wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 01:14 am BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

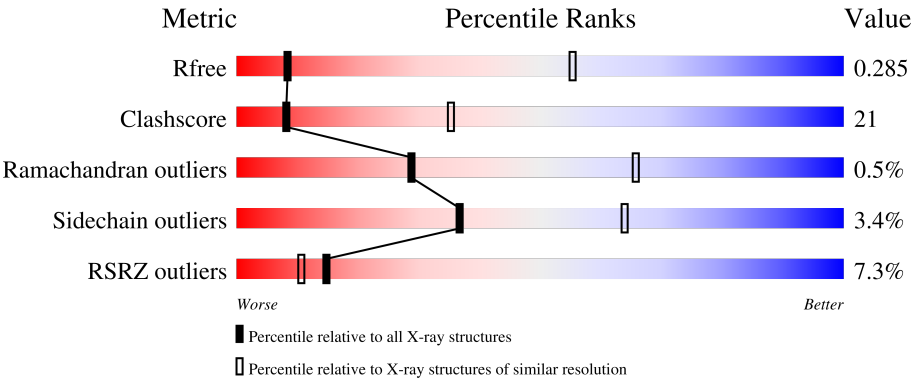
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	6% 66% 30%
1	B	2695	8% 68% 29%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	5094	-	-	X	-
3	SO4	A	5095	-	-	X	-
3	SO4	A	5096	-	-	X	-
3	SO4	B	5095	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

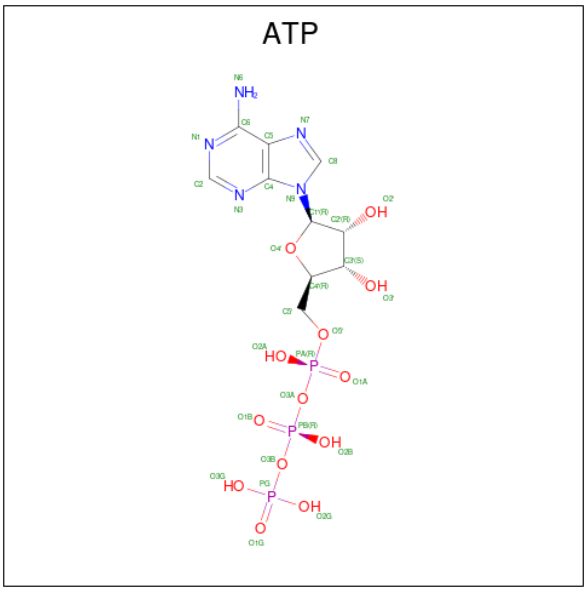
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

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

There are 8 discrepancies between the modelled and reference sequences:

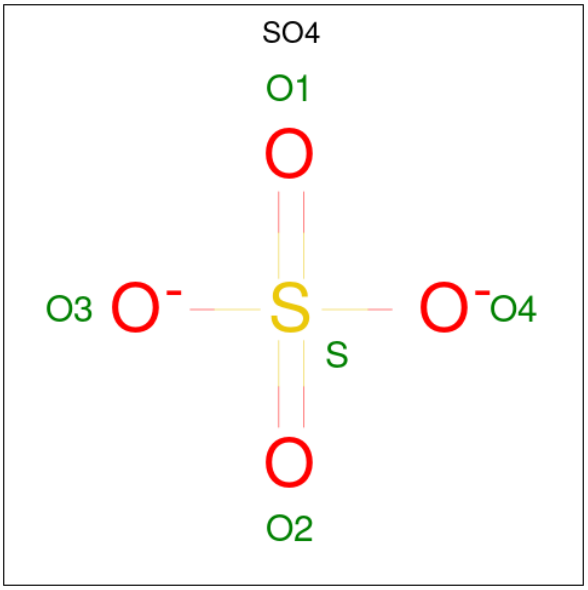
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	linker	UNP P36022
A	219	ASP	-	linker	UNP P36022
A	1630	ILE	LEU	conflict	UNP P36022
A	3782	ASP	GLU	conflict	UNP P36022
B	218	SER	-	linker	UNP P36022
B	219	ASP	-	linker	UNP P36022
B	1630	ILE	LEU	conflict	UNP P36022
B	3782	ASP	GLU	conflict	UNP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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

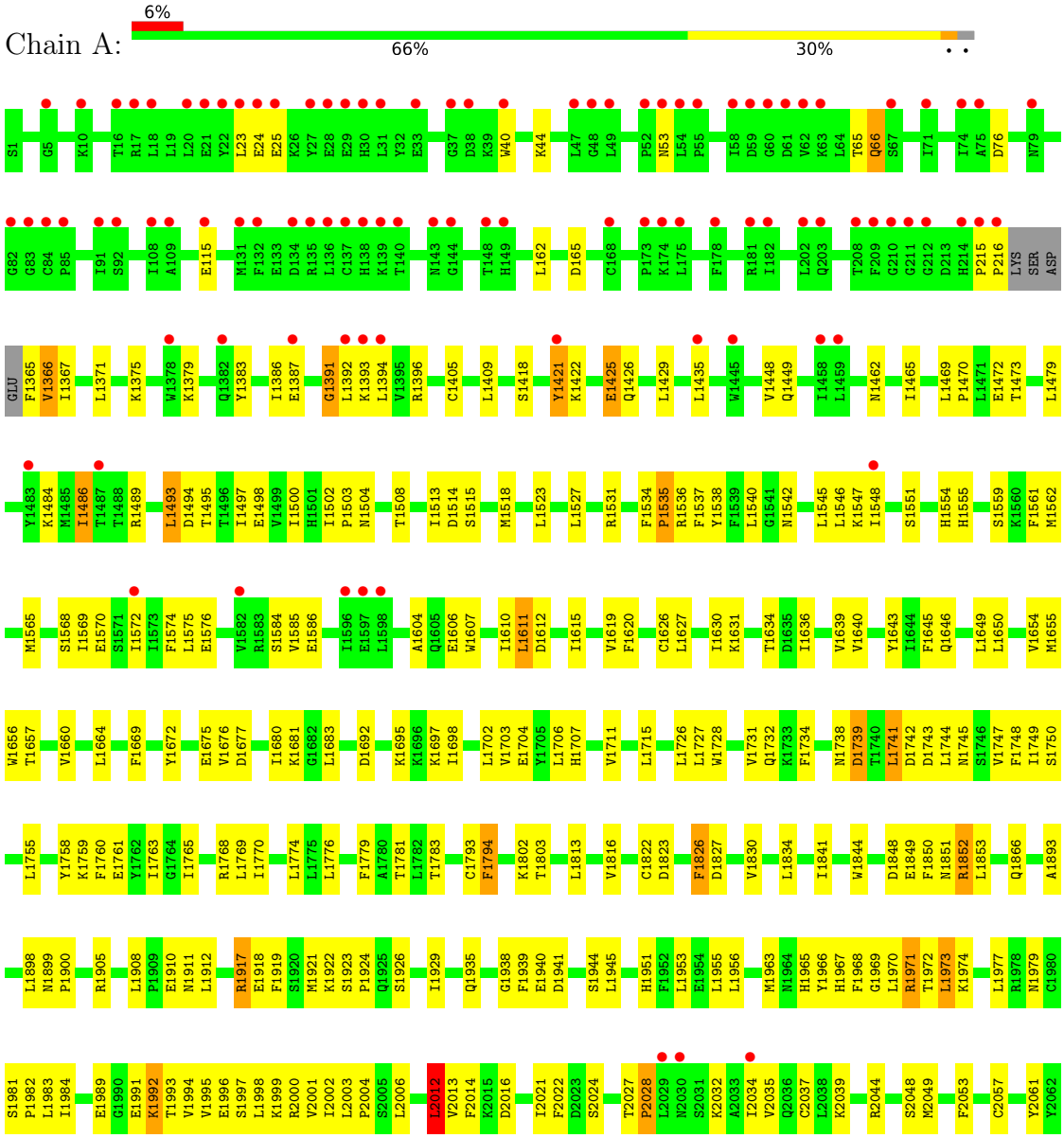
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

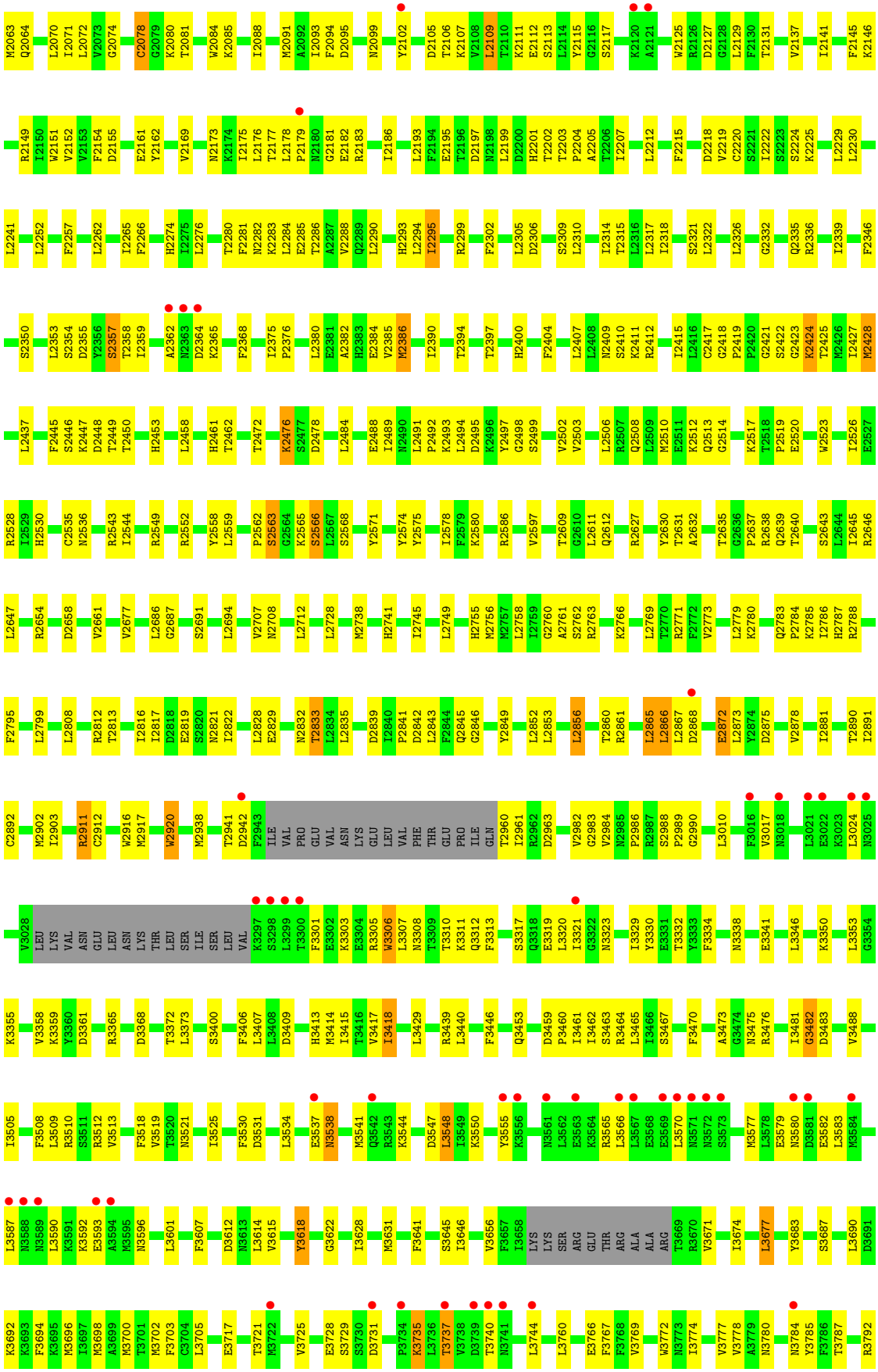
3 Residue-property plots (i)

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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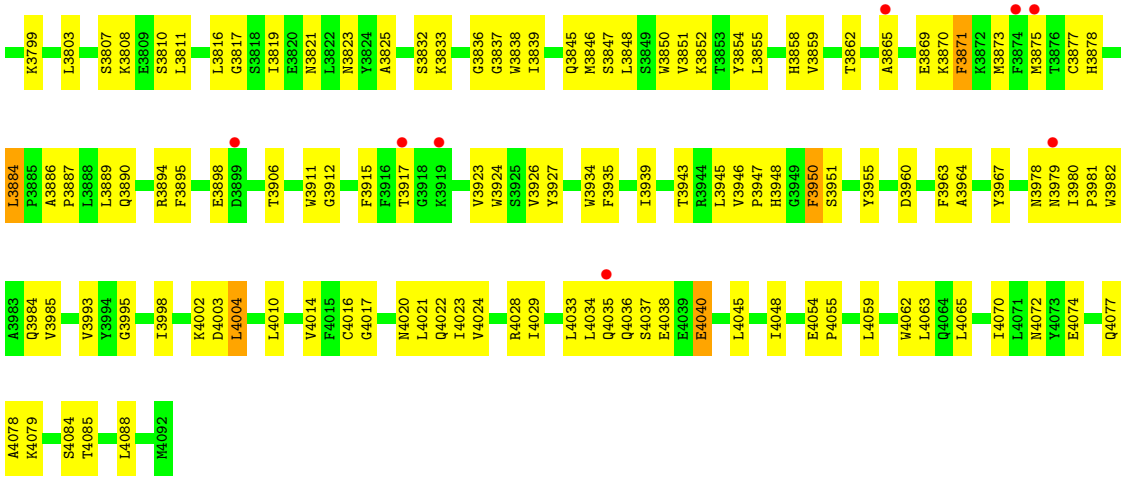
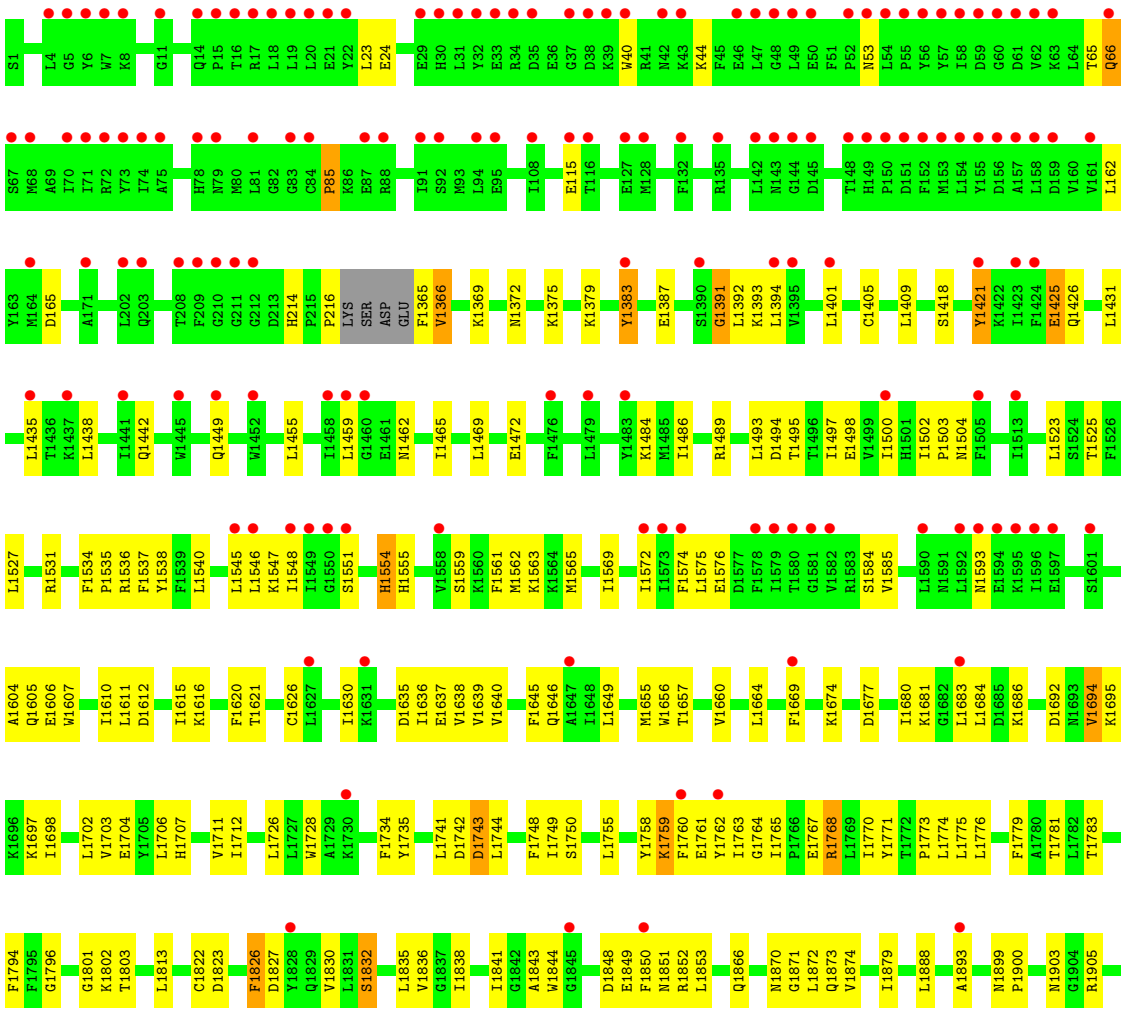
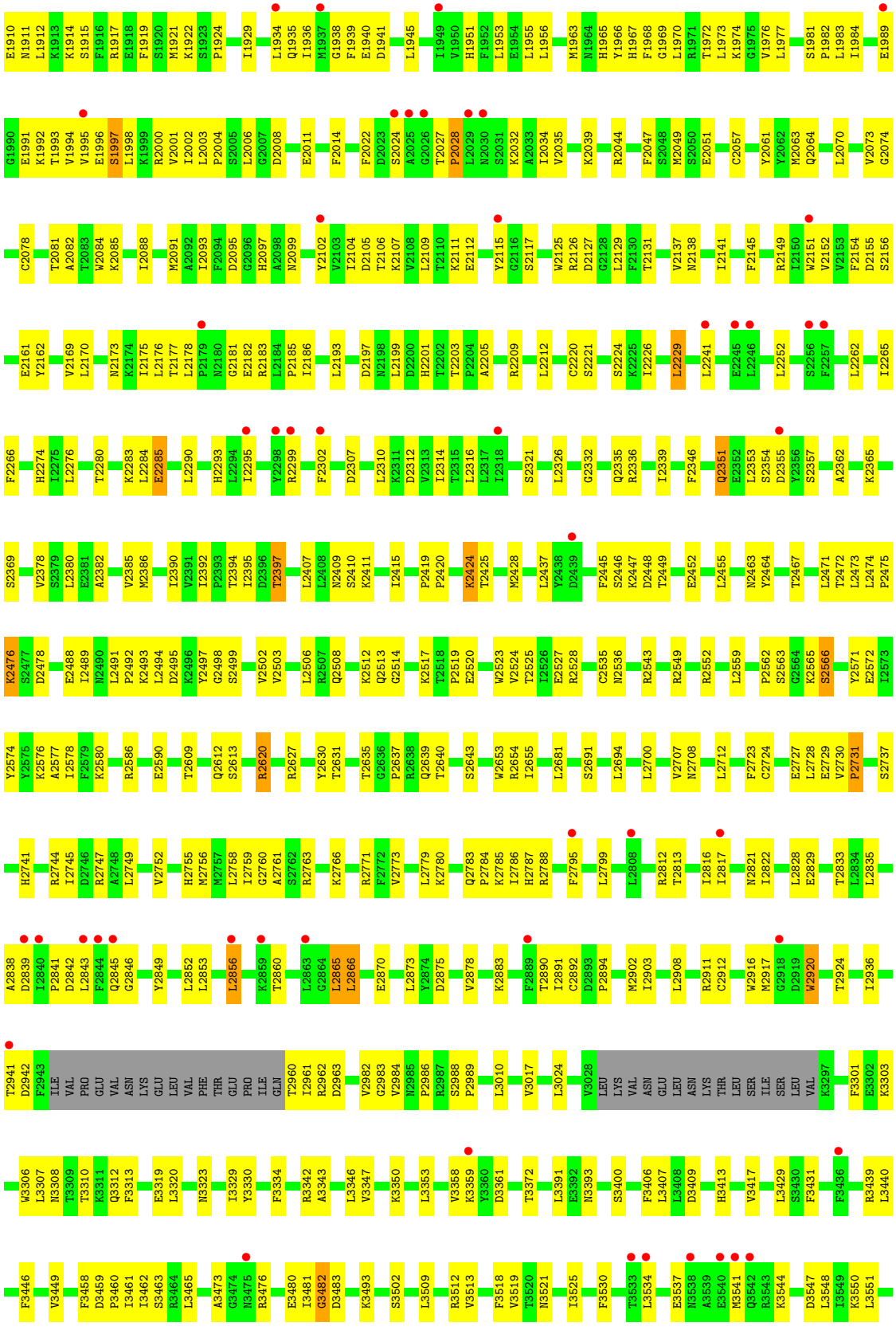
L2070 I2071 L2072 V2073 G2074
C2078 G2079 K2080 T2081
W2084 K2085
I2088
M2091 A2092 I2093 F2094 D2095
N2099
Y2102
D2105 T2106 K2107 V2108 L2109 T2110 K2111 E2112 S2113 L2114 Y2115 G2116 S2117
K2120 A2121
W2125 R2126 D2127 G2128 L2129 F2130 T2131
V2137
I2141
F2145 K2146
R2149 I2150 W2151 V2152 V2153 F2154 D2155
E2161 Y2162
V2169
N2173 K2174 I2175 L2176 T2177 L2178 P2179 N2180 G2181 E2182 R2183
I2186
L2193 F2194 E2195 T2196 D2197 N2198 L2199 D2200 H2201 T2202 T2203 P2204 A2205 T2206 I2207
L2212
F2215
D2218 V2219 C2220 S2221 I2222 S2223 S2224 K2225
L2229 L2230
L2241 L2252 F2257 L2262 I2265 F2266 H2274 I2275 L2276 T2280 F2281 N2282 K2283 L2284 E2285 T2286 A2287 V2288 Q2289 L2290 H2293 L2294 I2295 R2299 F2302 L2305 D2306 S2309 L2310 I2314 T2315 L2316 L2317 I2318 S2321 L2322 L2326 G2332 Q2335 R2336 I2339 F2346
S2350 L2353 S2354 D2355 Y2356 S2357 T2358 I2359 A2362 N2363 D2364 K2365 F2368 I2375 P2376 L2380 E2381 A2382 H2383 E2384 V2385 M2386 I2390 T2394 T2397 H2400 F2404 L2407 L2408 N2409 S2410 K2411 R2412 I2415 L2416 C2417 G2418 P2419 P2420 G2421 S2422 G2423 K2424 T2425 M2426 I2427 M2428
L2437 F2445 S2446 K2447 D2448 T2449 T2450 H2453 L2458 H2461 T2462 T2472 K2476 S2477 D2478 L2484 E2488 I2489 N2490 L2491 P2492 K2493 L2494 D2495 K2496 Y2497 G2498 S2499 V2502 V2503 L2506 R2507 Q2508 L2509 M2510 E2511 K2512 Q2513 G2514 K2517 T2518 P2519 E2520 W2523 I2526 E2527
R2528 I2529 H2530 C2535 N2536 R2543 I2544 R2549 R2552 Y2558 L2559 P2562 S2563 G2564 K2565 S2566 L2567 S2568 Y2571 Y2574 Y2575 I2578 F2579 K2580 R2586 V2597 T2609 G2610 L2611 Q2612 R2627 Y2630 T2631 A2632 T2635 G2636 P2637 R2638 Q2639 T2640 S2643 L2644 I2645 R2646
L2647 R2654 D2658 V2661 V2677 L2686 G2687 S2691 L2694 V2707 N2708 L2712 L2728 M2738 H2741 I2745 L2749 H2755 M2756 M2757 L2758 I2759 G2760 A2761 S2762 R2763 K2766 L2769 T2770 R2771 F2772 V2773 L2779 K2780 Q2783 P2784 K2785 I2786 H2787 R2788
F2795 L2799 L2808 R2812 T2813 I2816 I2817 D2818 E2819 S2820 N2821 I2822 L2828 E2829 N2832 T2833 L2834 L2835 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 Y2849 T2860 R2861 L2865 L2866 L2867 D2868 E2872 L2873 Y2874 D2875 V2878 I2881 T2890 I2891
C2892 M2902 I2903 R2911 C2912 W2916 M2917 W2920 M2938 T2941 D2942 F2943 T2960 I2961 R2962 D2963 V2982 G2983 V2984 N2985 P2986 R2987 S2988 P2989 G2990 L3010 F3016 V3017 N3018 L3021 E3022 K3023 L3024 N3025
V3028 LEU LYS VAL ASN GLU LEU ASN LYS THR LEU SER ILE SER LEU VAL K3297 S3298 L3299 T3300 F3301 E3302 K3303 E3304 R3305 W3306 L3307 N3308 T3309 T3310 K3311 Q3312 F3313 S3317 Q3318 E3319 L3320 I3321 G3322 N3323 I3329 Y3330 E3331 T3332 Y3333 F3334 N3338 E3341 L3346 K3350 L3353 G3354
K3355 V3358 K3359 Y3360 D3361 D3368 R3365 T3372 L3373 S3400 F3406 L3407 L3408 D3409 H3413 M3414 I3415 T3416 V3417 I3418 L3429 R3439 L3440 F3446 Q3453 D3459 P3460 I3461 I3462 S3463 R3464 L3465 I3466 S3467 F3470 A3473 G3474 N3475 R3476 I3481 G3482 D3483 V3488
I3505 F3508 L3509 R3510 S3511 R3512 V3513 F3518 V3519 T3520 N3521 I3525 F3530 D3531 L3534 E3537 N3538 M3541 Q3542 R3543 K3544 D3547 L3548 I3549 K3550 Y3555 K3556 N3561 L3562 E3563 K3564 R3565 L3566 L3567 E3568 E3569 L3570 N3571 N3572 S3573 M3577 L3578 E3579 N3580 D3581 E3582 L3583 M3584
L3587 N3588 N3589 L3590 K3591 K3592 E3593 A3594 M3595 N3596 L3601 F3607 D3612 N3613 L3614 V3615 Y3618 G3622 I3628 M3631 F3641 S3645 I3646 V3656 F3657 I3658 LYS LYS SER ARG GLU THR ARG ALA ALA ARG T3669 R3670 V3671 I3674 L3677 Y3683 S3687 L3690 D3691
K3692 K3693 F3694 K3695 M3696 I3697 M3698 A3699 M3700 T3701 M3702 F3703 C3704 L3705 E3717 T3721 M3722 V3725 E3728 S3729 S3730 D3731 P3734 K3735 L3736 T3737 V3738 D3739 T3740 N3741 L3744 L3760 E3766 F3767 F3768 V3769 W3772 N3773 I3774 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 R3792



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

Chain B:

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G1990 E1991 K1992 T1993 V1994 V1995 E1996 S1997 L1998 K1999 R2000 V2001 I2002 L2003 P2004 S2005 L2006 G2007 D2008 E2011 F2014 F2022 D2023 S2024 A2025 G2026 T2027 P2028 L2029 N2030 S2031 K2032 A2033 I2034 V2035 K2039 R2044 F2047 S2048 M2049 S2050 E2051 C2057 Y2061 Y2062 M2063 Q2064 L2070 V2073 G2074
C2078 T2081 A2082 T2083 W2084 K2085 I2088 M2091 A2092 I2093 F2094 D2095 G2096 H2097 A2098 N2099 Y2102 V2103 I2104 D2105 T2106 K2107 V2108 L2109 T2110 K2111 E2112 Y2115 G2116 S2117 W2125 R2126 D2127 G2128 L2129 F2130 T2131 V2137 N2138 I2141 F2145 R2149 I2150 W2151 V2152 V2153 F2154 D2155 S2156
E2161 Y2162 V2169 L2170 N2173 K2174 I2175 L2176 T2177 L2178 P2179 N2180 G2181 E2182 R2183 L2184 P2185 I2186 L2193 D2197 N2198 L2199 D2200 H2201 T2202 T2203 P2204 A2205 R2209 L2212 C2220 S2221 S2224 K2225 I2226 L2229 L2241 E2245 L2246 L2252 S2256 F2257 L2262 I2265
F2266 H2274 I2275 L2276 T2280 K2283 L2284 E2285 L2290 H2293 L2294 I2295 Y2298 R2299 F2302 D2307 L2310 K2311 D2312 V2313 I2314 I2315 L2316 I2317 I2318 S2321 L2326 G2332 Q2335 R2336 I2339 F2346 Q2351 E2352 L2353 S2354 D2355 Y2356 S2357 A2362 K2365
S2369 V2378 S2379 L2380 E2381 A2382 V2385 M2386 I2390 V2391 I2392 P2393 T2394 I2395 D2396 T2397 L2407 L2408 N2409 S2410 K2411 I2415 P2419 P2420 K2424 T2425 M2428 L2437 Y2438 D2439 F2445 S2446 K2447 D2448 T2449 E2452 L2455 N2463 Y2464 T2467 L2471 T2472 L2473 L2474 P2475
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A2838 D2839 I2840 P2841 D2842 L2843 F2844 Q2845 G2846 Y2849 L2852 L2853 L2856 K2859 T2860 L2863 G2864 L2865 L2866 E2870 L2873 Y2874 D2875 V2878 K2883 F2889 T2890 I2891 C2892 D2893 P2894 M2902 I2903 L2908 R2911 C2912 W2916 M2917 G2918 D2919 W2920 T2924 I2936
T2941 D2942 F2943 ILE VAL PRO GLU VAL ASN LYS GLU LEU VAL PHE THR GLU PRO ILE GLN T2960 I2961 R2962 D2963 V2982 G2983 V2984 N2985 P2986 R2987 S2988 P2989 L3010 V3017 L3024 V3028 LEU LYS VAL ASN GLU LEU ASN LYS THR LEU SER ILE SER LEU VAL K3297 F3301 E3302 K3303
W3306 L3307 N3308 T3309 T3310 K3311 Q3312 F3313 E3319 L3320 N3323 I3329 Y3330 F3334 R3342 A3343 L3346 V3347 K3350 L3353 V3358 K3359 Y3360 D3361 T3372 L3391 E3392 N3393 S3400 F3406 L3407 L3408 D3409 H3413 V3417 L3429 S3430 F3431 F3436 R3439 L3440
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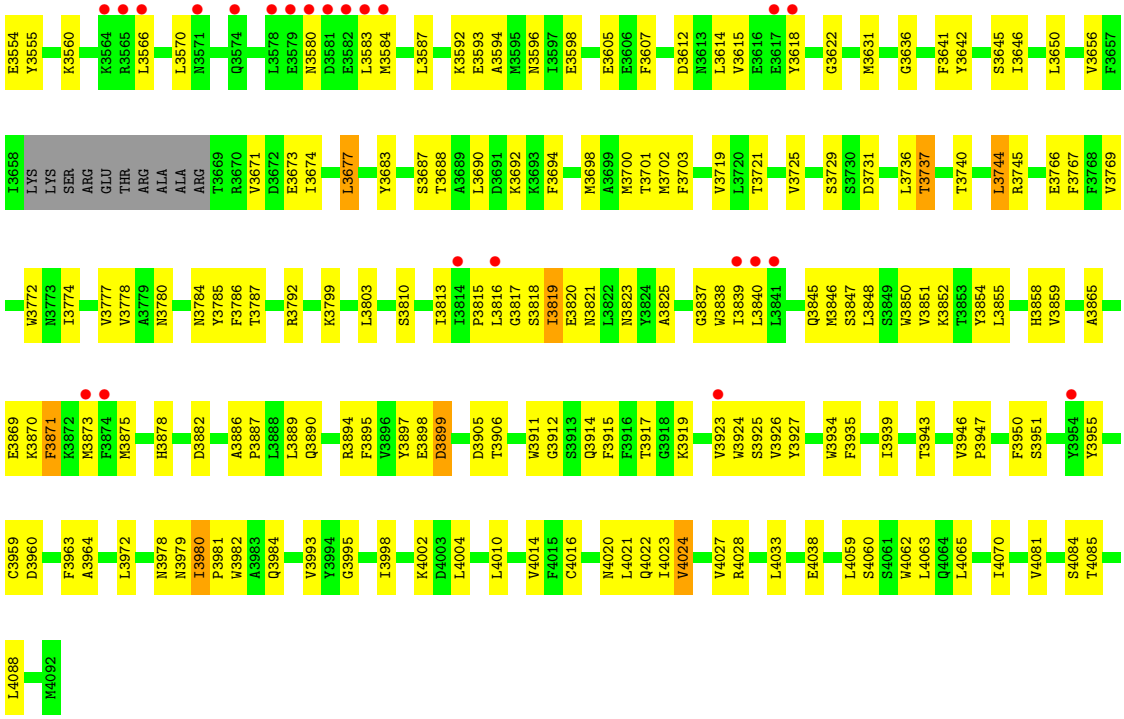
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W3772 N3773 I3774 V3777 V3778 A3779 N3780 N3784 Y3785 F3786 T3787 R3792 K3799 L3803 S3810 I3813 I3814 P3815 L3816 G3817 S3818 I3819 E3820 N3821 L3822 N3823 Y3824 A3825 G3837 W3838 I3839 L3840 L3841 Q3845 M3846 S3847 L3848 S3849 W3850 V3851 K3852 I3853 Y3854 L3855 H3858 V3859 A3865
E3869 K3870 F3871 K3872 M3873 F3874 M3875 H3878 D3882 A3886 P3887 L3888 L3889 Q3890 R3894 F3895 V3896 Y3897 E3898 D3899 D3905 T3906 W3911 G3912 S3913 Q3914 F3915 F3916 T3917 G3918 K3919 V3923 W3924 S3925 V3926 Y3927 W3934 F3935 I3939 T3943 V3946 P3947 F3950 S3951 Y3954 Y3955
C3959 D3960 F3963 A3964 L3972 N3978 N3979 I3980 P3981 W3982 A3983 Q3984 V3993 Y3994 G3995 I3998 K4002 D4003 L4004 L4010 V4014 F4015 C4016 N4020 L4021 Q4022 I4023 V4024 V4027 R4028 L4033 E4038 L4059 S4060 S4061 W4062 L4063 Q4064 L4065 I4070 V4081 S4084 T4085
L4088 M4092

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	175.77Å 118.19Å 202.68Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.14 – 3.70 49.09 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.14-3.70) 99.9 (49.09-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, R_{free}	0.231 , 0.289 0.226 , 0.285	Depositor DCC
R_{free} test set	4446 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	142.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 138.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ATP, MG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	1/21146 (0.0%)	0.80	12/28618 (0.0%)
1	B	0.47	0/21146	0.68	4/28618 (0.0%)
All	All	0.53	1/42292 (0.0%)	0.74	16/57236 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.57	1.63	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1741	LEU	CB-CG-CD1	8.44	125.34	111.00
1	A	1973	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	A	2866	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	1769	LEU	CA-CB-CG	6.06	129.24	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20748	0	20207	891	0
1	B	20748	0	20206	851	0
2	A	31	0	12	4	0
2	B	31	0	12	7	0
3	A	15	0	0	9	0
3	B	15	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	41590	0	40437	1741	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 21.

The worst 5 of 1741 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:C	1:A:3475:ASN:HB3	1.39	1.40
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.24
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.21
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.53	1.21
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.24	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2640/2695 (98%)	2519 (95%)	107 (4%)	14 (0%)	29	66
1	B	2640/2695 (98%)	2522 (96%)	104 (4%)	14 (0%)	29	66
All	All	5280/5390 (98%)	5041 (96%)	211 (4%)	28 (0%)	29	66

5 of 28 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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%)	2140 (96%)	78 (4%)	36	63
1	B	2218/2453 (90%)	2144 (97%)	74 (3%)	38	64
All	All	4436/4906 (90%)	4284 (97%)	152 (3%)	37	64

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2576	LYS
1	B	3905	ASP
1	B	2822	ILE
1	B	3391	LEU
1	B	4016	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2753	GLN
1	B	3336	HIS
1	B	3890	GLN
1	A	2688	ASN
1	A	2683	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	$\#\|Z\| > 2$
3	SO4	B	5094	-	4,4,4	0.38	0	6,6,6	0.46	0
3	SO4	B	5096	-	4,4,4	0.22	0	6,6,6	0.30	0
3	SO4	A	5096	-	4,4,4	0.28	0	6,6,6	0.30	0
3	SO4	B	5095	-	4,4,4	0.35	0	6,6,6	0.27	0
2	ATP	B	5093	4	26,33,33	0.95	2 (7%)	31,52,52	1.63	6 (19%)
3	SO4	A	5094	-	4,4,4	0.49	0	6,6,6	0.49	0
2	ATP	A	5093	4	26,33,33	1.13	1 (3%)	31,52,52	1.88	6 (19%)
3	SO4	A	5095	-	4,4,4	0.48	0	6,6,6	0.72	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
2	ATP	A	5093	4	-	3/18/38/38	0/3/3/3
2	ATP	B	5093	4	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5093	ATP	C5-C4	2.35	1.47	1.40
2	A	5093	ATP	C2'-C1'	-2.26	1.50	1.53
2	B	5093	ATP	O4'-C1'	2.18	1.44	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5093	ATP	PA-O3A-PB	-4.42	117.66	132.83
2	A	5093	ATP	PB-O3B-PG	-4.16	118.56	132.83
2	A	5093	ATP	N3-C2-N1	-4.11	122.25	128.68
2	A	5093	ATP	C3'-C2'-C1'	3.92	106.89	100.98
2	B	5093	ATP	PB-O3B-PG	-3.74	119.98	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5093	ATP	C5'-O5'-PA-O1A
2	B	5093	ATP	O4'-C4'-C5'-O5'
2	B	5093	ATP	C3'-C4'-C5'-O5'
2	A	5093	ATP	O4'-C4'-C5'-O5'
2	A	5093	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5096	SO4	1	0
3	A	5096	SO4	2	0
3	B	5095	SO4	2	0
2	B	5093	ATP	7	0

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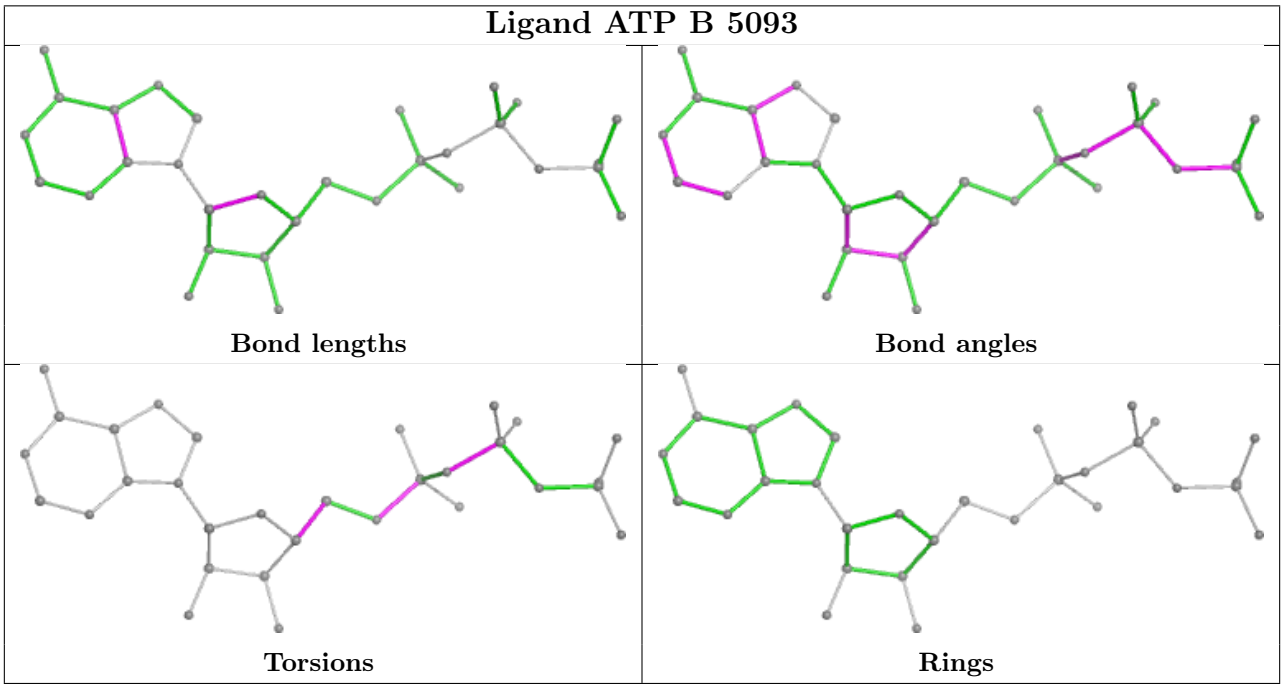
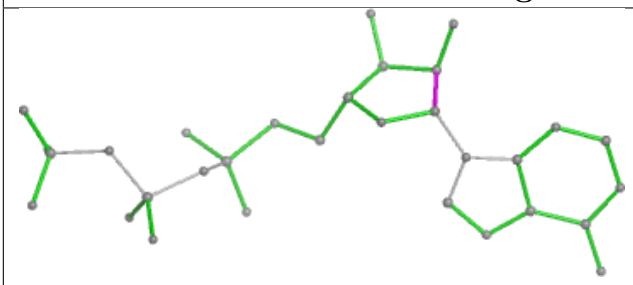
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5094	SO4	4	0
2	A	5093	ATP	4	0
3	A	5095	SO4	3	0

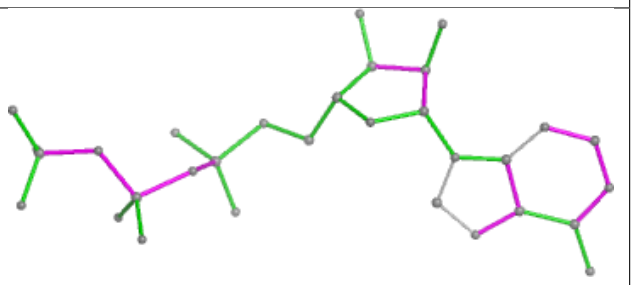
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



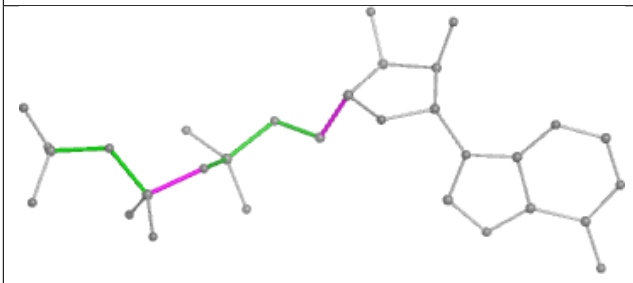
Ligand ATP A 5093



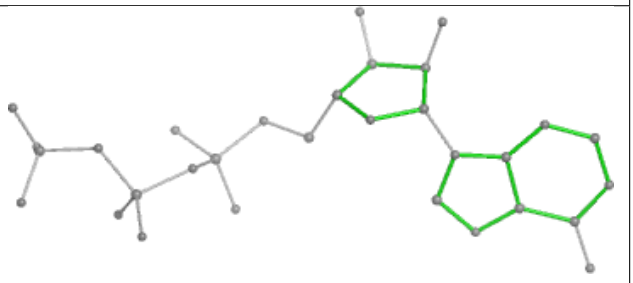
Bond lengths



Bond angles



Torsions



Rings

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%)	0.14	157 (5%)	22	15	80, 163, 325, 500	0
1	B	2650/2695 (98%)	0.37	228 (8%)	10	8	117, 210, 355, 500	0
All	All	5300/5390 (98%)	0.25	385 (7%)	15	11	80, 188, 342, 500	0

The worst 5 of 385 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	THR	18.1
1	B	35	ASP	17.2
1	B	155	TYR	17.2
1	B	31	LEU	16.5
1	B	67	SER	16.1

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

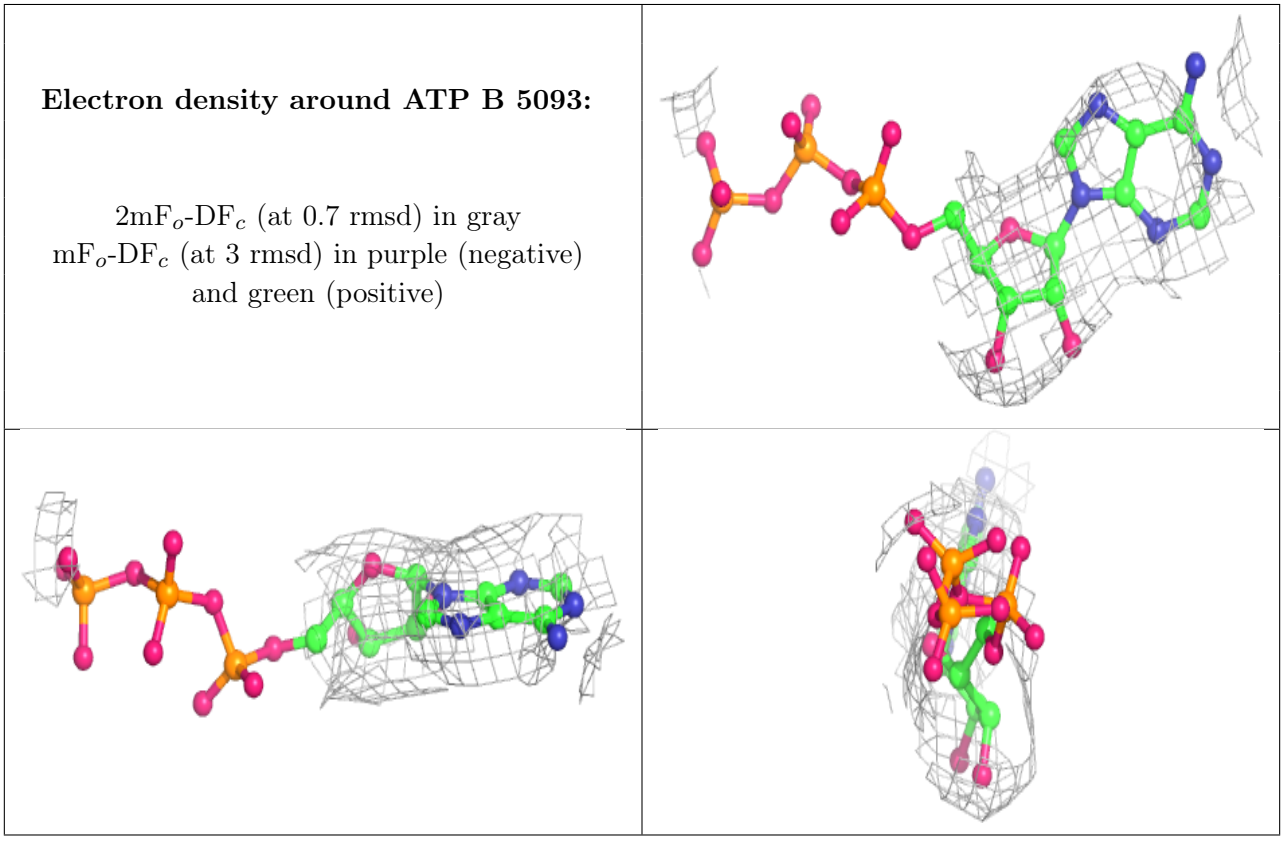
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	SO4	A	5096	5/5	0.83	0.22	128,136,144,154	0
3	SO4	B	5094	5/5	0.86	0.30	151,165,190,192	0
3	SO4	B	5095	5/5	0.90	0.24	155,178,186,207	0
2	ATP	B	5093	31/31	0.93	0.28	115,184,238,261	0
2	ATP	A	5093	31/31	0.95	0.32	72,125,180,196	0
3	SO4	A	5094	5/5	0.95	0.29	109,114,153,161	0
3	SO4	A	5095	5/5	0.95	0.40	108,128,132,133	0
3	SO4	B	5096	5/5	0.96	0.14	158,193,224,235	0
4	MG	B	5097	1/1	0.98	0.24	127,127,127,127	0
4	MG	A	5097	1/1	0.99	0.40	59,59,59,59	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.

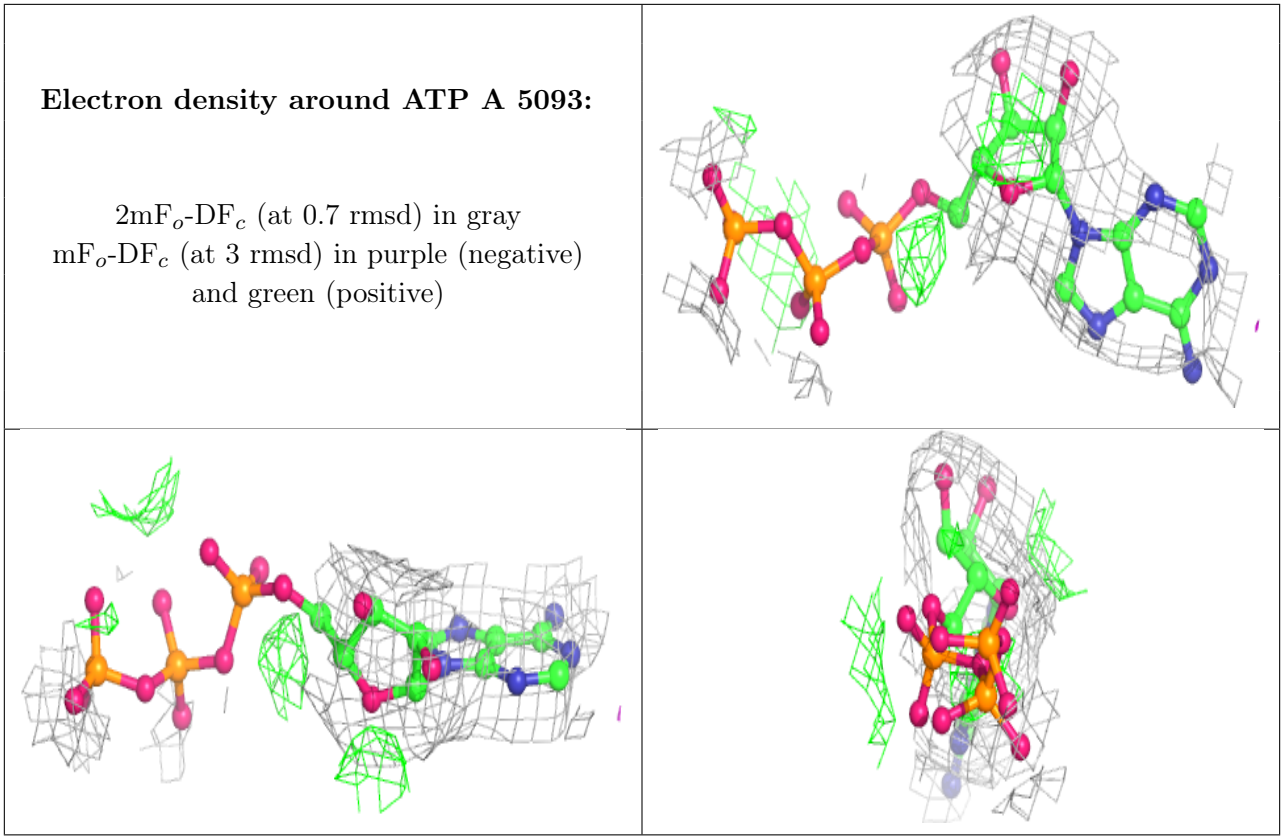
Electron density around ATP B 5093:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.