



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 10:17 AM BST

PDB ID : 4AKH
Title : Dynein Motor Domain - AMPPNP complex
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on : 2012-02-22
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

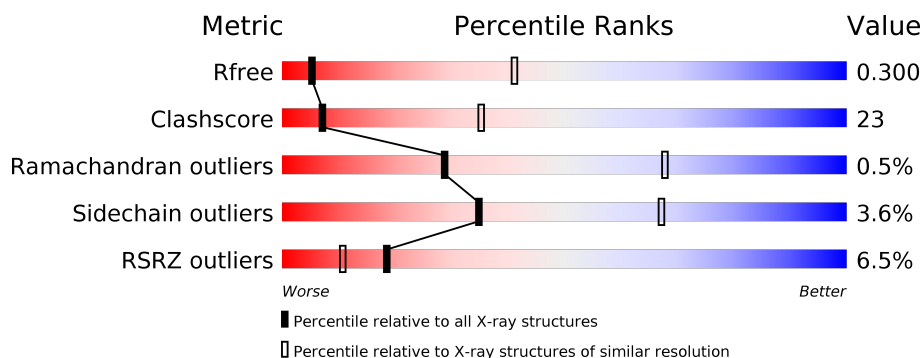
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	<div> <div>3%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	2695	<div> <div>10%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

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	5093	-	-	X	-
4	SO4	A	5095	-	-	X	-
4	SO4	B	5096	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 41642 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:

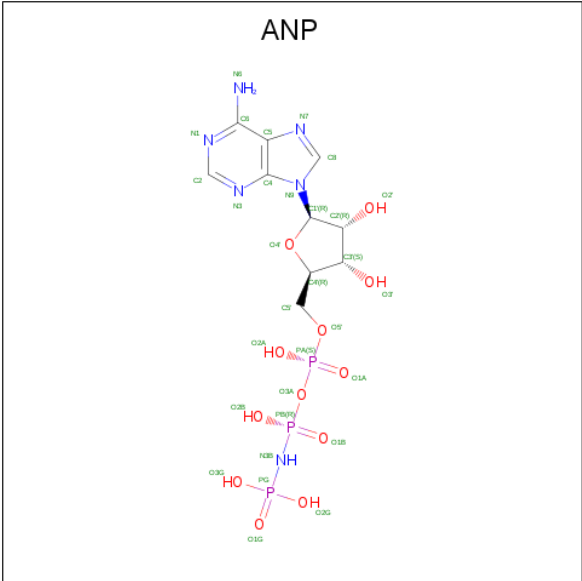
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

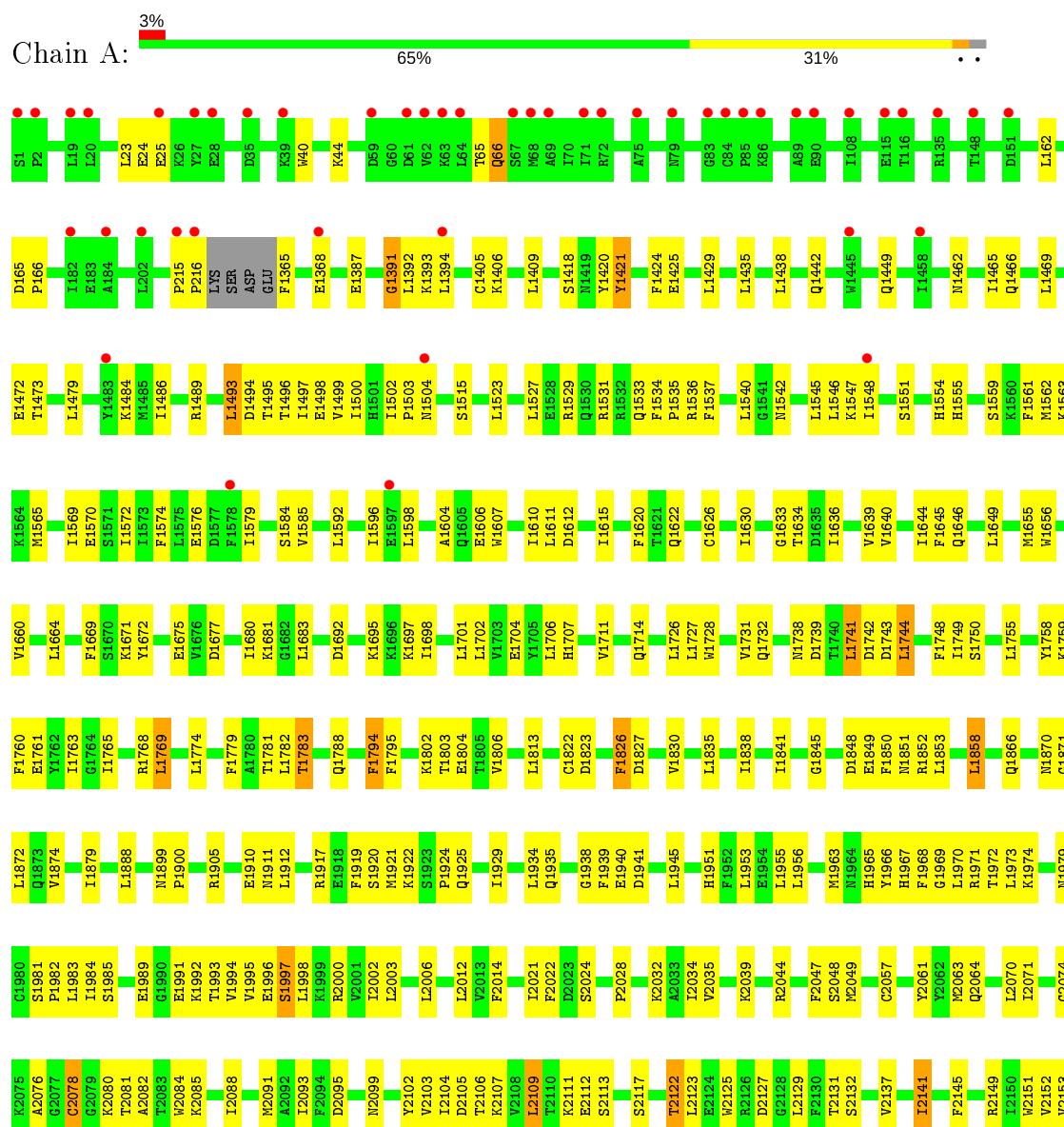
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

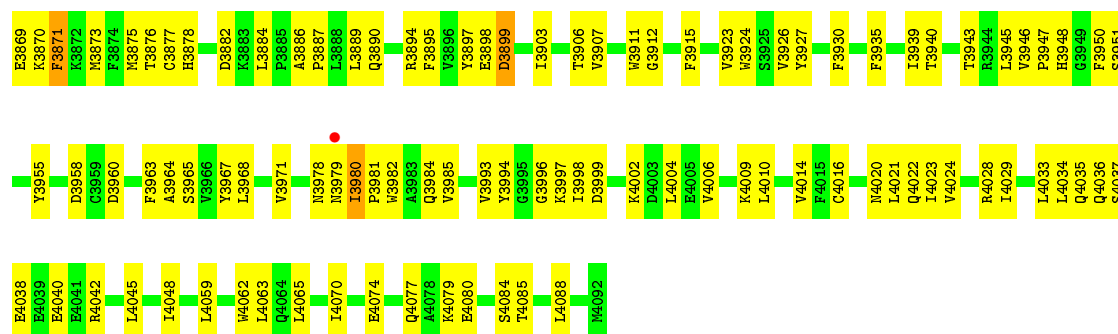
3 Residue-property plots

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.

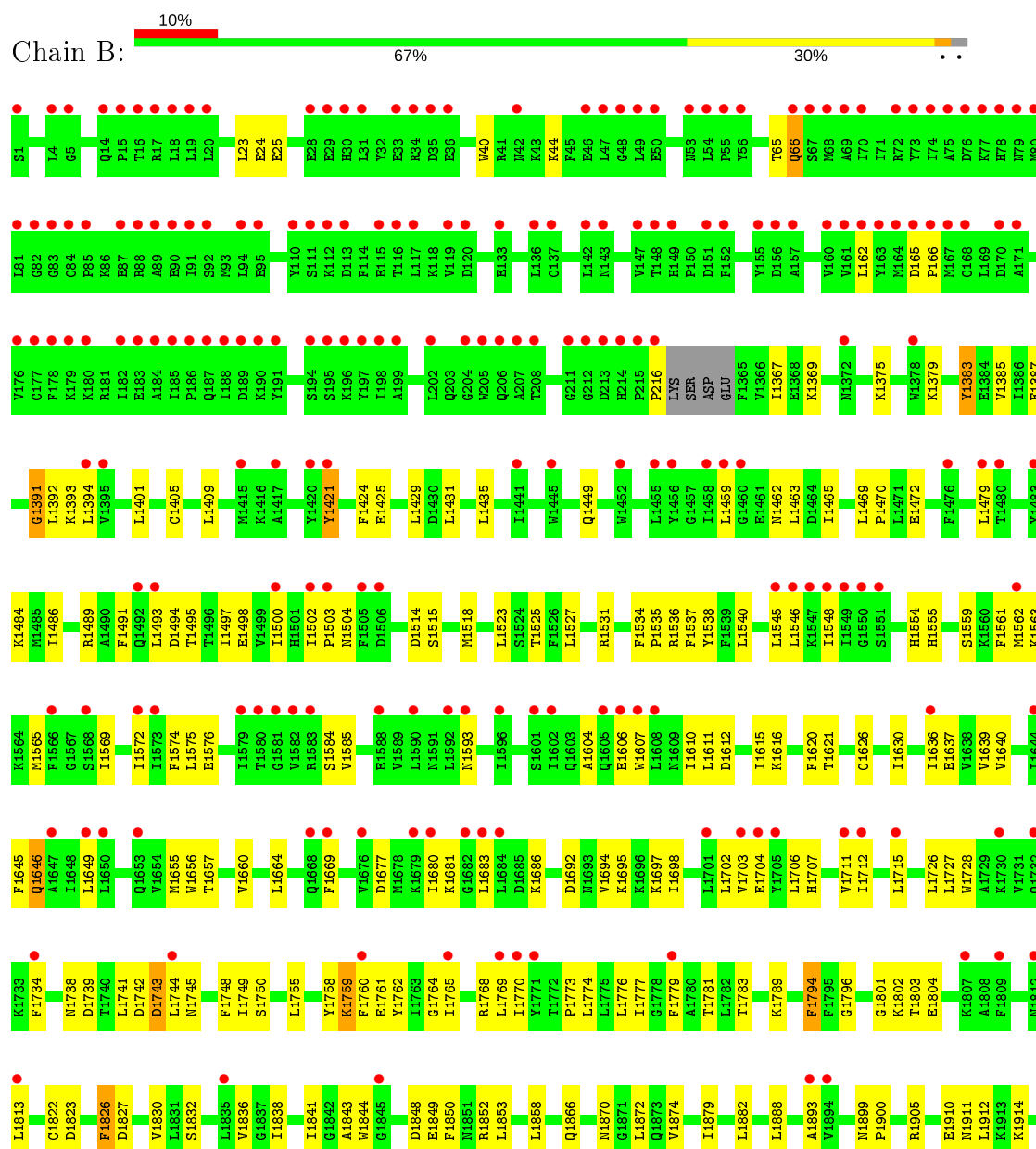
- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



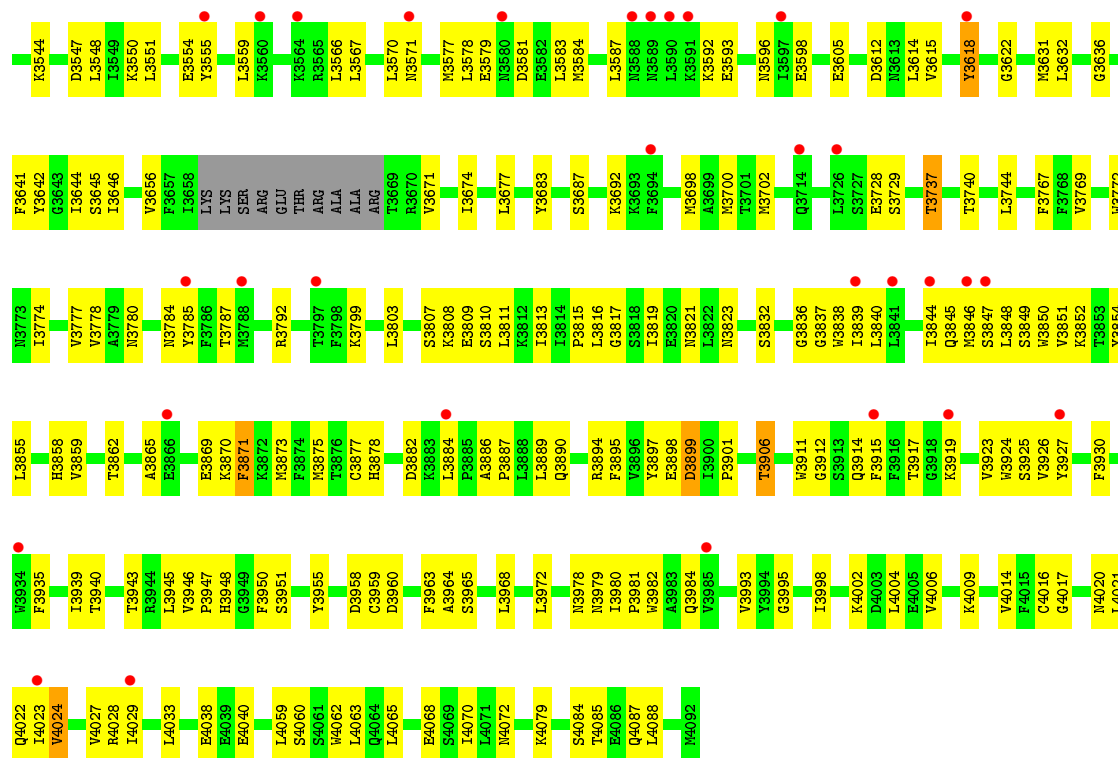




● Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



S5400	K3297	PRO	P2841	K2565	S2477	D3889	K2283	S2156	K2085	L1998	L1917
F3406	K3303	GLU	D2842	S2566	D2478	D3890	L2284	E2161	I2088	K1999	E1918
D3409	E3304	VAL	Q2845	Y2571	L2479	V2391	E2285	Y2162	I2088	R2001	F1919
K3425	K3305	LYS	Q2846	E2572	L2482	T2394	V2288	Y2169	M2091	L2003	M1921
K3426	K3306	GLU	R2747	L2573	L2483	L2395	V2289	L2169	A2092	L2002	K1922
K3427	K3307	LEU	A2748	Y2574	L2484	L2396	L2290	K2173	I2093	P2004	S1923
K3428	K3308	VAL	Y2849	Q2751	F2485	D3397	H2293	K2174	F2094	S2005	P1924
K3429	K3309	PHE	L2853	A2577	E2488	T2397	L2295	K2175	D2095	L2006	Q1925
S3430	K3310	THR	L2856	L2578	L2489	F2404	I2295	L2176	N2099	G2007	S1926
F3431	K3311	GLU	L2857	E2590	L2490	L2407	F2302	L2177	V2100	G2008	S1926
K3432	K3312	PRO	T2860	E2590	L2491	L2407	F2302	L2178	V2101	L2012	I1929
K3433	K3313	GLN	L2865	R2620	F2492	L2406	L2305	G2181	Y2102	V2013	E1933
K3434	K3314	T2960	L2866	T2623	K2493	N2409	L2306	E2182	V2103	F2014	L1934
K3435	K3315	T2961	L2867	G2760	L2494	S2410	D2307	E2183	I2104	Q1935	Q1935
K3436	K3316	R2962	L2867	A2761	D2495	K2411	D2307	E2183	D2105	F2022	I1936
K3437	K3317	D2963	E2870	R2627	K2496	R2412	L2310	E2186	T2106	D2023	M1937
K3438	K3318	A2964	E2871	Y2630	D2497	L2415	D2311	E2186	K2107	S2024	G1938
K3439	K3319	V2965	E2872	T2631	G2498	I2415	D2312	E2193	V2108	A2025	F1939
K3440	K3320	T2966	L2866	T2631	S2499	P2420	D2306	E2193	L2109	G2026	E1940
K3441	K3321	R2967	L2867	T2631	S2499	G2421	D2307	E2195	L2110	T2027	D1941
K3442	K3322	D2968	E2870	T2635	V2503	S2422	I2314	E2195	K2111	P2028	L1945
K3443	K3323	L2969	E2871	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3444	K3324	A2964	E2872	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3445	K3325	V2965	E2873	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3446	K3326	R2967	E2874	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3447	K3327	L2969	E2875	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3448	K3328	A2964	E2876	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3449	K3329	V2965	E2877	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3450	K3330	R2967	E2878	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3451	K3331	L2969	E2879	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3452	K3332	A2964	E2880	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3453	K3333	V2965	E2881	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3454	K3334	R2967	E2882	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3455	K3335	L2969	E2883	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3456	K3336	A2964	E2884	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3457	K3337	V2965	E2885	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3458	K3338	R2967	E2886	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3459	K3339	L2969	E2887	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3460	K3340	A2964	E2888	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3461	K3341	V2965	E2889	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3462	K3342	R2967	E2890	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3463	K3343	L2969	E2891	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3464	K3344	A2964	E2892	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3465	K3345	V2965	E2893	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3466	K3346	R2967	E2894	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3467	K3347	L2969	E2895	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3468	K3348	A2964	E2896	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3469	K3349	V2965	E2897	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3470	K3350	R2967	E2898	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3471	K3351	L2969	E2899	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3472	K3352	A2964	E2900	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3473	K3353	V2965	E2901	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3474	K3354	R2967	E2902	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3475	K3355	L2969	E2903	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3476	K3356	A2964	E2904	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3477	K3357	V2965	E2905	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3478	K3358	R2967	E2906	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3479	K3359	L2969	E2907	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3480	K3360	A2964	E2908	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3481	K3361	V2965	E2909	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3482	K3362	R2967	E2910	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3483	K3363	L2969	E2911	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3484	K3364	A2964	E2912	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3485	K3365	V2965	E2913	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3486	K3366	R2967	E2914	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3487	K3367	L2969	E2915	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3488	K3368	A2964	E2916	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3489	K3369	V2965	E2917	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3490	K3370	R2967	E2918	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3491	K3371	L2969	E2919	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3492	K3372	A2964	E2920	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3493	K3373	V2965	E2921	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3494	K3374	R2967	E2922	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3495	K3375	L2969	E2923	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3496	K3376	A2964	E2924	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3497	K3377	V2965	E2925	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3498	K3378	R2967	E2926	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3499	K3379	L2969	E2927	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3500	K3380	A2964	E2928	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3501	K3381	V2965	E2929	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3502	K3382	R2967	E2930	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3503	K3383	L2969	E2931	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3504	K3384	A2964	E2932	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3505	K3385	V2965	E2933	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3506	K3386	R2967	E2934	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3507	K3387	L2969	E2935	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3508	K3388	A2964	E2936	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3509	K3389	V2965	E2937	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3510	K3390	R2967	E2938	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3511	K3391	L2969	E2939	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3512	K3392	A2964	E2940	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3513	K3393	V2965	E2941	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3514	K3394	R2967	E2942	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3515	K3395	L2969	E2943	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3516	K3396	A2964	E2944	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3517	K3397	V2965	E2945	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3518	K3398	R2967	E2946	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3519	K3399	L2969	E2947	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3520	K3400	A2964	E2948	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3521	K3401	V2965	E2949	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3522	K3402	R2967	E2950	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3523	K3403	L2969	E2951	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3524	K3404	A2964	E2952	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3525	K3405	V2965	E2953	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3526	K3406	R2967	E2954	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3527	K3407	L2969	E2955	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3528	K3408	A2964	E2956	T2635	V2503	S2422	I2314	E2195	E2112	K2032	L1945
K3529	K3409	V2965	E2957	T2635	V2503	S2422	I23				



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	175.56Å 118.13Å 201.02Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 70.46 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.60) 99.2 (70.46-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.302 0.236 , 0.300	Depositor DCC
R_{free} test set	4767 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	127.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41642	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, ANP, SO4, 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	0.53	0/21146	0.77	7/28618 (0.0%)
1	B	0.46	2/21146 (0.0%)	0.68	5/28618 (0.0%)
All	All	0.49	2/42292 (0.0%)	0.73	12/57236 (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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3306	TRP	CE3-CZ3	-6.25	1.27	1.38
1	B	3306	TRP	CE2-CZ2	-5.22	1.30	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2012	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	1741	LEU	CB-CG-CD1	6.69	122.38	111.00
1	A	3792	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	1782	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	2460	ARG	NE-CZ-NH2	-5.52	117.54	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2119	LEU	Peptide
1	B	2620	ARG	Sidechain

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	952	0
1	B	20748	0	20206	909	0
2	A	31	0	12	8	0
2	B	31	0	12	17	0
3	A	31	0	13	7	0
3	B	31	0	13	7	0
4	A	10	0	0	3	0
4	B	10	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41642	0	40462	1861	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 1861 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:CB	1:A:1365:PHE:CE1	2.05	1.38
1:B:3303:LYS:HD2	1:B:3306:TRP:CD1	1.67	1.28
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.25
1:A:1368:GLU:HG2	1:A:1424:PHE:CZ	1.69	1.24
1:B:2467:THR:HB	1:B:2473:LEU:CD1	1.66	1.23

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%)	2518 (95%)	110 (4%)	12 (0%)	29	68
1	B	2640/2695 (98%)	2515 (95%)	111 (4%)	14 (0%)	29	68
All	All	5280/5390 (98%)	5033 (95%)	221 (4%)	26 (0%)	29	68

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	1391	GLY
1	B	3578	LEU
1	A	24	GLU
1	A	1633	GLY

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%)	2138 (96%)	80 (4%)	35	67
1	B	2218/2453 (90%)	2137 (96%)	81 (4%)	34	66
All	All	4436/4906 (90%)	4275 (96%)	161 (4%)	35	67

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3940	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1826	PHE
1	B	3899	ASP
1	A	3958	ASP
1	B	1421	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3962	GLN
1	B	1736	GLN
1	B	3783	ASN
1	A	3970	ASN
1	B	1501	HIS

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 monosaccharides 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	5	26,33,33	1.01	1 (3%)	31,52,52	1.65	5 (16%)
2	ATP	B	5093	5	26,33,33	1.02	2 (7%)	31,52,52	1.65	5 (16%)
4	SO4	B	5095	-	4,4,4	0.33	0	6,6,6	0.46	0
4	SO4	A	5095	-	4,4,4	0.52	0	6,6,6	0.69	0
3	ANP	A	5094	-	29,33,33	2.43	5 (17%)	31,52,52	1.56	7 (22%)
3	ANP	B	5094	-	29,33,33	2.48	5 (17%)	31,52,52	1.52	4 (12%)
4	SO4	A	5096	-	4,4,4	0.45	0	6,6,6	0.24	0
4	SO4	B	5096	-	4,4,4	0.35	0	6,6,6	0.20	0

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	ANP	A	5094	-	-	8/14/38/38	0/3/3/3
3	ANP	B	5094	-	-	6/14/38/38	0/3/3/3
2	ATP	B	5093	5	-	7/18/38/38	0/3/3/3
2	ATP	A	5093	5	-	5/18/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5094	ANP	PG-O1G	9.66	1.61	1.46
3	A	5094	ANP	PG-O1G	9.47	1.61	1.46
3	B	5094	ANP	PG-N3B	4.66	1.75	1.63
3	A	5094	ANP	PG-N3B	4.66	1.75	1.63
3	B	5094	ANP	PB-N3B	4.60	1.75	1.63

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5093	ATP	C3'-C2'-C1'	3.97	106.96	100.98
2	B	5093	ATP	C3'-C2'-C1'	3.77	106.65	100.98
2	B	5093	ATP	PB-O3B-PG	-3.71	120.08	132.83
2	B	5093	ATP	PA-O3A-PB	-3.69	120.16	132.83
2	A	5093	ATP	PB-O3B-PG	-3.60	120.49	132.83

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

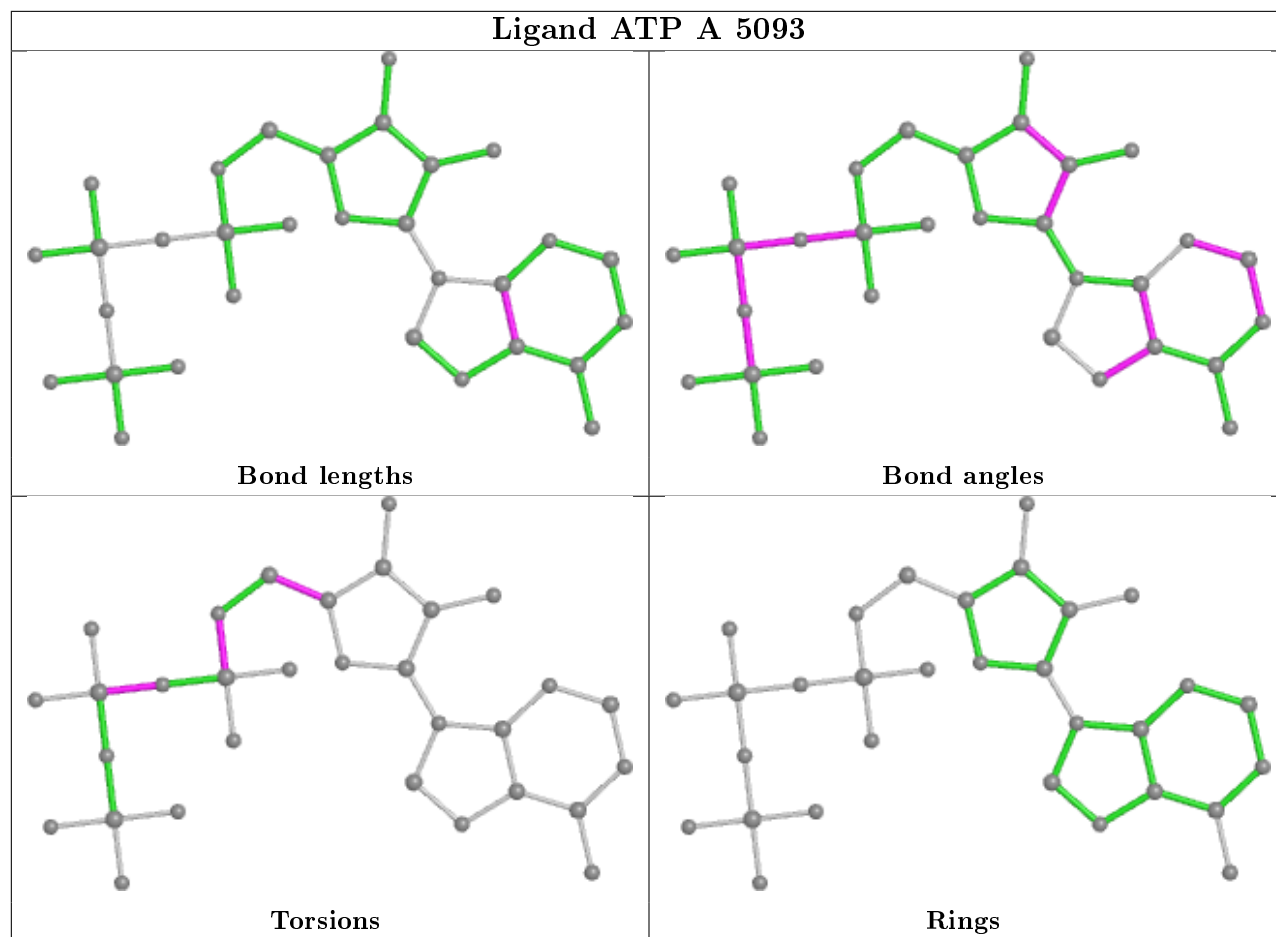
Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	C5'-O5'-PA-O1A
3	A	5094	ANP	PB-N3B-PG-O1G
3	A	5094	ANP	C5'-O5'-PA-O2A
3	B	5094	ANP	PB-N3B-PG-O1G
3	B	5094	ANP	C5'-O5'-PA-O1A

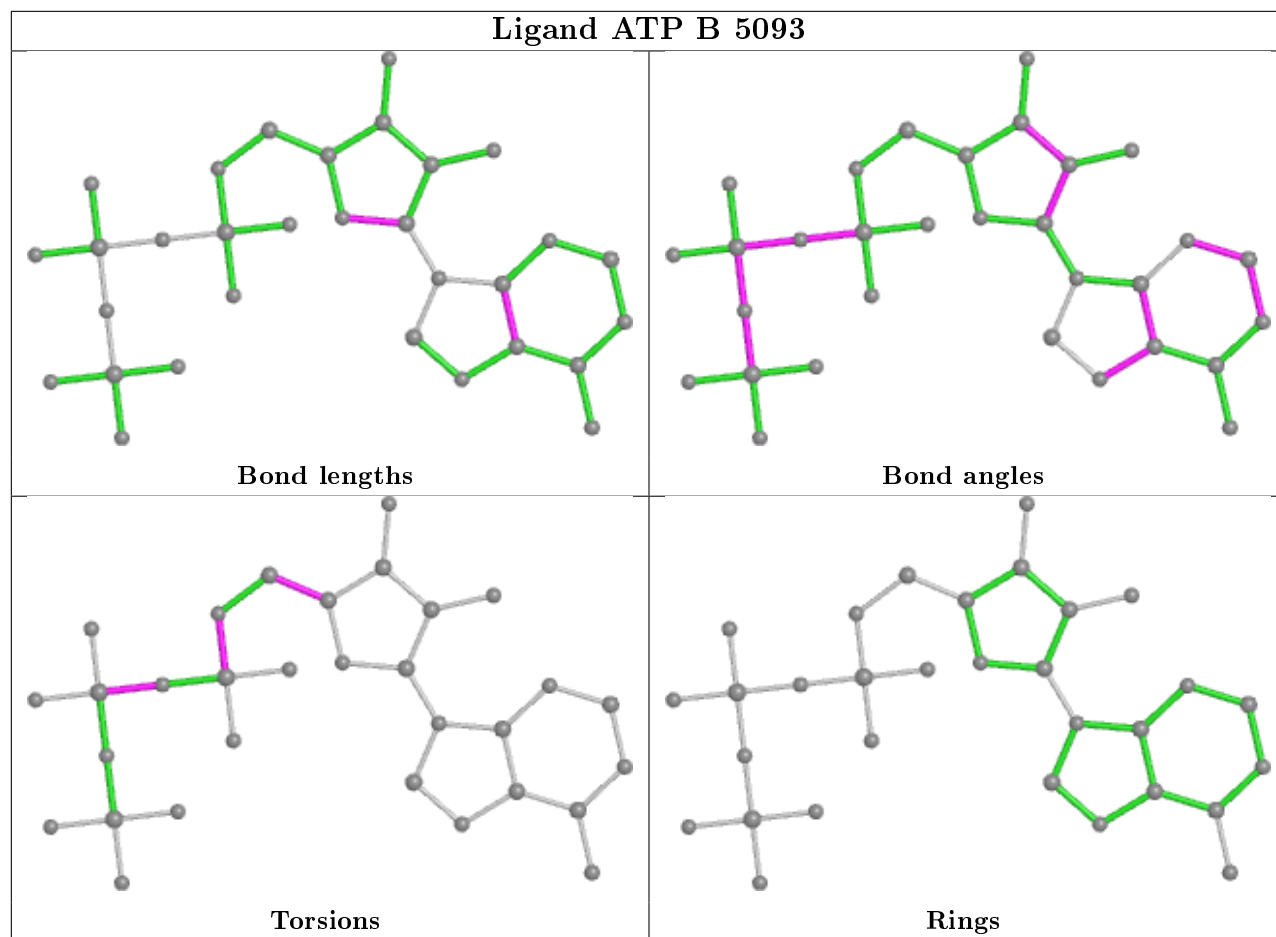
There are no ring outliers.

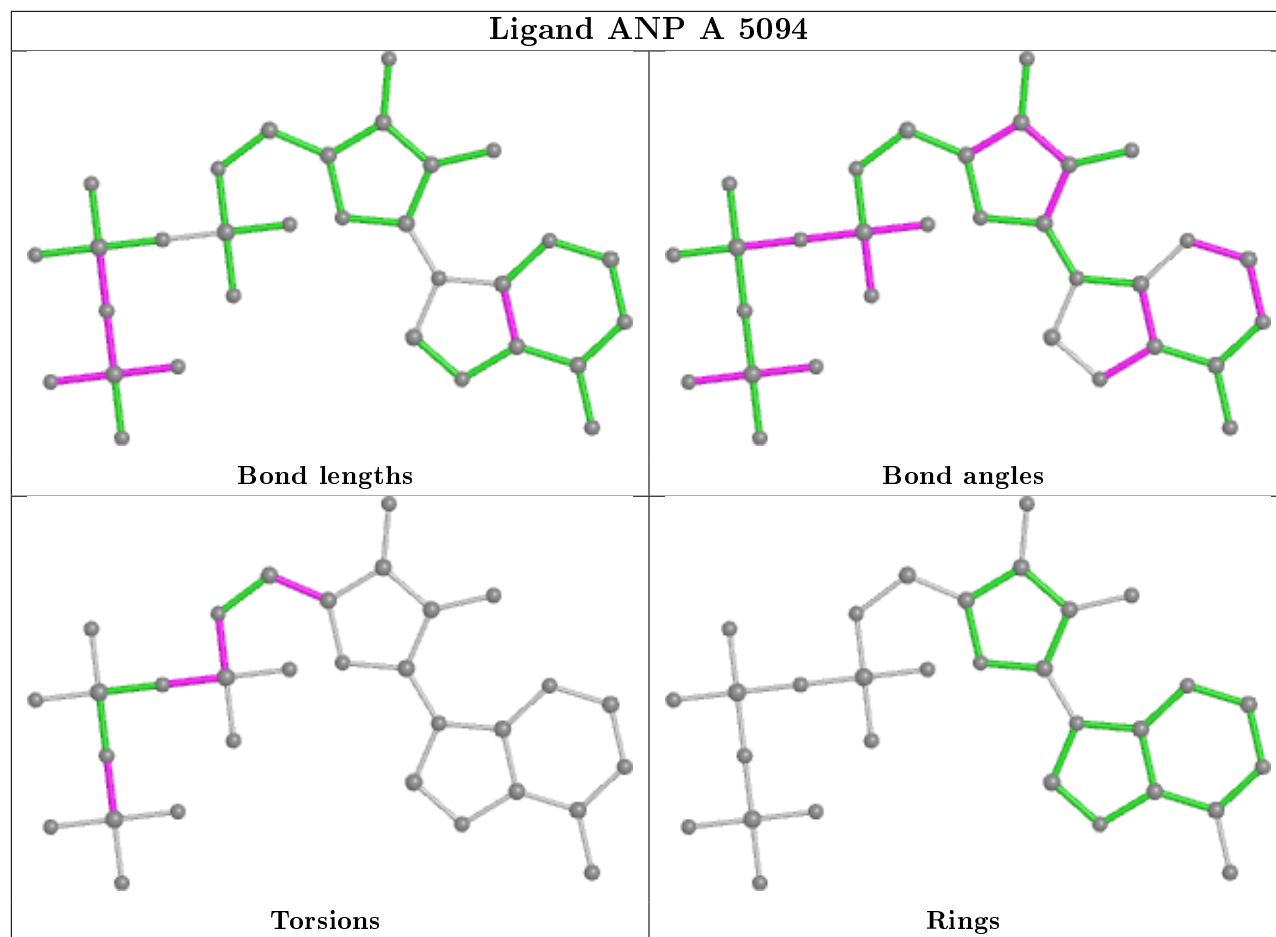
6 monomers are involved in 45 short contacts:

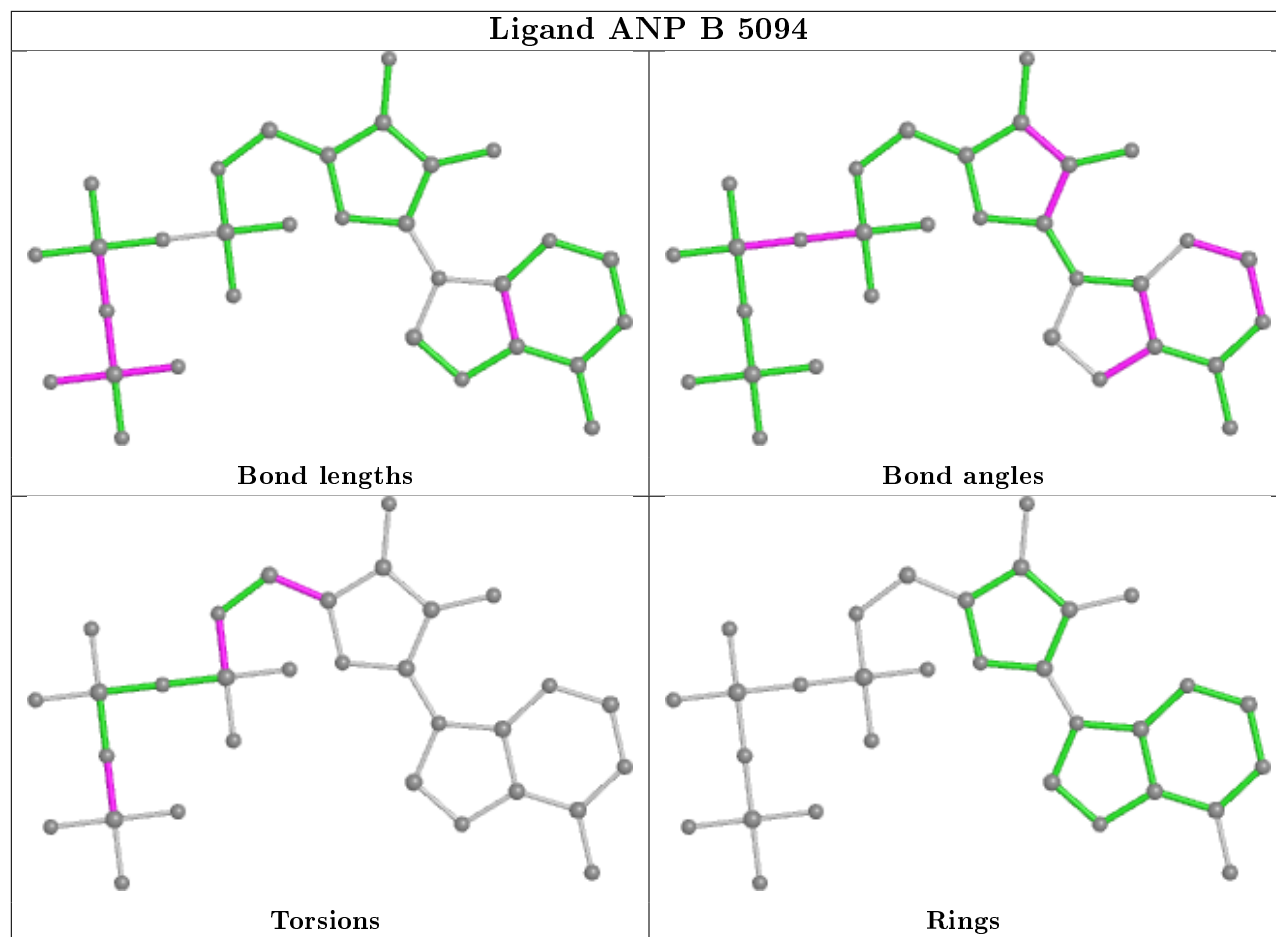
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	8	0
2	B	5093	ATP	17	0
4	A	5095	SO4	3	0
3	A	5094	ANP	7	0
3	B	5094	ANP	7	0
4	B	5096	SO4	3	0

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%)	0.11	69 (2%) 56 40	69, 151, 281, 423	0
1	B	2650/2695 (98%)	0.64	277 (10%) 6 3	92, 193, 357, 500	0
All	All	5300/5390 (98%)	0.37	346 (6%) 18 11	69, 172, 321, 500	0

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	24.7
1	B	164	MET	22.6
1	B	213	ASP	20.8
1	B	29	GLU	19.9
1	B	163	TYR	19.7

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](#)

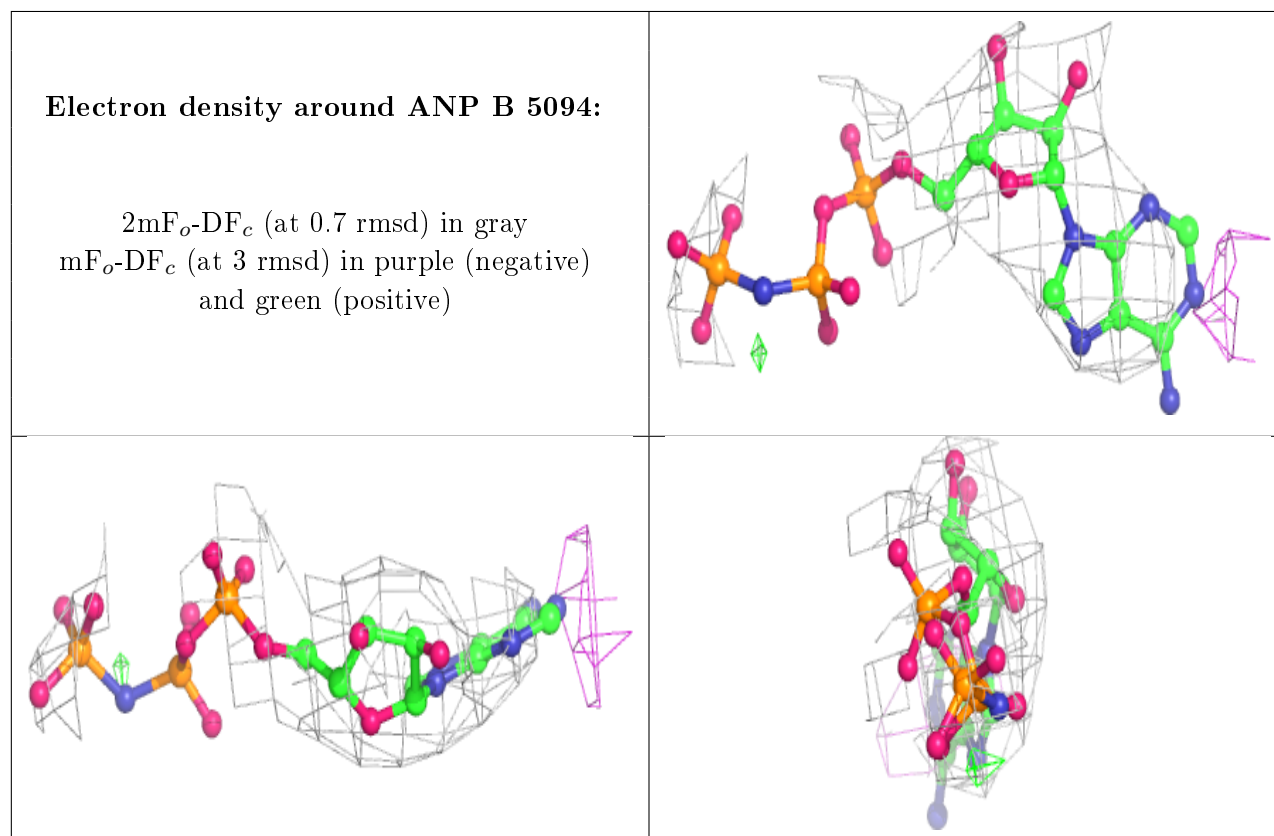
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

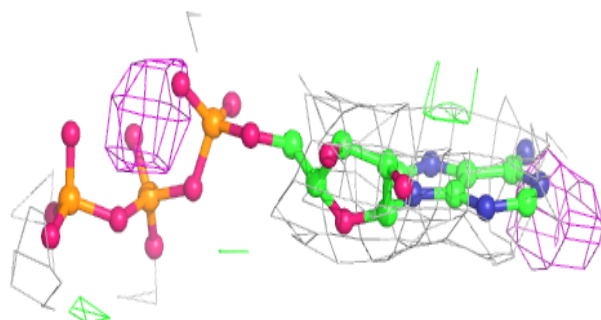
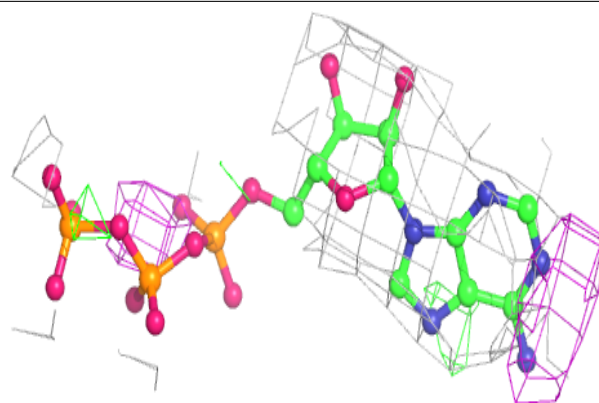
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	5095	5/5	0.84	0.18	152,154,166,167	0
3	ANP	B	5094	31/31	0.89	0.29	112,145,237,257	0
2	ATP	B	5093	31/31	0.92	0.24	99,141,184,200	0
3	ANP	A	5094	31/31	0.94	0.27	111,140,238,248	0
2	ATP	A	5093	31/31	0.95	0.29	88,123,185,204	0
4	SO4	B	5096	5/5	0.95	0.14	155,168,174,176	0
4	SO4	A	5096	5/5	0.96	0.20	115,130,143,145	0
4	SO4	A	5095	5/5	0.96	0.25	84,98,104,105	0
5	MG	B	5097	1/1	0.97	0.18	66,66,66,66	0
5	MG	A	5097	1/1	0.99	0.22	62,62,62,62	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.

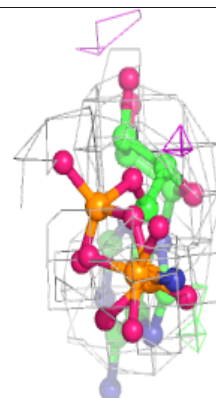
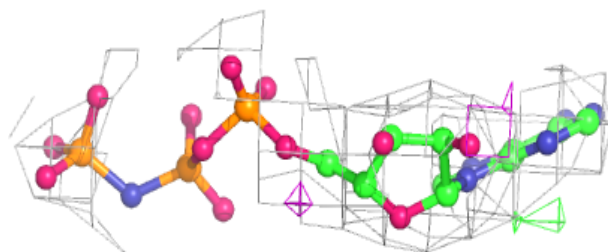
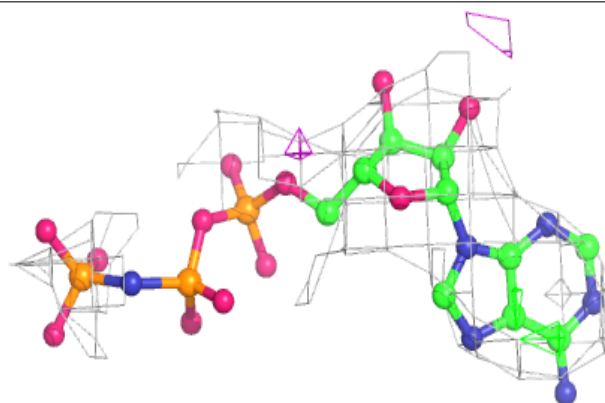


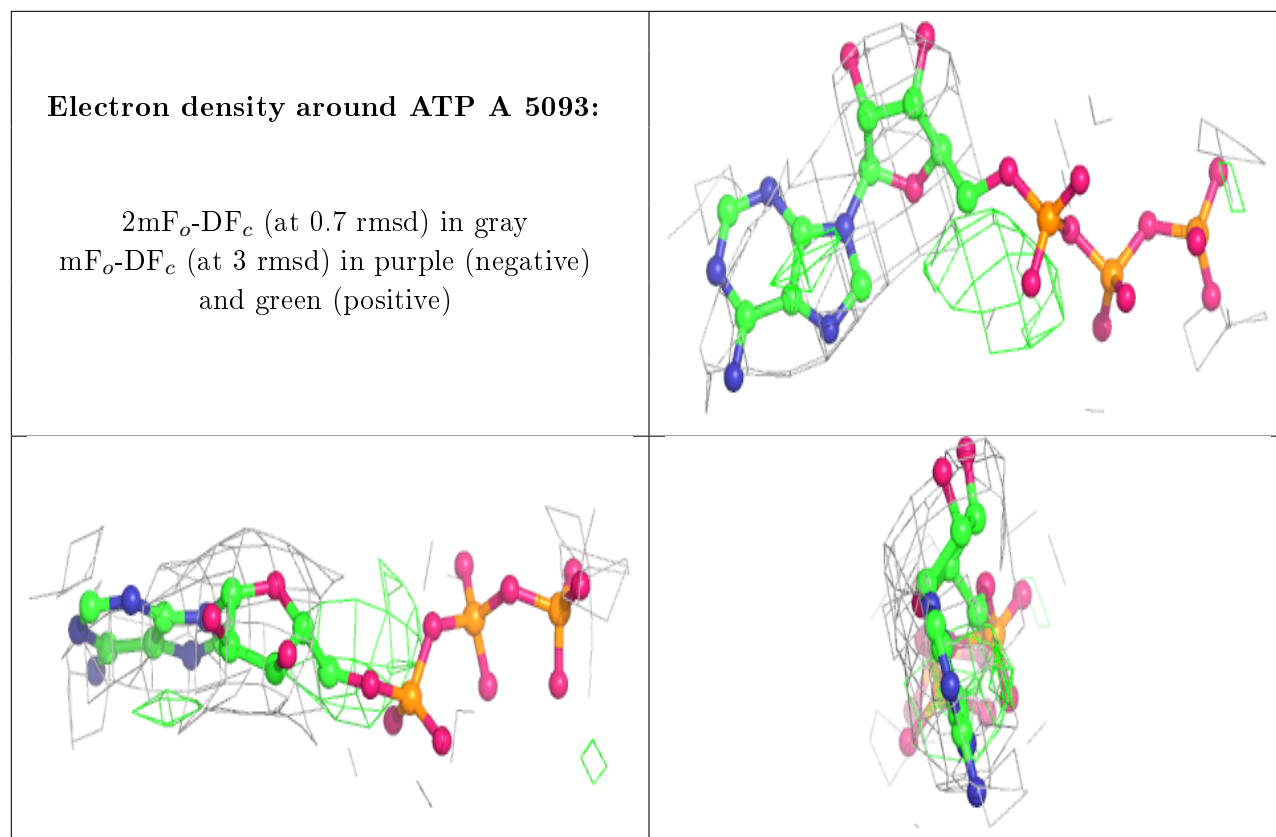
Electron density around ATP B 5093:

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

**Electron density around ANP 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.