wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 07:47 am GMT

PDB ID	:	6H78
Title	:	E1 enzyme for ubiquitin like protein activation.
Authors	:	Soudah, N.; Padala, P.; Hassouna, F.; Mashahreh, B.; Lebedev, A.A.; Isupov, M.N.; Cohen-Kfir, E.; Wiener, R.
Deposited on	:	2018-07-30
Resolution	:	2.70 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:

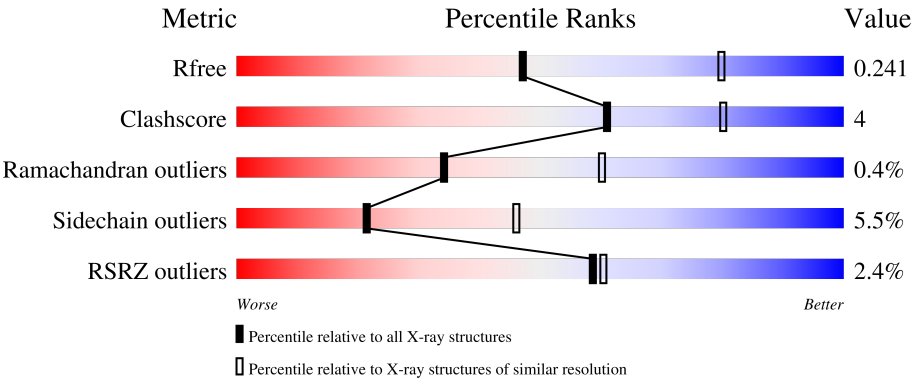
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	300	2% 82% 11% • 6%
1	B	300	3% 80% 12% • 7%
1	C	300	2% 79% 15% • 5%
1	D	300	2% 78% 11% • 9%
1	E	300	% 80% 14% • 5%

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Mol	Chain	Length	Quality of chain
1	F	300	2% 79% 12% 10%
1	G	300	% 80% 11% • 8%
1	H	300	2% 80% 13% 7%
1	I	300	% 86% 7% • 7%
1	J	300	5% 77% 15% • 7%
1	K	300	3% 79% 11% • 8%
1	L	300	% 77% 15% • 7%
1	M	300	2% 79% 9% • 10%
1	N	300	4% 82% 12% • 5%
1	O	300	2% 78% 11% • 10%
1	P	300	3% 82% 13% • 5%

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	MG	O	404	-	-	-	X
5	EDO	P	405	-	-	-	X

2 Entry composition (i)

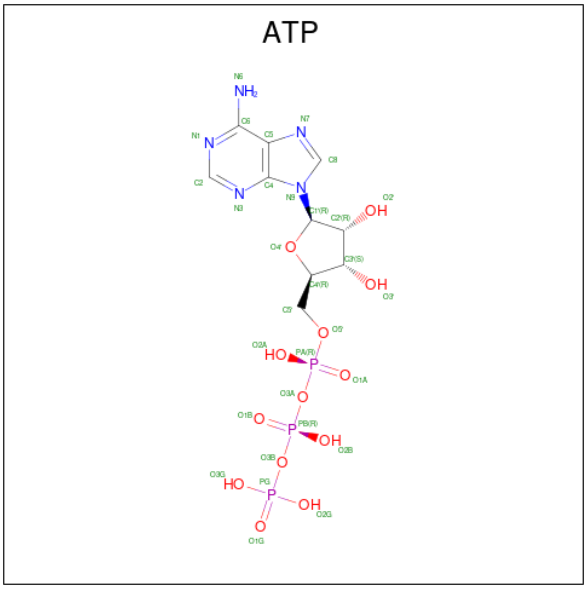
There are 7 unique types of molecules in this entry. The entry contains 36069 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ubiquitin-like modifier-activating enzyme 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	2	0
			2194	1384	380	410	20			
1	B	278	Total	C	N	O	S	0	0	0
			2138	1348	368	402	20			
1	C	286	Total	C	N	O	S	0	0	0
			2207	1391	381	415	20			
1	D	272	Total	C	N	O	S	0	0	0
			2098	1322	361	395	20			
1	E	286	Total	C	N	O	S	0	2	0
			2221	1400	385	416	20			
1	F	271	Total	C	N	O	S	0	1	0
			2097	1322	363	392	20			
1	G	276	Total	C	N	O	S	0	0	0
			2125	1341	366	398	20			
1	H	280	Total	C	N	O	S	0	2	0
			2173	1371	374	407	21			
1	I	280	Total	C	N	O	S	0	3	0
			2183	1378	377	407	21			
1	J	279	Total	C	N	O	S	0	2	0
			2165	1364	378	403	20			
1	K	276	Total	C	N	O	S	0	1	0
			2130	1346	365	399	20			
1	L	280	Total	C	N	O	S	0	1	0
			2169	1368	374	407	20			
1	M	270	Total	C	N	O	S	0	0	0
			2085	1315	359	391	20			
1	N	286	Total	C	N	O	S	0	1	0
			2215	1396	384	415	20			
1	O	271	Total	C	N	O	S	0	2	0
			2102	1325	364	393	20			
1	P	286	Total	C	N	O	S	0	0	0
			2207	1391	381	415	20			

- 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		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- 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		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		
3	G	2	Total	Mg	0	0
			2	2		
3	H	2	Total	Mg	0	0
			2	2		
3	I	2	Total	Mg	0	0
			2	2		
3	J	2	Total	Mg	0	0
			2	2		
3	K	2	Total	Mg	0	0
			2	2		
3	L	2	Total	Mg	0	0
			2	2		
3	M	2	Total	Mg	0	0
			2	2		
3	N	2	Total	Mg	0	0
			2	2		
3	O	2	Total	Mg	0	0
			2	2		

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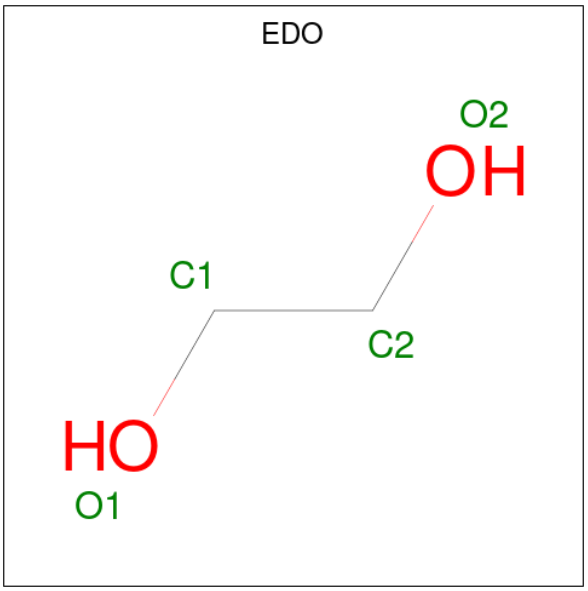
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	2	Total Mg 2 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0
4	M	1	Total Zn 1 1	0	0
4	N	1	Total Zn 1 1	0	0
4	O	1	Total Zn 1 1	0	0
4	P	1	Total Zn 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	79	Total O 79 79	0	0
7	B	49	Total O 49 49	0	0
7	C	40	Total O 40 40	0	0
7	D	57	Total O 57 57	0	0
7	E	56	Total O 56 56	0	0
7	F	57	Total O 57 57	0	0
7	G	55	Total O 55 55	0	0
7	H	53	Total O 53 53	0	0
7	I	67	Total O 67 67	0	0

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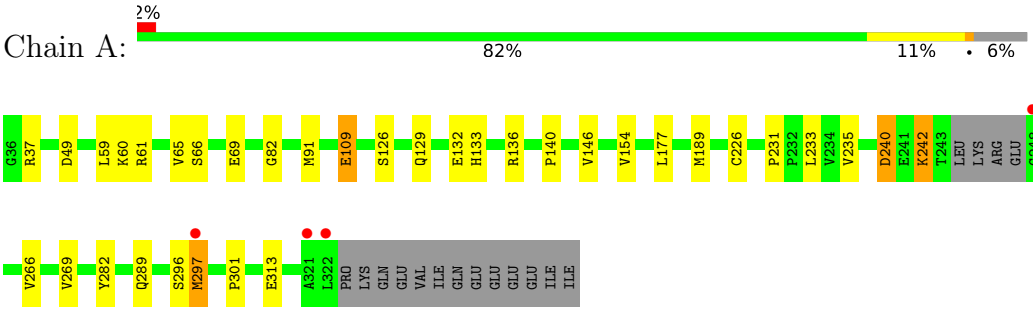
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	60	Total O 60 60	0	0
7	K	52	Total O 52 52	0	0
7	L	64	Total O 64 64	0	0
7	M	45	Total O 45 45	0	0
7	N	37	Total O 37 37	0	0
7	O	42	Total O 42 42	0	0
7	P	34	Total O 34 34	0	0

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.

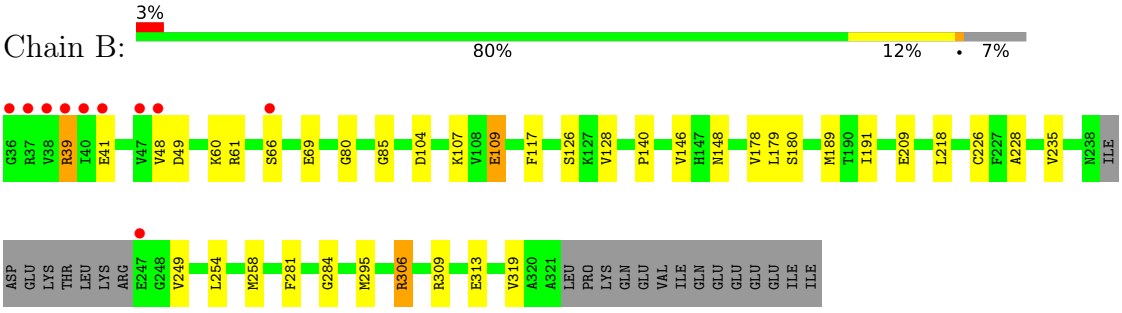
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain A:



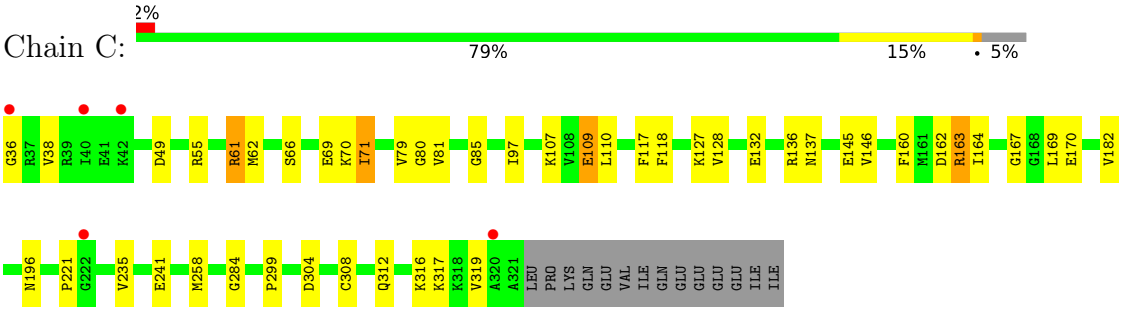
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain B:



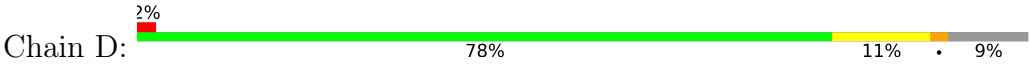
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

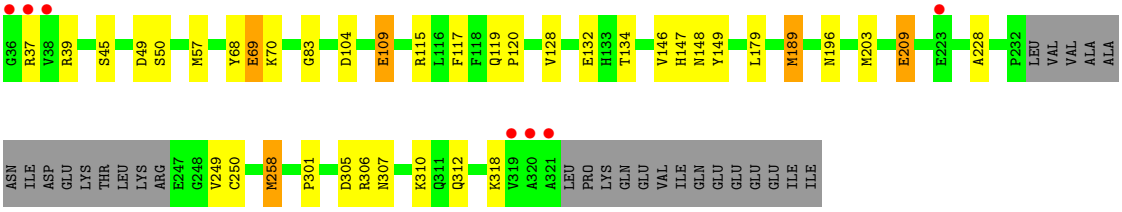
Chain C:



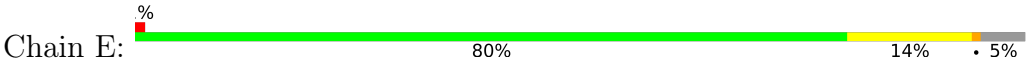
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

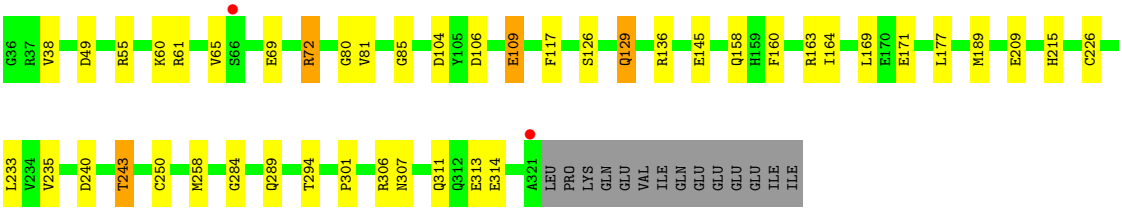
Chain D:



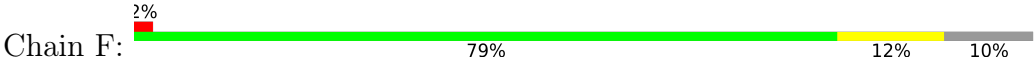


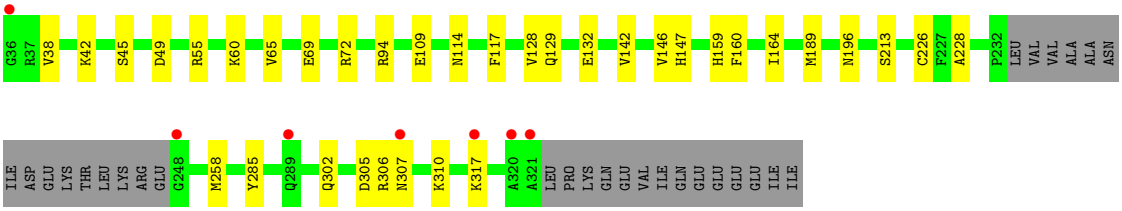
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5



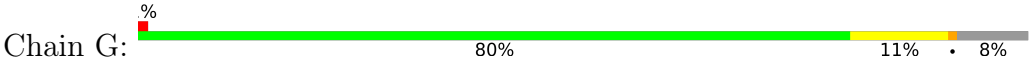


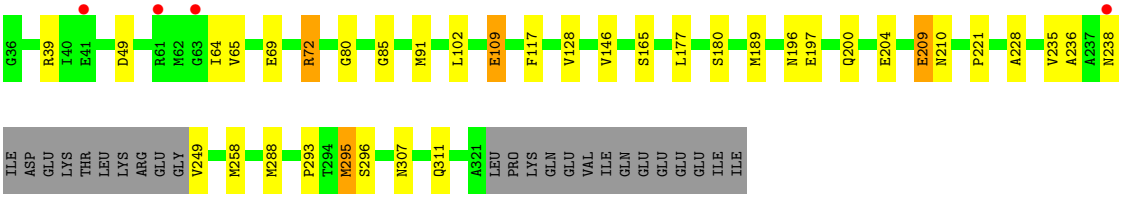
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5



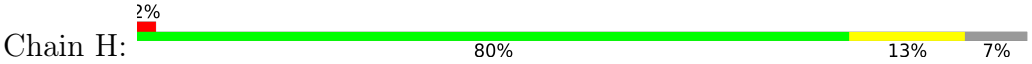


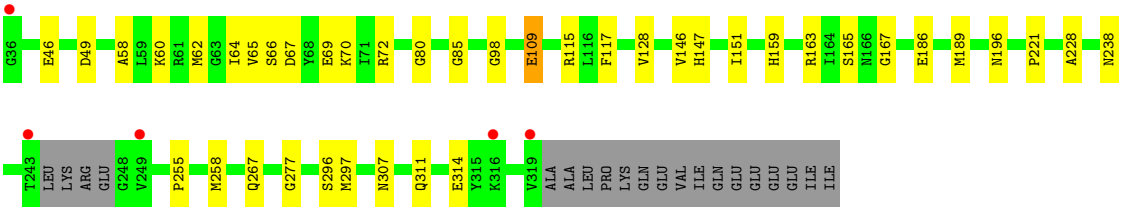
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5





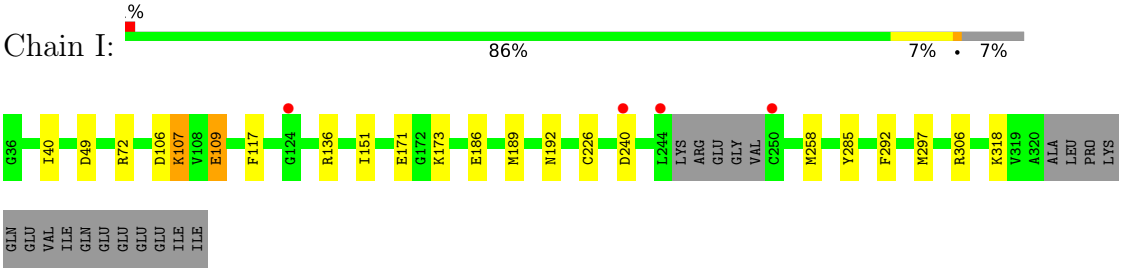
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5





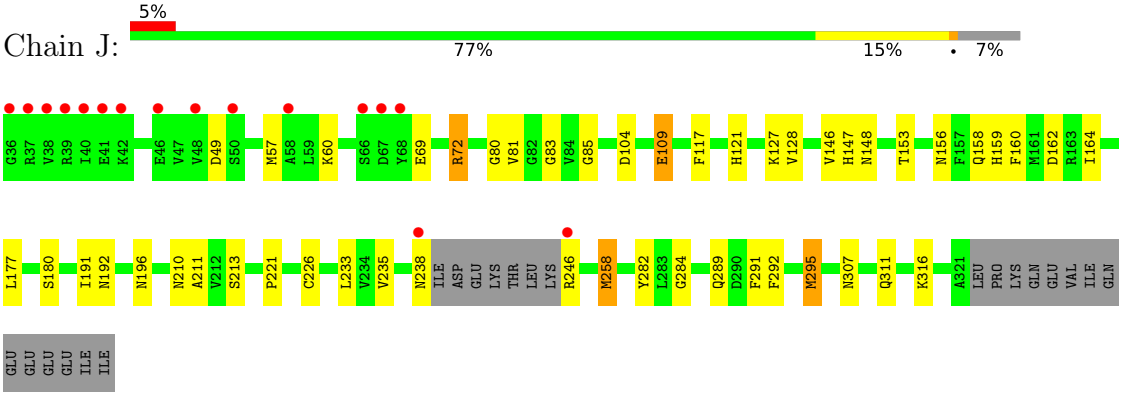
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain I:



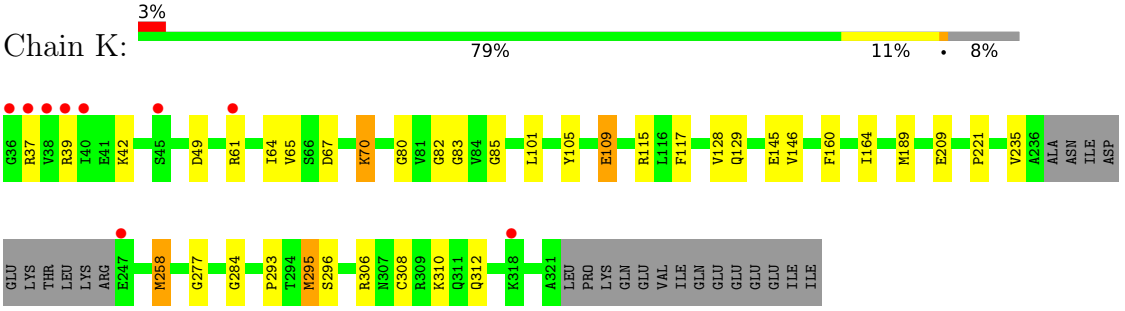
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain J:



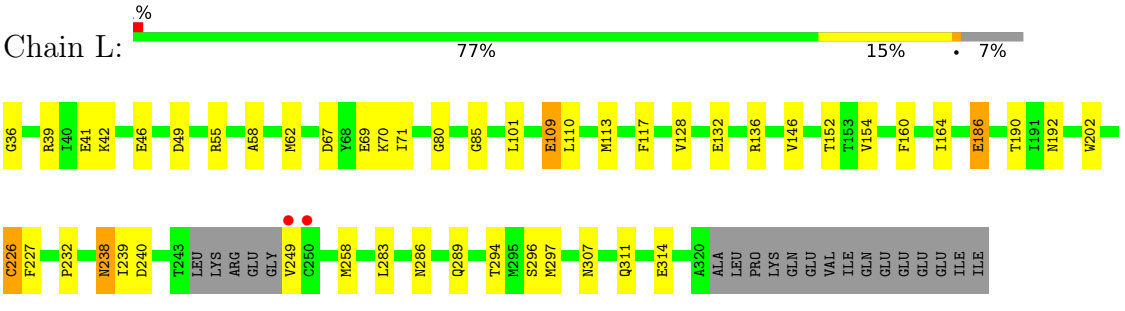
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain K:



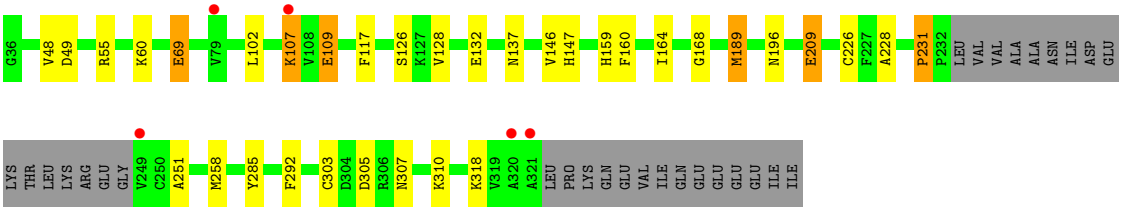
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain L:

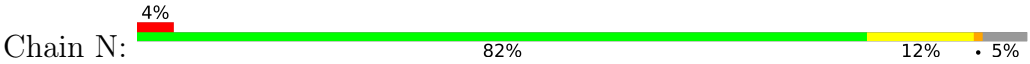


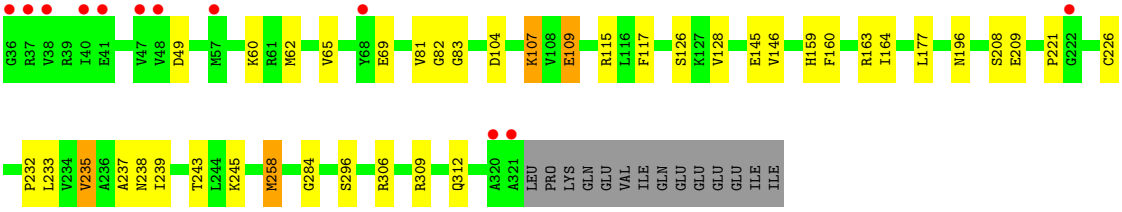
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5

Chain M:

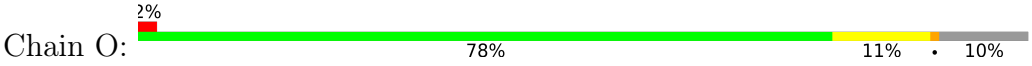


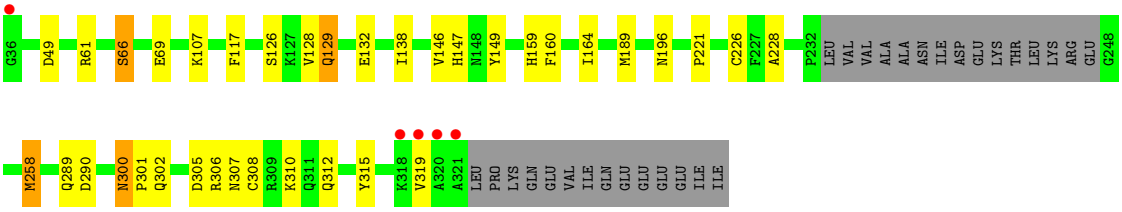
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5



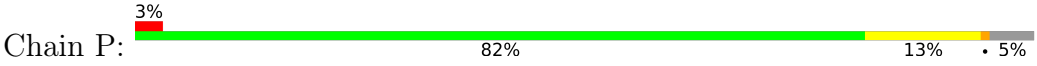


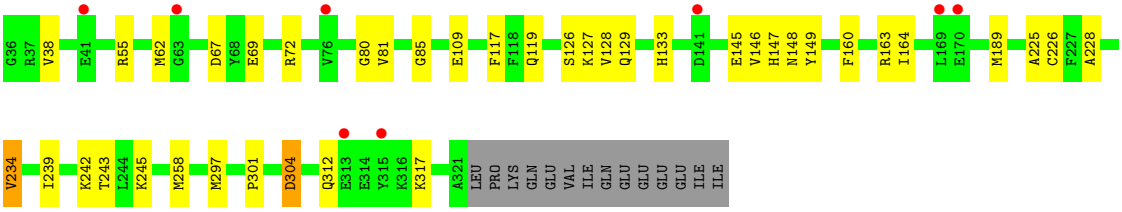
• Molecule 1: Ubiquitin-like modifier-activating enzyme 5





• Molecule 1: Ubiquitin-like modifier-activating enzyme 5





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	143.86Å 151.93Å 153.54Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	107.98 – 2.70 107.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.4 (107.98-2.70) 87.4 (107.75-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.190 , 0.242 0.189 , 0.241	Depositor DCC
R_{free} test set	1693 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	36069	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: ZN, EDO, ATP, CL, MG

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	0.35	0/2237	0.71	0/3022
1	B	0.37	0/2175	0.72	0/2940
1	C	0.35	0/2245	0.73	0/3034
1	D	0.39	0/2135	0.73	0/2884
1	E	0.35	0/2265	0.73	1/3060 (0.0%)
1	F	0.39	0/2137	0.75	0/2886
1	G	0.36	0/2162	0.72	0/2923
1	H	0.36	0/2216	0.70	0/2993
1	I	0.35	0/2229	0.72	0/3010
1	J	0.36	0/2208	0.72	0/2982
1	K	0.35	0/2170	0.71	0/2933
1	L	0.38	0/2209	0.72	0/2985
1	M	0.37	0/2122	0.72	0/2867
1	N	0.33	0/2256	0.69	0/3048
1	O	0.38	0/2145	0.71	0/2897
1	P	0.34	0/2245	0.68	0/3034
All	All	0.36	0/35156	0.72	1/47498 (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	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	K	0	1
1	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	129	GLN	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136[A]	ARG	Sidechain
1	A	136[B]	ARG	Sidechain
1	E	72	ARG	Sidechain
1	F	94	ARG	Sidechain
1	G	39	ARG	Sidechain

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	2194	0	2196	21	0
1	B	2138	0	2124	21	0
1	C	2207	0	2203	27	0
1	D	2098	0	2079	29	0
1	E	2221	0	2224	21	0
1	F	2097	0	2086	18	0
1	G	2125	0	2115	23	0
1	H	2173	0	2171	18	0
1	I	2183	0	2188	10	0
1	J	2165	0	2163	32	0
1	K	2130	0	2124	27	0
1	L	2169	0	2164	28	0
1	M	2085	0	2070	22	0
1	N	2215	0	2216	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2102	0	2092	22	0
1	P	2207	0	2203	18	0
2	A	31	0	12	1	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
2	I	31	0	12	0	0
2	J	31	0	12	0	0
2	K	31	0	12	1	0
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	1	0
2	O	31	0	12	0	0
2	P	31	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	A	12	0	18	1	0
5	B	20	0	30	0	0
5	C	4	0	6	0	0
5	D	12	0	18	1	0
5	E	8	0	12	1	0
5	F	12	0	18	0	0
5	G	12	0	18	1	0
5	H	4	0	6	0	0
5	J	24	0	36	1	0
5	K	8	0	12	0	0
5	L	12	0	18	0	0
5	M	8	0	12	0	0
5	N	4	0	6	1	0
5	O	12	0	18	0	0
5	P	16	0	24	1	0
6	K	1	0	0	0	0
7	A	79	0	0	1	0
7	B	49	0	0	0	0
7	C	40	0	0	2	0
7	D	57	0	0	1	0
7	E	56	0	0	2	0
7	F	57	0	0	0	0
7	G	55	0	0	1	0
7	H	53	0	0	1	0
7	I	67	0	0	1	0
7	J	60	0	0	2	0
7	K	52	0	0	3	0
7	L	64	0	0	3	0
7	M	45	0	0	2	0
7	N	37	0	0	3	0
7	O	42	0	0	2	0
7	P	34	0	0	1	0
All	All	36069	0	34862	312	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 4.

The worst 5 of 312 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:J:72[B]:ARG:HH21	1:J:72[B]:ARG:HG2	1.05	1.08
1:A:49:ASP:HB3	1:B:109:GLU:HG2	1.48	0.95
1:M:49:ASP:HB3	1:N:109:GLU:HG2	1.52	0.91
1:C:49:ASP:HB3	1:D:109:GLU:HG2	1.52	0.91
1:A:301:PRO:HB3	5:A:406:EDO:H11	1.54	0.89

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	281/300 (94%)	271 (96%)	10 (4%)	0	100	100
1	B	274/300 (91%)	260 (95%)	13 (5%)	1 (0%)	34	60
1	C	284/300 (95%)	269 (95%)	14 (5%)	1 (0%)	34	60
1	D	268/300 (89%)	259 (97%)	8 (3%)	1 (0%)	34	60
1	E	286/300 (95%)	276 (96%)	9 (3%)	1 (0%)	41	66
1	F	268/300 (89%)	257 (96%)	10 (4%)	1 (0%)	34	60
1	G	272/300 (91%)	260 (96%)	11 (4%)	1 (0%)	34	60
1	H	278/300 (93%)	269 (97%)	8 (3%)	1 (0%)	34	60
1	I	279/300 (93%)	271 (97%)	7 (2%)	1 (0%)	34	60
1	J	277/300 (92%)	267 (96%)	9 (3%)	1 (0%)	34	60
1	K	273/300 (91%)	259 (95%)	13 (5%)	1 (0%)	34	60
1	L	277/300 (92%)	268 (97%)	8 (3%)	1 (0%)	34	60
1	M	266/300 (89%)	258 (97%)	5 (2%)	3 (1%)	14	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	285/300 (95%)	272 (95%)	12 (4%)	1 (0%)	34 60
1	O	269/300 (90%)	261 (97%)	7 (3%)	1 (0%)	34 60
1	P	284/300 (95%)	271 (95%)	12 (4%)	1 (0%)	34 60
All	All	4421/4800 (92%)	4248 (96%)	156 (4%)	17 (0%)	34 60

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	117	PHE
1	E	117	PHE
1	H	117	PHE
1	I	117	PHE
1	J	117	PHE

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	242/257 (94%)	229 (95%)	13 (5%)	22 47
1	B	235/257 (91%)	221 (94%)	14 (6%)	19 42
1	C	243/257 (95%)	224 (92%)	19 (8%)	12 29
1	D	231/257 (90%)	219 (95%)	12 (5%)	23 49
1	E	245/257 (95%)	225 (92%)	20 (8%)	11 26
1	F	231/257 (90%)	220 (95%)	11 (5%)	25 53
1	G	234/257 (91%)	224 (96%)	10 (4%)	29 57
1	H	241/257 (94%)	229 (95%)	12 (5%)	24 51
1	I	242/257 (94%)	229 (95%)	13 (5%)	22 47
1	J	238/257 (93%)	227 (95%)	11 (5%)	27 54
1	K	235/257 (91%)	225 (96%)	10 (4%)	29 57
1	L	240/257 (93%)	222 (92%)	18 (8%)	13 31
1	M	230/257 (90%)	219 (95%)	11 (5%)	25 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	244/257 (95%)	231 (95%)	13 (5%)	22 48
1	O	232/257 (90%)	223 (96%)	9 (4%)	32 61
1	P	243/257 (95%)	228 (94%)	15 (6%)	18 40
All	All	3806/4112 (93%)	3595 (94%)	211 (6%)	21 46

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	173	LYS
1	K	295	MET
1	P	69	GLU
1	I	258	MET
1	J	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	312	GLN
1	P	148	ASN
1	J	312	GLN
1	P	137	ASN
1	O	300	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 107 ligands modelled in this entry, 49 are monoatomic - leaving 58 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	EDO	J	405	-	3,3,3	0.68	0	2,2,2	0.45	0
5	EDO	G	405	-	3,3,3	0.45	0	2,2,2	0.44	0
2	ATP	L	401	3	26,33,33	0.93	1 (3%)	31,52,52	1.31	3 (9%)
2	ATP	N	401	3	26,33,33	0.82	0	31,52,52	1.61	6 (19%)
5	EDO	P	405	-	3,3,3	0.56	0	2,2,2	0.24	0
5	EDO	E	405	-	3,3,3	0.59	0	2,2,2	0.22	0
5	EDO	O	407	-	3,3,3	0.59	0	2,2,2	0.21	0
5	EDO	P	408	-	3,3,3	0.50	0	2,2,2	0.35	0
5	EDO	M	406	-	3,3,3	0.56	0	2,2,2	0.32	0
2	ATP	H	401	3	26,33,33	1.02	1 (3%)	31,52,52	1.43	4 (12%)
5	EDO	K	405	-	3,3,3	0.43	0	2,2,2	0.57	0
5	EDO	A	406	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EDO	D	405	-	3,3,3	0.60	0	2,2,2	0.16	0
5	EDO	O	406	-	3,3,3	0.48	0	2,2,2	0.43	0
5	EDO	O	405	-	3,3,3	0.41	0	2,2,2	0.70	0
2	ATP	K	401	3	26,33,33	0.92	0	31,52,52	1.62	8 (25%)
2	ATP	D	401	3	26,33,33	0.99	1 (3%)	31,52,52	1.44	4 (12%)
5	EDO	M	405	-	3,3,3	0.49	0	2,2,2	0.79	0
5	EDO	N	405	-	3,3,3	0.48	0	2,2,2	0.25	0
2	ATP	O	401	3	26,33,33	0.99	2 (7%)	31,52,52	1.31	3 (9%)
5	EDO	P	406	-	3,3,3	0.60	0	2,2,2	0.14	0
5	EDO	E	406	-	3,3,3	0.42	0	2,2,2	0.50	0
2	ATP	G	401	3	26,33,33	1.00	2 (7%)	31,52,52	1.37	6 (19%)
5	EDO	H	405	-	3,3,3	0.43	0	2,2,2	0.50	0
5	EDO	B	406	-	3,3,3	0.34	0	2,2,2	0.80	0
5	EDO	C	405	-	3,3,3	0.53	0	2,2,2	0.37	0
2	ATP	I	400	3	26,33,33	0.98	2 (7%)	31,52,52	1.64	9 (29%)
5	EDO	K	406	-	3,3,3	0.57	0	2,2,2	0.24	0
2	ATP	A	401	3	26,33,33	0.98	1 (3%)	31,52,52	1.49	5 (16%)
5	EDO	A	407	-	3,3,3	0.61	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	J	407	-	3,3,3	0.45	0	2,2,2	0.54	0
5	EDO	L	405	-	3,3,3	0.45	0	2,2,2	0.55	0
2	ATP	M	401	3	26,33,33	1.08	3 (11%)	31,52,52	1.40	4 (12%)
5	EDO	L	406	-	3,3,3	0.47	0	2,2,2	0.44	0
5	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.66	0
5	EDO	G	407	-	3,3,3	0.38	0	2,2,2	0.59	0
5	EDO	B	409	-	3,3,3	0.53	0	2,2,2	0.29	0
5	EDO	F	407	-	3,3,3	0.54	0	2,2,2	0.33	0
5	EDO	B	407	-	3,3,3	0.39	0	2,2,2	0.71	0
5	EDO	F	405	-	3,3,3	0.62	0	2,2,2	0.10	0
2	ATP	J	401	3	26,33,33	0.79	0	31,52,52	1.46	3 (9%)
5	EDO	A	405	-	3,3,3	0.39	0	2,2,2	0.58	0
5	EDO	F	406	-	3,3,3	0.35	0	2,2,2	0.68	0
5	EDO	L	407	-	3,3,3	0.49	0	2,2,2	0.51	0
2	ATP	E	401	3	26,33,33	1.06	2 (7%)	31,52,52	1.65	6 (19%)
5	EDO	D	406	-	3,3,3	0.50	0	2,2,2	0.53	0
5	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.42	0
2	ATP	F	401	3	26,33,33	0.96	2 (7%)	31,52,52	1.40	3 (9%)
5	EDO	J	406	-	3,3,3	0.41	0	2,2,2	0.59	0
2	ATP	B	401	3	26,33,33	0.85	2 (7%)	31,52,52	1.78	7 (22%)
5	EDO	G	406	-	3,3,3	0.44	0	2,2,2	0.46	0
5	EDO	J	409	-	3,3,3	0.52	0	2,2,2	0.14	0
2	ATP	C	401	3	26,33,33	0.89	1 (3%)	31,52,52	1.53	6 (19%)
5	EDO	D	407	-	3,3,3	0.46	0	2,2,2	0.57	0
5	EDO	J	408	-	3,3,3	0.56	0	2,2,2	0.38	0
5	EDO	J	410	-	3,3,3	0.53	0	2,2,2	0.36	0
5	EDO	P	407	-	3,3,3	0.55	0	2,2,2	0.32	0
2	ATP	P	401	3	26,33,33	0.99	2 (7%)	31,52,52	1.17	3 (9%)

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	EDO	J	405	-	-	1/1/1/1	-
5	EDO	G	405	-	-	0/1/1/1	-
2	ATP	L	401	3	-	5/18/38/38	0/3/3/3
2	ATP	N	401	3	-	4/18/38/38	0/3/3/3
5	EDO	P	405	-	-	1/1/1/1	-
5	EDO	E	405	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	O	407	-	-	0/1/1/1	-
5	EDO	P	408	-	-	1/1/1/1	-
5	EDO	M	406	-	-	1/1/1/1	-
2	ATP	H	401	3	-	8/18/38/38	0/3/3/3
5	EDO	K	405	-	-	0/1/1/1	-
5	EDO	A	406	-	-	0/1/1/1	-
5	EDO	D	405	-	-	0/1/1/1	-
5	EDO	O	406	-	-	1/1/1/1	-
5	EDO	O	405	-	-	0/1/1/1	-
2	ATP	K	401	3	-	3/18/38/38	0/3/3/3
2	ATP	D	401	3	-	2/18/38/38	0/3/3/3
5	EDO	M	405	-	-	1/1/1/1	-
5	EDO	N	405	-	-	1/1/1/1	-
2	ATP	O	401	3	-	5/18/38/38	0/3/3/3
5	EDO	P	406	-	-	1/1/1/1	-
5	EDO	E	406	-	-	1/1/1/1	-
2	ATP	G	401	3	-	5/18/38/38	0/3/3/3
5	EDO	H	405	-	-	0/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	C	405	-	-	1/1/1/1	-
2	ATP	I	400	3	-	6/18/38/38	0/3/3/3
5	EDO	K	406	-	-	1/1/1/1	-
2	ATP	A	401	3	-	6/18/38/38	0/3/3/3
5	EDO	A	407	-	-	0/1/1/1	-
5	EDO	J	407	-	-	1/1/1/1	-
5	EDO	L	405	-	-	1/1/1/1	-
2	ATP	M	401	3	-	3/18/38/38	0/3/3/3
5	EDO	L	406	-	-	1/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
5	EDO	G	407	-	-	1/1/1/1	-
5	EDO	B	409	-	-	0/1/1/1	-
5	EDO	F	407	-	-	1/1/1/1	-
5	EDO	B	407	-	-	1/1/1/1	-
5	EDO	F	405	-	-	1/1/1/1	-
2	ATP	J	401	3	-	4/18/38/38	0/3/3/3
5	EDO	A	405	-	-	1/1/1/1	-
5	EDO	F	406	-	-	1/1/1/1	-
5	EDO	L	407	-	-	1/1/1/1	-
2	ATP	E	401	3	-	5/18/38/38	0/3/3/3
5	EDO	D	406	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	408	-	-	1/1/1/1	-
2	ATP	F	401	3	-	6/18/38/38	0/3/3/3
5	EDO	J	406	-	-	0/1/1/1	-
2	ATP	B	401	3	-	6/18/38/38	0/3/3/3
5	EDO	G	406	-	-	1/1/1/1	-
5	EDO	J	409	-	-	0/1/1/1	-
2	ATP	C	401	3	-	6/18/38/38	0/3/3/3
5	EDO	D	407	-	-	0/1/1/1	-
5	EDO	J	408	-	-	1/1/1/1	-
5	EDO	J	410	-	-	1/1/1/1	-
5	EDO	P	407	-	-	1/1/1/1	-
2	ATP	P	401	3	-	6/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ATP	C5-C4	2.76	1.48	1.40
2	O	401	ATP	C5-C4	2.62	1.47	1.40
2	F	401	ATP	C5-C4	2.59	1.47	1.40
2	H	401	ATP	C5-C4	2.58	1.47	1.40
2	P	401	ATP	C2-N3	2.57	1.36	1.32

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	ATP	C4-C5-N7	-5.18	104.00	109.40
2	E	401	ATP	C4-C5-N7	-4.65	104.56	109.40
2	E	401	ATP	O4'-C1'-C2'	-4.47	100.40	106.93
2	N	401	ATP	C4-C5-N7	-4.27	104.94	109.40
2	K	401	ATP	O4'-C1'-C2'	-3.89	101.24	106.93

There are no chirality outliers.

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ATP	C5'-O5'-PA-O2A
2	B	401	ATP	C5'-O5'-PA-O1A
2	C	401	ATP	C5'-O5'-PA-O1A
2	C	401	ATP	C5'-O5'-PA-O2A
2	E	401	ATP	C5'-O5'-PA-O1A

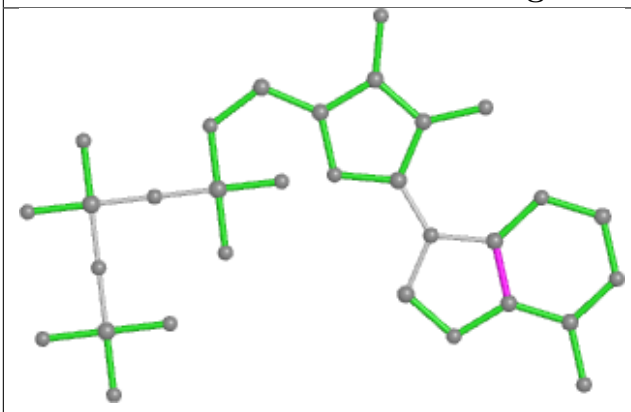
There are no ring outliers.

10 monomers are involved in 10 short contacts:

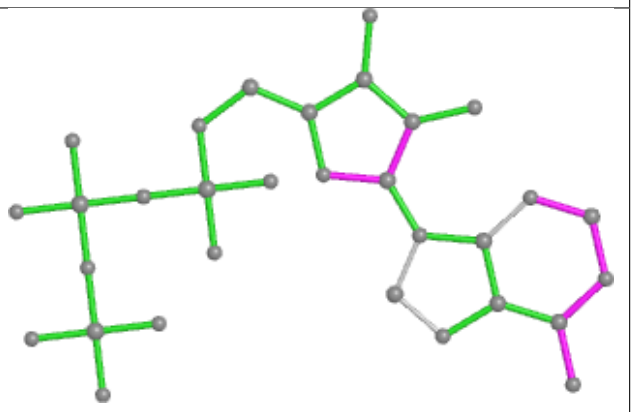
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	405	EDO	1	0
2	N	401	ATP	1	0
5	A	406	EDO	1	0
2	K	401	ATP	1	0
5	N	405	EDO	1	0
5	P	406	EDO	1	0
5	E	406	EDO	1	0
2	A	401	ATP	1	0
5	G	406	EDO	1	0
5	D	407	EDO	1	0

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.

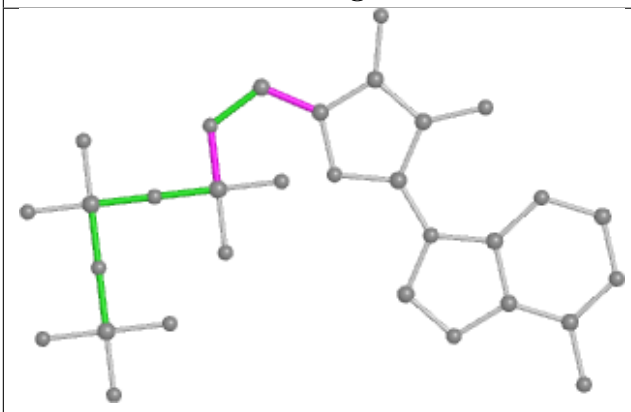
Ligand ATP L 401



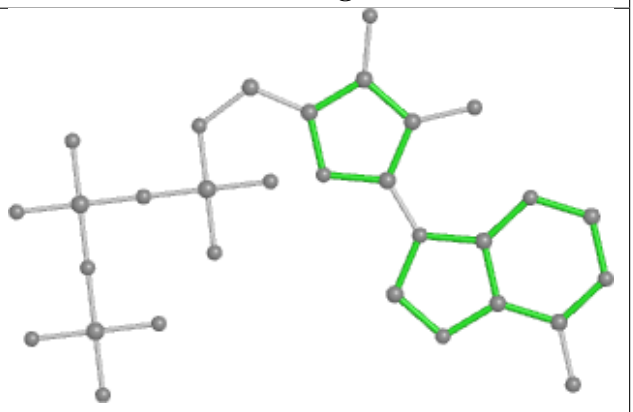
Bond lengths



Bond angles

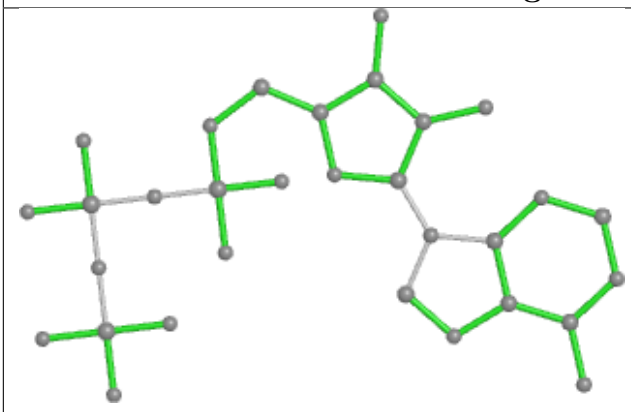


Torsions



Rings

Ligand ATP N 401



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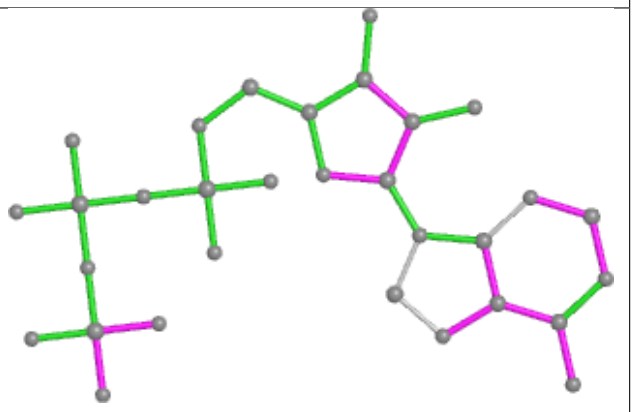

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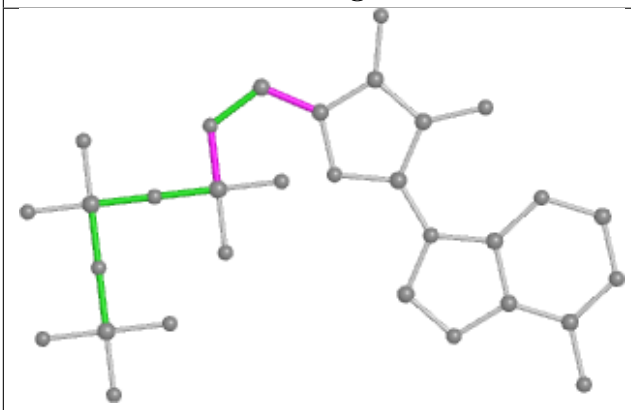

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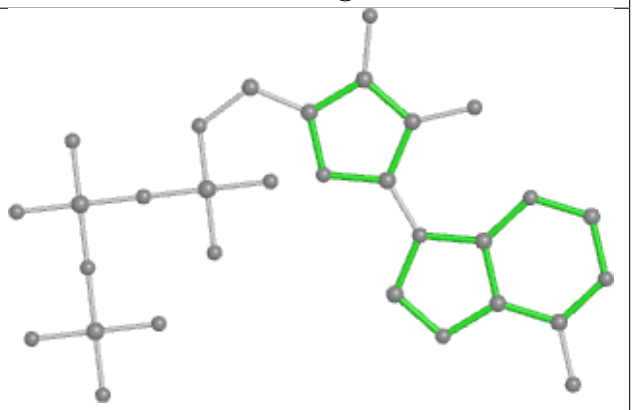
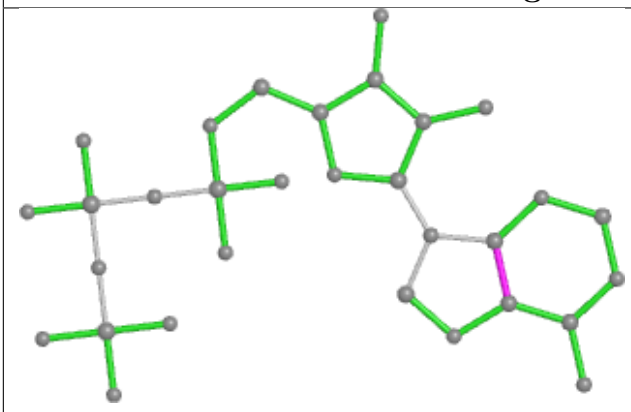
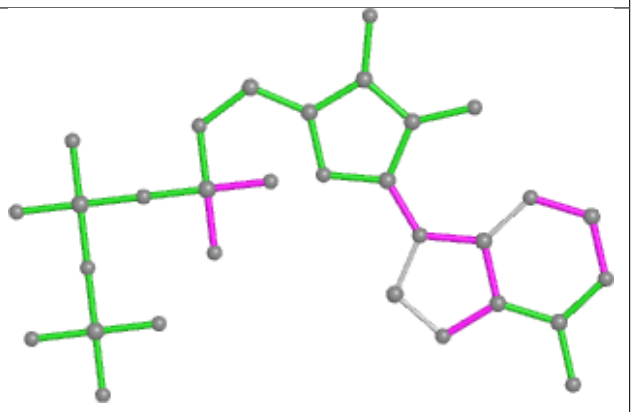


Rings

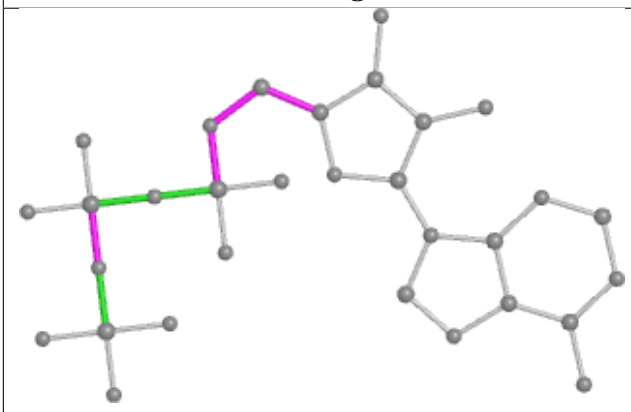
Ligand ATP H 401



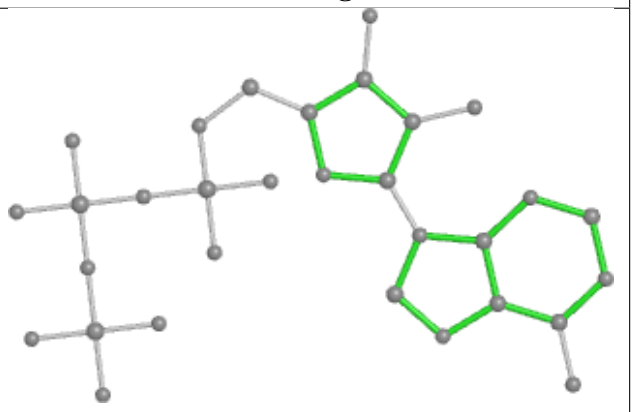
Bond lengths



Bond angles

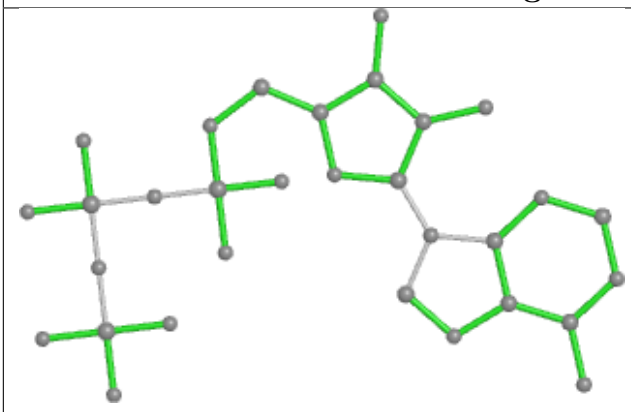


Torsions



Rings

Ligand ATP K 401



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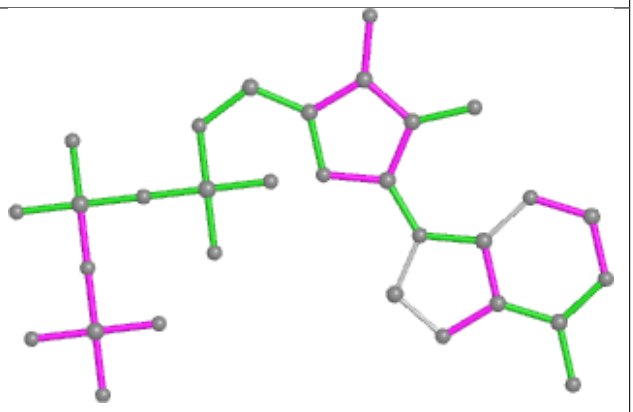
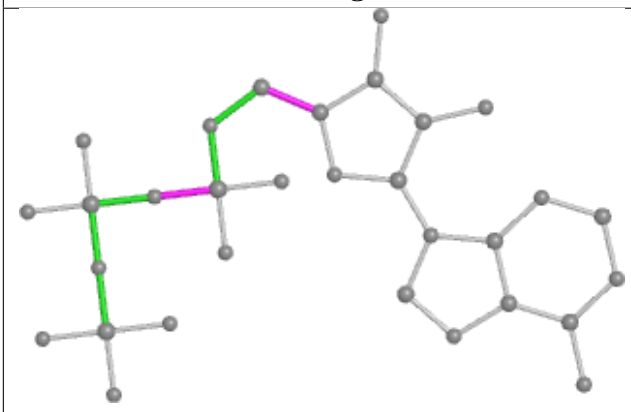


Bond angles



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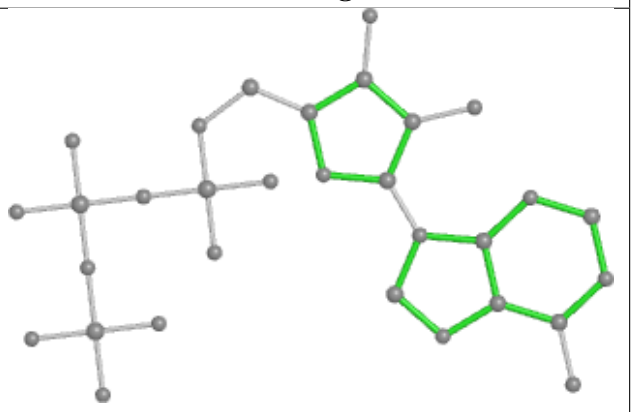
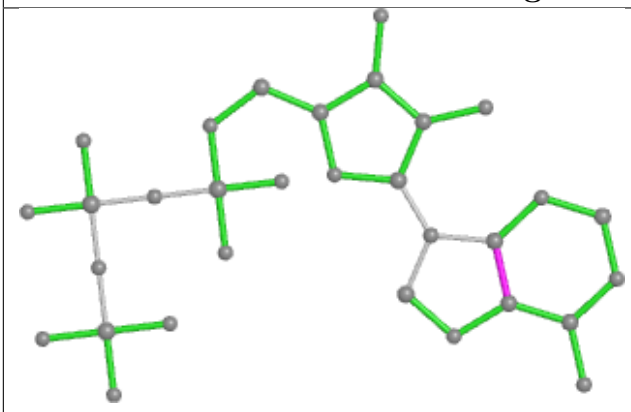
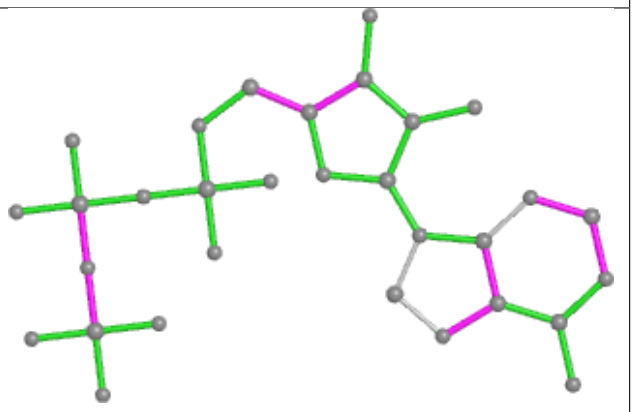


Rings

Ligand ATP D 401



Bond lengths



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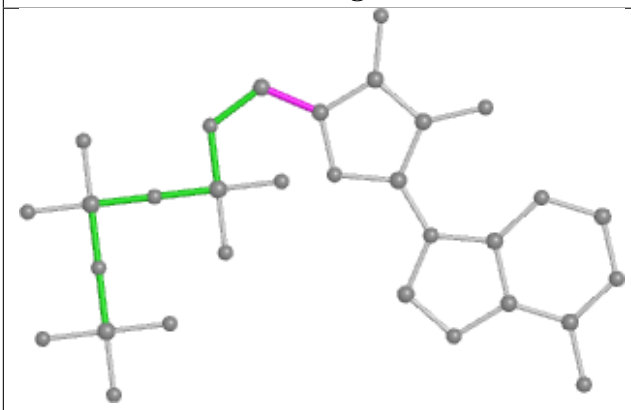
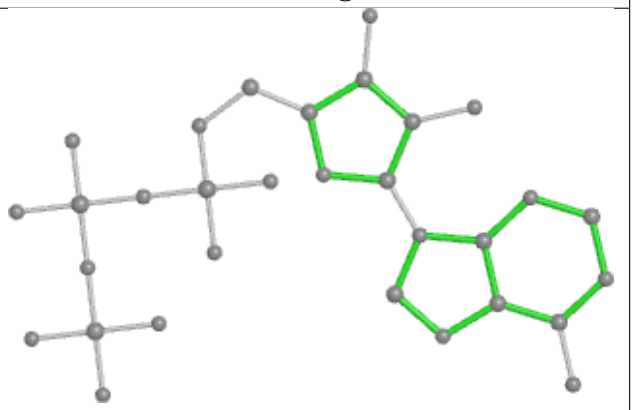
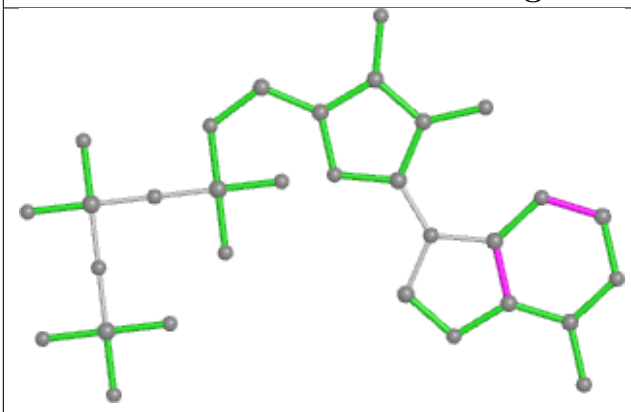


Torsions

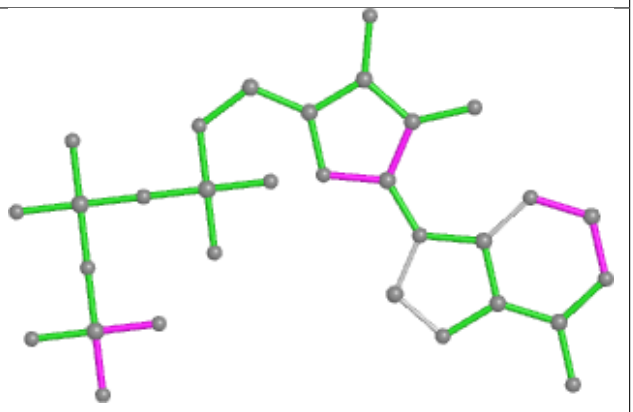


Rings

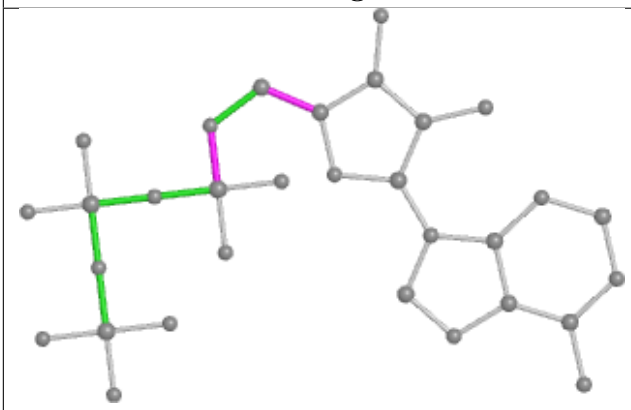
Ligand ATP O 401



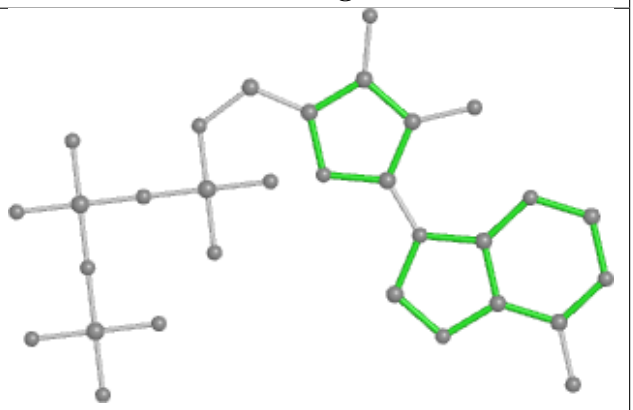
Bond lengths



Bond angles



Torsions



Rings

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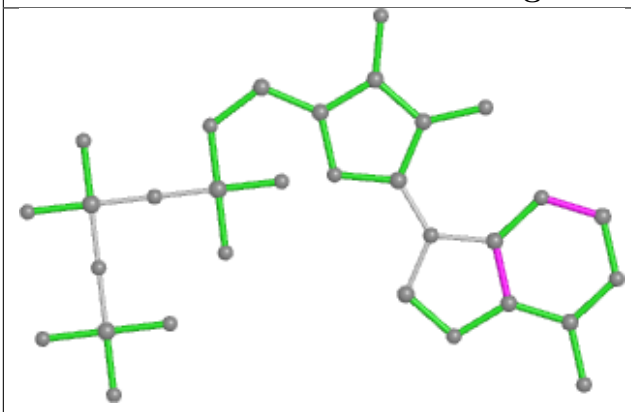

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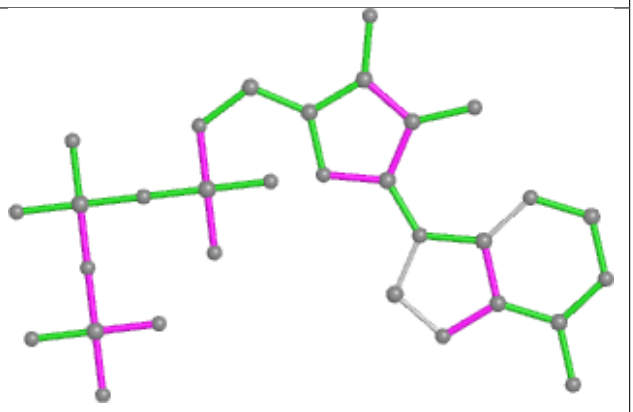

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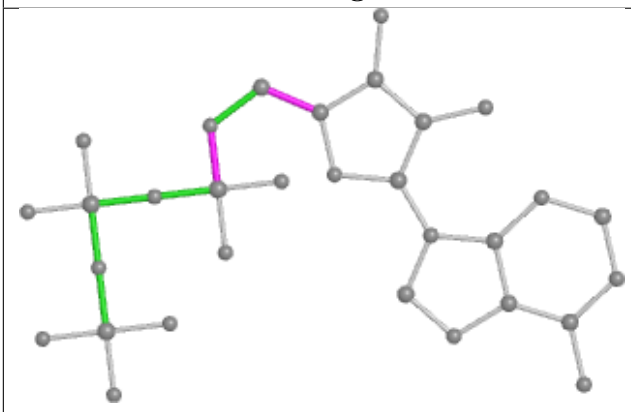

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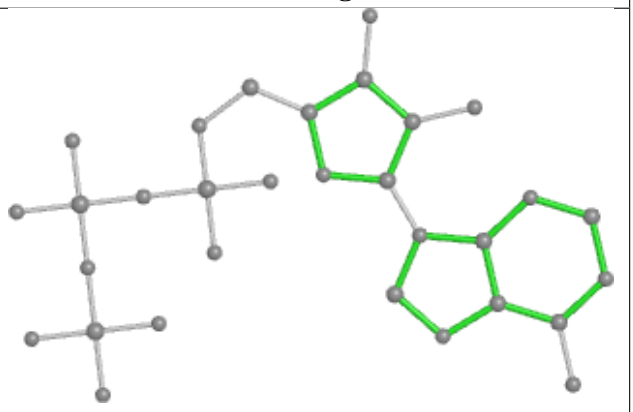
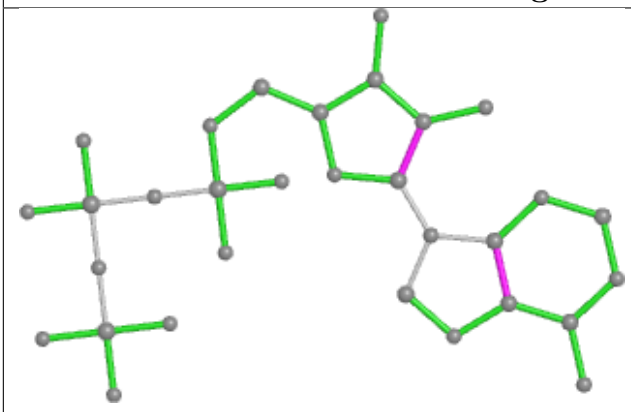


Rings

Ligand ATP I 400



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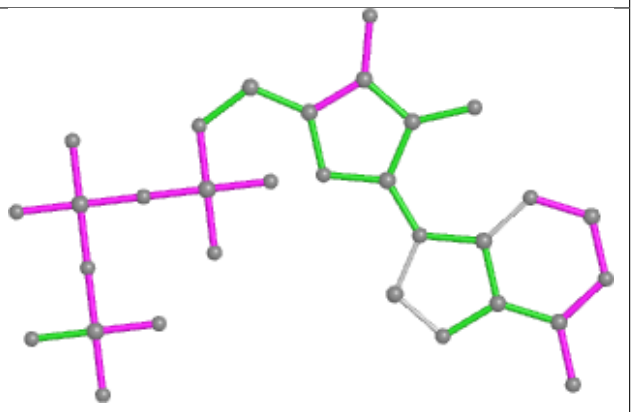

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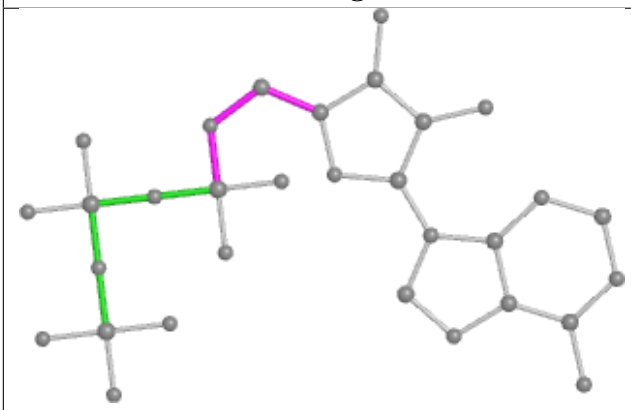

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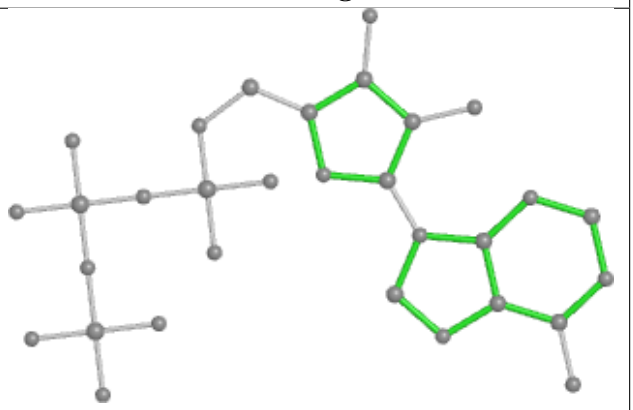
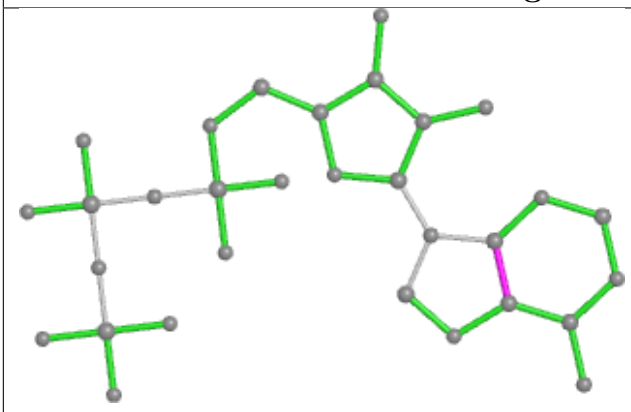


Rings

Ligand ATP A 401



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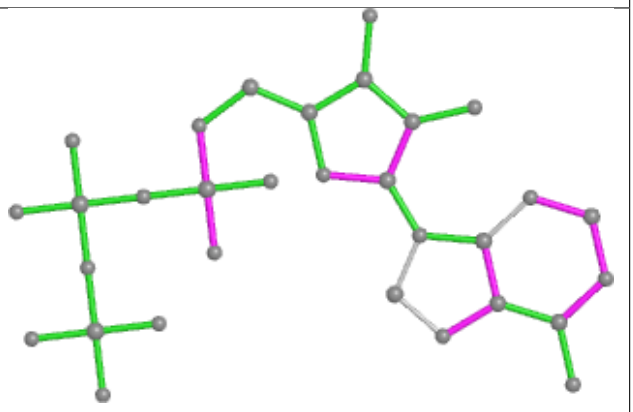
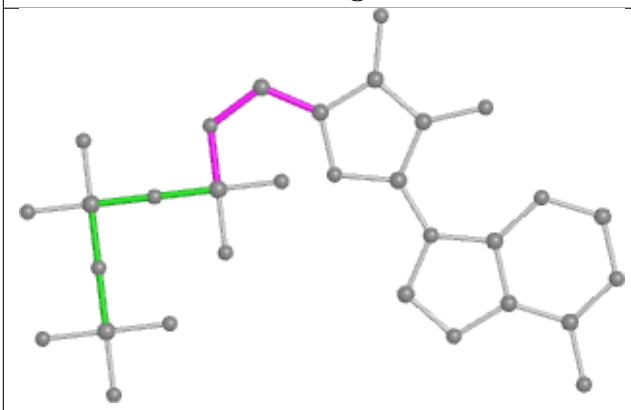
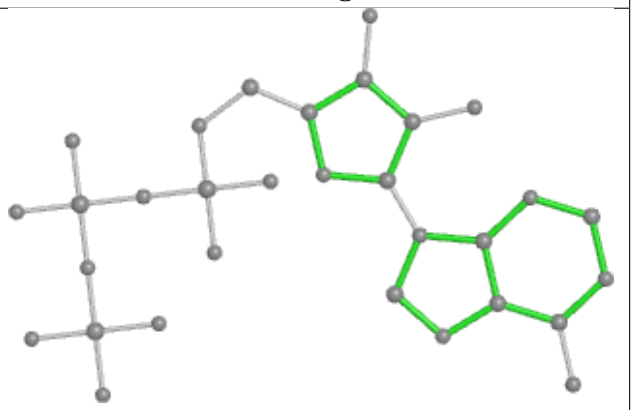


Bond angles

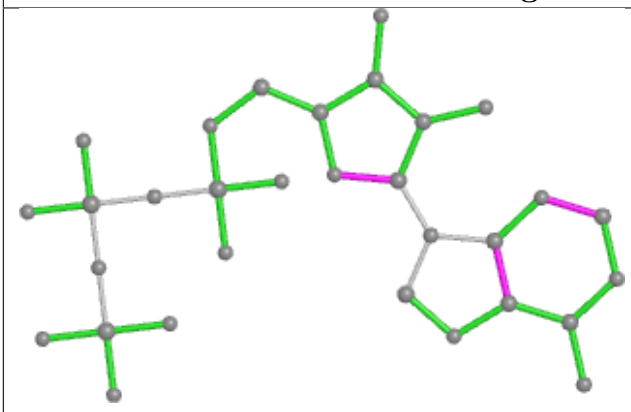


Torsions

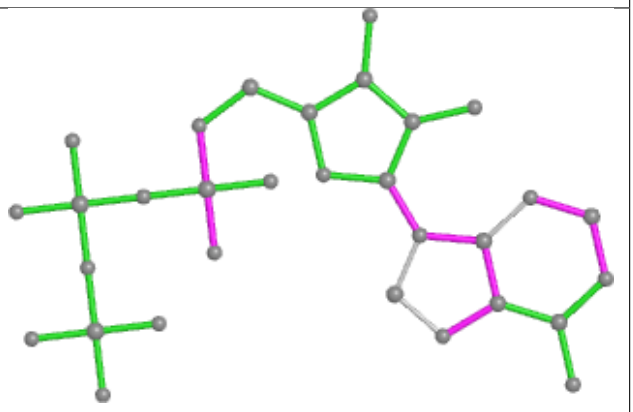


Rings

Ligand ATP M 401



Bond lengths



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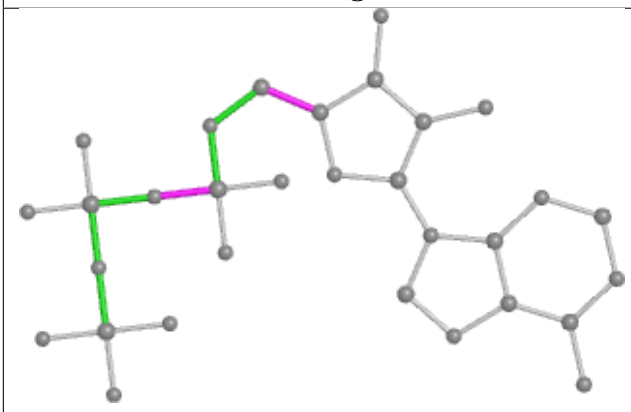
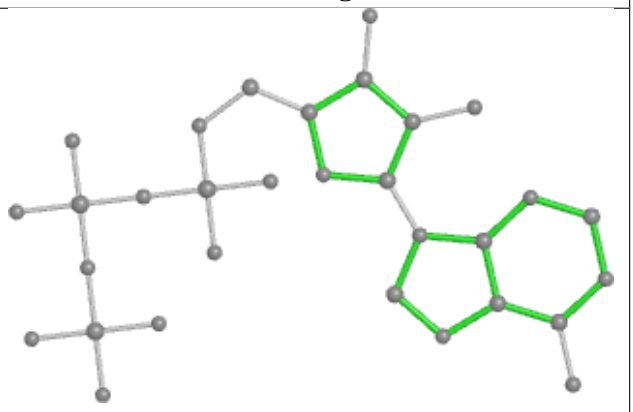
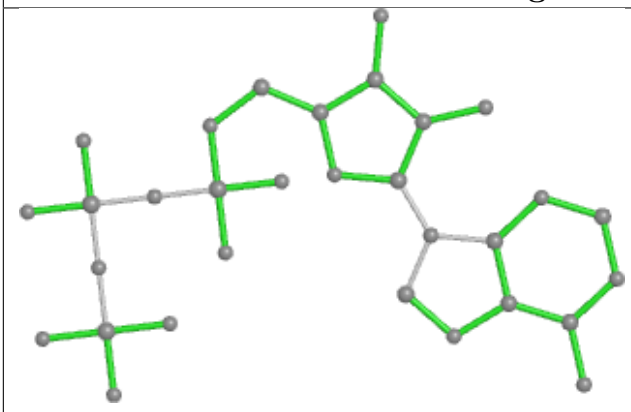


Torsions

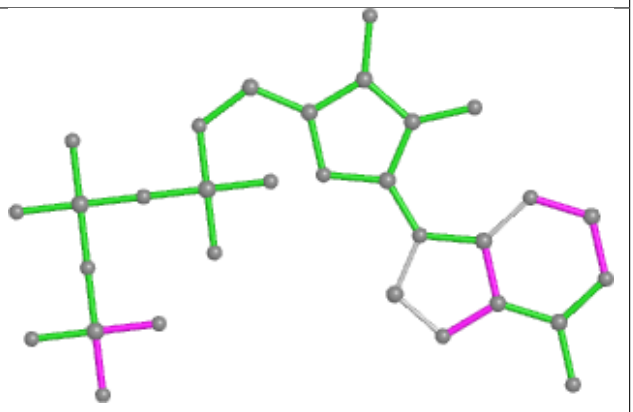


Rings

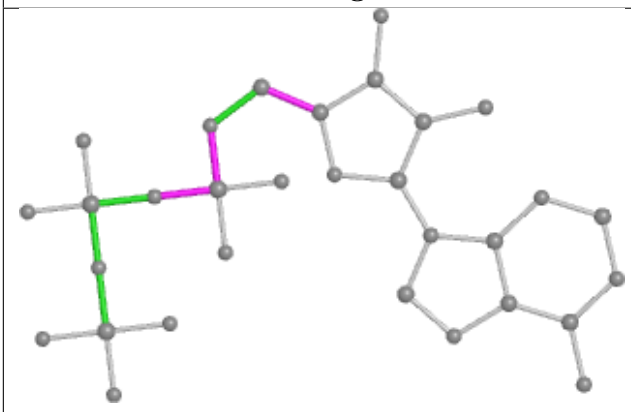
Ligand ATP J 401



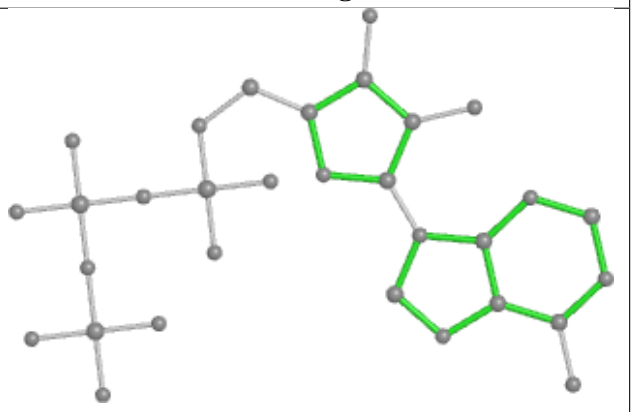
Bond lengths



Bond angles

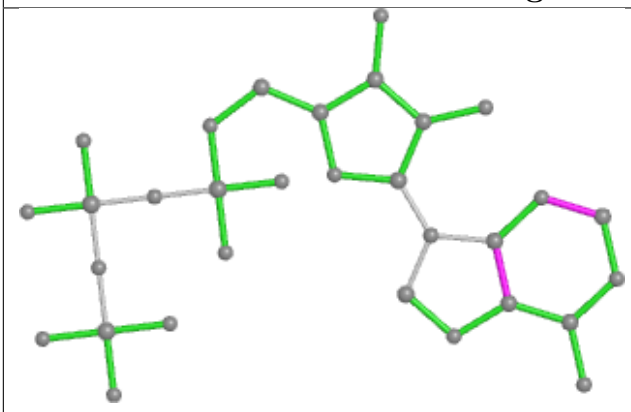


Torsions

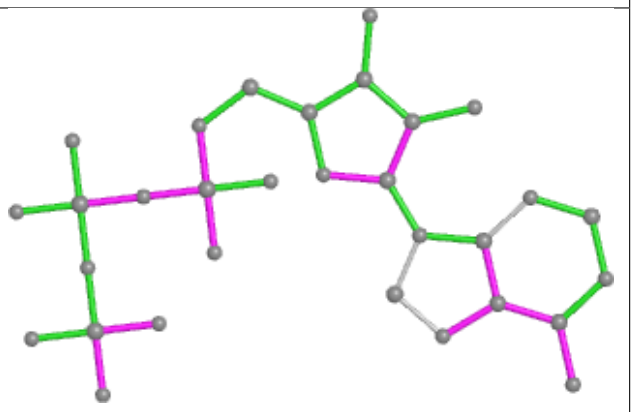


Rings

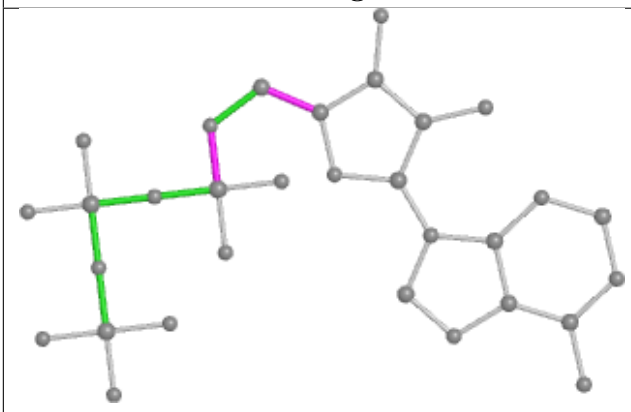
Ligand ATP E 401



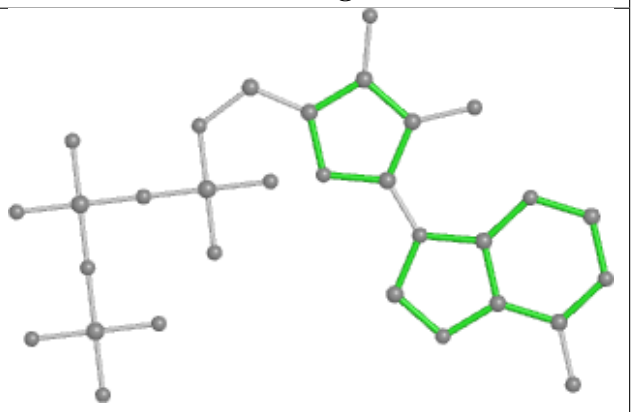
Bond lengths



Bond angles

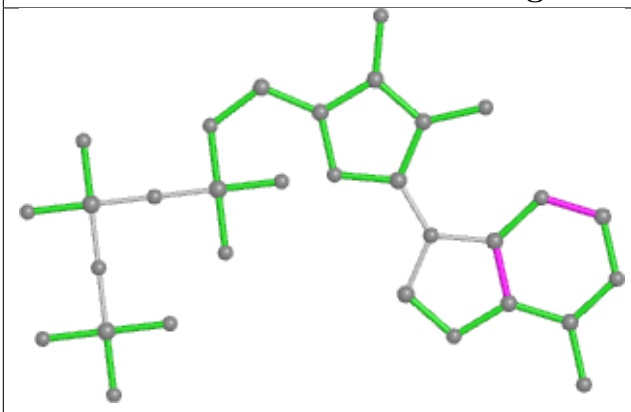


Torsions

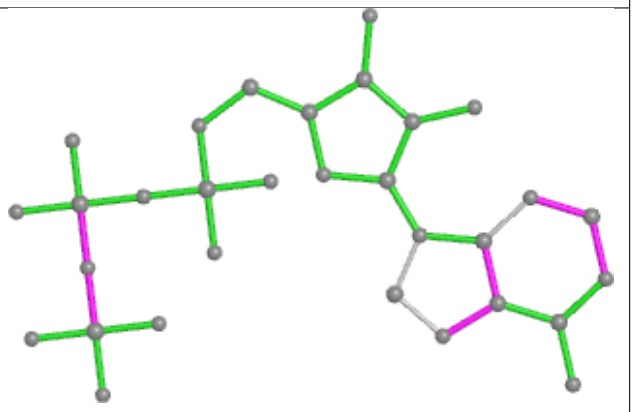


Rings

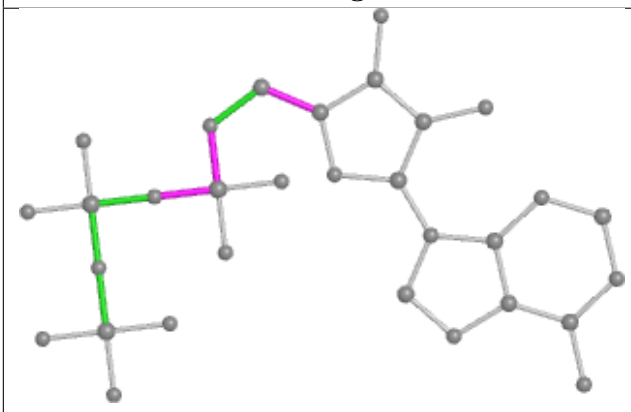
Ligand ATP F 401



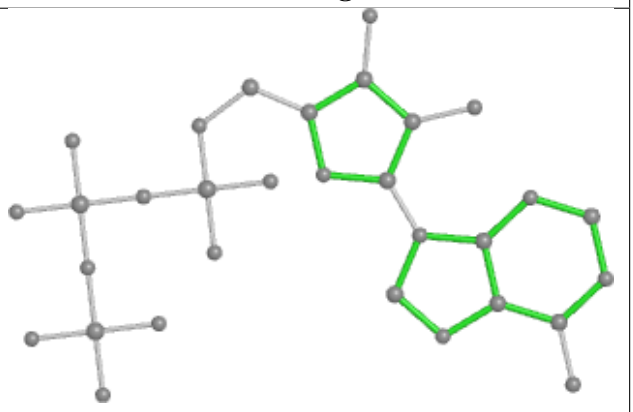
Bond lengths



Bond angles

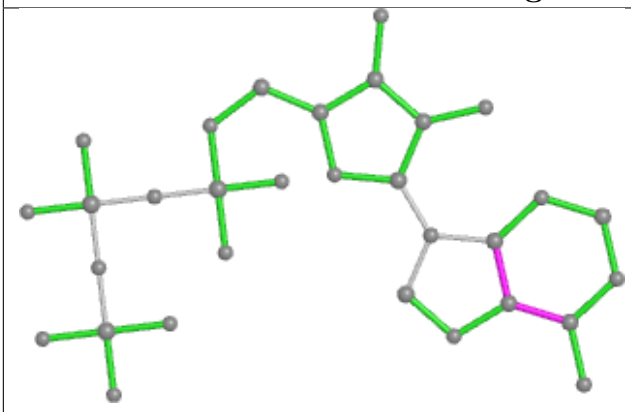


Torsions

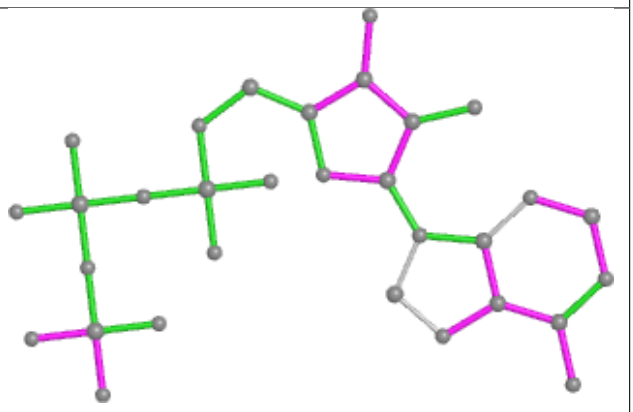


Rings

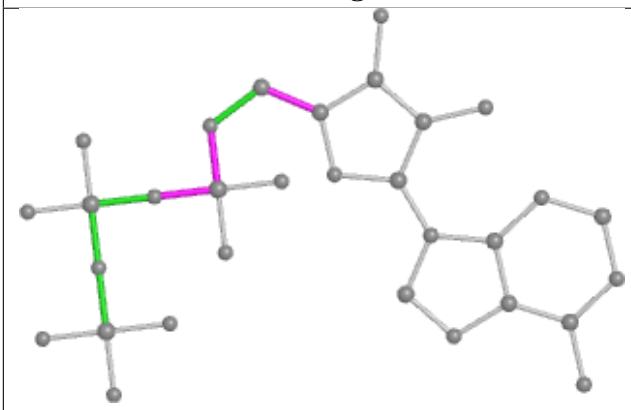
Ligand ATP B 401



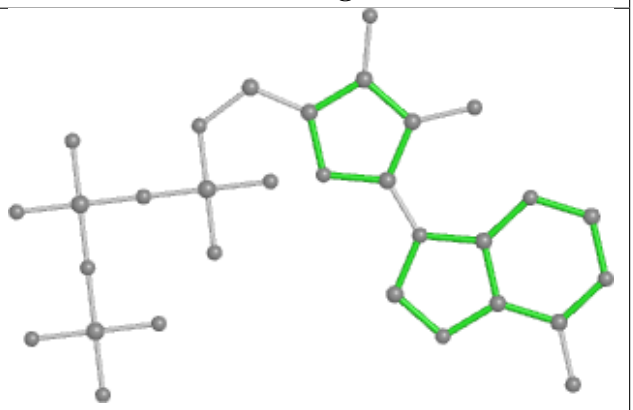
Bond lengths



Bond angles

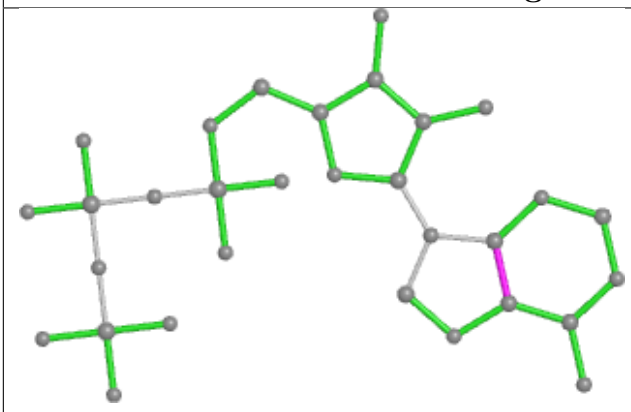


Torsions

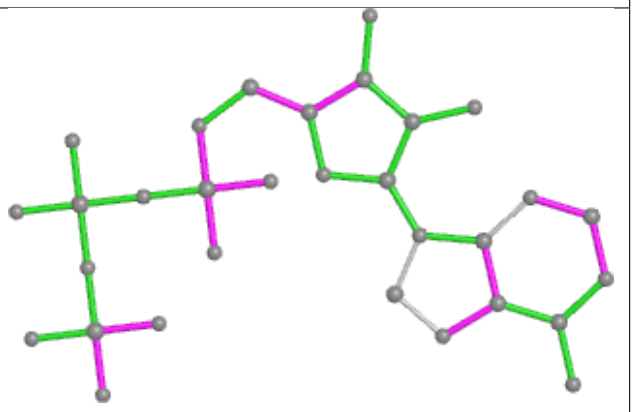


Rings

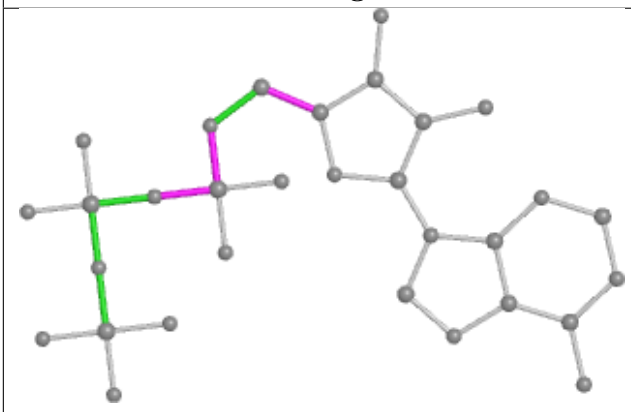
Ligand ATP C 401



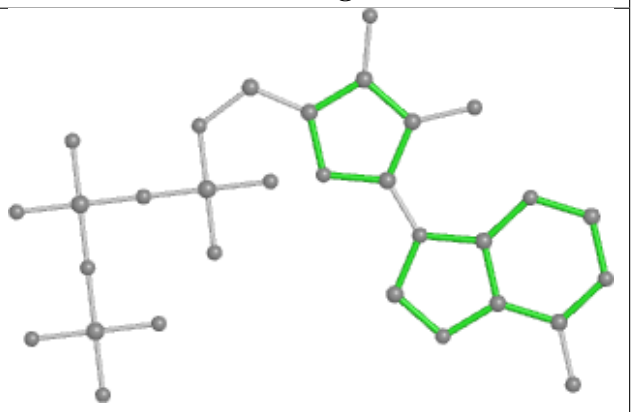
Bond lengths



Bond angles

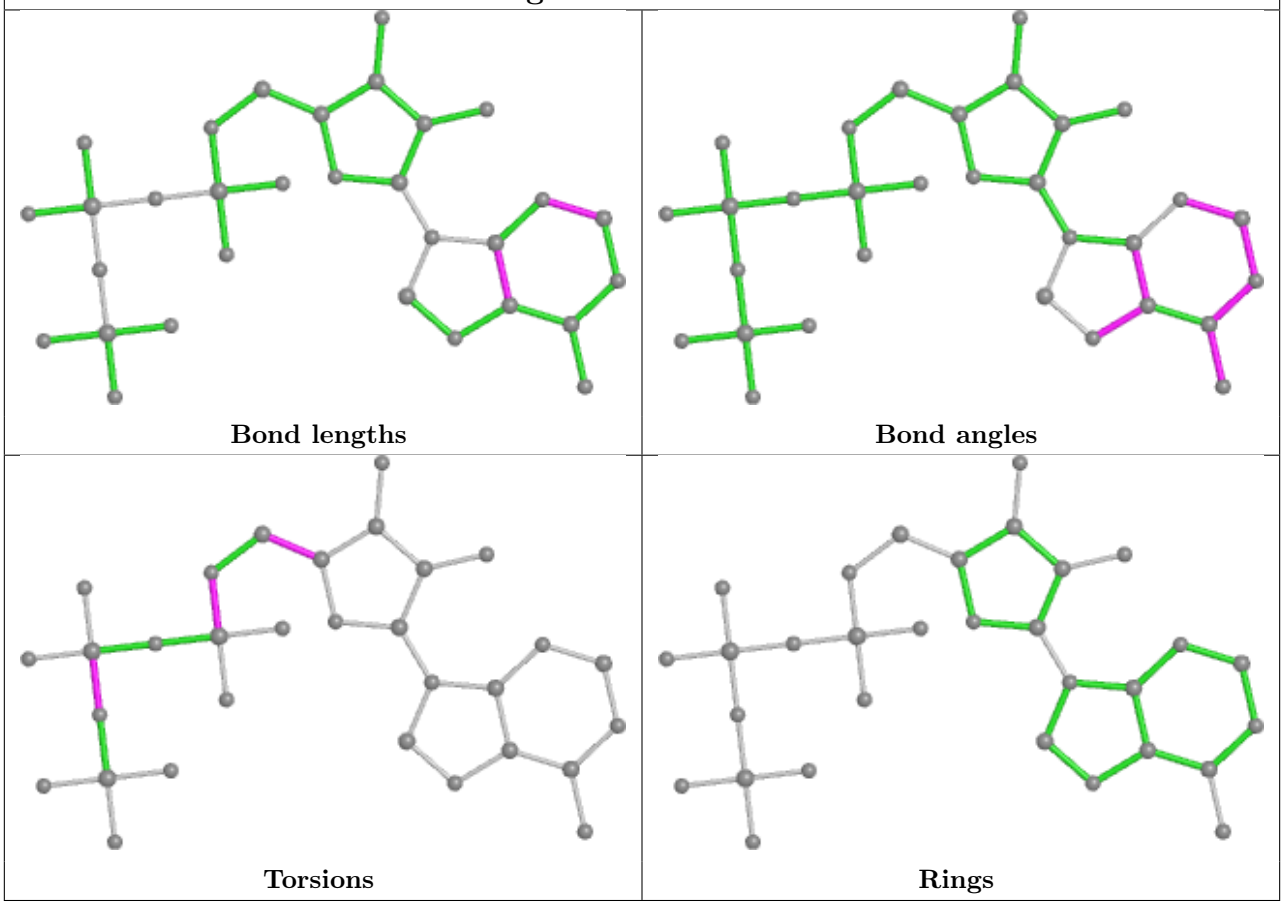


Torsions



Rings

Ligand ATP P 401



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	283/300 (94%)	-0.01	5 (1%)	68	70	27, 44, 88, 138	0
1	B	278/300 (92%)	0.15	10 (3%)	42	42	28, 45, 93, 146	0
1	C	286/300 (95%)	0.20	5 (1%)	70	72	31, 53, 96, 142	0
1	D	272/300 (90%)	0.12	7 (2%)	56	57	27, 42, 104, 129	0
1	E	286/300 (95%)	0.12	2 (0%)	87	89	28, 49, 92, 137	0
1	F	271/300 (90%)	0.15	7 (2%)	56	57	26, 41, 85, 128	0
1	G	276/300 (92%)	0.06	4 (1%)	75	77	27, 44, 85, 134	0
1	H	280/300 (93%)	0.06	5 (1%)	68	70	23, 44, 85, 134	0
1	I	280/300 (93%)	0.04	4 (1%)	75	77	29, 44, 83, 153	0
1	J	279/300 (93%)	0.28	16 (5%)	23	22	29, 44, 100, 144	0
1	K	276/300 (92%)	0.12	9 (3%)	46	46	26, 43, 92, 145	0
1	L	280/300 (93%)	-0.03	2 (0%)	87	89	27, 42, 82, 117	0
1	M	270/300 (90%)	0.13	5 (1%)	66	69	27, 43, 80, 129	0
1	N	286/300 (95%)	0.31	12 (4%)	36	35	28, 55, 109, 149	0
1	O	271/300 (90%)	0.11	5 (1%)	68	70	25, 41, 89, 139	0
1	P	286/300 (95%)	0.26	8 (2%)	53	54	28, 59, 113, 138	0
All	All	4460/4800 (92%)	0.13	106 (2%)	59	60	23, 45, 96, 153	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	36	GLY	8.0
1	N	40	ILE	7.7
1	O	320	ALA	6.8
1	I	244	LEU	5.9
1	B	38	VAL	5.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MG	O	404	1/1	0.69	0.40	110,110,110,110	0
5	EDO	L	407	4/4	0.69	0.26	63,67,91,93	0
5	EDO	J	408	4/4	0.73	0.20	65,66,70,81	0
5	EDO	P	405	4/4	0.73	0.40	72,72,73,98	0
3	MG	P	402	1/1	0.74	0.12	121,121,121,121	0
3	MG	E	404	1/1	0.76	0.11	115,115,115,115	0
3	MG	F	402	1/1	0.76	0.11	91,91,91,91	0
5	EDO	G	406	4/4	0.76	0.21	73,85,86,98	0
5	EDO	J	405	4/4	0.77	0.21	65,85,89,109	0
5	EDO	O	407	4/4	0.79	0.38	63,67,109,112	0
5	EDO	B	409	4/4	0.79	0.23	69,83,91,104	0
5	EDO	N	405	4/4	0.80	0.24	58,69,94,96	0
5	EDO	K	406	4/4	0.81	0.24	87,92,98,106	0
3	MG	F	404	1/1	0.82	0.54	96,96,96,96	0
5	EDO	F	406	4/4	0.82	0.20	81,85,90,95	0
5	EDO	M	405	4/4	0.83	0.33	88,90,97,124	0
3	MG	H	404	1/1	0.83	0.19	106,106,106,106	0
5	EDO	G	407	4/4	0.83	0.20	68,81,82,88	0
5	EDO	B	406	4/4	0.83	0.23	61,66,70,94	0
5	EDO	J	407	4/4	0.84	0.31	78,89,101,105	0
3	MG	G	404	1/1	0.84	0.16	98,98,98,98	0
3	MG	M	404	1/1	0.85	0.27	94,94,94,94	0
5	EDO	A	407	4/4	0.85	0.27	46,59,65,106	0
3	MG	B	404	1/1	0.86	0.11	88,88,88,88	0
3	MG	N	402	1/1	0.88	0.14	82,82,82,82	0
3	MG	B	402	1/1	0.88	0.10	106,106,106,106	0
3	MG	D	404	1/1	0.88	0.21	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	G	405	4/4	0.88	0.19	57,64,71,73	0
3	MG	E	402	1/1	0.88	0.18	74,74,74,74	0
5	EDO	D	407	4/4	0.89	0.18	62,62,77,86	0
5	EDO	E	406	4/4	0.89	0.17	61,64,77,79	0
3	MG	J	404	1/1	0.89	0.07	90,90,90,90	0
5	EDO	P	407	4/4	0.89	0.23	72,82,85,101	0
3	MG	I	403	1/1	0.90	0.16	89,89,89,89	0
3	MG	H	402	1/1	0.90	0.07	82,82,82,82	0
5	EDO	B	407	4/4	0.90	0.26	63,68,74,83	0
5	EDO	A	405	4/4	0.90	0.13	60,61,92,114	0
5	EDO	J	410	4/4	0.91	0.20	65,67,77,98	0
5	EDO	O	406	4/4	0.91	0.27	55,60,68,78	0
5	EDO	B	405	4/4	0.91	0.19	60,62,74,85	0
5	EDO	B	408	4/4	0.91	0.17	66,79,87,94	0
3	MG	M	402	1/1	0.91	0.17	104,104,104,104	0
5	EDO	O	405	4/4	0.92	0.17	55,57,58,72	0
5	EDO	J	409	4/4	0.92	0.43	53,69,71,71	0
3	MG	L	404	1/1	0.92	0.12	86,86,86,86	0
5	EDO	M	406	4/4	0.92	0.38	55,56,56,70	0
3	MG	N	404	1/1	0.92	0.09	112,112,112,112	0
5	EDO	L	405	4/4	0.93	0.17	59,64,68,69	0
3	MG	I	401	1/1	0.93	0.08	66,66,66,66	0
3	MG	C	404	1/1	0.93	0.06	85,85,85,85	0
3	MG	O	402	1/1	0.93	0.19	104,104,104,104	0
5	EDO	C	405	4/4	0.93	0.21	56,57,73,78	0
5	EDO	K	405	4/4	0.94	0.19	56,63,69,70	0
5	EDO	F	405	4/4	0.94	0.20	46,67,73,88	0
5	EDO	F	407	4/4	0.94	0.21	47,53,60,66	0
3	MG	L	402	1/1	0.95	0.07	106,106,106,106	0
5	EDO	A	406	4/4	0.95	0.13	61,63,68,82	0
3	MG	D	402	1/1	0.95	0.09	110,110,110,110	0
3	MG	A	402	1/1	0.95	0.14	90,90,90,90	0
5	EDO	D	406	4/4	0.95	0.28	66,75,78,92	0
3	MG	P	404	1/1	0.95	0.12	106,106,106,106	0
5	EDO	E	405	4/4	0.95	0.15	56,60,62,71	0
5	EDO	H	405	4/4	0.95	0.22	65,70,74,77	0
5	EDO	P	406	4/4	0.95	0.26	69,70,82,96	0
5	EDO	L	406	4/4	0.95	0.33	72,72,73,85	0
5	EDO	P	408	4/4	0.95	0.35	54,59,69,81	0
3	MG	K	404	1/1	0.96	0.11	100,100,100,100	0
3	MG	A	404	1/1	0.96	0.06	61,61,61,61	0
3	MG	G	402	1/1	0.96	0.18	138,138,138,138	0

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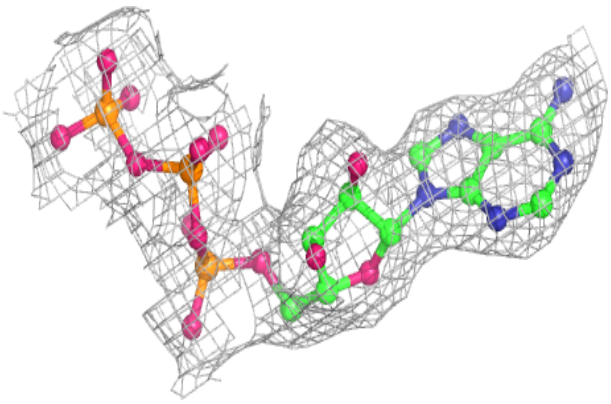
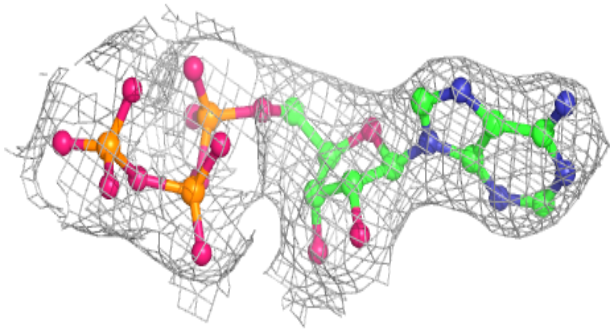
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	J	406	4/4	0.97	0.20	59,61,66,70	0
2	ATP	E	401	31/31	0.97	0.17	37,46,59,87	0
2	ATP	F	401	31/31	0.97	0.14	24,39,56,102	0
4	ZN	C	403	1/1	0.97	0.14	70,70,70,70	0
4	ZN	P	403	1/1	0.97	0.13	70,70,70,70	0
3	MG	K	402	1/1	0.97	0.21	153,153,153,153	0
5	EDO	D	405	4/4	0.97	0.17	42,54,61,62	0
2	ATP	I	400	31/31	0.97	0.14	34,43,63,69	0
2	ATP	N	401	31/31	0.97	0.16	38,51,68,80	0
2	ATP	B	401	31/31	0.97	0.16	32,42,64,78	0
6	CL	K	407	1/1	0.97	0.27	47,47,47,47	1
2	ATP	J	401	31/31	0.98	0.15	29,42,69,88	0
3	MG	J	402	1/1	0.98	0.09	95,95,95,95	0
4	ZN	A	403	1/1	0.98	0.15	44,44,44,44	0
2	ATP	K	401	31/31	0.98	0.18	26,39,59,93	0
4	ZN	F	403	1/1	0.98	0.10	47,47,47,47	0
4	ZN	K	403	1/1	0.98	0.18	44,44,44,44	0
4	ZN	N	403	1/1	0.98	0.11	67,67,67,67	0
2	ATP	L	401	31/31	0.98	0.14	33,45,69,72	0
2	ATP	M	401	31/31	0.98	0.16	30,45,74,94	0
2	ATP	A	401	31/31	0.98	0.13	33,42,67,79	0
2	ATP	O	401	31/31	0.98	0.14	24,38,60,81	0
2	ATP	P	401	31/31	0.98	0.15	39,52,65,79	0
2	ATP	C	401	31/31	0.98	0.17	36,45,58,67	0
2	ATP	G	401	31/31	0.98	0.17	31,44,66,82	0
2	ATP	H	401	31/31	0.98	0.13	32,39,67,93	0
2	ATP	D	401	31/31	0.98	0.15	34,43,67,73	0
3	MG	C	402	1/1	0.98	0.08	70,70,70,70	0
4	ZN	L	403	1/1	0.99	0.13	40,40,40,40	0
4	ZN	M	403	1/1	0.99	0.13	45,45,45,45	0
4	ZN	E	403	1/1	0.99	0.12	58,58,58,58	0
4	ZN	O	403	1/1	0.99	0.14	43,43,43,43	0
4	ZN	B	403	1/1	0.99	0.16	44,44,44,44	0
4	ZN	G	403	1/1	0.99	0.15	46,46,46,46	0
4	ZN	J	403	1/1	0.99	0.14	40,40,40,40	0
4	ZN	D	403	1/1	0.99	0.14	50,50,50,50	0
4	ZN	H	403	1/1	1.00	0.13	47,47,47,47	0
4	ZN	I	402	1/1	1.00	0.14	44,44,44,44	0

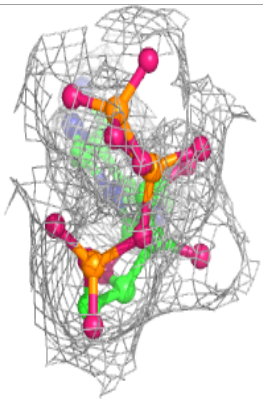
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP E 401:

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

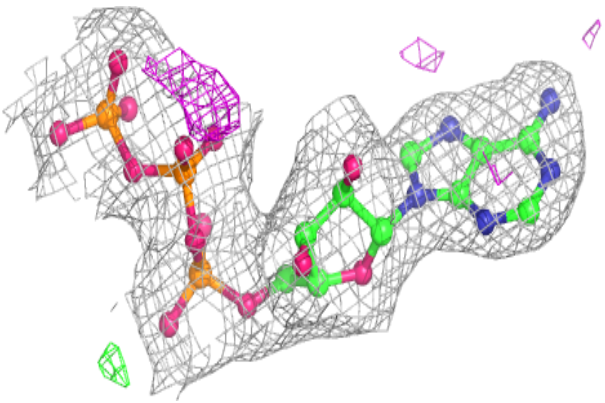


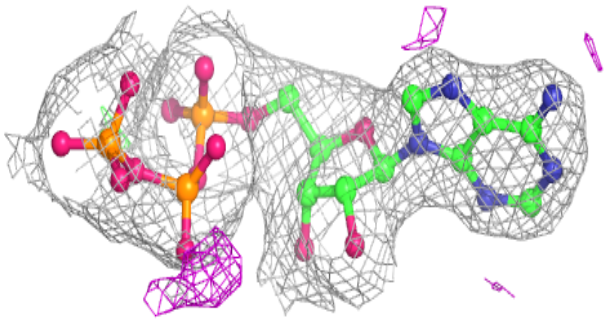


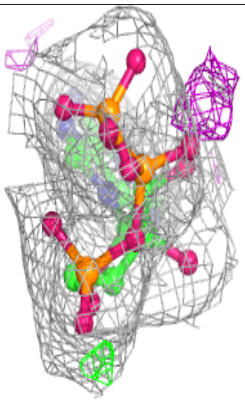


Electron density around ATP F 401:

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

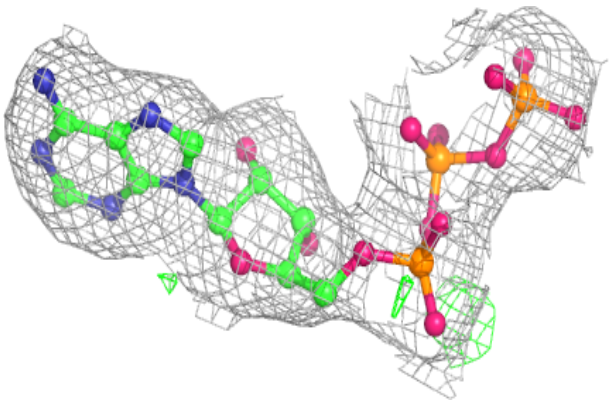


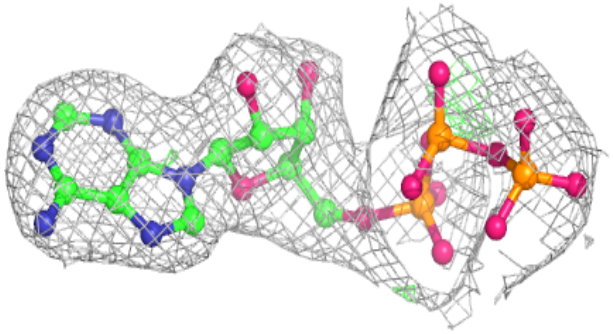


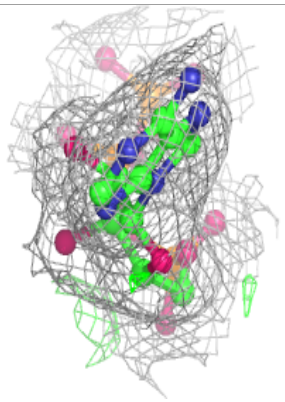


Electron density around ATP I 400:

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

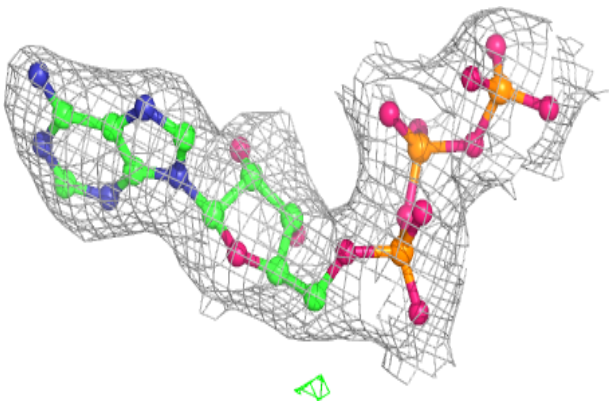


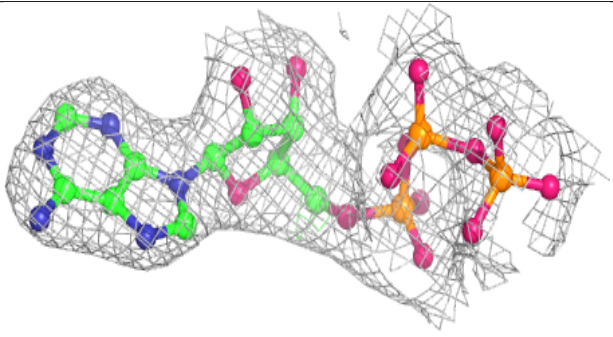


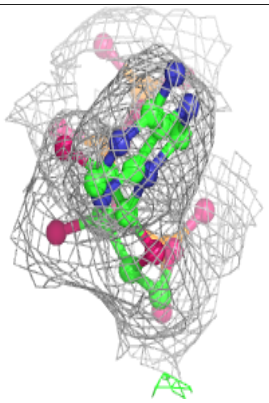


Electron density around ATP N 401:

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

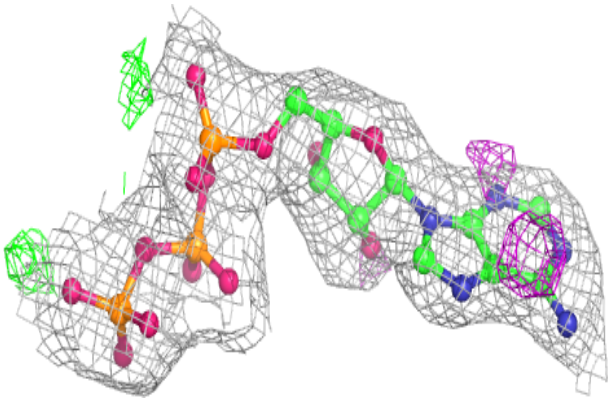


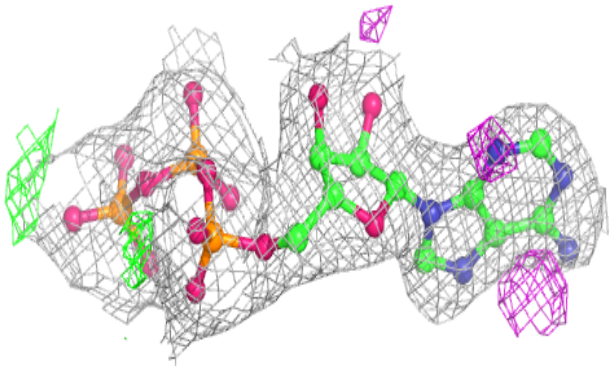


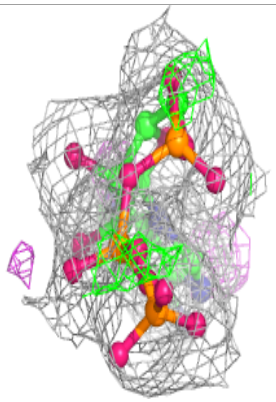


Electron density around ATP B 401:

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

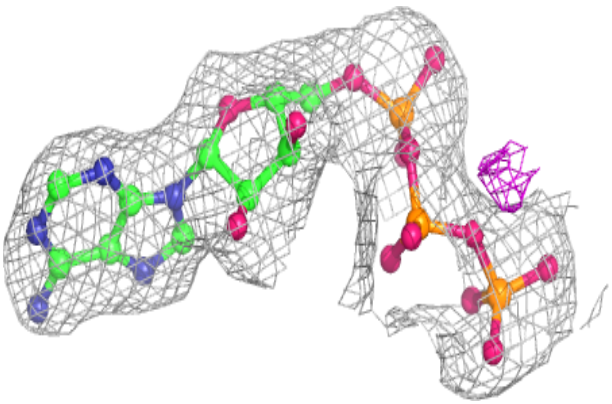


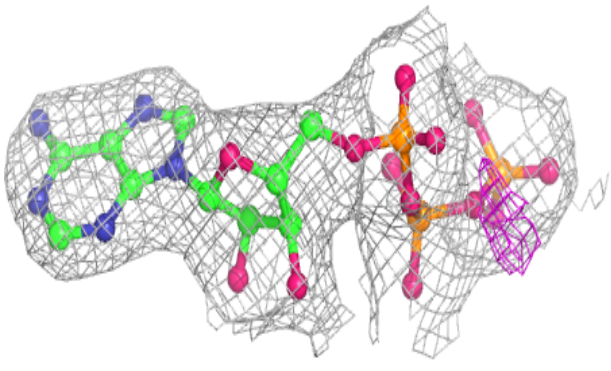


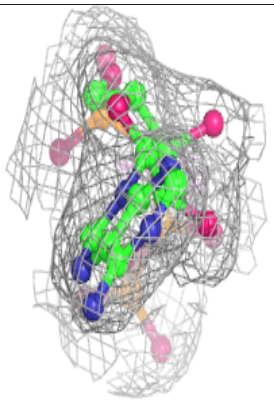


Electron density around ATP J 401:

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

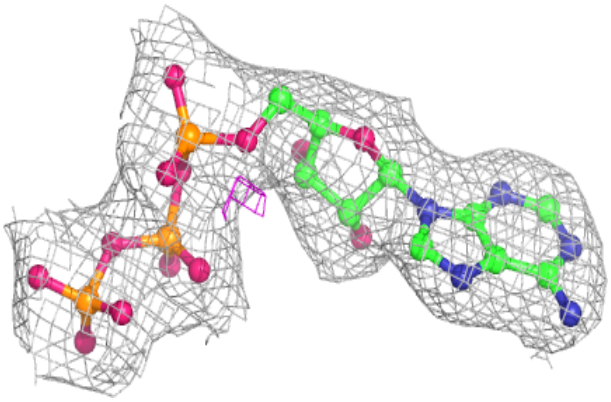


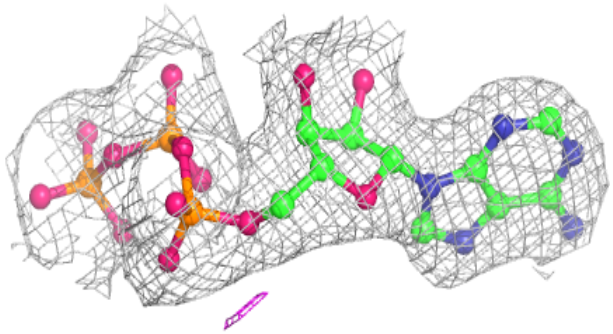


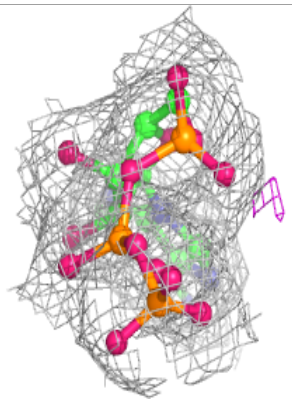


Electron density around ATP K 401:

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

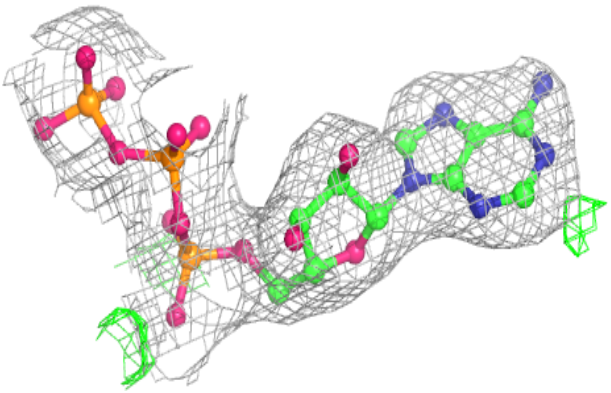


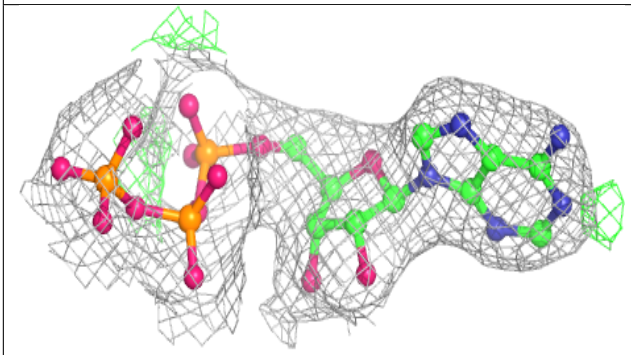


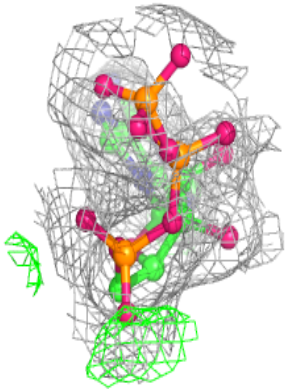


Electron density around ATP L 401:

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

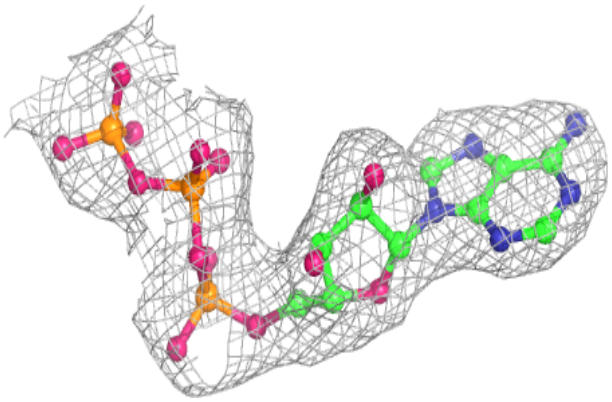


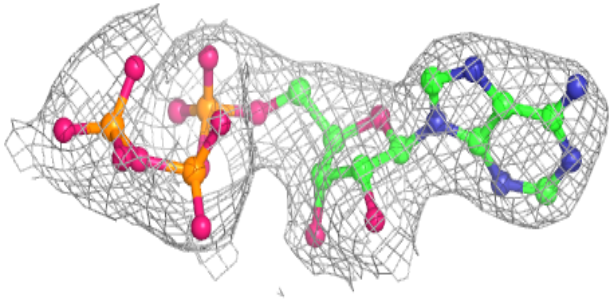


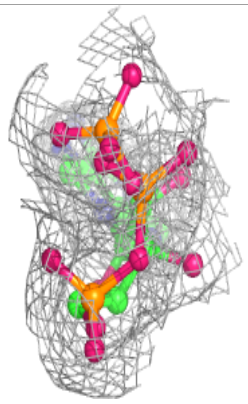


Electron density around ATP M 401:

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

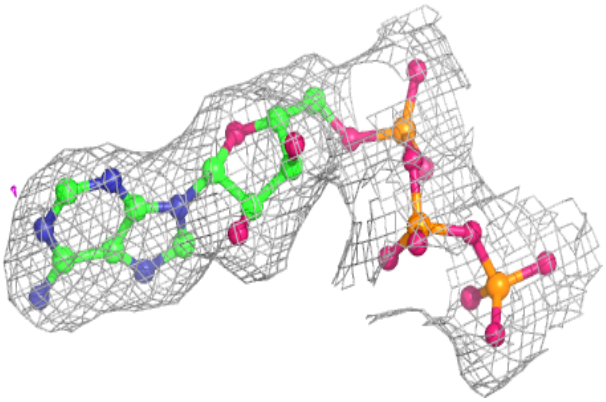


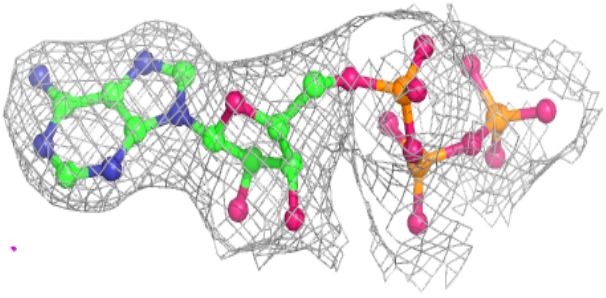


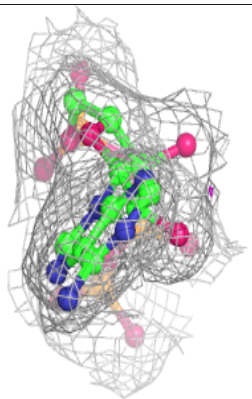


Electron density around ATP A 401:

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

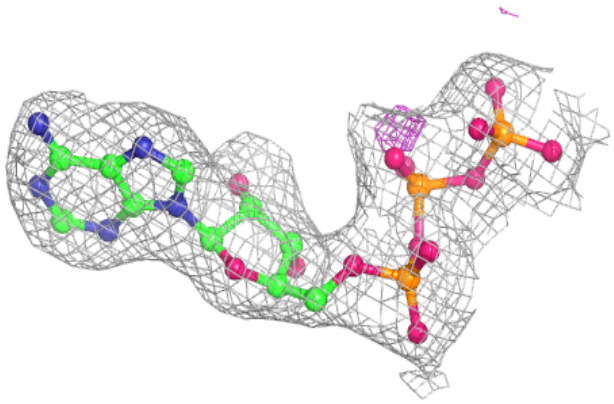


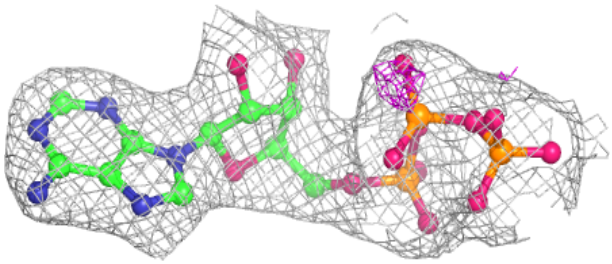


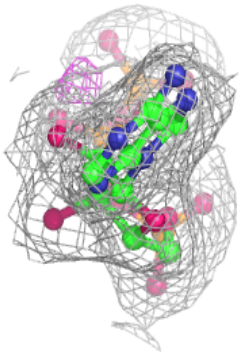


Electron density around ATP O 401:

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

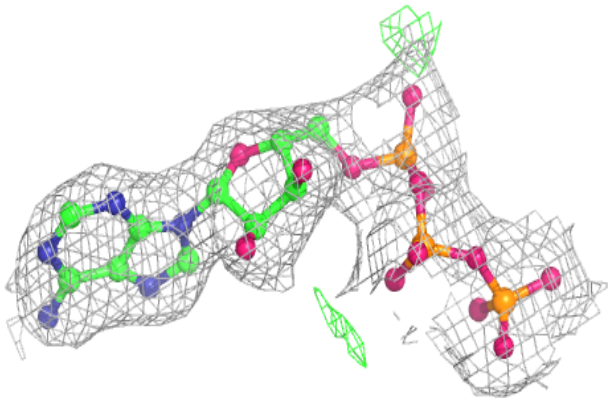


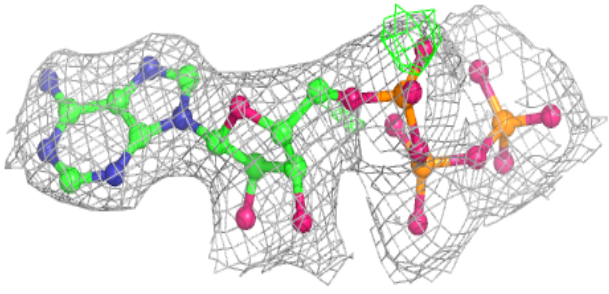


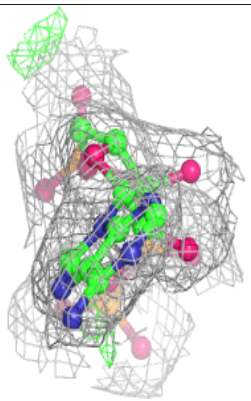


Electron density around ATP P 401:

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

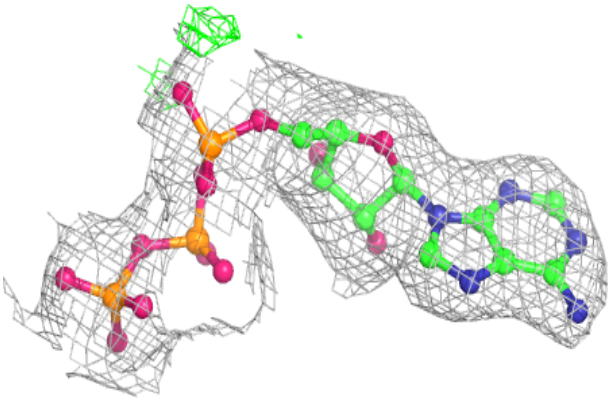


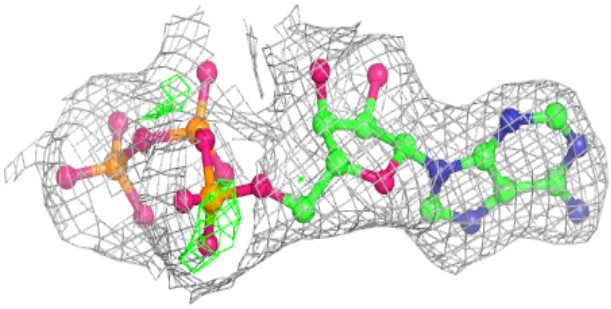


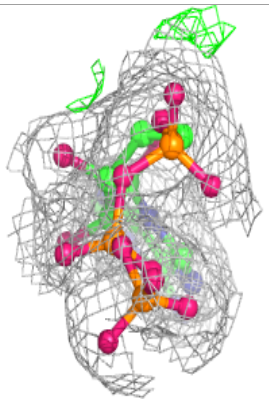


Electron density around ATP C 401:

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

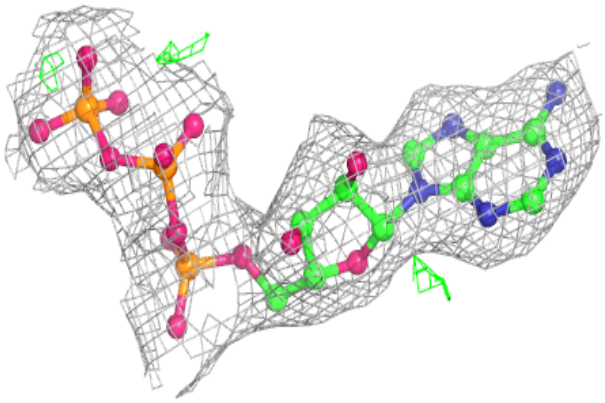


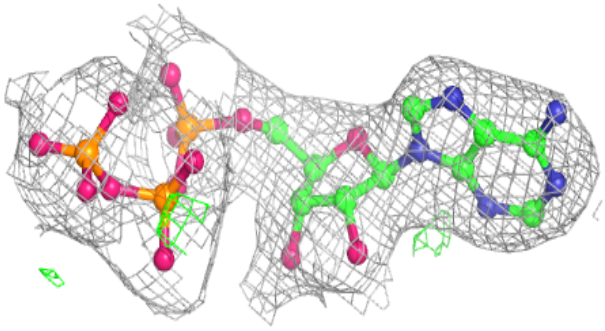


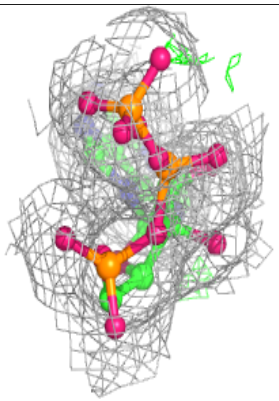


Electron density around ATP G 401:

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

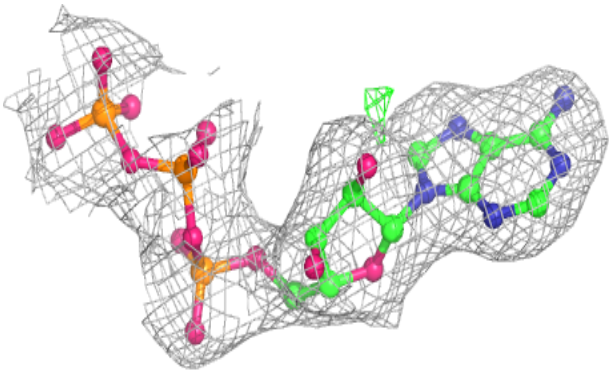


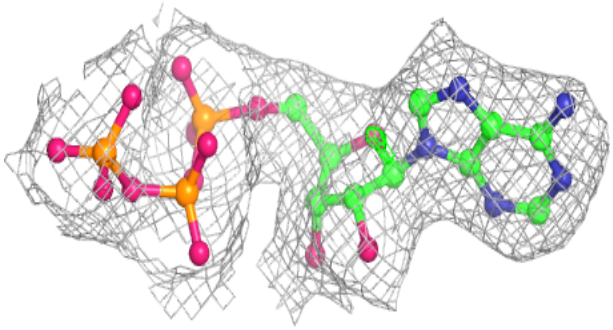


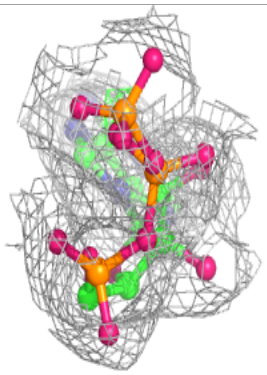


Electron density around ATP H 401:

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

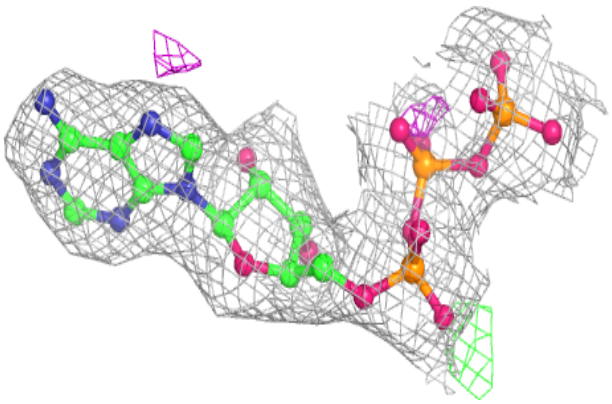


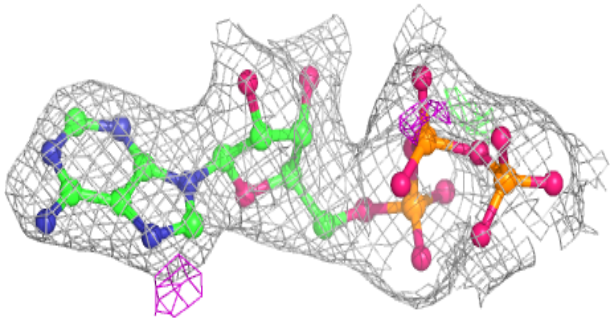


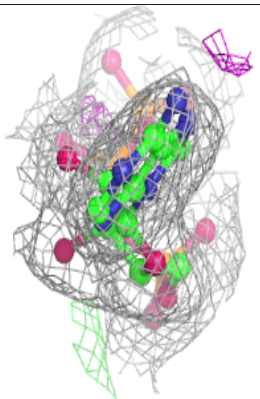


Electron density around ATP D 401:

$2mF_o$-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.