



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:53 pm BST

PDB ID : 4RH7  
Title : Crystal structure of human cytoplasmic dynein 2 motor domain in complex with ADP.Vi  
Authors : Schmidt, H.; Zalyte, R.; Urnavicius, L.; Carter, A.P.  
Deposited on : 2014-10-01  
Resolution : 3.41 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

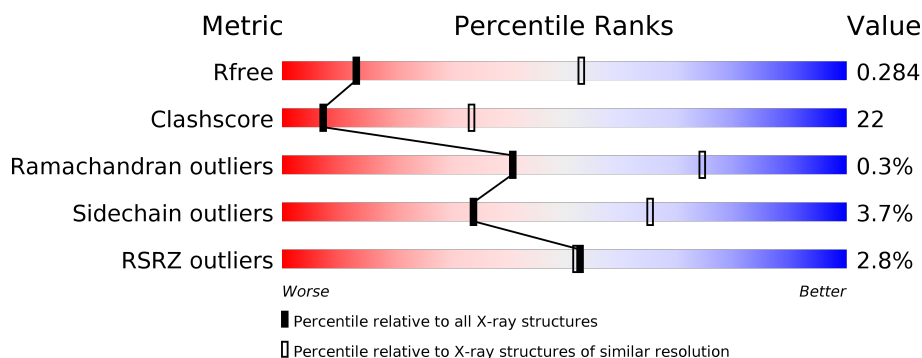
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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  $\geq 3$ , 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	3450	

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	AOV	A	4401	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22816 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.

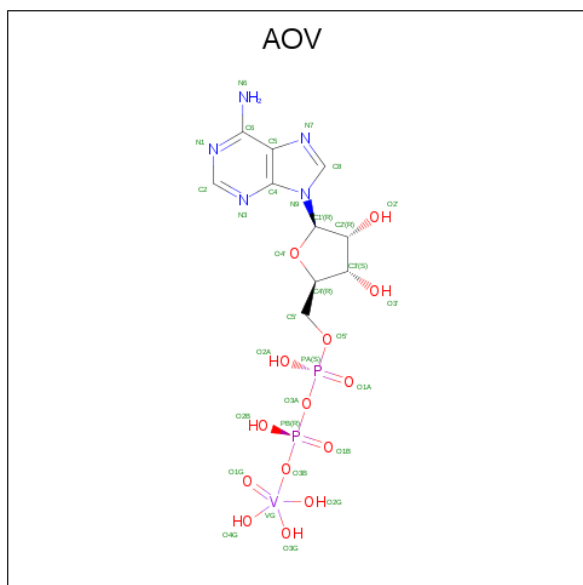
- Molecule 1 is a protein called Green fluorescent protein/Cytoplasmic dynein 2 heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	3005	22697	14414	3922	4263	98	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	GLY	-	LINKER	UNP Q8NCM8
A	1090	SER	-	LINKER	UNP Q8NCM8
A	1413	ARG	LYS	VARIANT	UNP Q8NCM8
A	2871	GLN	ARG	VARIANT	UNP Q8NCM8
A	3680	VAL	ALA	VARIANT	UNP Q8NCM8
A	4308	VAL	-	EXPRESSION TAG	UNP Q8NCM8

- Molecule 2 is ADP ORTHOVANADATE (three-letter code: AOV) (formula:  $C_{10}H_{17}N_5O_{14}P_2V$ ).

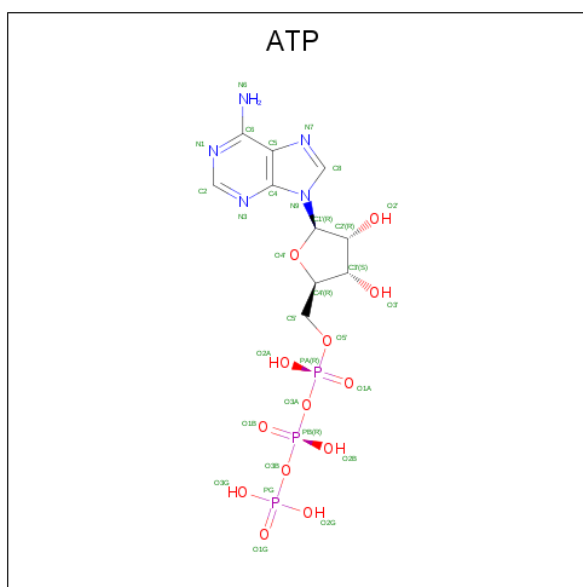


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	0	0
			32	10	5	14	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





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



S3136	V2943	LYS	L2723	A2531	S2429	V2346	D2243	V2163	S2049	L1939	H1819	S1723
V3137	Q2944	GLU	L2723	R2532	I2430	R2347	L2249	V2164	S2050	L1939	H1820	F1728
Q3138	D2945	GLU	L2626	R2533	I2431	P2348	L2249	E2165	W2051	L1943	D1821	F1728
A2946	A2946	LYS	L2730	L2534	Y2432	P2348	D2253	T2166	I2052	K1944	N1822	N1729
S2947	S2947	LYS	L2628	F2535	R2435	C2351	F2254	S2167	D2055	I1955	E1823	G1730
E2948	E2948	LYS	L2629	R2536	R2435	E2352	S2255	L2168	D2055	I1955	L1824	L1731
Q2949	Q2949	ASN	L2632	E2544	I2441	R2353	N2256	V2169	E2064	P1956	L1825	V1732
K2950	K2950	SER	E2632	L2545	Y2442	L2355	G2257	G2170	S2065	A1962	V1828	W1737
L2951	E2745	D2848	V2633	F2548	G2444	L2356	L2258	V2172	L2066	L1963	I1829	G1738
E2952	P2746	P2849	E2635	D2549	L2445	L2357	Q2264	N2174	N2067	L1964	F1740	F1739
L2953	L2749	P2750	R2639	L2550	E2447	D2360	Q2264	G2175	L2070	L1965	S1832	D1741
L2956	P2764	F2765	R2642	L2552	P2448	I2361	P2261	E2178	D2071	M1973	F1835	E1742
E2962	F2765	N2766	V2643	L2553	V2449	L2362	P2266	D2072	N2073	I1977	F1849	F1743
E2963	L2856	L2857	V2644	L2553	L2450	L2363	P2266	D2073	R2074	P1980	L1855	L1746
V2964	L2857	L2858	S2645	Q2557	N2453	V2365	Q2269	E2187	L2076	S1981	L1862	L1751
V2965	S2645	F2768	S2645	Q2557	N2453	V2365	Q2269	E2187	L2076	S1981	W1864	S1752
V2975	S2850	T2769	S2857	W2580	I2469	L2366	R2270	I2196	F2092	C1997	G1865	I1758
K2979	L2651	Y2770	G2658	V2573	L2468	L2367	R2270	I2196	E2095	R1993	L1866	W1781
G3019	L2652	R2771	G2660	V2574	L2469	V2384	F2287	N2199	E2095	A1994	R1867	F1781
G3025	L2653	L2772	L2653	T2575	L2565	V2375	I2288	N2201	A2105	A1995	L1869	N1784
F3037	R2656	Q2773	R2656	G2577	D2566	V2375	P2292	R2205	R2109	C1997	L1879	I1787
F3037	S2857	Q2774	S2857	G2577	D2566	V2375	E2293	R2205	E2293	C1997	Q1882	F1788
L3067	G2658	M2782	G2659	V2573	L2468	L2383	F2287	N2199	E2095	R1993	Q1882	F1788
K3071	G2661	K2802	R2661	T2575	L2565	V2384	I2288	N2201	A2105	A1995	L1869	N1784
P3076	R2662	C2803	R2662	G2577	D2566	V2375	P2292	R2205	E2293	C1997	L1879	I1787
K3080	L2664	Q2804	L2664	A2578	V2486	E2390	G2294	F2208	M2112	T1999	Q1882	F1788
A3087	T2665	V2805	T2665	H2580	P2496	E2391	G2294	F2208	I2113	G2000	L1790	I1789
Y3099	V2668	L2806	V2668	G2583	C2497	L2397	G2296	T2209	F2114	V2002	E1894	W1791
L3103	L2676	G2810	L2676	ALA	I2493	L2397	L2301	V2212	S2116	Q2005	S1895	N1792
H3119	R2683	W2811	R2683	ALA	I2493	E2398	L2301	V2212	S2116	Q2005	S1895	N1792
L3120	G2684	S2812	G2684	ALA	I2493	E2398	L2301	V2212	S2116	Q2005	S1895	N1792
K3121	V2685	M2816	V2685	A2587	W2502	L2399	Q2307	W2215	R2131	Y2006	Q1900	G1796
K3122	V2685	L2819	V2685	A2587	W2502	L2399	Q2307	W2215	R2131	Y2006	Q1900	G1796
K3123	Q2699	P2820	Q2699	Q2590	D2510	L2402	S2310	S2219	R2132	K2011	L1902	G1799
K3124	E2704	E2826	E2704	P2591	D2510	L2402	S2310	S2219	R2132	K2011	L1902	G1799
K3125	A2705	GLY	A2705	L2592	L2511	W2406	Q2312	A2152	Q2133	T1906	T1906	A1801
K3126	Q2706	GLY	Q2706	P2593	E2512	R2441	F2223	A2152	Q2133	T1906	T1906	A1801
K3127	Q2706	GLY	Q2706	P2593	E2512	R2441	F2223	A2152	Q2133	T1906	T1906	A1801
K3128	E2704	GLY	E2704	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3129	A2705	GLY	A2705	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3130	Q2706	GLY	Q2706	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3131	Q2706	GLY	Q2706	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3132	Q2706	GLY	Q2706	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3133	Q2706	GLY	Q2706	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3134	Q2706	GLY	Q2706	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
K3135	Q2706	GLY	Q2706	L2595	H2517	R2444	C2318	Q2154	E2136	M1907	M1907	Q1802
F3238	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
D3239	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
L3240	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
L3241	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
L3242	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
L3243	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
L3244	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235
L3245	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235	L3235

S4239	I4150	R4033	D3932	Y3830	K3711	ILE	R3525	D3357	S3248
P4240	I4151	E4034	R3953	E3831	L3718	ARG	R3525	D3357	E3249
S4241	Q4152		Y3934	L3836	E3719	R3612	N3533	N3363	I3252
V4245	N4153	S4037	Y3939	L3837	I3720	E3621	D3536	F3366	E3256
L4246	N4154	N4038	Y3943	L3840	E3721	R3622	R3543	R3367	D3261
P4247	K4157	E4039	L3944	M3841	Q3730	L3629	I3544	L3368	D3262
C4248	L4164	S4041	L3944	R3842	A3731	A3632	Q3546	F3369	D3370
P4249	S4165	P4042	Y3952	T3843	D3732	A3633	Q3546	S3371	
W4252	E4166	V4043	Y3953	Y3844	P3733	P3634	I3548	T3372	V3270
I4253	T4167	L4046	ASP	W3847	E3736	S3635	L3551	R3373	I3271
P4254	S4171		VAL	K3854	L3740	L3636	Q3552	N3374	L3272
Q4255	E4172	N4051	PHE	K3854	L3740	L3636	Q3552	P3375	Q3273
E4265	E4172	Q4052	ASN	K3854	L3740	L3636	Q3552	N3376	
C4266	D4177	N4053	GLN	N3857	Y3750	T3639	V3555	P3377	V3276
I4267	S4054	S4054	ARG	T3858	Y3750	C3641	V3555	C3277	C3277
S4268	N4055	N4055	ASN	H3859	M3755	P3642	C3560	I3379	P3278
L4269	L4056	L4057	LYS	R3860	Q3756	P3642	C3560	P3380	F3279
P4270	R4184	I4072	SER	L3864	Q3759	W3648	I3563	L3280	I3281
V4271	Q4185	L4073	F3965	L3864	A3760	Y3652	D3567	A3383	S3285
V4281	E4186	S4074	P3966	H3871	D3761	N3653	D3567	A3384	
T4282	T4187	F4075	P3966	H3871	L3762	N3654	M3570	S3385	
N4283	A4188	I4076	Y3869	Q3875	A3771	C3657	F3575	V3387	T3288
I4284	G4192	I4077	S3970	E3876	Q3759	C3657	F3575	T3388	E3289
D4285	T4187	L4078	C3975	R3877	W3776	E3658	V3576	W3290	W3290
V4286	K4199	E4079	C3975	T3881	P3662	P3662	R3577	K3292	K3292
P4287	F4200	Q4080	S3976	P3882	K3780	K3667	G3578	T3293	H3294
C4288	V4201	V4090	I3984	W3885	N3781	K3667	R3579	S3298	L3295
Q4289	A4202	L4094	E3989	Y3900	V3785	S3670	R3580	D3297	L3296
N4291	S4203	L4094	D3990	Y3900	V3785	S3670	P3581	I3451	
Q4292	W4204	L4097	D3991	I3903	W3788	F3672	L3583	D3486	
D4293	L4208	V4100	F3996	D3904	L3789	F3673	F3584		
Q4294	Q4214	T4105	P3999	R3905	P3790	Q3674	Q3585	D3490	
W4295	I4215	L4106	P3999	L3906	V3791	L3675	E3586	A3491	
I4296	K4216	L4106	A4000	F3907	L3792	L3676	N3587	Y3492	
Q4297	I4217	N4001	N4001	D3908	E3793	V3677	E3588	L3493	
C4298		I4002	I4002	G3909	K3794		W3589	P3494	
L4302	L4220	V4111	L4002	A3910	K3802	V3680	D3590	N3309	
F4303	L4221	L4118	Q4007	K3911		L3681	T3591	L3495	
L4304	L4222	P4124	Q4017	Q3914	F3805	R3682	V3595	F3320	
N4306	E4223	W4127	Q4017	W3915	T3810	R3685	VAL	G3321	
Q4307	G4224	W4127	L4021	E3916	T3810	L3686	VAL	K3322	
V4308	C4225	W4127	L4021	F3917	H3814	Q3687	GLY	L3324	
	S4226	P4134	L4022	V3918	P3815	S3688	ASP	I3325	
	F4227	P4134	R4023	V3918	P3815	A3689	MET	I3326	
	D4228	P4137	S4024	H3919	P3819	K3690	LEU	L3336	
	G4229	L4138	L4025	G3920	P3819	P3693	ARG	Y3337	
	N4230	Y4139	T4026	L3921	L3821	F3693	LYS	P3338	
	Q4231	Y4140	A4027	L3922	L3822	K3701	ALA	N3513	
	L4232	S4029	G4028	A3925	L3822	K3701	ASP	N3514	
	Q4236	R4147	S4029	A3925	L3822	K3701	SER	N3515	
	L4237	F4031	R4030	G3929	P3705	P3705	GLN	Y3516	
	D4238	L4149	D4032	G3929	L3826	L3710	LYS	R3517	
					T3829			F3518	



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.03Å 487.15Å 276.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.60 – 3.41 56.54 – 3.41	Depositor EDS
% Data completeness (in resolution range)	62.2 (56.60-3.41) 62.2 (56.54-3.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.237 , 0.285 0.239 , 0.284	Depositor DCC
$R_{free}$ test set	3915 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 110.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AOV, MG, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.61	2/23147 (0.0%)	0.78	5/31474 (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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2275	PHE	CB-CG	-5.18	1.42	1.51
1	A	2826	GLU	CD-OE2	5.06	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2426	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	2275	PHE	CB-CA-C	-5.82	98.76	110.40
1	A	1915	CYS	CA-CB-SG	5.68	124.22	114.00
1	A	4253	ILE	CB-CA-C	-5.50	100.59	111.60
1	A	2426	ARG	NE-CZ-NH2	5.42	123.01	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	LEU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	2247	GLU	Peptide
1	A	2275	PHE	Peptide
1	A	2310	SER	Peptide
1	A	2416	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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	22697	0	21503	995	0
2	A	32	0	12	12	0
3	A	2	0	0	0	0
4	A	31	0	12	4	0
5	A	54	0	24	10	0
All	All	22816	0	21551	996	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 22.

The worst 5 of 996 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:3581:PRO:HA	1:A:3584:PHE:CE1	1.16	1.63
1:A:2284:LYS:CE	1:A:2401:GLN:HG3	1.33	1.55
1:A:2284:LYS:HE3	1:A:2401:GLN:CG	1.49	1.40
1:A:3291:LEU:O	1:A:3294:HIS:CE1	1.75	1.39
1:A:3581:PRO:CA	1:A:3584:PHE:CE1	2.04	1.38

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2995/3450 (87%)	2834 (95%)	153 (5%)	8 (0%)	41 74

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1820	PRO
1	A	3965	PHE
1	A	1589	SER
1	A	1645	VAL
1	A	3375	PRO

### 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	2286/3065 (75%)	2201 (96%)	85 (4%)	34 65

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3336	LEU
1	A	3584	PHE
1	A	4215	ILE
1	A	3343	ASP
1	A	3495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2362	ASN
1	A	2391	ASN

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Mol	Chain	Res	Type
1	A	3738	GLN
1	A	2269	GLN
1	A	2777	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	ADP	A	4405	-	24,29,29	1.07	1 (4%)	29,45,45	1.67	7 (24%)
5	ADP	A	4406	-	24,29,29	1.12	1 (4%)	29,45,45	1.65	7 (24%)
4	ATP	A	4403	3	26,33,33	0.88	1 (3%)	31,52,52	1.99	5 (16%)
2	AOV	A	4401	3	27,34,34	5.35	3 (11%)	26,56,56	1.55	3 (11%)

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
5	ADP	A	4405	-	-	3/12/32/32	0/3/3/3
5	ADP	A	4406	-	-	0/12/32/32	0/3/3/3
4	ATP	A	4403	3	-	0/18/38/38	0/3/3/3
2	AOV	A	4401	3	-	0/12/39/39	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4401	AOV	O1G-VG	27.32	2.10	1.61
5	A	4406	ADP	PB-O1B	3.16	1.60	1.50
2	A	4401	AOV	C5-C4	2.50	1.47	1.40
2	A	4401	AOV	C2-N3	2.37	1.35	1.32
5	A	4405	ADP	C4-N3	-2.31	1.32	1.35

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4403	ATP	PA-O3A-PB	-6.39	110.88	132.83
4	A	4403	ATP	PB-O3B-PG	-6.11	111.86	132.83
2	A	4401	AOV	PA-O3A-PB	-4.77	116.47	132.83
5	A	4405	ADP	C4-C5-N7	-4.16	105.06	109.40
2	A	4401	AOV	C4-C5-N7	-3.87	105.36	109.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4405	ADP	C5'-O5'-PA-O2A
5	A	4405	ADP	C5'-O5'-PA-O3A
5	A	4405	ADP	O4'-C4'-C5'-O5'

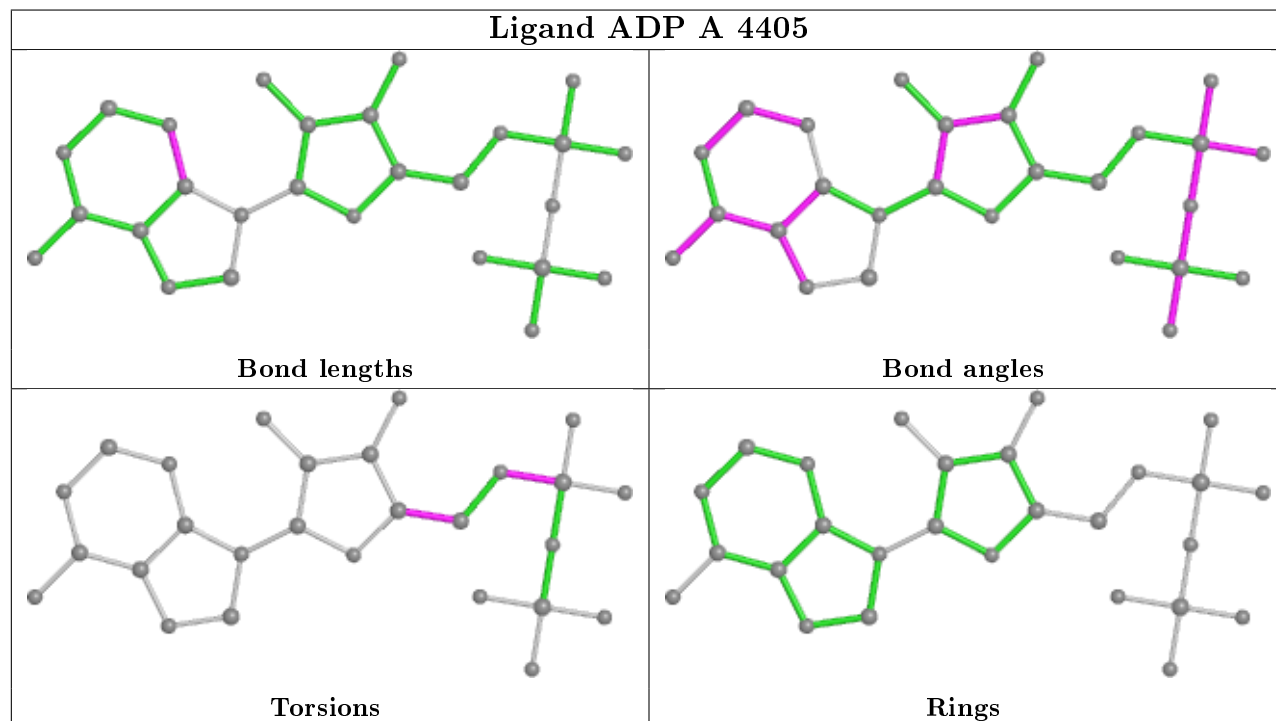
There are no ring outliers.

4 monomers are involved in 26 short contacts:

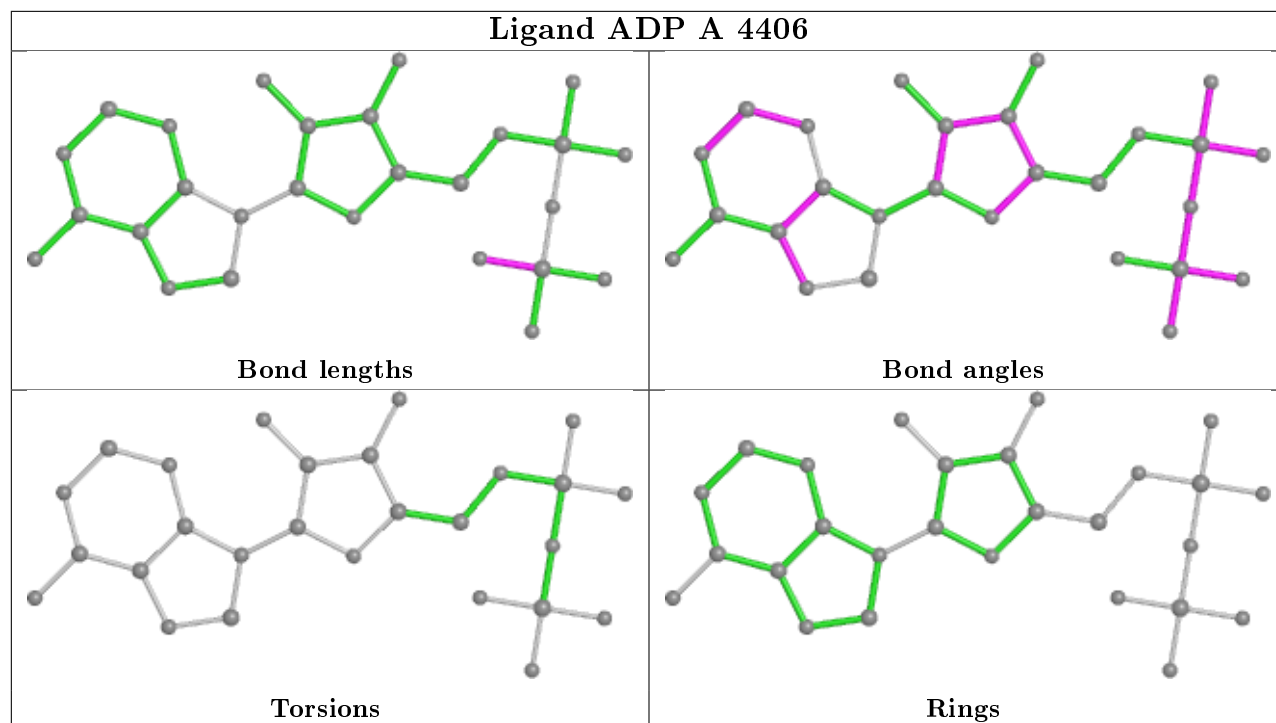
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4405	ADP	5	0
5	A	4406	ADP	5	0
4	A	4403	ATP	4	0
2	A	4401	AOV	12	0

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

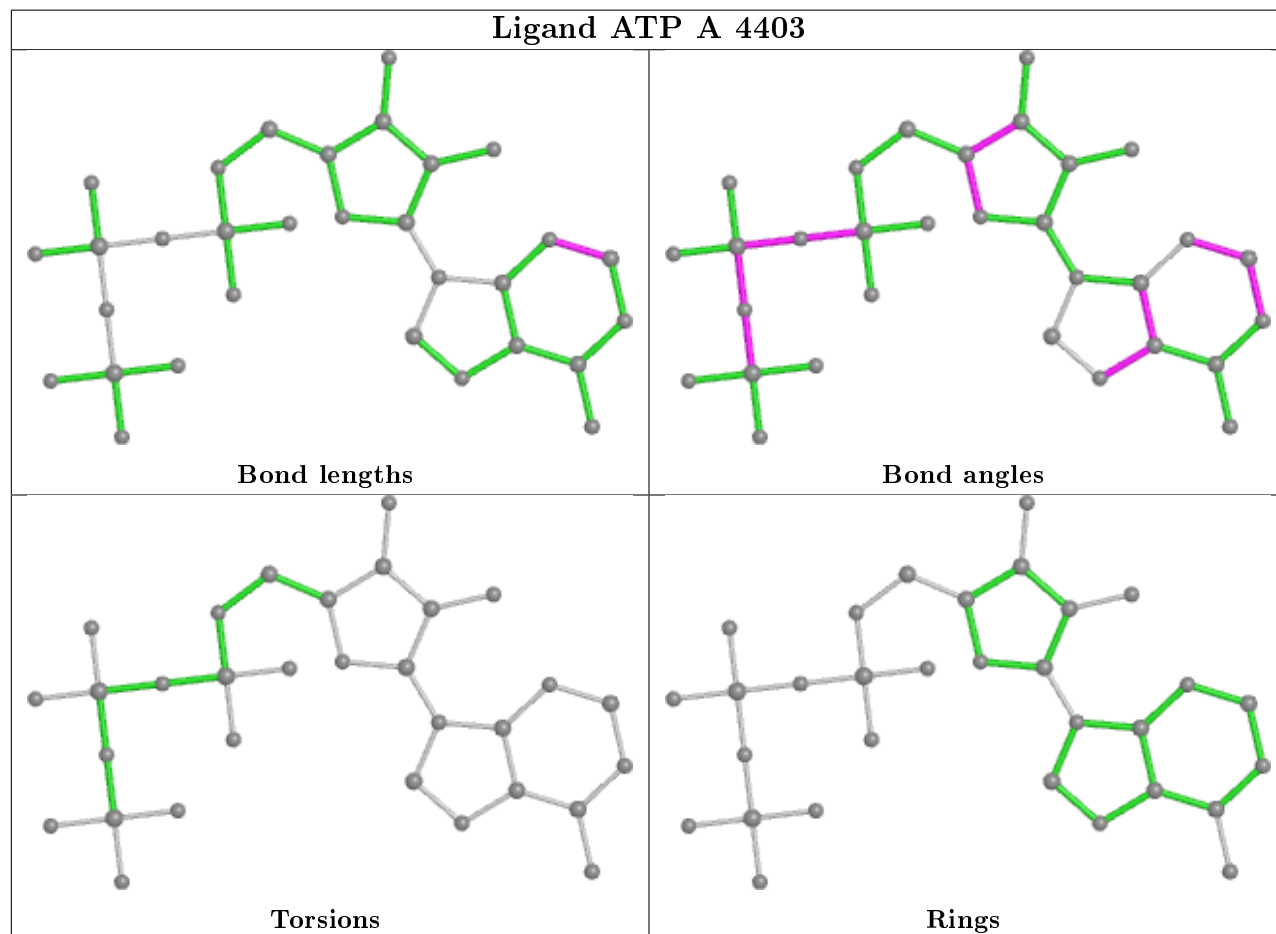
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



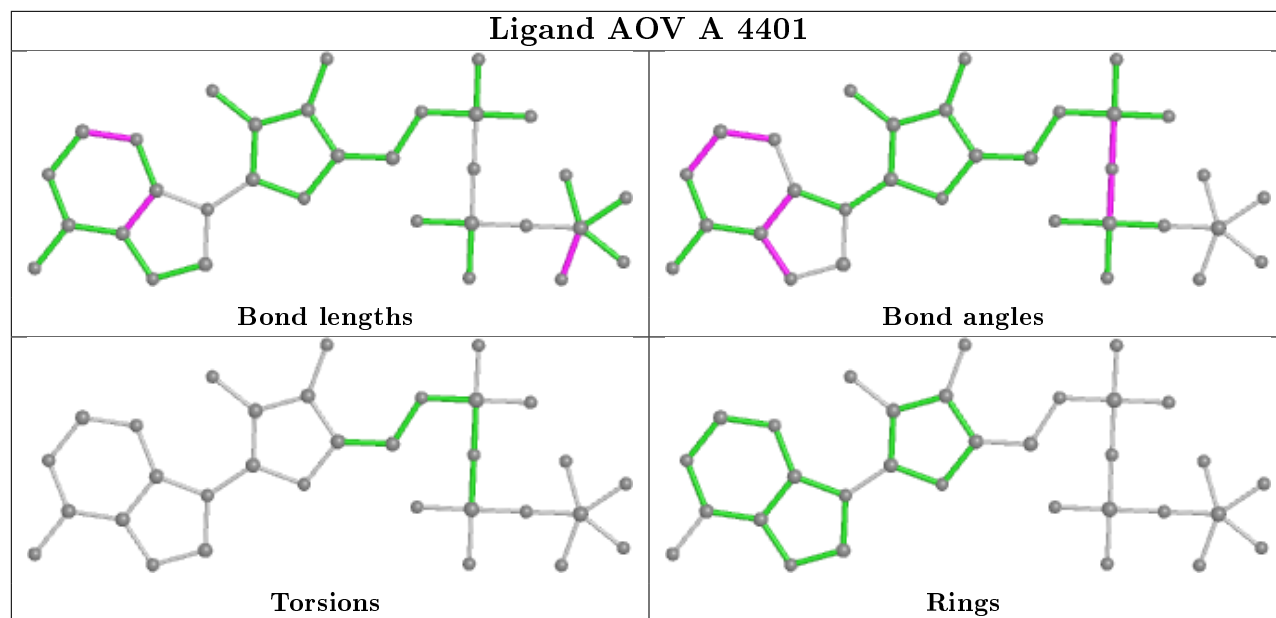
## Ligand ADP A 4406



## Ligand ATP A 4403







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	3005/3450 (87%)	-0.31	85 (2%) 53 52	39, 110, 274, 477	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3130	LEU	8.1
1	A	2975	ASP	5.9
1	A	3136	SER	5.5
1	A	2942	SER	4.7
1	A	2946	ALA	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

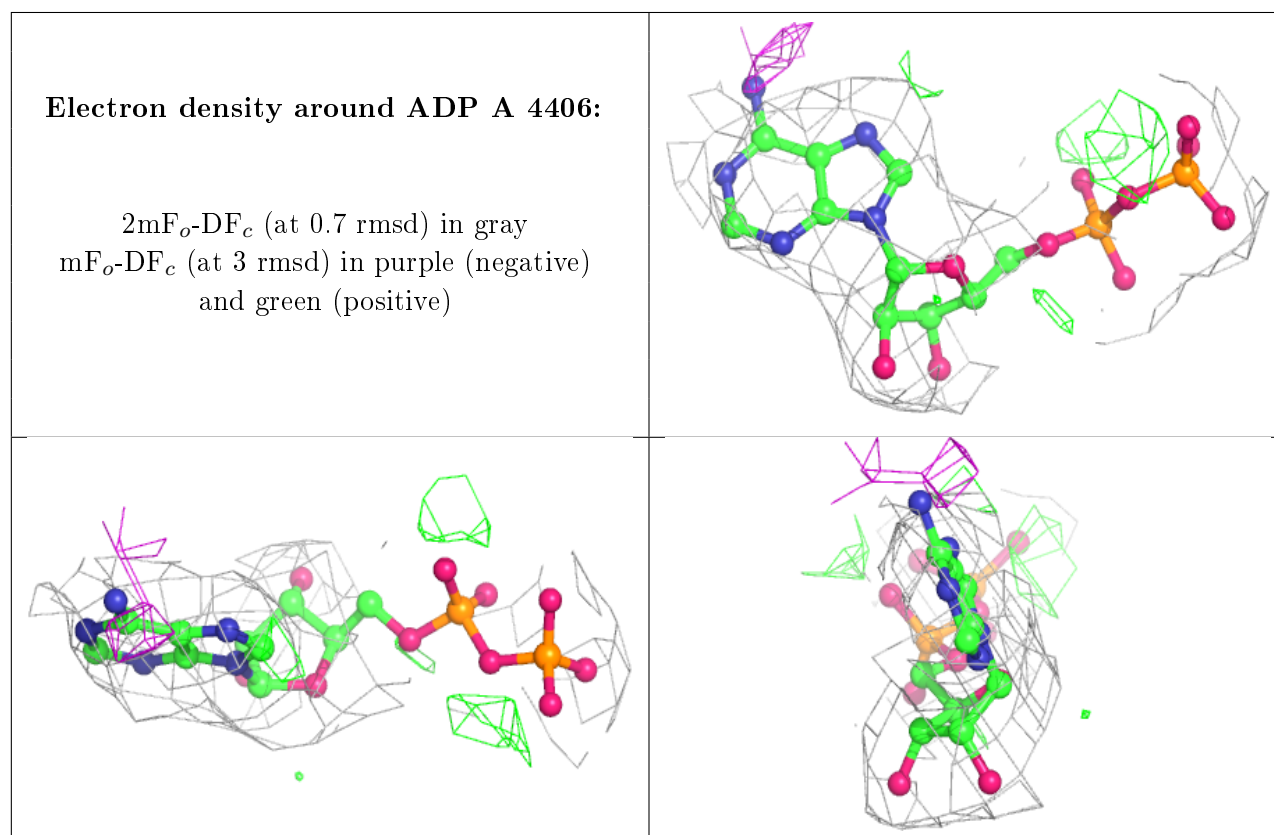
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ADP	A	4406	27/27	0.95	0.20	66,85,103,111	0
5	ADP	A	4405	27/27	0.97	0.18	42,46,57,61	0

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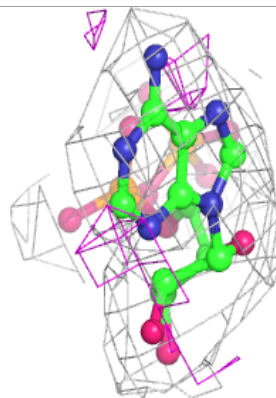
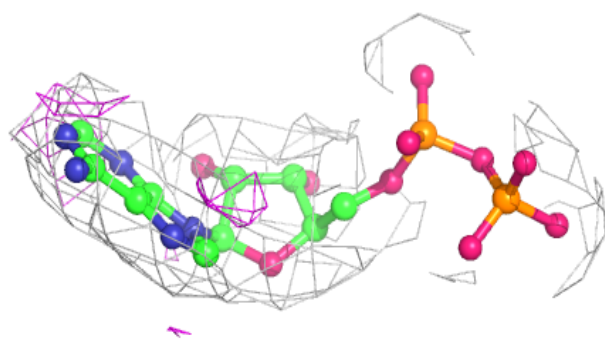
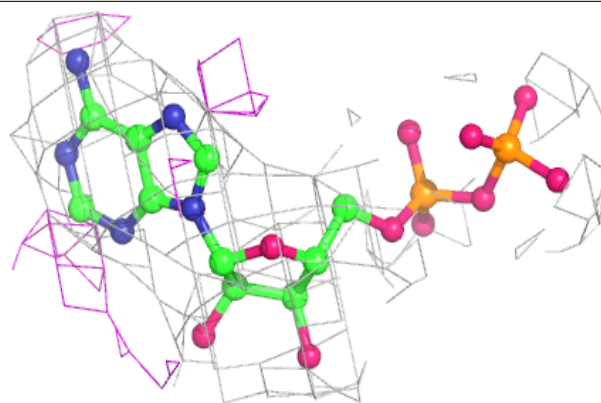
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	A	4403	31/31	0.97	0.18	49,80,97,108	0
2	AOV	A	4401	32/32	0.98	0.20	41,69,88,93	0
3	MG	A	4402	1/1	0.99	0.21	31,31,31,31	0
3	MG	A	4404	1/1	1.00	0.22	22,22,22,22	0

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.

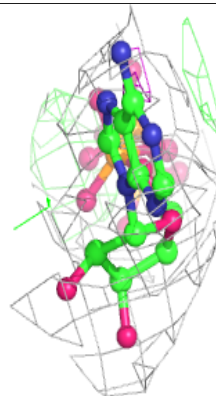
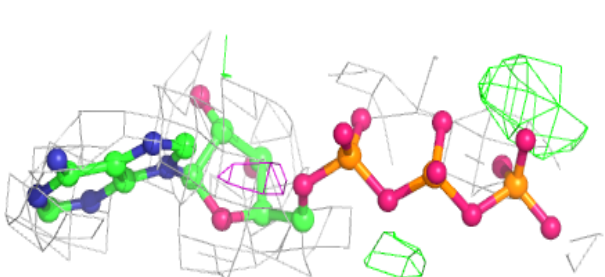
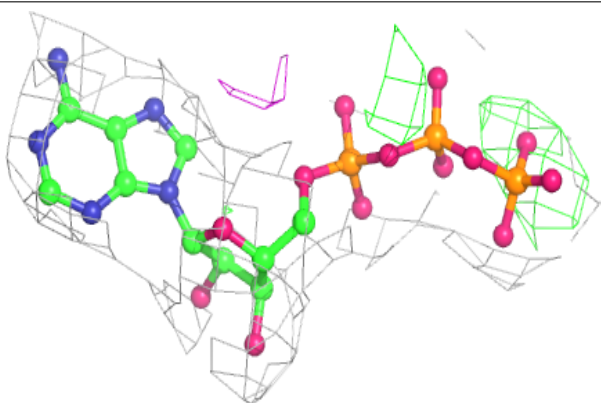


**Electron density around ADP A 4405:**

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

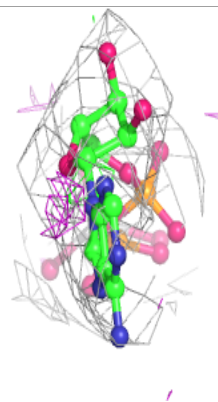
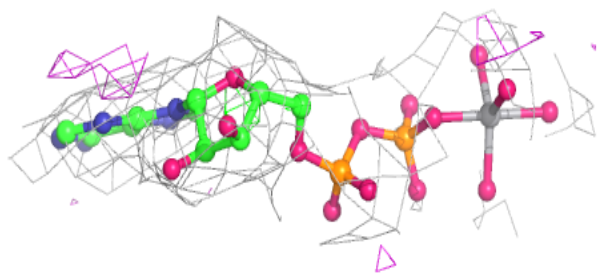
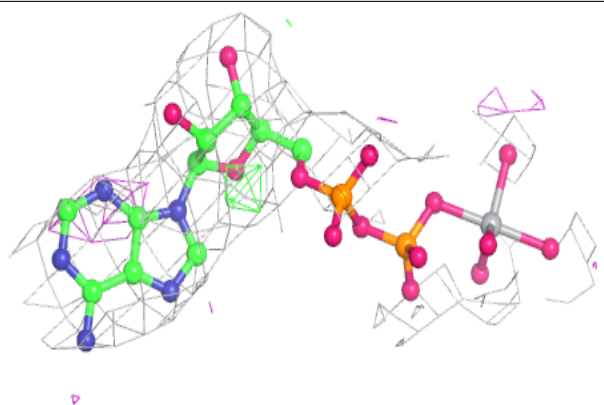
**Electron density around ATP A 4403:**

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



**Electron density around AOV A 4401:**

$2mF_o-DF_c$  (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.