wwPDB X-ray Structure Validation Summary Report (i)

Apr 27, 2024 – 10:06 pm BST

PDB ID	:	4AI6
Title	:	Dynein Motor Domain - ADP complex
Authors	:	Schmidt, H.; Gleave, E.S.; Carter, A.P.
Deposited on	:	2012-02-08
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

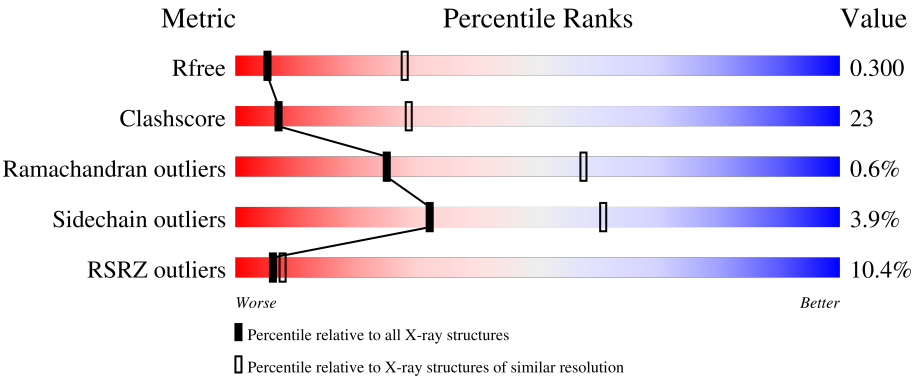
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	11% 66% 31%
1	B	2695	9% 67% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	B	5400	-	-	X	-
3	ADP	A	5401	-	-	X	-
3	ADP	A	5402	-	-	X	-
3	ADP	B	5402	-	-	X	-
4	SO4	A	5403	-	-	X	-
4	SO4	B	5403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41678 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

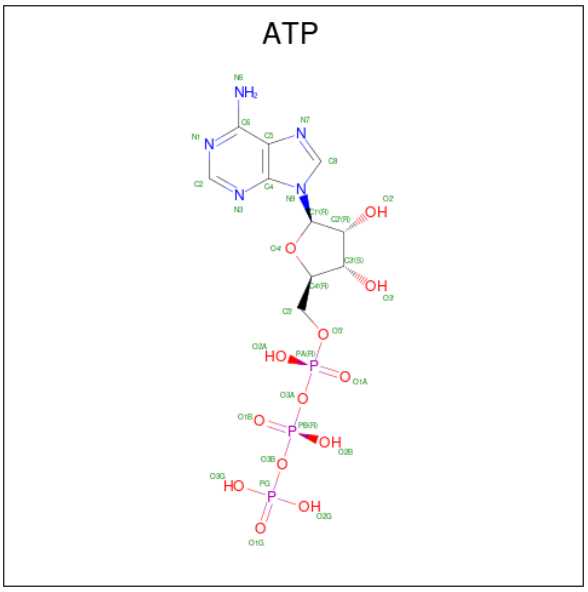
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 10 discrepancies between the modelled and reference sequences:

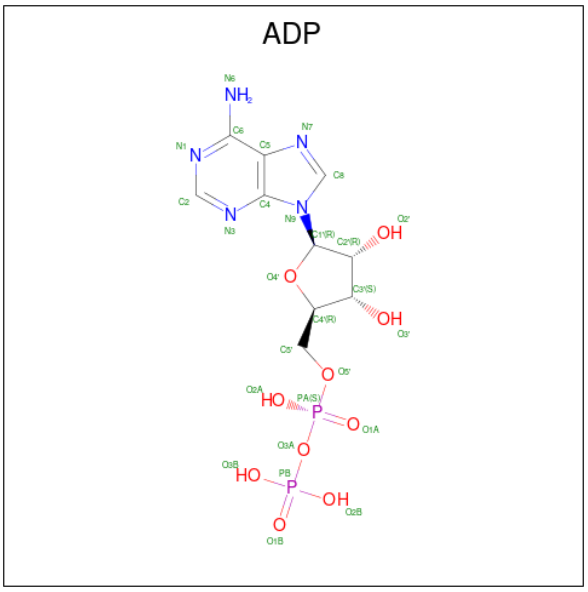
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	linker	UNP P36022
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	217	LYS	-	linker	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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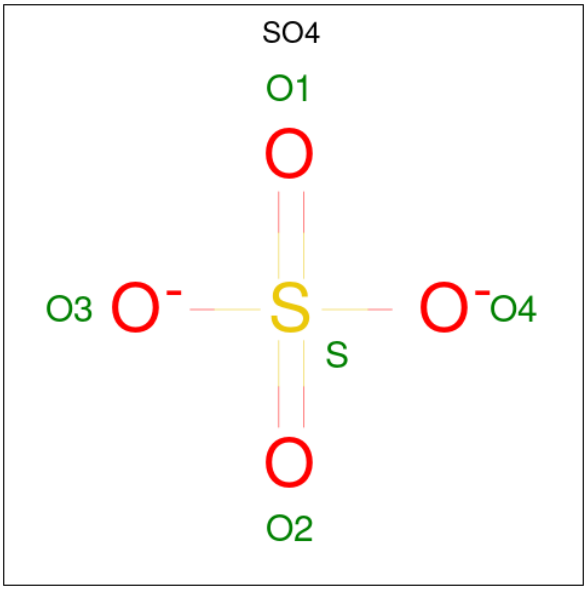
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

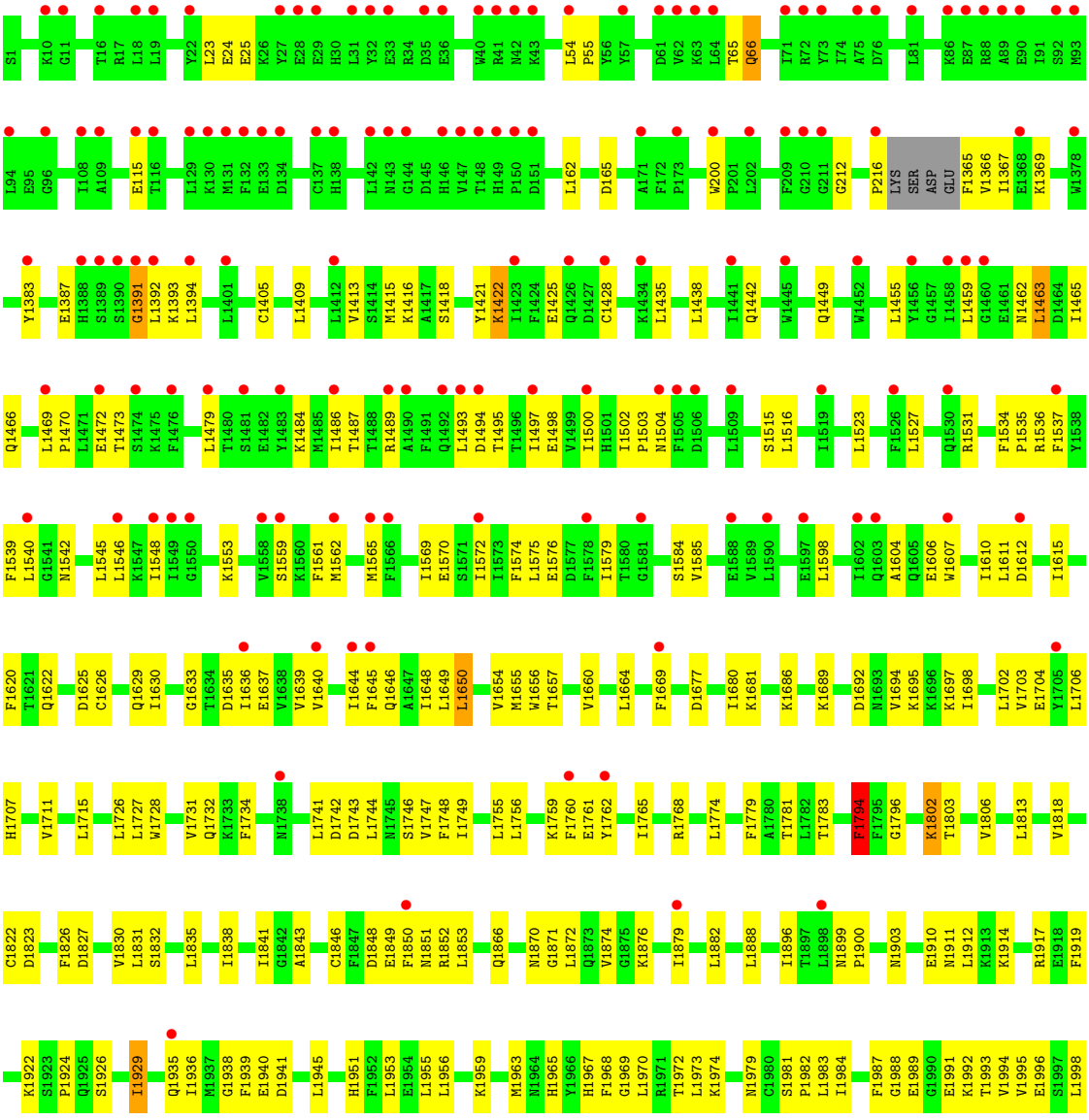
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0

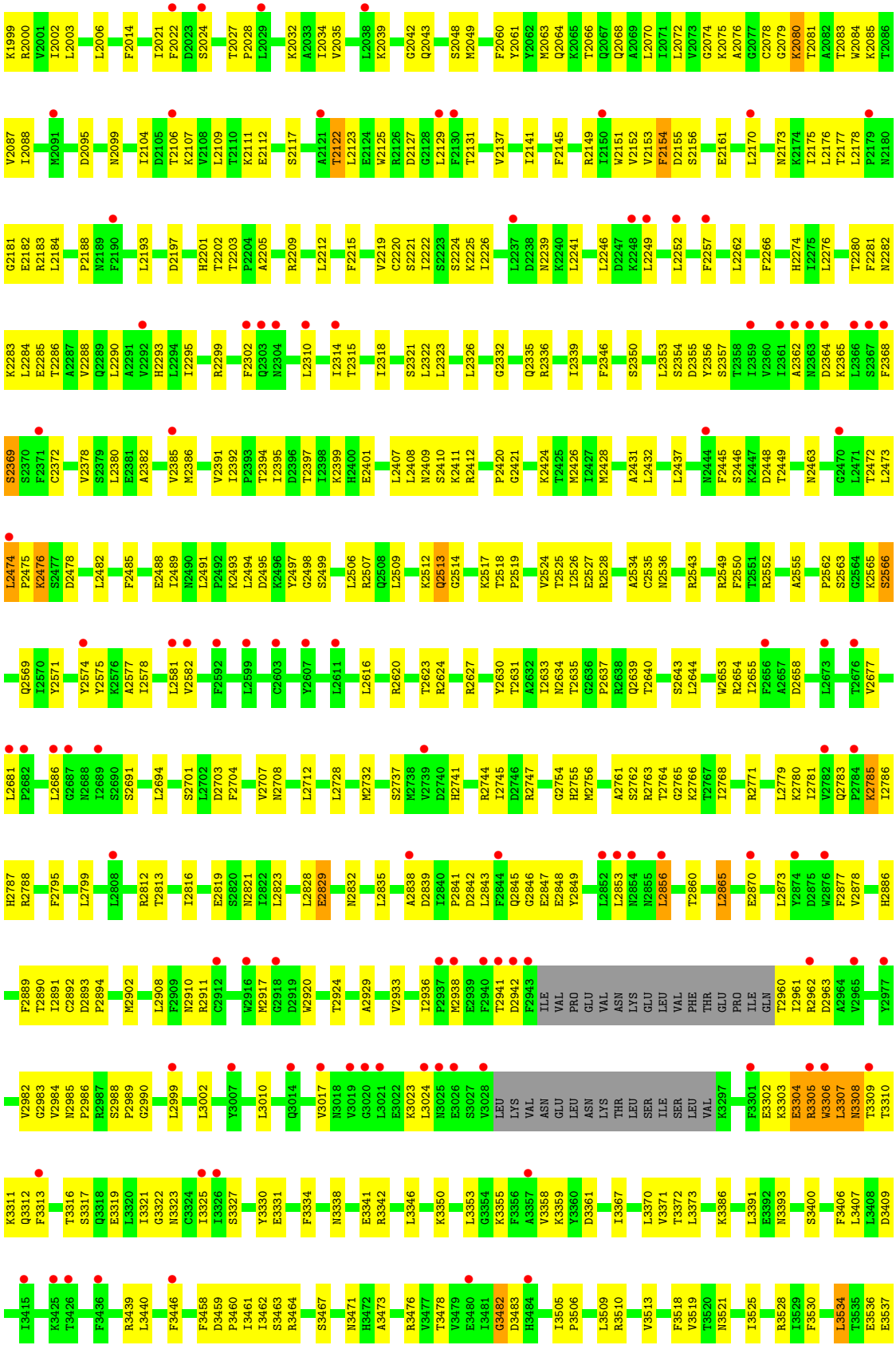
3 Residue-property plots (i)

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

Chain A:

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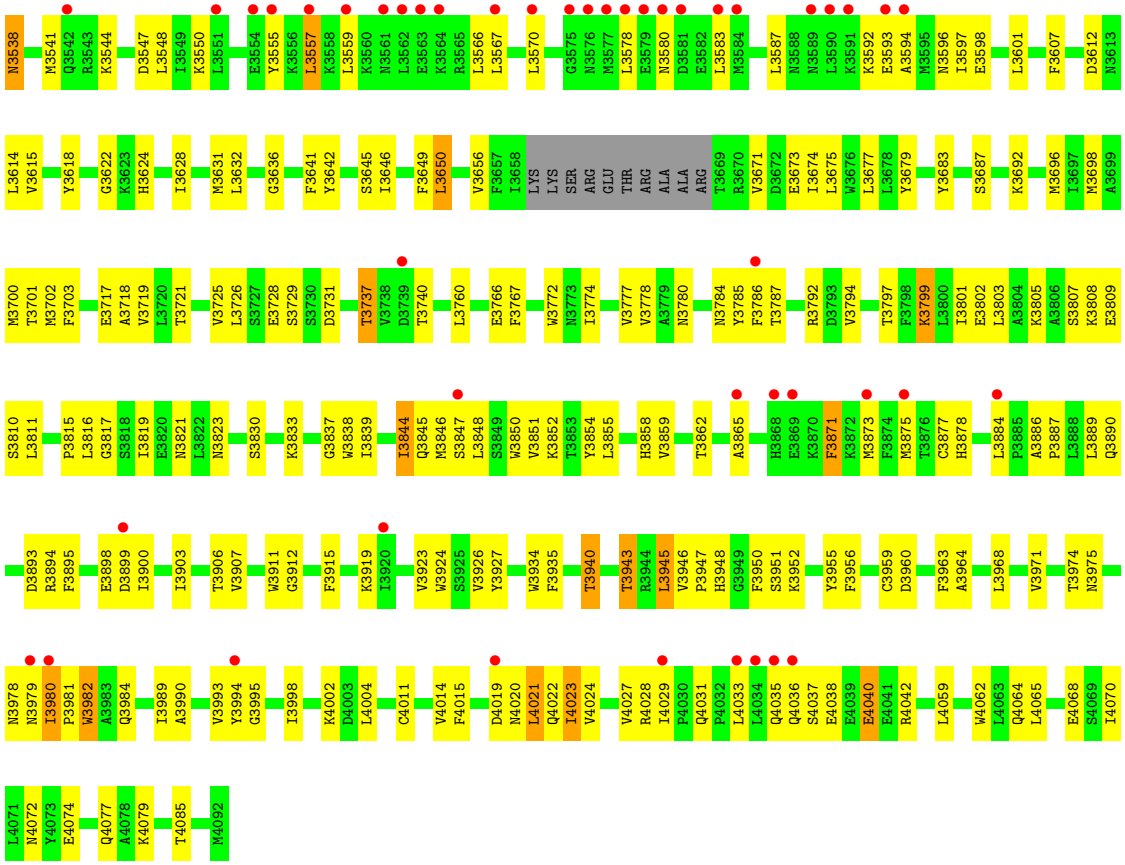
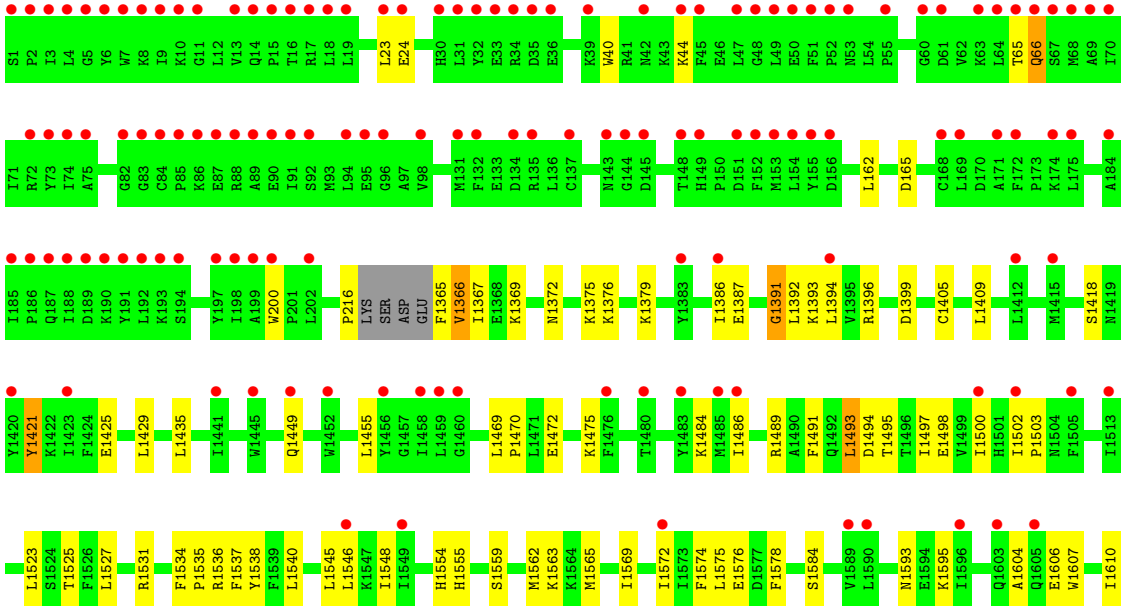
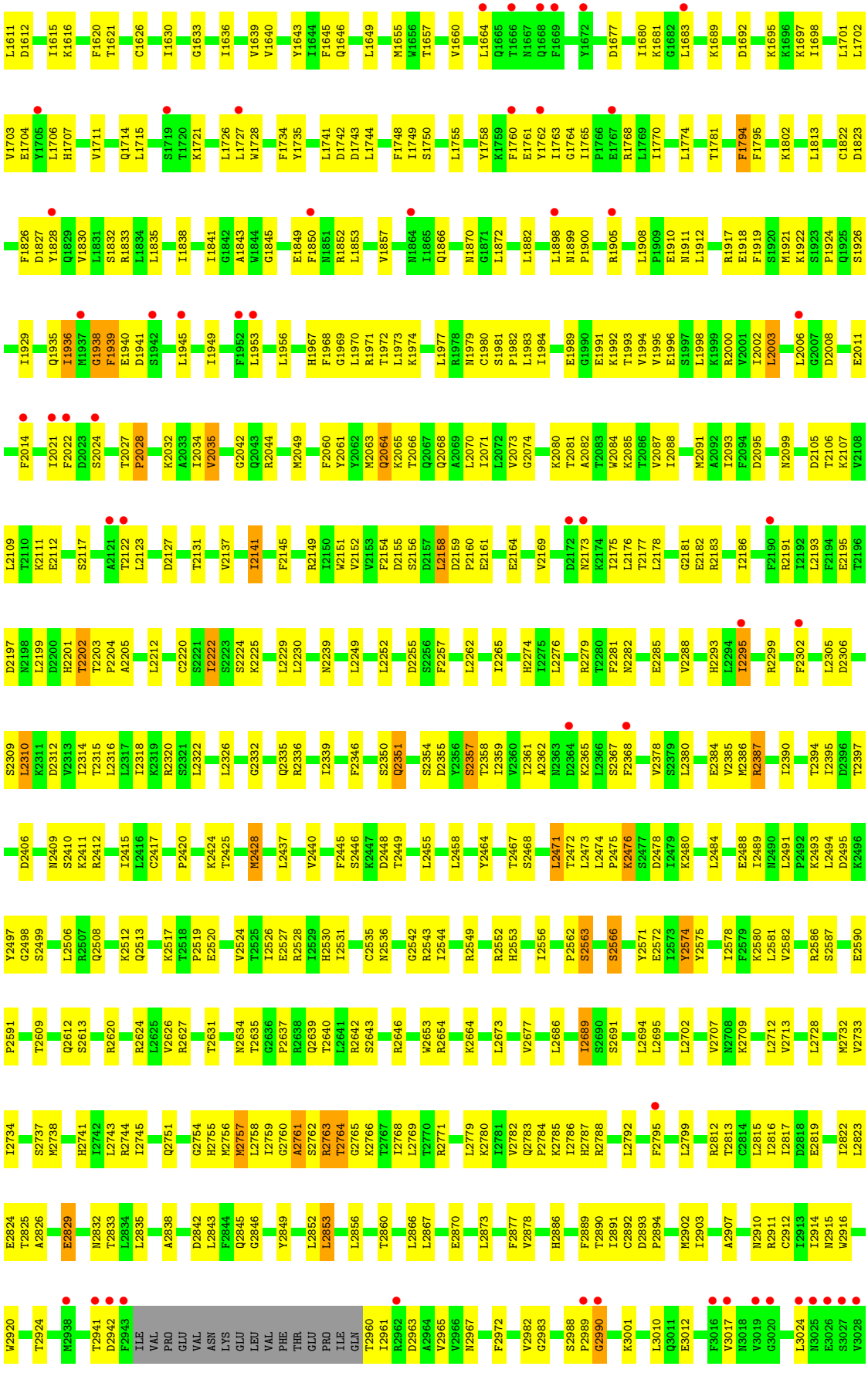
V2087 I2088 M2091 D2095 N2099 I2104 D2105 T2106 K2107 V2108 L2109 T2110 K2111 E2112 S2117 A2121 T2122 L2123 E2124 W2125 R2126 D2127 G2128 L2129 F2130 T2131 V2137 I2141 F2145 R2149 I2150 W2151 V2152 V2153 F2154 D2155 S2156 E2161 L2170 N2173 K2174 I2175 L2176 T2177 L2178 P2179 N2180
G2181 E2182 R2183 L2184 P2188 N2189 F2190 L2193 D2197 H2201 T2202 T2203 P2204 A2205 R2209 L2212 F2215 V2219 C2220 S2221 I2222 S2223 S2224 K2225 I2226 L2237 D2238 N2239 K2240 L2241 L2246 D2247 K2248 L2249 L2252 F2257 L2262 F2266 H2274 T2275 L2276 T2280 F2281 N2282
K2283 L2284 E2285 T2286 A2287 V2288 Q2289 L2290 A2291 V2292 H2293 L2294 I2295 R2299 F2302 Q2303 N2304 L2310 I2314 T2315 I2318 S2321 I2322 L2323 L2326 G2332 Q2335 R2336 I2339 F2346 S2350 L2353 S2354 D2355 Y2356 S2357 T2358 I2359 V2360 I2361 A2362 N2363 D2364 K2365 L2366 S2367 F2368
S2369 S2370 F2371 C2372 V2378 S2379 L2380 E2381 A2382 V2385 M2386 Y2391 I2392 P2393 T2394 I2395 D2396 T2397 I2398 K2399 H2400 E2401 L2407 L2408 N2409 S2410 K2411 R2412 P2420 G2421 K2424 T2425 M2426 I2427 M2428 A2431 L2432 L2437 N2444 F2445 S2446 K2447 D2448 T2449 N2463 G2470 L2471 T2472 L2473
L2474 P2475 K2476 S2477 D2478 L2482 F2485 E2488 I2489 N2490 L2491 P2492 K2493 L2494 D2495 K2496 Y2497 G2498 S2499 L2506 R2507 Q2508 L2509 K2512 Q2513 G2514 K2517 T2518 P2519 V2524 T2525 I2526 E2527 R2528 A2534 C2535 N2536 R2543 R2549 F2550 T2551 R2552 A2555 P2562 S2563 G2564 K2565 S2566
Q2569 I2570 Y2571 Y2574 Y2575 K2576 A2577 I2578 L2581 V2582 F2592 L2599 C2603 Y2607 L2611 L2616 R2620 T2623 R2624 R2627 Y2630 T2631 A2632 I2633 N2634 T2635 G2636 P2637 R2638 Q2639 T2640 S2643 L2644 W2653 R2654 I2655 F2656 A2657 D2658 L2673 T2676 V2677
L2681 P2682 L2686 G2687 N2688 I2689 S2690 S2691 L2694 S2701 L2702 D2703 F2704 V2707 N2708 L2712 L2728 M2732 S2737 M2738 V2739 D2740 H2741 R2744 I2745 D2746 R2747 G2754 H2755 M2756 A2761 S2762 R2763 T2764 G2765 K2766 T2767 I2768 R2771 L2779 K2780 I2781 V2782 Q2783 P2784 K2785 I2786
H2787 R2788 F2795 L2799 L2808 R2812 T2813 I2816 E2819 S2820 N2821 I2822 L2823 L2828 E2829 N2832 L2835 A2838 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 E2847 E2848 Y2849 L2852 L2853 W2854 N2855 L2856 T2860 L2865 E2870 L2873 Y2874 D2875 W2876 F2877 V2878 H2886
F2889 T2890 I2891 C2892 D2893 P2894 M2902 L2908 F2909 N2910 R2911 C2912 W2916 M2917 G2918 D2919 W2920 T2924 A2929 V2933 I2936 P2937 M2938 E2939 F2940 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 A2964 V2965 Y2977
V2982 G2983 V2984 N2985 P2986 R2987 S2988 P2989 G2990 L2999 L3002 Y3007 L3010 Q3014 V3017 N3018 V3019 G3020 L3021 E3022 K3023 L3024 N3025 E3026 S3027 V3028 LEU LYS VAL ASN GLU LEU ASN LYS THR LEU SER ILE SER LEU VAL K3297 E3301 E3302 K3303 E3304 R3305 W3306 L3307 N3308 T3309 T3310
K3311 Q3312 F3313 T3316 S3317 Q3318 E3319 L3320 I3321 G3322 N3323 C3324 I3325 I3326 S3327 Y3330 E3331 F3334 N3338 E3341 R3342 L3346 K3350 L3353 G3354 K3355 F3356 A3357 V3358 K3359 Y3360 D3361 I3367 L3370 V3371 T3372 L3373 K3386 L3391 E3392 N3393 S3400 F3406 L3407 L3408 D3409
I3415 K3425 T3426 F3436 R3439 L3440 F3446 F3458 D3459 P3460 I3461 I3462 S3463 R3464 S3467 N3471 H3472 A3473 R3476 V3477 T3478 V3479 E3480 I3481 G3482 D3483 H3484 I3505 P3506 L3509 R3510 V3513 F3518 V3519 T3520 N3521 I3525 R3528 I3529 F3530 L3534 T3535 E3536 E3537



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

Chain B:

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V1703 E1704 Y1705 L1706 H1707 V1711 Q1714 L1715 S1719 T1720 K1721 L1726 L1727 W1728 F1734 Y1735 L1741 D1742 D1743 L1744 F1748 I1749 S1750 L1755 Y1758 K1759 F1760 E1761 Y1762 I1763 G1764 I1765 P1766 E1767 R1768 L1769 I1770 L1774 T1781 F1794 F1795 K1802 L1813 C1822 D1823
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I1929 Q1935 I1936 M1937 G1938 F1939 E1940 D1941 S1942 L1945 I1949 F1952 L1953 L1956 H1967 F1968 G1969 L1970 R1971 T1972 L1973 K1974 L1977 R1978 N1979 C1980 S1981 P1982 L1983 I1984 E1989 G1990 E1991 K1992 T1993 V1994 V1995 E1996 S1997 L1998 K1999 R2000 V2001 I2002 L2003 L2006 G2007 D2008 E2011
F2014 I2021 F2022 D2023 S2024 T2027 P2028 K2032 A2033 I2034 V2035 G2042 Q2043 R2044 M2049 H2060 Y2061 Y2062 M2063 Q2064 K2065 T2066 Q2067 Q2068 A2069 L2070 I2071 L2072 V2073 G2074 K2080 T2081 A2082 T2083 W2084 K2085 T2086 V2087 I2088 M2091 A2092 I2093 F2094 D2095 N2099 D2105 T2106 K2107 V2108
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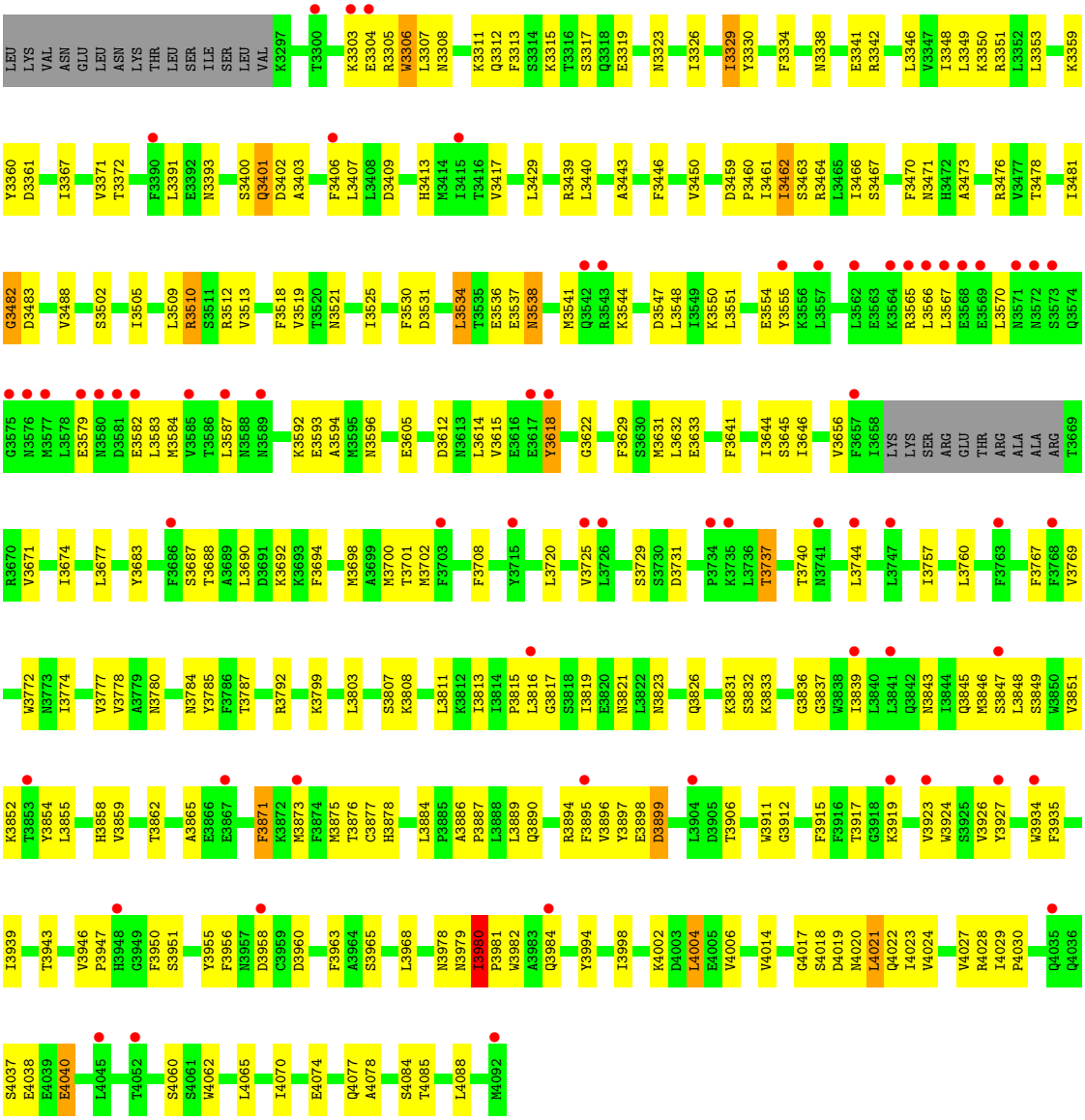
E2824 T2825 A2826 E2829 N2832 T2833 L2834 L2835 A2838 D2842 L2843 F2844 Q2845 G2846 Y2849 L2852 L2853 L2856 T2860 L2866 L2867 E2870 L2873 F2877 V2878 H2886 F2889 T2890 I2891 C2892 D2893 P2894 M2902 I2903 A2907 N2910 R2911 C2912 I2913 I2914 N2915 W2916
W2920 T2924 M2938 T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 A2964 V2965 V2966 N2967 F2972 V2982 G2983 S2988 P2989 G2990 K3001 L3010 Q3011 E3012 F3016 V3017 N3018 V3019 G3020 L3024 N3025 E3026 S3027 V3028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G3482 D3483 V3488 S3502 I3505 L3509 R3510 S3511 R3512 V3513 F3518 V3519 T3520 N3521 I3525 F3530 D3531 L3534 T3535 E3536 E3537 N3538 M3541 Q3542 R3543 K3544 D3547 L3548 I3549 K3550 L3551 E3554 Y3555 K3556 L3557 L3562 E3563 K3564 R3565 L3566 L3567 E3568 E3569 L3570 N3571 N3572 S3573 Q3574
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R3670 V3671 I3674 L3677 Y3683 F3686 S3687 T3688 A3689 L3690 D3691 K3692 K3693 F3694 M3698 A3699 M3700 T3701 M3702 F3703 F3708 Y3715 L3720 V3725 L3726 S3729 S3730 D3731 P3734 K3735 L3736 T3737 T3740 N3741 L3744 L3747 I3757 L3760 F3763 F3767 F3768 V3769
W3772 N3773 I3774 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 R3792 K3799 L3803 S3807 K3808 L3811 K3812 I3813 I3814 P3815 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823 Q3826 K3831 S3832 K3833 G3836 G3837 W3838 I3839 L3840 L3841 Q3842 N3843 I3844 Q3845 M3846 S3847 L3848 S3849 W3850 V3851
K3852 T3853 Y3854 L3855 H3858 V3859 T3862 A3865 E3866 E3867 F3871 K3872 M3873 F3874 M3875 T3876 C3877 H3878 L3884 P3885 A3886 P3887 L3888 L3889 Q3890 R3894 F3895 V3896 Y3897 E3898 D3899 L3904 D3905 T3906 W3911 G3912 F3915 F3916 T3917 G3918 K3919 V3923 W3924 S3925 V3926 Y3927 W3934 F3935
I3939 T3943 V3946 P3947 H3948 G3949 F3950 S3951 Y3955 F3956 N3957 D3958 C3959 D3960 F3963 A3964 S3965 L3968 N3978 N3979 I3980 P3981 W3982 A3983 Q3984 Y3994 I3998 K4002 D4003 L4004 E4005 V4006 V4014 G4017 S4018 D4019 N4020 L4021 Q4022 I4023 V4024 V4027 R4028 I4029 P4030 Q4035 Q4036
S4037 E4038 E4039 E4040 L4045 T4052 S4060 S4061 W4062 L4065 I4070 E4074 Q4077 A4078 S4084 T4085 L4088 N4092

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	174.89Å 119.17Å 193.97Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	49.29 – 3.40 49.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-3.40) 99.9 (49.24-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.241 , 0.303 0.236 , 0.300	Depositor DCC
R_{free} test set	5512 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	133.4	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 132.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41678	wwPDB-VP
Average B, all atoms (Å^2)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, ADP, 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	0.54	0/21146	0.77	12/28618 (0.0%)
1	B	0.52	0/21146	0.76	9/28618 (0.0%)
All	All	0.53	0/42292	0.77	21/57236 (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	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2455	LEU	CB-CG-CD1	-8.01	97.38	111.00
1	A	3650	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	A	1882	LEU	CA-CB-CG	6.87	131.09	115.30
1	A	1463	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	3945	LEU	CB-CG-CD2	-6.48	99.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3308	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20206	934	0
1	B	20748	0	20207	930	0
2	A	31	0	12	6	0
2	B	31	0	12	22	0
3	A	54	0	24	28	0
3	B	54	0	24	29	0
4	A	5	0	0	2	0
4	B	5	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	41678	0	40485	1867	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 1867 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2732:MET:HB2	3:B:5402:ADP:C6	1.40	1.57
1:B:1365:PHE:CD1	1:B:1366:VAL:HG23	1.34	1.57
1:A:1365:PHE:CE2	1:A:1366:VAL:HG23	1.55	1.39
1:A:1365:PHE:CD2	1:A:1366:VAL:HG23	1.68	1.27
1:B:1365:PHE:CE1	1:B:1366:VAL:HG23	1.70	1.27

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%)	2503 (95%)	121 (5%)	16 (1%)	25 57
1	B	2640/2695 (98%)	2506 (95%)	116 (4%)	18 (1%)	22 55
All	All	5280/5390 (98%)	5009 (95%)	237 (4%)	34 (1%)	25 57

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	1391	GLY
1	A	2369	SER
1	A	3309	THR
1	B	1391	GLY

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%)	2128 (96%)	90 (4%)	30 59
1	B	2218/2453 (90%)	2133 (96%)	85 (4%)	33 61
All	All	4436/4906 (90%)	4261 (96%)	175 (4%)	32 61

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2346	PHE
1	B	3391	LEU
1	B	2395	ILE
1	B	2702	LEU
1	B	3536	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3521	ASN
1	B	3780	ASN
1	A	3323	ASN
1	A	2753	GLN
1	B	3783	ASN

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	$\#\|Z\| > 2$
4	SO4	B	5403	-	4,4,4	0.34	0	6,6,6	0.45	0
3	ADP	B	5402	-	24,29,29	0.98	1 (4%)	29,45,45	1.53	5 (17%)
3	ADP	A	5402	-	24,29,29	1.02	1 (4%)	29,45,45	1.58	5 (17%)
2	ATP	A	5400	-	26,33,33	1.02	1 (3%)	31,52,52	1.62	6 (19%)
2	ATP	B	5400	-	26,33,33	1.02	1 (3%)	31,52,52	1.61	6 (19%)
4	SO4	A	5403	-	4,4,4	0.36	0	6,6,6	0.74	0
3	ADP	B	5401	-	24,29,29	1.22	2 (8%)	29,45,45	1.56	6 (20%)
3	ADP	A	5401	-	24,29,29	1.20	2 (8%)	29,45,45	1.46	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	5402	-	-	1/12/32/32	0/3/3/3
3	ADP	A	5402	-	-	5/12/32/32	0/3/3/3
2	ATP	A	5400	-	-	5/18/38/38	0/3/3/3
2	ATP	B	5400	-	-	5/18/38/38	0/3/3/3
3	ADP	B	5401	-	-	5/12/32/32	0/3/3/3
3	ADP	A	5401	-	-	6/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5401	ADP	C5-C4	2.91	1.48	1.40
3	A	5401	ADP	C2-N3	2.69	1.36	1.32
3	B	5401	ADP	C5-C4	2.63	1.47	1.40
3	B	5402	ADP	C5-C4	2.60	1.47	1.40
2	B	5400	ATP	C5-C4	2.45	1.47	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5402	ADP	C3'-C2'-C1'	4.03	107.04	100.98
3	A	5402	ADP	N3-C2-N1	-3.88	122.61	128.68
3	B	5401	ADP	PA-O3A-PB	-3.74	119.99	132.83
3	B	5401	ADP	N3-C2-N1	-3.72	122.86	128.68
2	B	5400	ATP	C3'-C2'-C1'	3.64	106.46	100.98

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

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

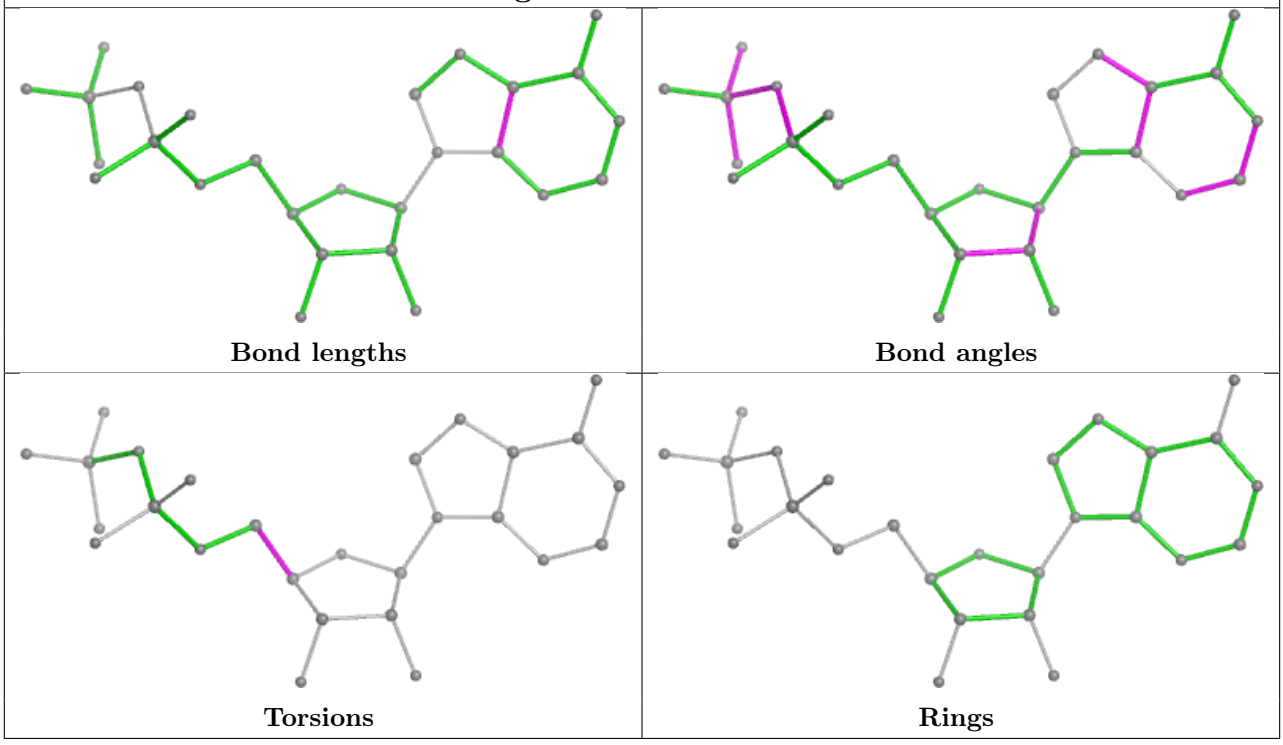
There are no ring outliers.

8 monomers are involved in 89 short contacts:

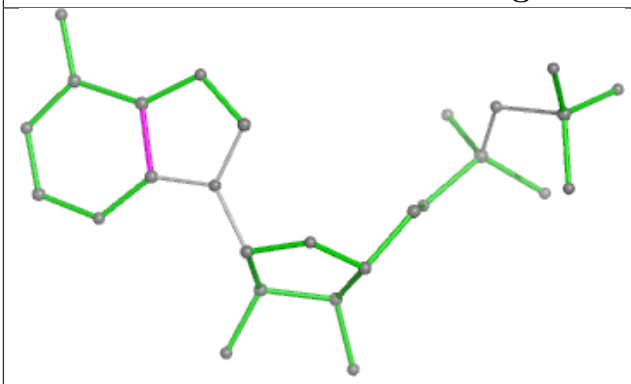
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5403	SO4	2	0
3	B	5402	ADP	23	0
3	A	5402	ADP	17	0
2	A	5400	ATP	6	0
2	B	5400	ATP	22	0
4	A	5403	SO4	2	0
3	B	5401	ADP	6	0
3	A	5401	ADP	11	0

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 then 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.

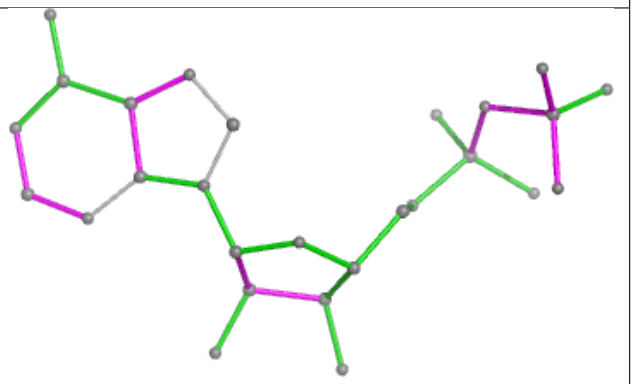
Ligand ADP B 5402



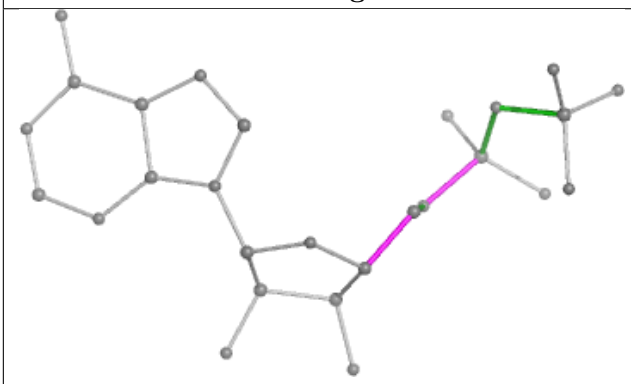
Ligand ADP A 5402



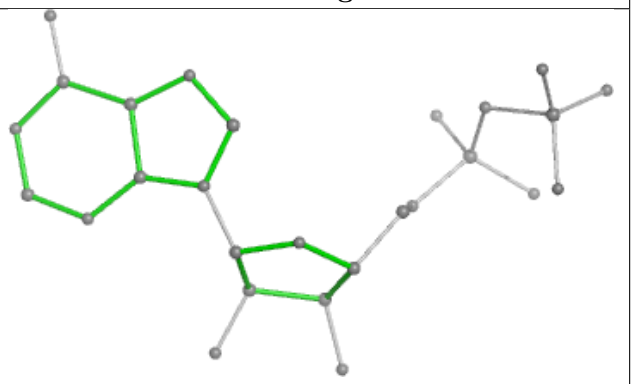
Bond lengths



Bond angles

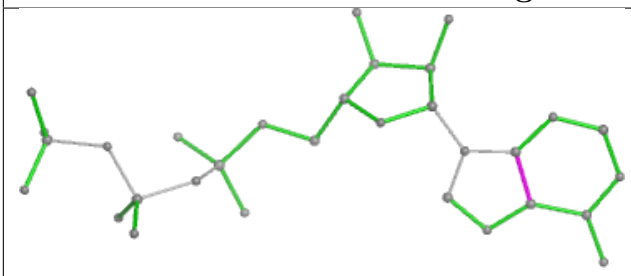


Torsions

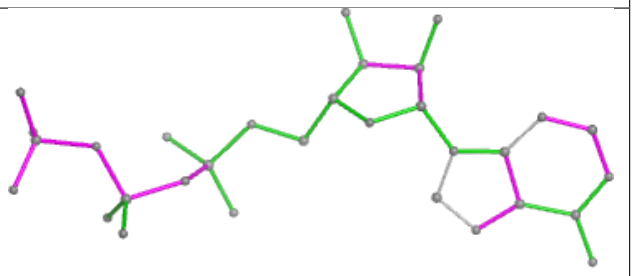


Rings

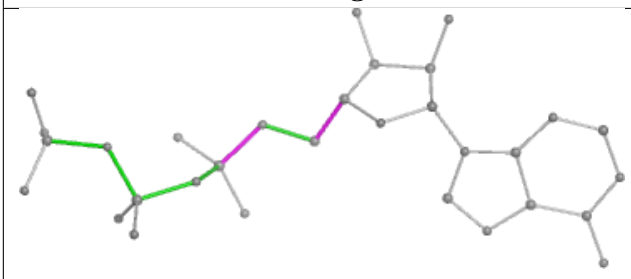
Ligand ATP A 5400



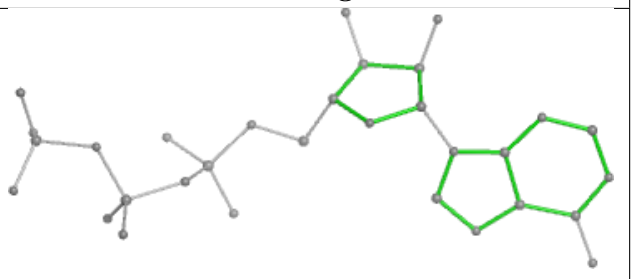
Bond lengths



Bond angles



Torsions



Rings

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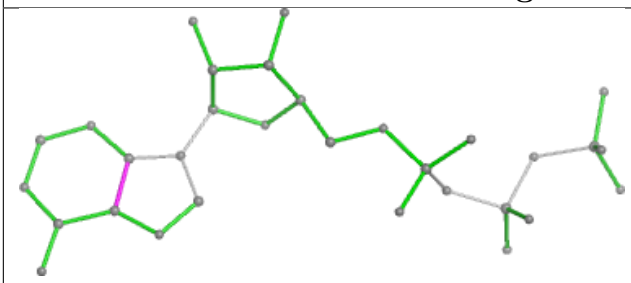
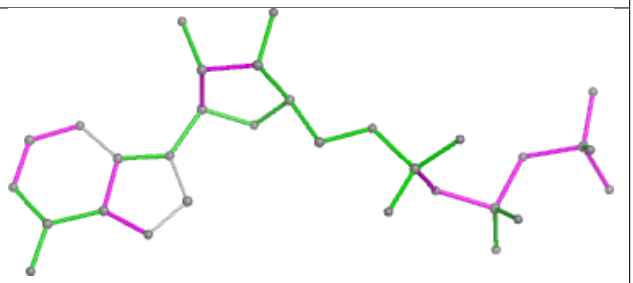
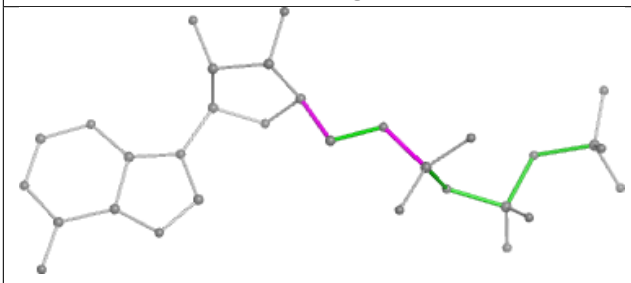


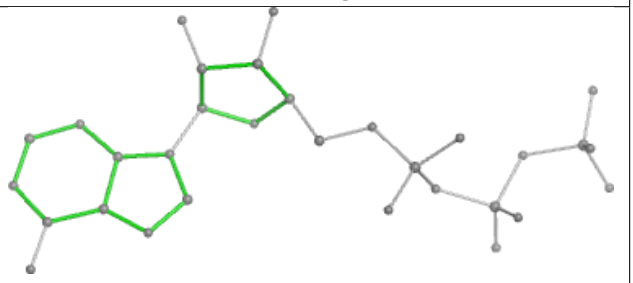
Bond lengths



Bond angles

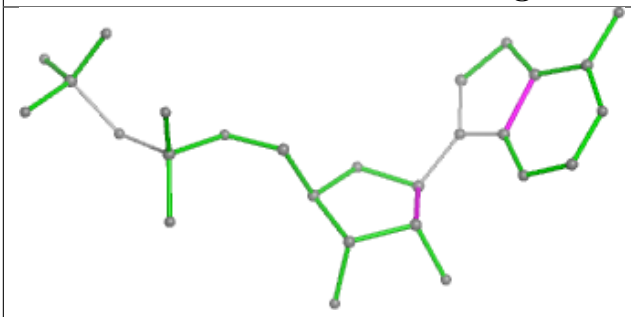


Torsions

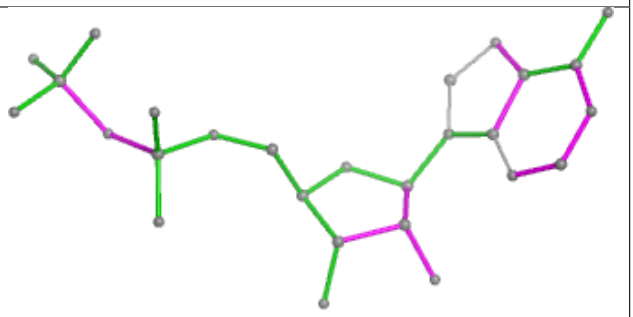


Rings

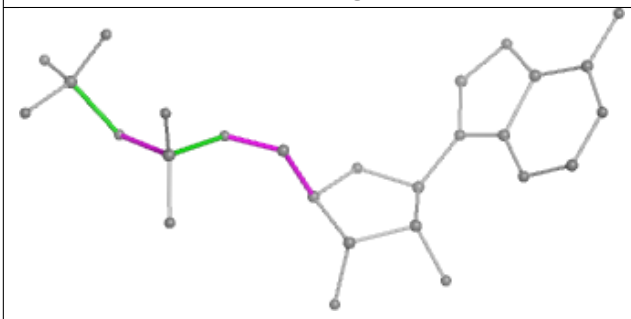
Ligand ADP B 5401



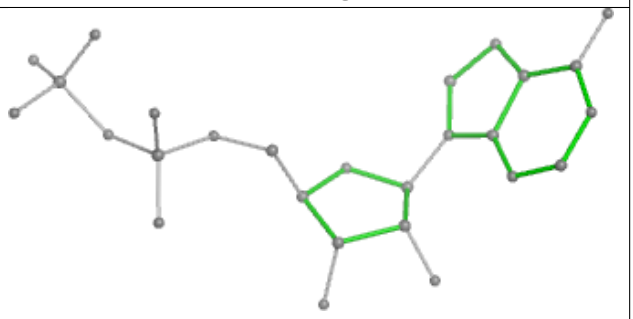
Bond lengths



Bond angles

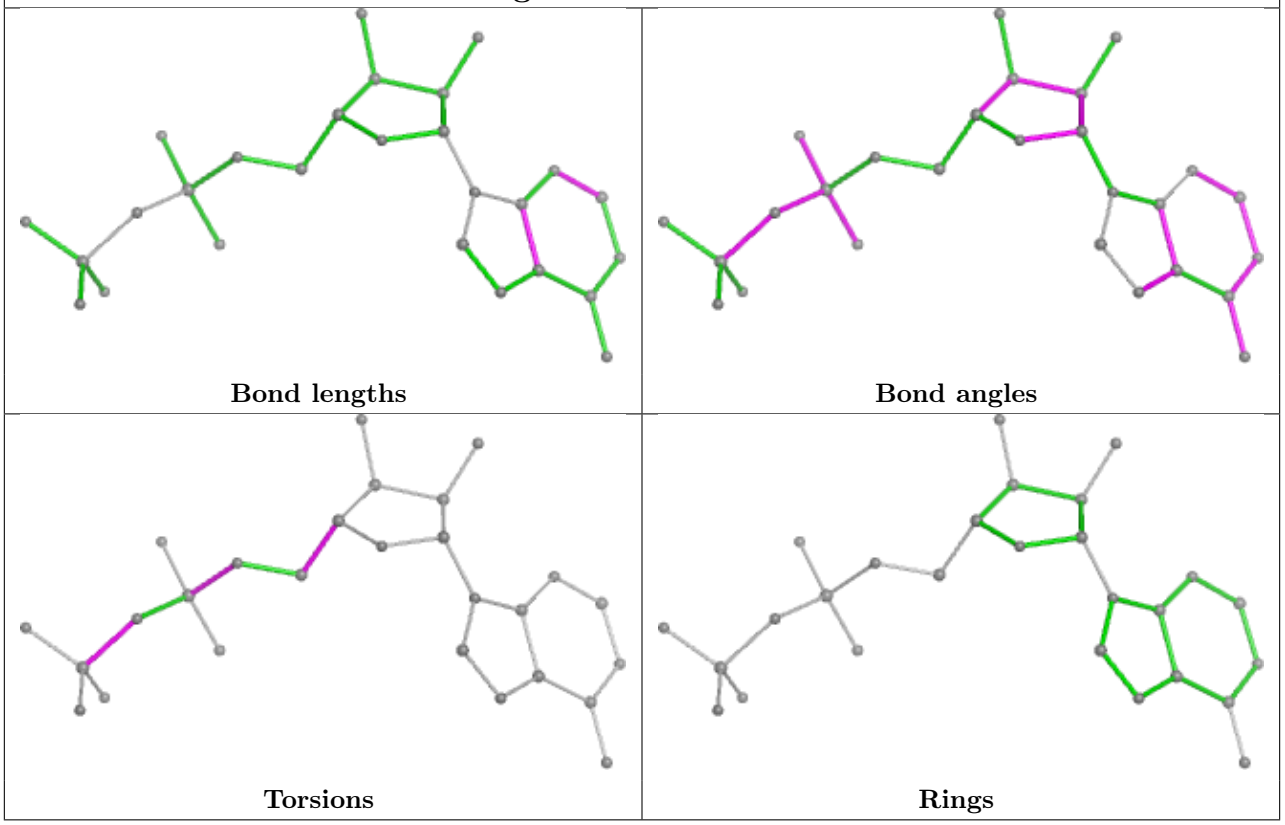


Torsions



Rings

Ligand ADP A 5401



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.60	296 (11%) 5 6	88, 185, 310, 500	1 (0%)
1	B	2650/2695 (98%)	0.70	256 (9%) 7 9	96, 180, 317, 500	1 (0%)
All	All	5300/5390 (98%)	0.65	552 (10%) 6 8	88, 183, 311, 500	2 (0%)

The worst 5 of 552 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	35.4
1	B	33	GLU	29.6
1	B	83	GLY	28.0
1	B	69	ALA	26.8
1	A	131	MET	25.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

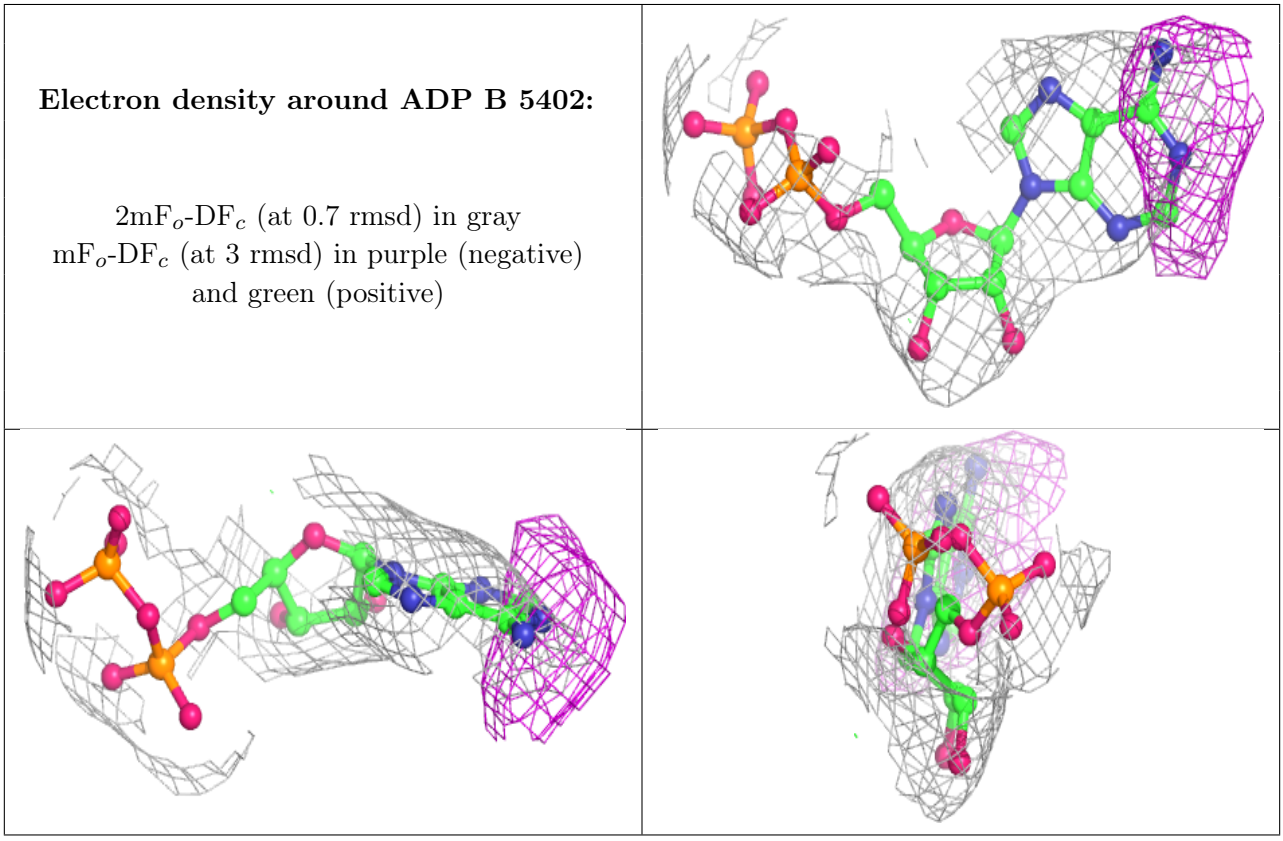
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	5404	1/1	0.77	0.17	97,97,97,97	0
3	ADP	B	5402	27/27	0.87	0.33	108,145,183,194	0
3	ADP	A	5401	27/27	0.89	0.28	126,146,191,198	0
5	MG	B	5404	1/1	0.90	0.30	107,107,107,107	0
2	ATP	B	5400	31/31	0.91	0.27	124,160,195,221	0
4	SO4	B	5403	5/5	0.91	0.16	139,143,171,171	0
4	SO4	A	5403	5/5	0.92	0.23	101,136,142,145	0
3	ADP	A	5402	27/27	0.93	0.25	134,176,208,218	0
3	ADP	B	5401	27/27	0.94	0.27	98,121,138,153	0
2	ATP	A	5400	31/31	0.94	0.31	122,147,224,246	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.

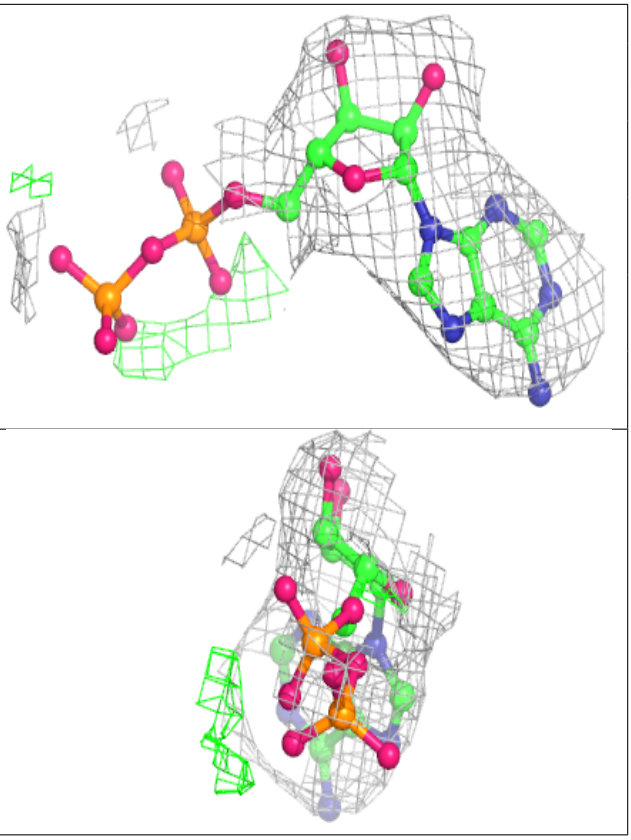
Electron density around ADP B 5402:

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



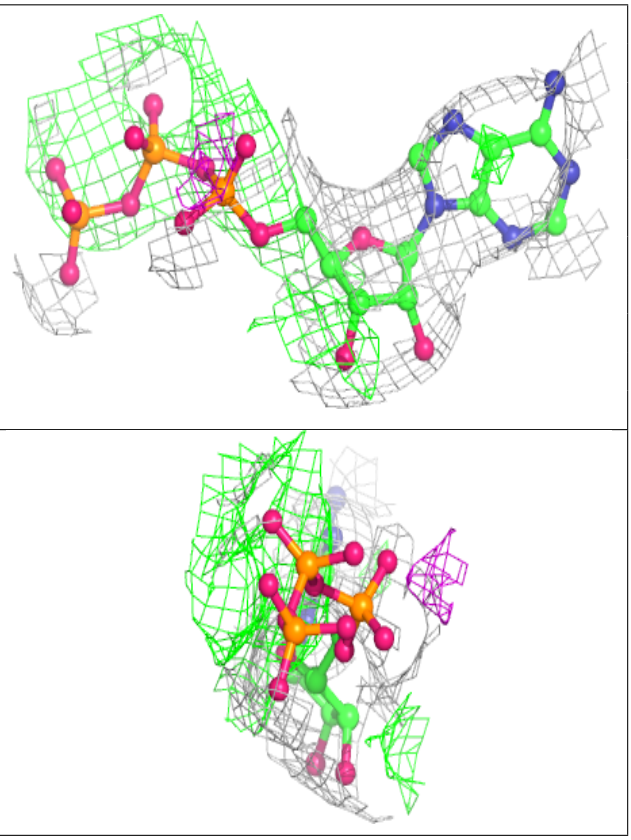
Electron density around ADP A 5401:

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



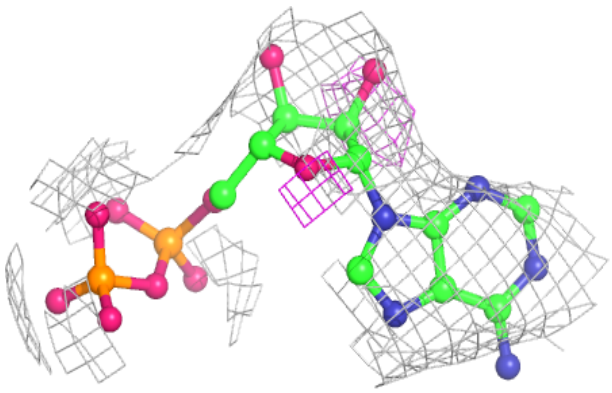
Electron density around ATP B 5400:

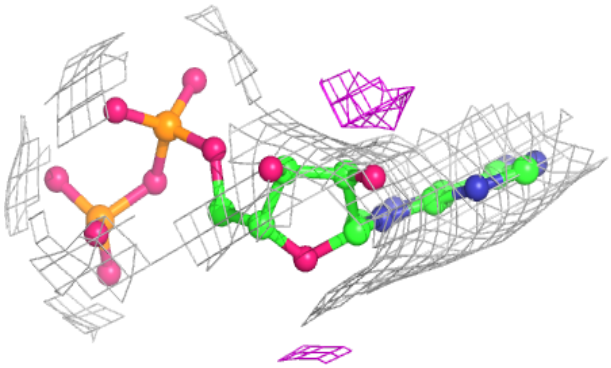
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

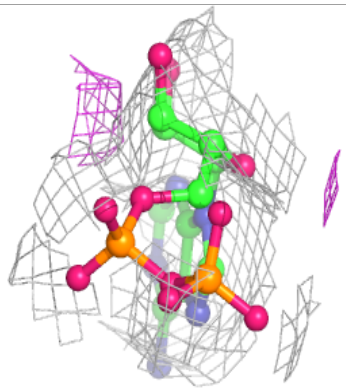


Electron density around ADP A 5402:

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

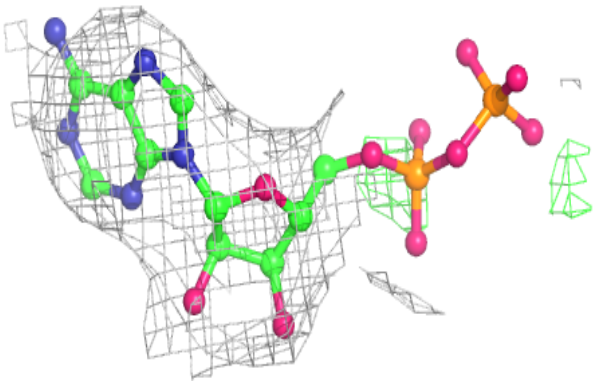


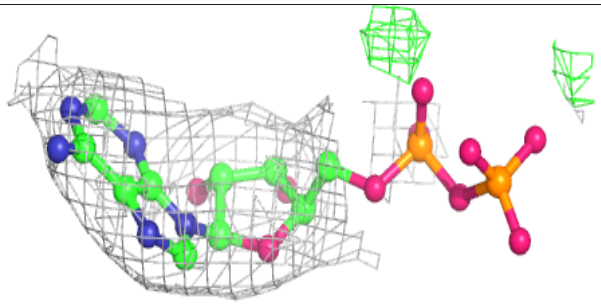


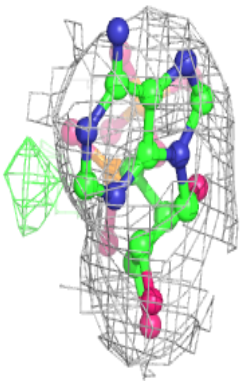


Electron density around ADP B 5401:

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

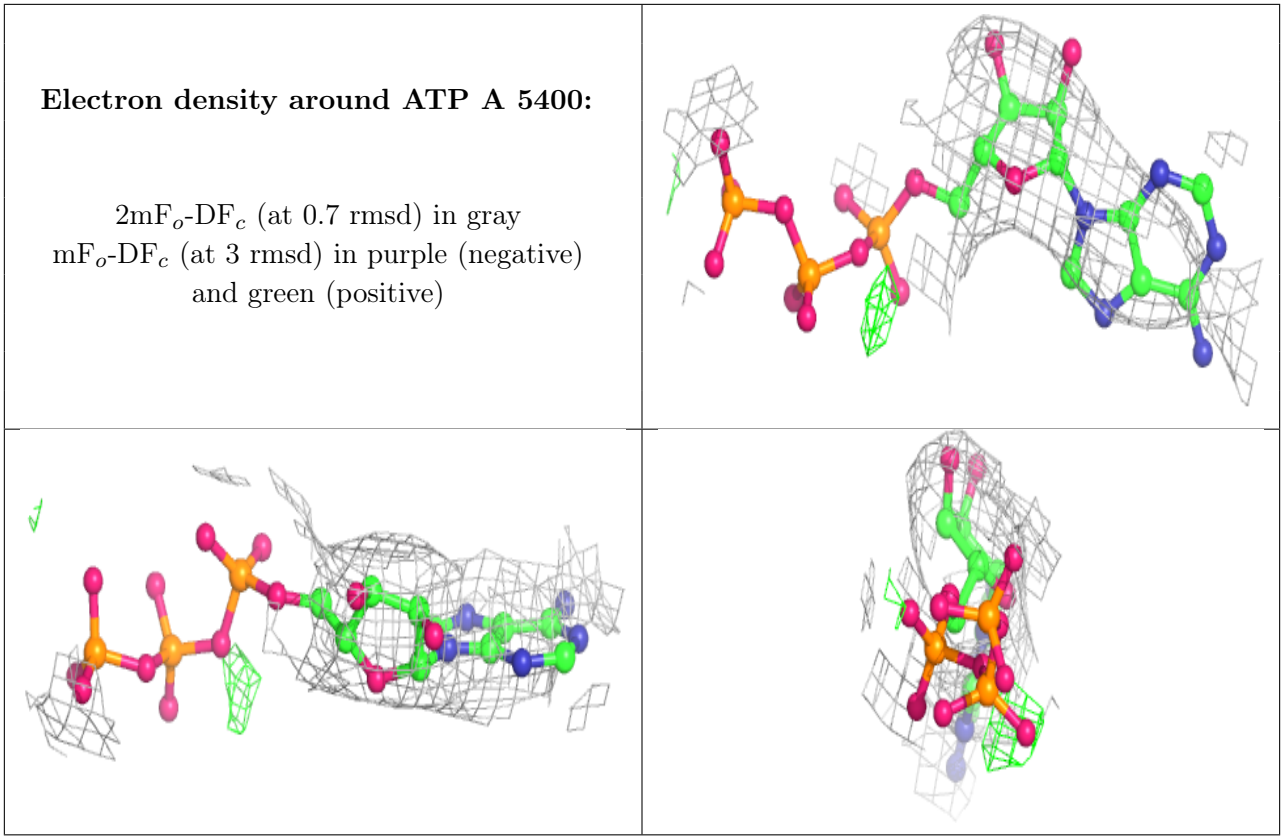






Electron density around ATP A 5400:

$2mF_o$-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.