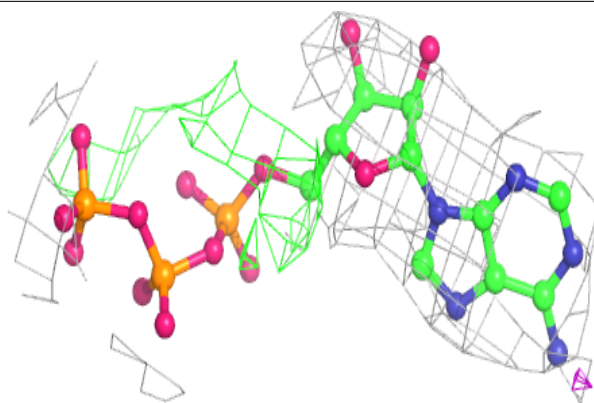
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	B	5096	5/5	0.87	0.53	86,103,146,179	0
4	MG	A	5095	1/1	0.89	0.40	76,76,76,76	0
3	ADP	B	5094	27/27	0.90	0.27	81,114,155,168	0
2	ATP	B	5093	31/31	0.92	0.26	93,138,174,217	0
5	SO4	A	5096	5/5	0.92	0.45	77,106,130,132	0
2	ATP	A	5093	31/31	0.93	0.29	78,92,129,144	0
3	ADP	A	5094	27/27	0.94	0.25	91,101,113,131	0
4	MG	B	5095	1/1	0.97	0.34	86,86,86,86	0
5	SO4	B	5097	5/5	0.97	0.17	157,162,176,183	0
5	SO4	A	5097	5/5	0.97	0.22	82,93,104,115	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.

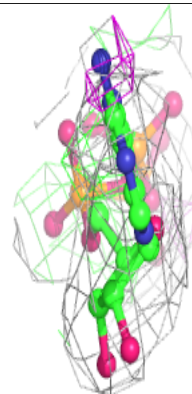
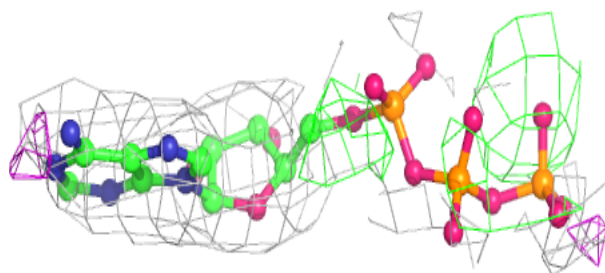
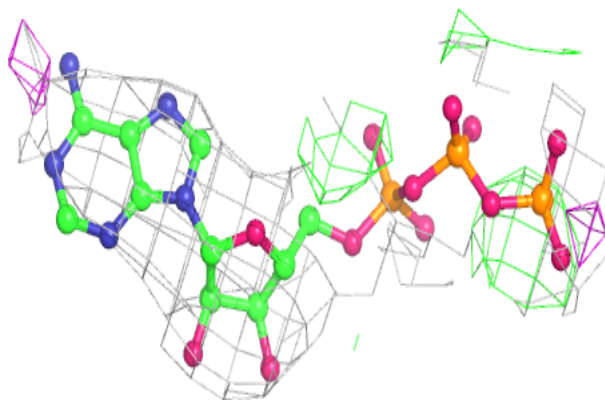


Electron density around ATP B 5093:

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

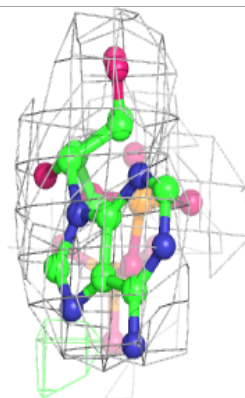
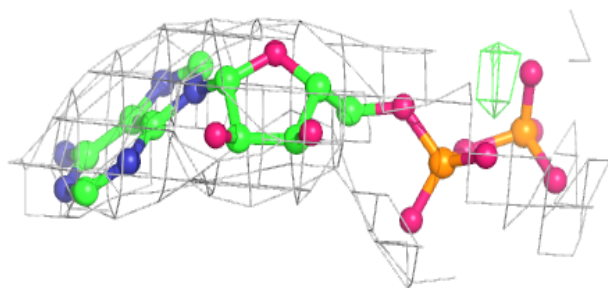
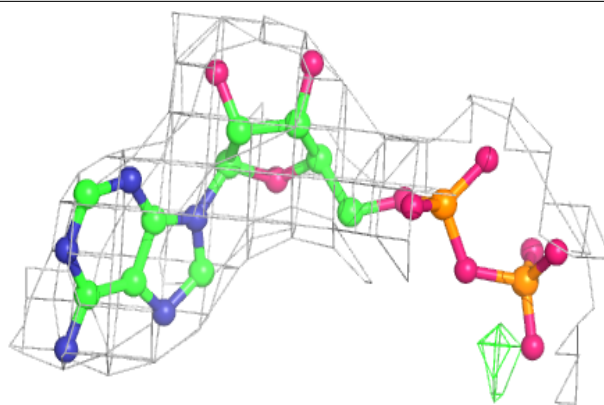
**Electron density around ATP A 5093:**

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



Electron density around ADP 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.