wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 04:06 AM EDT

PDB ID	:	6PJW
Title	:	Adenylate kinase from Methanococcus igneus - AMP bound form
Authors	:	Moon, S.; Kim, J.; Olmos, J.L.; Bae, E.; Phillips Jr., G.N.
Deposited on	:	2019-06-28
Resolution	:	2.40 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

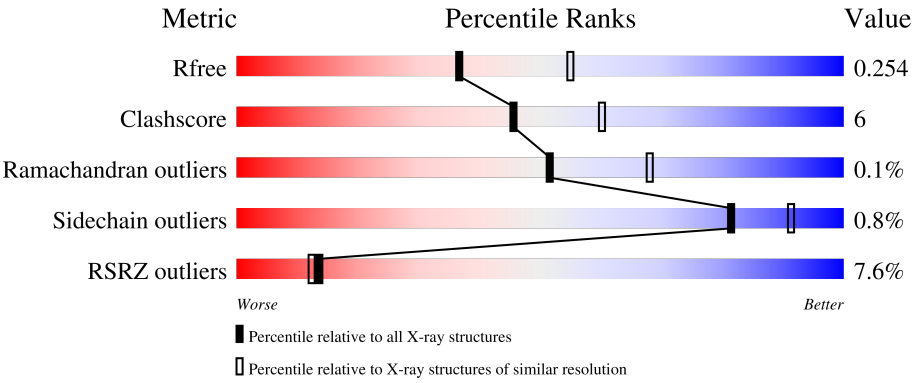
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	200	8% 79% 15%
1	B	200	2% 84% 10%
1	C	200	8% 82% 13%
1	D	200	2% 83% 12%
1	E	200	2% 80% 15%

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Mol	Chain	Length	Quality of chain
1	F	200	8% 84% 10%
1	G	200	12% 81% 14%
1	H	200	6% 74% 20%
1	I	200	10% 88% 8%
1	J	200	9% 81% 14%
1	K	200	12% 80% 14%
1	L	200	9% 79% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 37566 atoms, of which 18934 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 Adenylate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	B	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	C	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	D	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	E	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	F	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	G	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	H	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	I	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	J	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	K	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			
1	L	191	Total	C	H	N	O	S	0	0	0
			3037	934	1550	256	289	8			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	LEU	-	expression tag	UNP P43408
A	194	GLU	-	expression tag	UNP P43408
A	195	HIS	-	expression tag	UNP P43408
A	196	HIS	-	expression tag	UNP P43408
A	197	HIS	-	expression tag	UNP P43408

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Chain	Residue	Modelled	Actual	Comment	Reference
A	198	HIS	-	expression tag	UNP P43408
A	199	HIS	-	expression tag	UNP P43408
A	200	HIS	-	expression tag	UNP P43408
B	193	LEU	-	expression tag	UNP P43408
B	194	GLU	-	expression tag	UNP P43408
B	195	HIS	-	expression tag	UNP P43408
B	196	HIS	-	expression tag	UNP P43408
B	197	HIS	-	expression tag	UNP P43408
B	198	HIS	-	expression tag	UNP P43408
B	199	HIS	-	expression tag	UNP P43408
B	200	HIS	-	expression tag	UNP P43408
C	193	LEU	-	expression tag	UNP P43408
C	194	GLU	-	expression tag	UNP P43408
C	195	HIS	-	expression tag	UNP P43408
C	196	HIS	-	expression tag	UNP P43408
C	197	HIS	-	expression tag	UNP P43408
C	198	HIS	-	expression tag	UNP P43408
C	199	HIS	-	expression tag	UNP P43408
C	200	HIS	-	expression tag	UNP P43408
D	193	LEU	-	expression tag	UNP P43408
D	194	GLU	-	expression tag	UNP P43408
D	195	HIS	-	expression tag	UNP P43408
D	196	HIS	-	expression tag	UNP P43408
D	197	HIS	-	expression tag	UNP P43408
D	198	HIS	-	expression tag	UNP P43408
D	199	HIS	-	expression tag	UNP P43408
D	200	HIS	-	expression tag	UNP P43408
E	193	LEU	-	expression tag	UNP P43408
E	194	GLU	-	expression tag	UNP P43408
E	195	HIS	-	expression tag	UNP P43408
E	196	HIS	-	expression tag	UNP P43408
E	197	HIS	-	expression tag	UNP P43408
E	198	HIS	-	expression tag	UNP P43408
E	199	HIS	-	expression tag	UNP P43408
E	200	HIS	-	expression tag	UNP P43408
F	193	LEU	-	expression tag	UNP P43408
F	194	GLU	-	expression tag	UNP P43408
F	195	HIS	-	expression tag	UNP P43408
F	196	HIS	-	expression tag	UNP P43408
F	197	HIS	-	expression tag	UNP P43408
F	198	HIS	-	expression tag	UNP P43408
F	199	HIS	-	expression tag	UNP P43408

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Chain	Residue	Modelled	Actual	Comment	Reference
F	200	HIS	-	expression tag	UNP P43408
G	193	LEU	-	expression tag	UNP P43408
G	194	GLU	-	expression tag	UNP P43408
G	195	HIS	-	expression tag	UNP P43408
G	196	HIS	-	expression tag	UNP P43408
G	197	HIS	-	expression tag	UNP P43408
G	198	HIS	-	expression tag	UNP P43408
G	199	HIS	-	expression tag	UNP P43408
G	200	HIS	-	expression tag	UNP P43408
H	193	LEU	-	expression tag	UNP P43408
H	194	GLU	-	expression tag	UNP P43408
H	195	HIS	-	expression tag	UNP P43408
H	196	HIS	-	expression tag	UNP P43408
H	197	HIS	-	expression tag	UNP P43408
H	198	HIS	-	expression tag	UNP P43408
H	199	HIS	-	expression tag	UNP P43408
H	200	HIS	-	expression tag	UNP P43408
I	193	LEU	-	expression tag	UNP P43408
I	194	GLU	-	expression tag	UNP P43408
I	195	HIS	-	expression tag	UNP P43408
I	196	HIS	-	expression tag	UNP P43408
I	197	HIS	-	expression tag	UNP P43408
I	198	HIS	-	expression tag	UNP P43408
I	199	HIS	-	expression tag	UNP P43408
I	200	HIS	-	expression tag	UNP P43408
J	193	LEU	-	expression tag	UNP P43408
J	194	GLU	-	expression tag	UNP P43408
J	195	HIS	-	expression tag	UNP P43408
J	196	HIS	-	expression tag	UNP P43408
J	197	HIS	-	expression tag	UNP P43408
J	198	HIS	-	expression tag	UNP P43408
J	199	HIS	-	expression tag	UNP P43408
J	200	HIS	-	expression tag	UNP P43408
K	193	LEU	-	expression tag	UNP P43408
K	194	GLU	-	expression tag	UNP P43408
K	195	HIS	-	expression tag	UNP P43408
K	196	HIS	-	expression tag	UNP P43408
K	197	HIS	-	expression tag	UNP P43408
K	198	HIS	-	expression tag	UNP P43408
K	199	HIS	-	expression tag	UNP P43408
K	200	HIS	-	expression tag	UNP P43408
L	193	LEU	-	expression tag	UNP P43408

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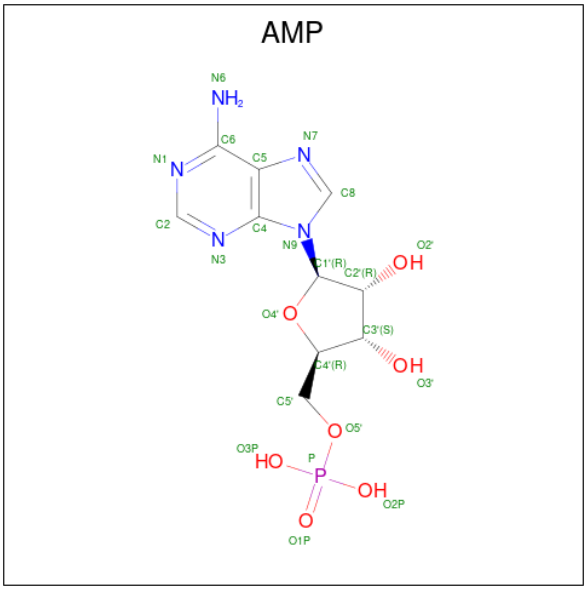
Chain	Residue	Modelled	Actual	Comment	Reference
L	194	GLU	-	expression tag	UNP P43408
L	195	HIS	-	expression tag	UNP P43408
L	196	HIS	-	expression tag	UNP P43408
L	197	HIS	-	expression tag	UNP P43408
L	198	HIS	-	expression tag	UNP P43408
L	199	HIS	-	expression tag	UNP P43408
L	200	HIS	-	expression tag	UNP P43408

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	B	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	B	1	Total	C	H	N	O	P	0	0
			36	10	13	5	7	1		
2	C	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	C	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	D	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	D	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	E	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	F	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	F	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	G	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	G	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	H	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	H	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	I	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	I	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	J	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	J	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	K	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	K	1	Total	C	H	N	O	P	0	0
			36	10	13	5	7	1		
2	L	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		
2	L	1	Total	C	H	N	O	P	0	0
			37	10	14	5	7	1		

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	36	Total O 36 36	0	0
4	C	20	Total O 20 20	0	0
4	D	25	Total O 25 25	0	0
4	E	18	Total O 18 18	0	0
4	F	16	Total O 16 16	0	0
4	G	11	Total O 11 11	0	0
4	H	16	Total O 16 16	0	0
4	I	9	Total O 9 9	0	0
4	J	18	Total O 18 18	0	0

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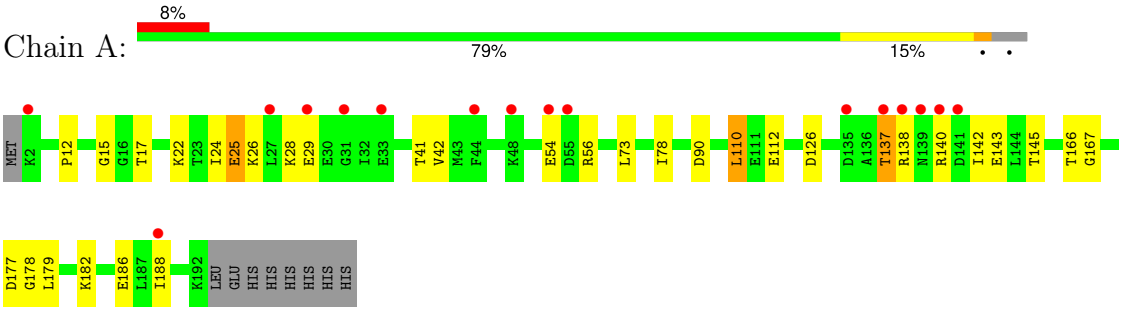
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	14	Total O 14 14	0	0
4	L	22	Total O 22 22	0	0

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.

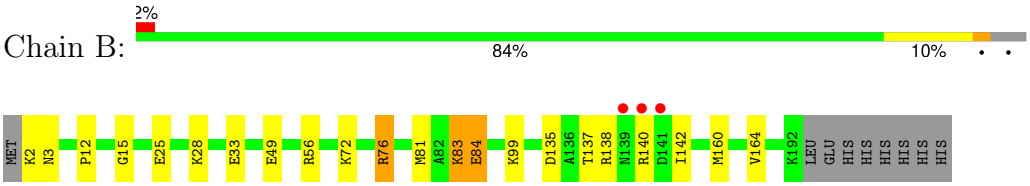
- Molecule 1: Adenylate kinase

Chain A:



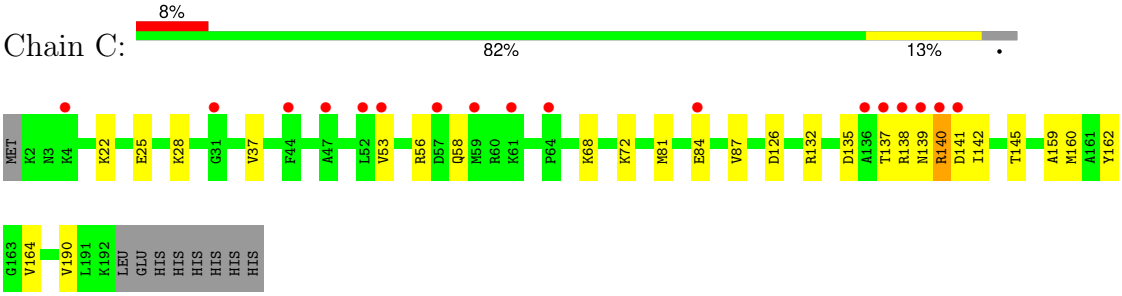
- Molecule 1: Adenylate kinase

Chain B:



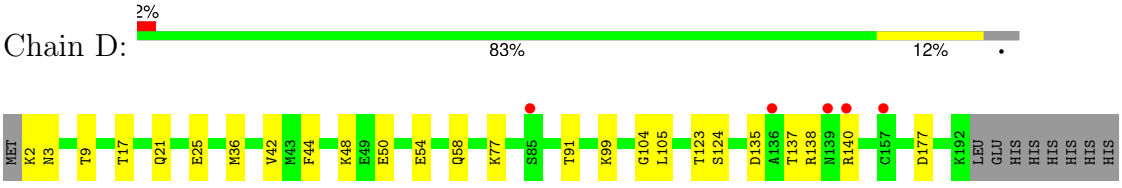
- Molecule 1: Adenylate kinase

Chain C:



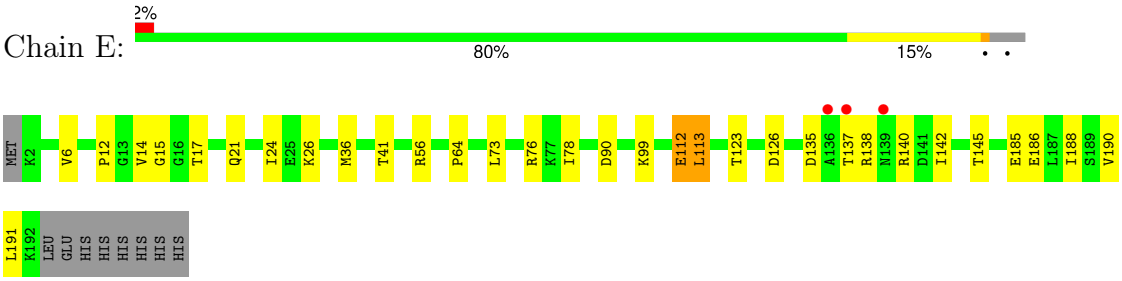
- Molecule 1: Adenylate kinase

Chain D:



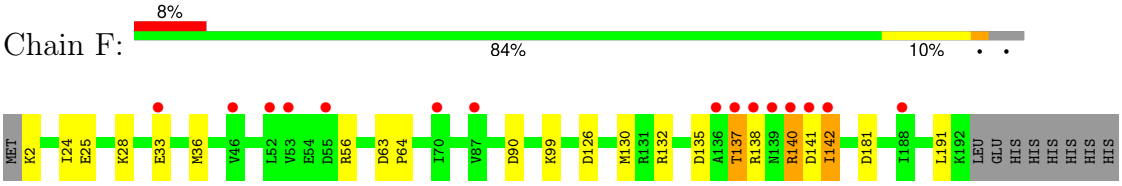
- Molecule 1: Adenylate kinase

Chain E:



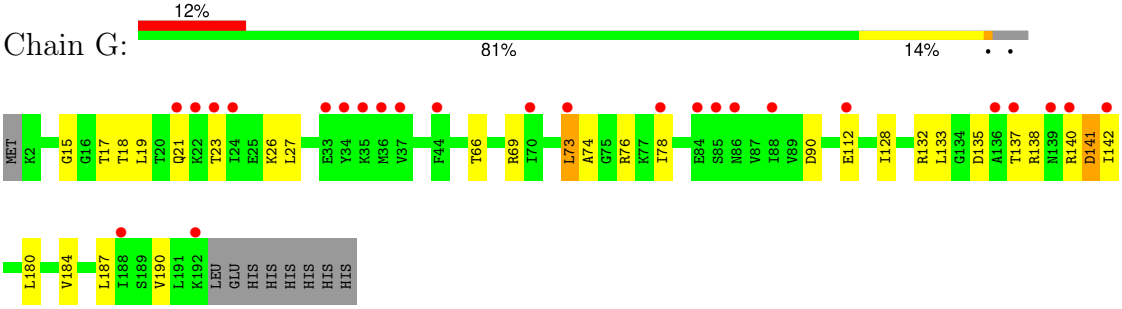
• Molecule 1: Adenylate kinase

Chain F:



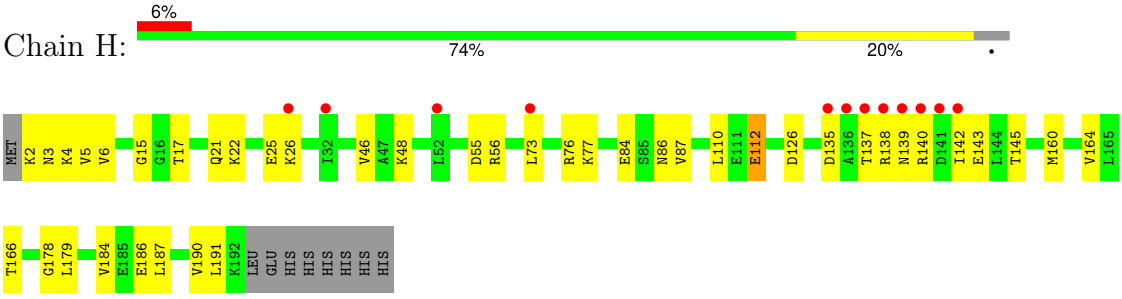
• Molecule 1: Adenylate kinase

Chain G:



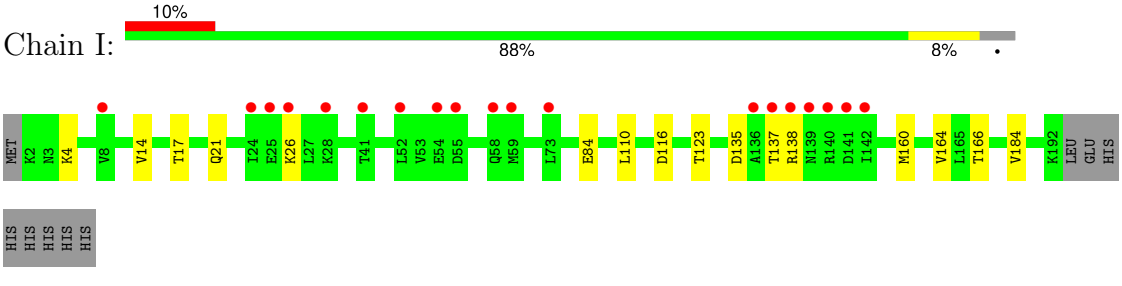
• Molecule 1: Adenylate kinase

Chain H:



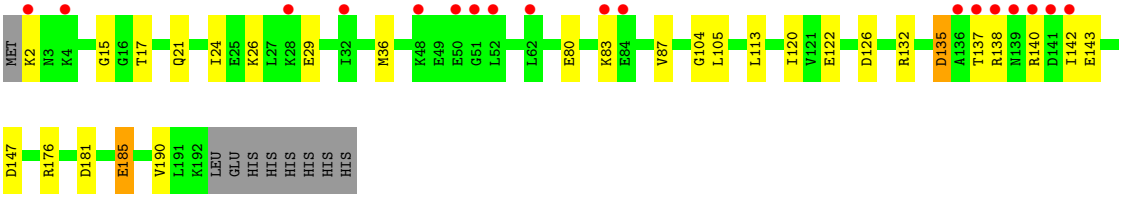
• Molecule 1: Adenylate kinase

Chain I:

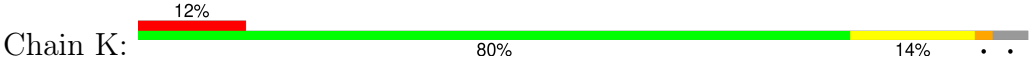


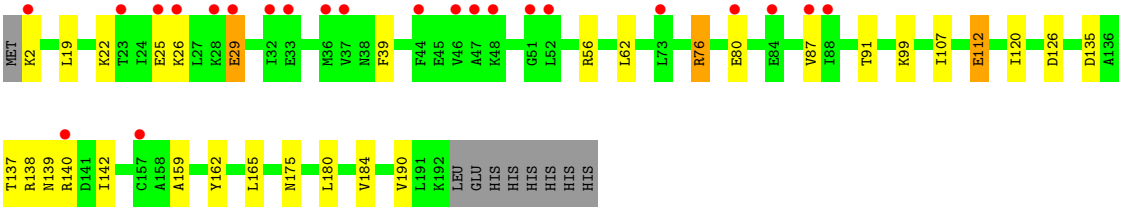
• Molecule 1: Adenylate kinase

Chain J:

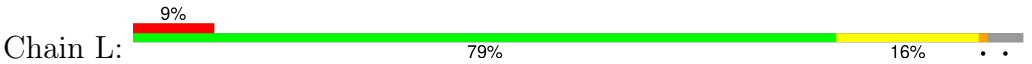


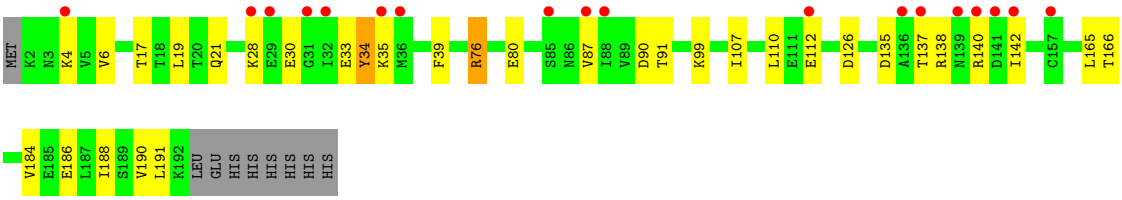
• Molecule 1: Adenylate kinase





• Molecule 1: Adenylate kinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.77Å 121.39Å 121.04Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	44.33 – 2.40 48.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (44.33-2.40) 86.5 (48.06-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.39 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.200 , 0.248 0.204 , 0.254	Depositor DCC
R_{free} test set	2020 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	37566	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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: MG, AMP

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	0.77	2/1501 (0.1%)	0.90	3/2021 (0.1%)
1	B	0.81	3/1501 (0.2%)	0.94	1/2021 (0.0%)
1	C	0.82	1/1501 (0.1%)	0.93	1/2021 (0.0%)
1	D	0.80	0/1501	0.90	1/2021 (0.0%)
1	E	0.89	5/1501 (0.3%)	0.93	5/2021 (0.2%)
1	F	0.79	2/1501 (0.1%)	0.93	6/2021 (0.3%)
1	G	0.63	0/1501	0.79	1/2021 (0.0%)
1	H	0.69	1/1501 (0.1%)	0.87	2/2021 (0.1%)
1	I	0.67	0/1501	0.77	0/2021
1	J	0.77	1/1501 (0.1%)	0.87	3/2021 (0.1%)
1	K	0.73	3/1501 (0.2%)	0.82	2/2021 (0.1%)
1	L	0.75	1/1501 (0.1%)	0.89	2/2021 (0.1%)
All	All	0.76	19/18012 (0.1%)	0.88	27/24252 (0.1%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	112	GLU	CG-CD	-14.09	1.30	1.51
1	B	84	GLU	CB-CG	8.38	1.68	1.52
1	K	112	GLU	CD-OE2	-7.86	1.17	1.25
1	H	112	GLU	CD-OE2	-7.67	1.17	1.25
1	L	34	TYR	CZ-OH	-7.56	1.25	1.37

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	112	GLU	OE1-CD-OE2	9.92	135.20	123.30
1	E	112	GLU	CG-CD-OE2	-8.75	100.80	118.30
1	K	76	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	110	LEU	CB-CG-CD2	-7.33	98.54	111.00
1	A	126	ASP	CB-CG-OD1	-7.08	111.93	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1487	1550	1549	27	2
1	B	1487	1550	1549	19	1
1	C	1487	1550	1549	20	1
1	D	1487	1550	1549	18	0
1	E	1487	1550	1549	21	2
1	F	1487	1550	1549	8	0
1	G	1487	1550	1549	23	0
1	H	1487	1550	1549	35	3
1	I	1487	1550	1549	13	0
1	J	1487	1550	1549	16	0
1	K	1487	1550	1549	22	1
1	L	1487	1550	1549	26	1
2	A	46	28	24	2	0
2	B	46	27	24	3	0
2	C	46	28	24	1	1
2	D	46	28	24	1	0
2	E	46	28	24	2	0
2	F	46	28	24	0	0
2	G	46	28	24	2	0
2	H	46	28	24	1	0
2	I	46	28	24	0	0
2	J	46	28	24	1	0
2	K	46	27	24	3	0
2	L	46	28	24	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	19	0	0	4	0
4	B	36	0	0	2	0
4	C	20	0	0	1	0
4	D	25	0	0	3	0
4	E	18	0	0	0	0
4	F	16	0	0	0	0
4	G	11	0	0	2	0
4	H	16	0	0	1	0
4	I	9	0	0	0	0
4	J	18	0	0	0	0
4	K	14	0	0	2	0
4	L	22	0	0	0	0
All	All	18632	18934	18876	239	6

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 6.

The worst 5 of 239 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:L:107:ILE:HD13	1:L:165:LEU:HD13	1.39	1.04
1:B:135:ASP:OD1	1:B:137:THR:HG22	1.59	1.03
1:B:140:ARG:NH2	4:B:401:HOH:O	1.94	0.99
1:K:135:ASP:OD1	1:K:137:THR:HG22	1.64	0.98
1:J:135:ASP:OD1	1:J:137:THR:HG22	1.67	0.94

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ASP:OD1	1:H:145:THR:OG1[1_556]	1.98	0.22
1:B:25:GLU:OE1	2:C:302:AMP:O3'[2_646]	1.99	0.21
1:A:137:THR:OG1	1:H:139:ASN:OD1[1_455]	2.00	0.20
1:A:145:THR:OG1	1:K:126:ASP:OD1[1_455]	2.05	0.15
1:C:145:THR:OG1	1:L:126:ASP:OD1[1_455]	2.09	0.11

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	189/200 (94%)	184 (97%)	5 (3%)	0	100	100
1	B	189/200 (94%)	187 (99%)	2 (1%)	0	100	100
1	C	189/200 (94%)	185 (98%)	3 (2%)	1 (0%)	29	41
1	D	189/200 (94%)	188 (100%)	1 (0%)	0	100	100
1	E	189/200 (94%)	187 (99%)	2 (1%)	0	100	100
1	F	189/200 (94%)	185 (98%)	4 (2%)	0	100	100
1	G	189/200 (94%)	186 (98%)	3 (2%)	0	100	100
1	H	189/200 (94%)	186 (98%)	3 (2%)	0	100	100
1	I	189/200 (94%)	185 (98%)	4 (2%)	0	100	100
1	J	189/200 (94%)	186 (98%)	3 (2%)	0	100	100
1	K	189/200 (94%)	185 (98%)	3 (2%)	1 (0%)	29	41
1	L	189/200 (94%)	186 (98%)	3 (2%)	0	100	100
All	All	2268/2400 (94%)	2230 (98%)	36 (2%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	140	ARG
1	K	139	ASN

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	166/175 (95%)	165 (99%)	1 (1%)	86 94
1	B	166/175 (95%)	166 (100%)	0	100 100
1	C	166/175 (95%)	166 (100%)	0	100 100
1	D	166/175 (95%)	166 (100%)	0	100 100
1	E	166/175 (95%)	166 (100%)	0	100 100
1	F	166/175 (95%)	160 (96%)	6 (4%)	35 54
1	G	166/175 (95%)	165 (99%)	1 (1%)	86 94
1	H	166/175 (95%)	165 (99%)	1 (1%)	86 94
1	I	166/175 (95%)	166 (100%)	0	100 100
1	J	166/175 (95%)	163 (98%)	3 (2%)	59 76
1	K	166/175 (95%)	164 (99%)	2 (1%)	71 85
1	L	166/175 (95%)	165 (99%)	1 (1%)	86 94
All	All	1992/2100 (95%)	1977 (99%)	15 (1%)	81 91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	141	ASP
1	K	87	VAL
1	H	55	ASP
1	L	142	ILE
1	J	113	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AMP	B	301	-	21,25,25	1.06	1 (4%)	23,38,38	1.55	4 (17%)
2	AMP	K	301	-	21,25,25	0.70	0	23,38,38	1.01	2 (8%)
2	AMP	G	301	-	21,25,25	0.72	0	23,38,38	0.91	2 (8%)
2	AMP	J	301	-	21,25,25	0.69	0	23,38,38	1.16	3 (13%)
2	AMP	E	302	-	21,25,25	0.85	0	23,38,38	0.96	2 (8%)
2	AMP	K	302	-	21,25,25	0.74	0	23,38,38	1.25	4 (17%)
2	AMP	A	301	-	21,25,25	0.68	0	23,38,38	1.07	1 (4%)
2	AMP	J	302	-	21,25,25	0.73	0	23,38,38	1.33	3 (13%)
2	AMP	B	302	-	21,25,25	1.17	2 (9%)	23,38,38	1.26	3 (13%)
2	AMP	C	302	-	21,25,25	1.38	2 (9%)	23,38,38	1.18	2 (8%)
2	AMP	G	302	-	21,25,25	0.86	0	23,38,38	1.05	2 (8%)
2	AMP	D	302	-	21,25,25	0.82	1 (4%)	23,38,38	1.21	4 (17%)
2	AMP	I	302	-	21,25,25	0.77	0	23,38,38	1.18	2 (8%)
2	AMP	L	301	-	21,25,25	1.15	3 (14%)	23,38,38	1.04	2 (8%)
2	AMP	F	301	-	21,25,25	0.88	0	23,38,38	1.15	3 (13%)
2	AMP	L	302	-	21,25,25	0.96	1 (4%)	23,38,38	0.98	2 (8%)
2	AMP	E	301	-	21,25,25	0.81	0	23,38,38	1.12	2 (8%)
2	AMP	C	301	-	21,25,25	0.80	0	23,38,38	0.98	1 (4%)
2	AMP	H	301	-	21,25,25	0.79	0	23,38,38	0.94	2 (8%)
2	AMP	H	302	-	21,25,25	0.81	0	23,38,38	1.02	2 (8%)
2	AMP	A	302	-	21,25,25	0.76	0	23,38,38	1.24	3 (13%)
2	AMP	F	302	-	21,25,25	0.84	1 (4%)	23,38,38	1.43	4 (17%)
2	AMP	D	301	-	21,25,25	1.01	1 (4%)	23,38,38	1.24	2 (8%)
2	AMP	I	301	-	21,25,25	0.81	1 (4%)	23,38,38	1.10	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	B	301	-	-	0/6/26/26	0/3/3/3
2	AMP	K	301	-	-	0/6/26/26	0/3/3/3
2	AMP	G	301	-	-	0/6/26/26	0/3/3/3
2	AMP	J	301	-	-	2/6/26/26	0/3/3/3
2	AMP	E	302	-	-	5/6/26/26	0/3/3/3
2	AMP	K	302	-	-	5/6/26/26	0/3/3/3
2	AMP	A	301	-	-	1/6/26/26	0/3/3/3
2	AMP	J	302	-	-	5/6/26/26	0/3/3/3
2	AMP	B	302	-	-	5/6/26/26	0/3/3/3
2	AMP	C	302	-	-	0/6/26/26	0/3/3/3
2	AMP	G	302	-	-	3/6/26/26	0/3/3/3
2	AMP	D	302	-	-	5/6/26/26	0/3/3/3
2	AMP	I	302	-	-	5/6/26/26	0/3/3/3
2	AMP	L	301	-	-	2/6/26/26	0/3/3/3
2	AMP	F	301	-	-	1/6/26/26	0/3/3/3
2	AMP	L	302	-	-	0/6/26/26	0/3/3/3
2	AMP	E	301	-	-	0/6/26/26	0/3/3/3
2	AMP	C	301	-	-	2/6/26/26	0/3/3/3
2	AMP	H	301	-	-	1/6/26/26	0/3/3/3
2	AMP	H	302	-	-	1/6/26/26	0/3/3/3
2	AMP	A	302	-	-	5/6/26/26	0/3/3/3
2	AMP	F	302	-	-	5/6/26/26	0/3/3/3
2	AMP	D	301	-	-	1/6/26/26	0/3/3/3
2	AMP	I	301	-	-	0/6/26/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	AMP	P-O1P	4.51	1.64	1.50
2	B	301	AMP	C4-N3	-3.52	1.30	1.35
2	B	302	AMP	P-O2P	-3.25	1.42	1.54
2	C	302	AMP	P-O3P	-2.87	1.44	1.54
2	L	301	AMP	P-O3P	-2.75	1.44	1.54

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	AMP	C4-C5-N7	4.78	114.39	109.34
2	F	302	AMP	O3P-P-O5'	-4.11	95.94	106.67
2	D	301	AMP	O2P-P-O1P	3.66	125.11	110.83
2	J	302	AMP	O2P-P-O1P	3.63	124.97	110.83
2	A	301	AMP	O2P-P-O1P	3.40	124.09	110.83

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	AMP	C5'-O5'-P-O2P
2	A	302	AMP	C5'-O5'-P-O3P
2	B	302	AMP	C5'-O5'-P-O2P
2	B	302	AMP	C5'-O5'-P-O3P
2	D	301	AMP	C5'-O5'-P-O2P

There are no ring outliers.

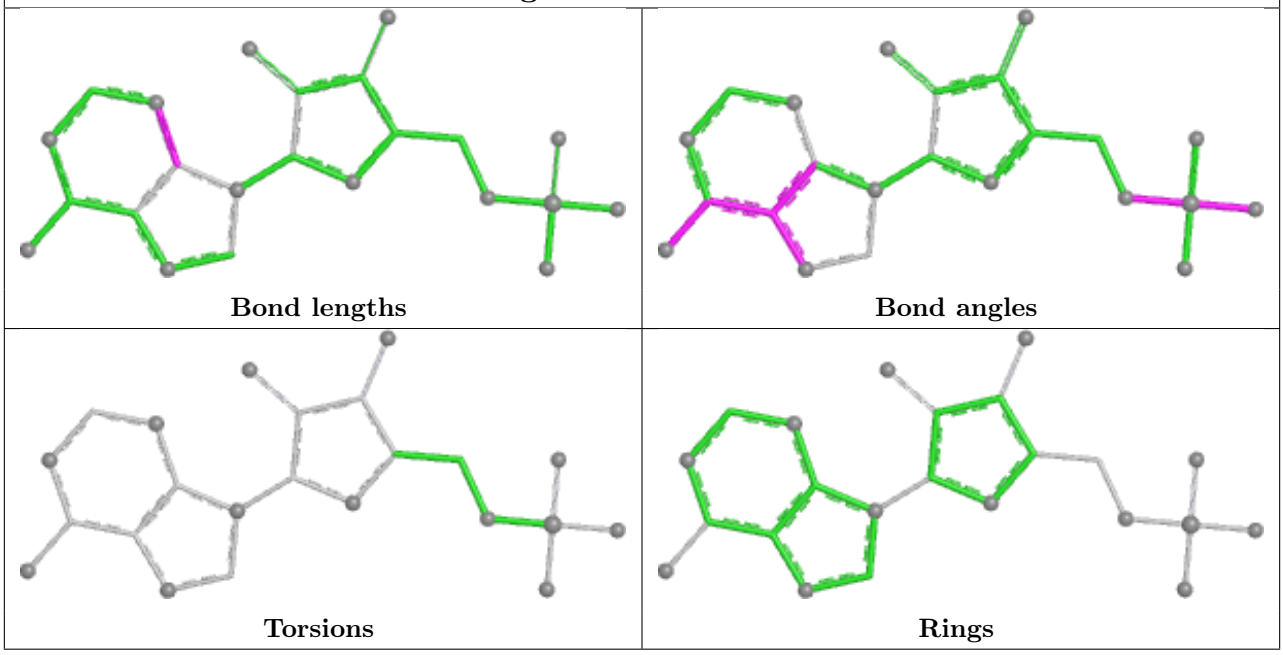
13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	AMP	1	0
2	K	301	AMP	1	0
2	E	302	AMP	1	0
2	K	302	AMP	2	0
2	A	301	AMP	1	0
2	J	302	AMP	1	0
2	B	302	AMP	2	0
2	C	302	AMP	1	1
2	G	302	AMP	2	0
2	D	302	AMP	1	0
2	E	301	AMP	1	0
2	H	302	AMP	1	0
2	A	302	AMP	1	0

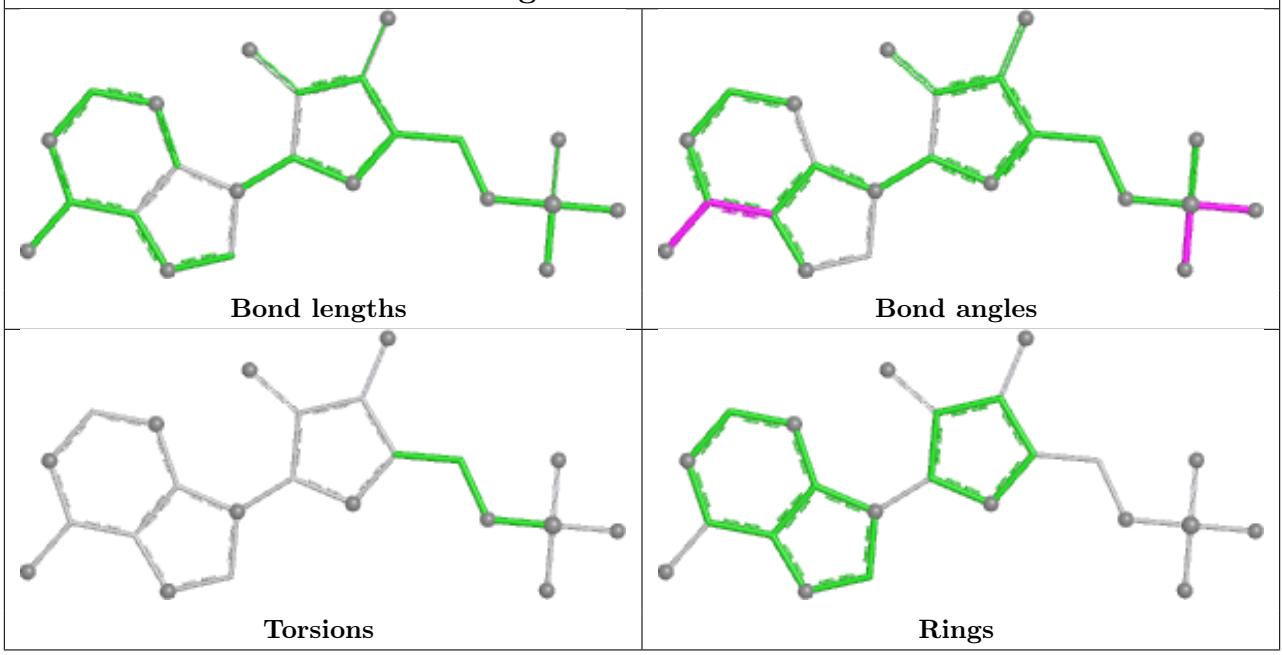
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

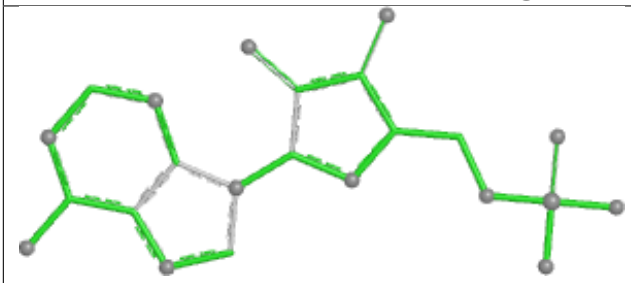
Ligand AMP B 301



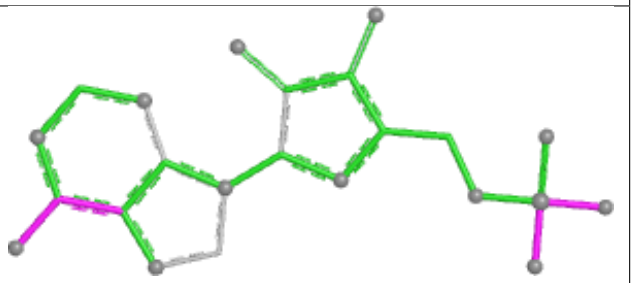
Ligand AMP K 301



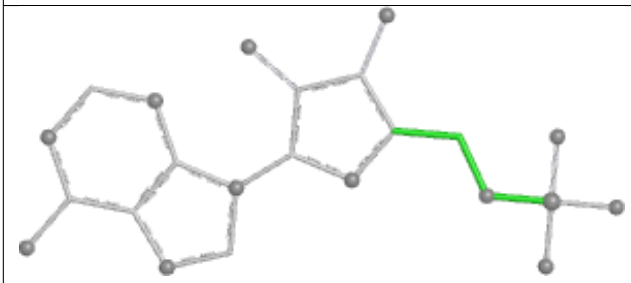
Ligand AMP G 301



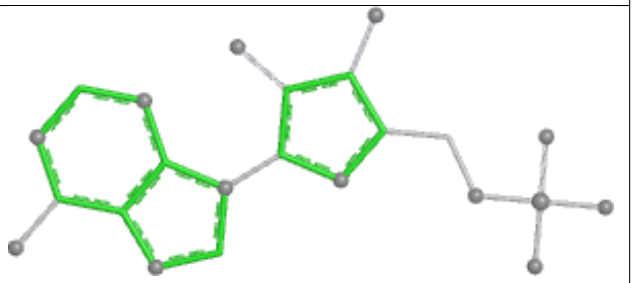
Bond lengths



Bond angles

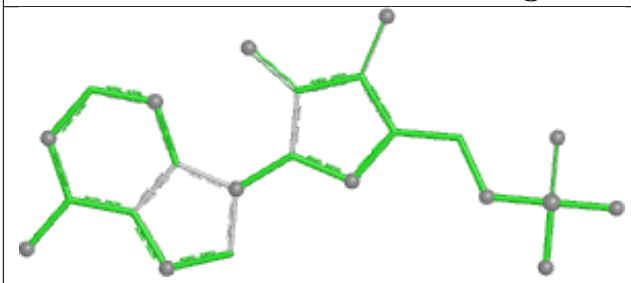


Torsions

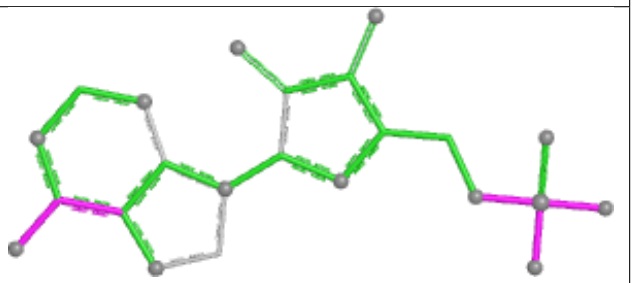


Rings

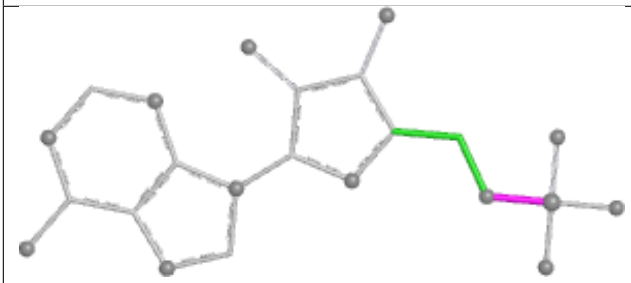
Ligand AMP J 301



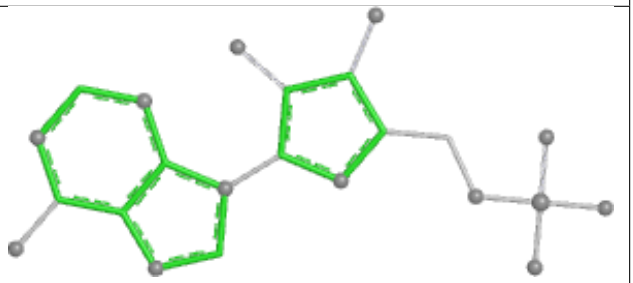
Bond lengths



Bond angles

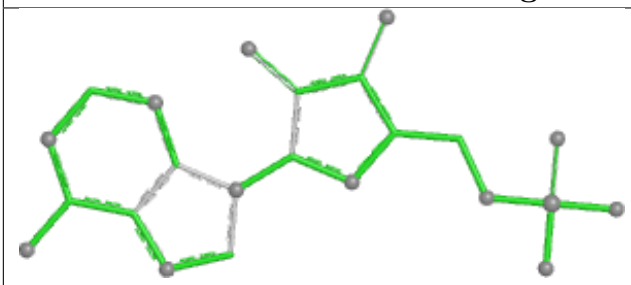


Torsions

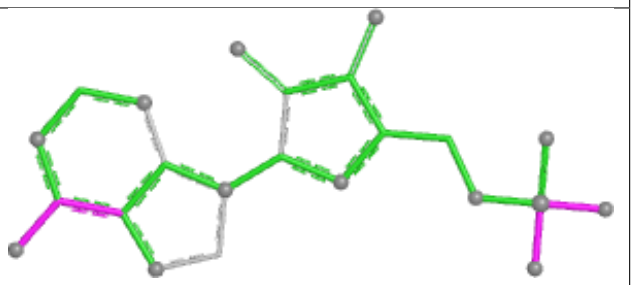


Rings

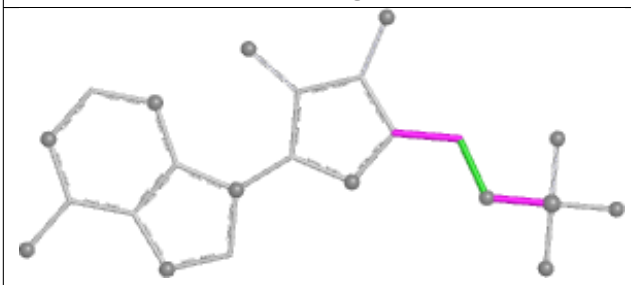
Ligand AMP E 302



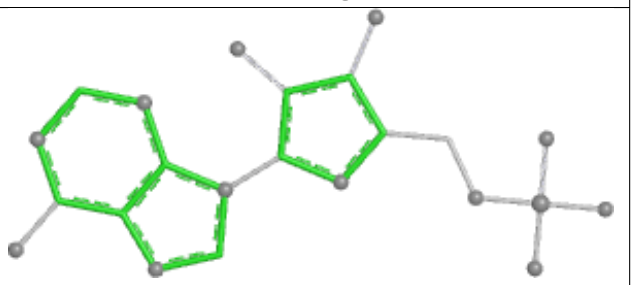
Bond lengths



Bond angles

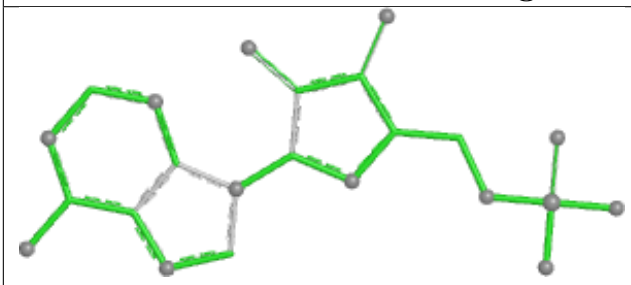


Torsions



Rings

Ligand AMP K 302



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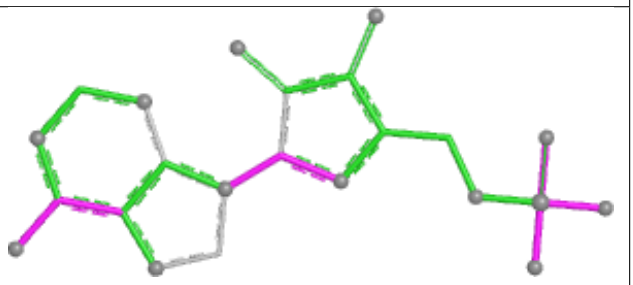

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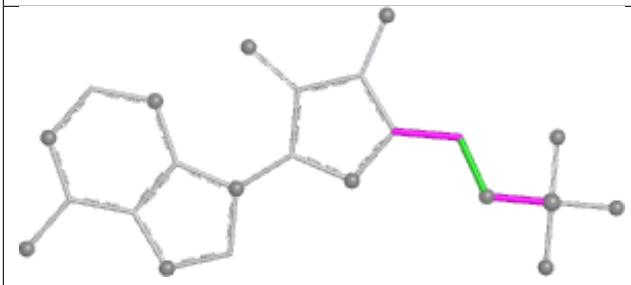

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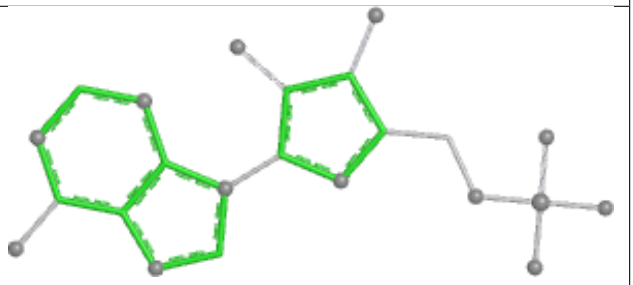
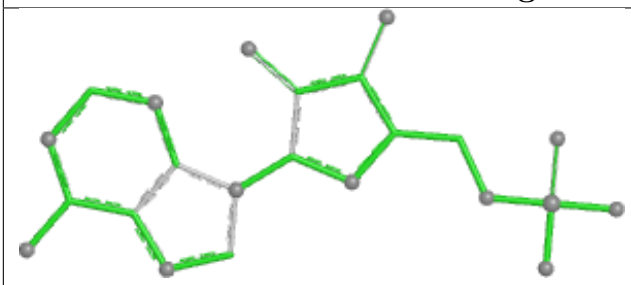


Rings

Ligand AMP A 301



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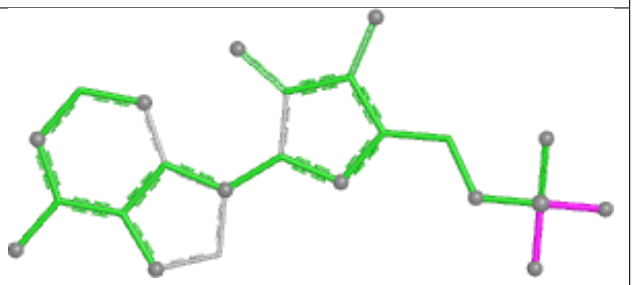

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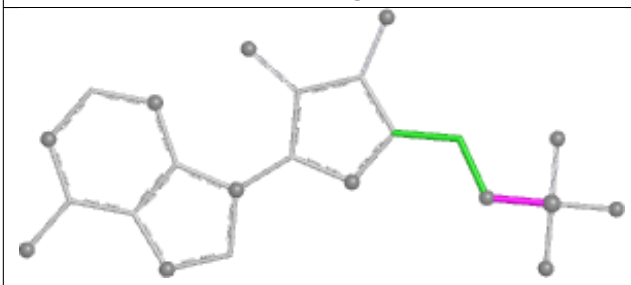

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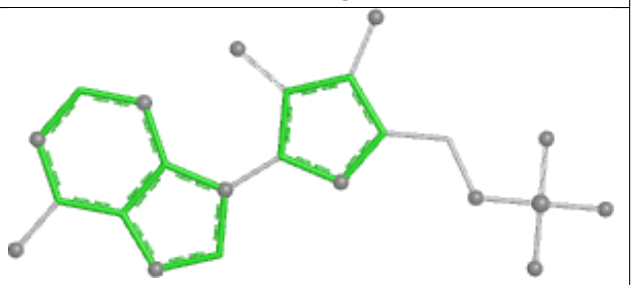
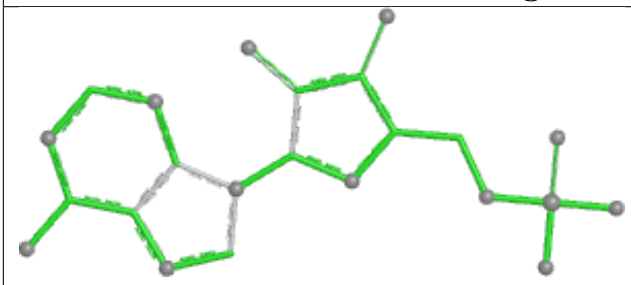


Rings

Ligand AMP J 302



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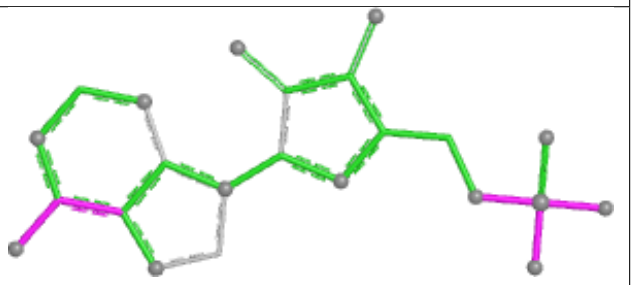

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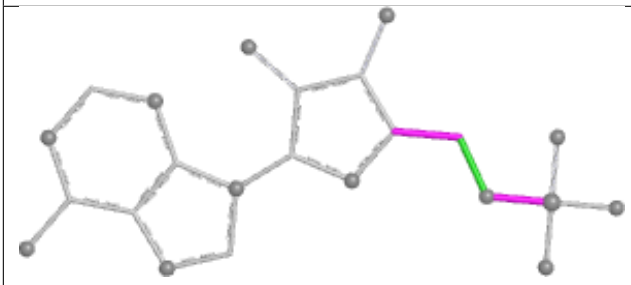

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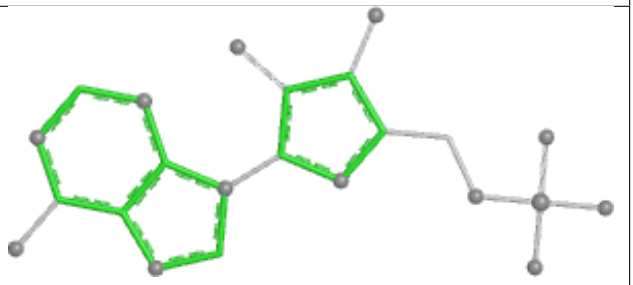
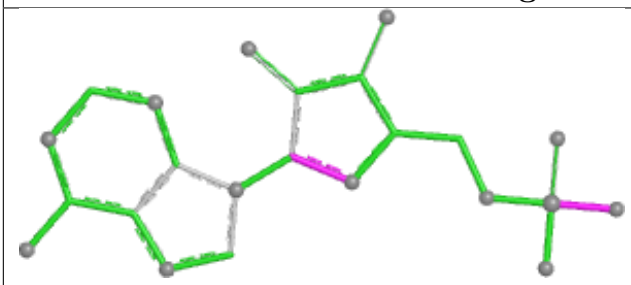


Rings

Ligand AMP B 302



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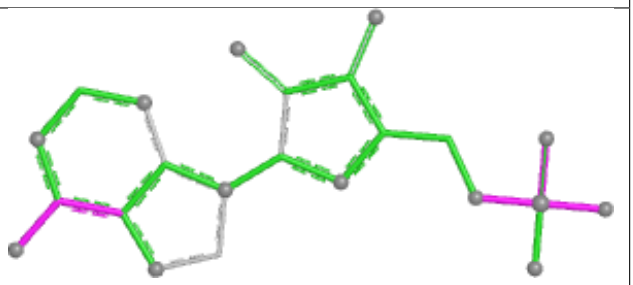

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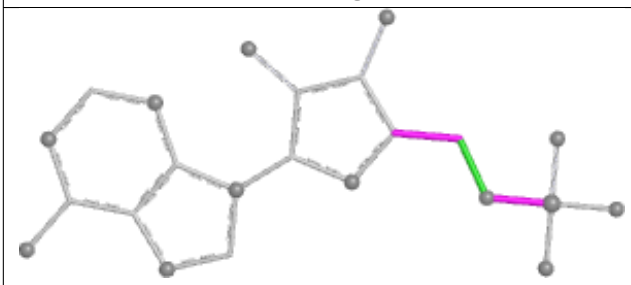

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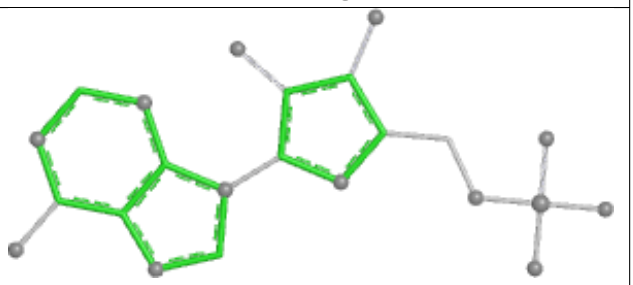
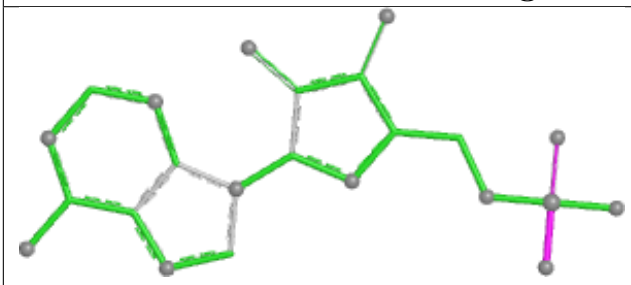


Rings

Ligand AMP C 302



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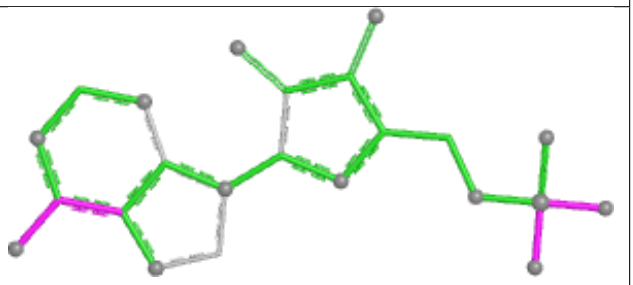

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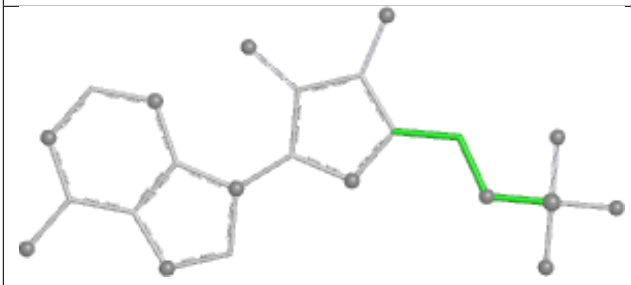

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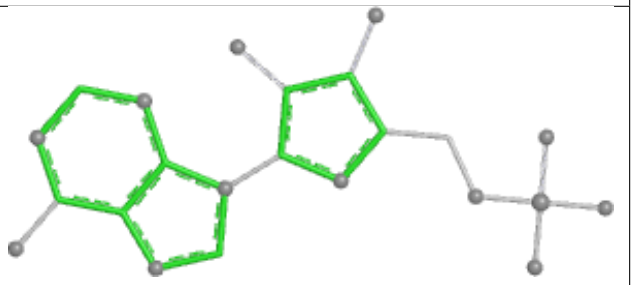
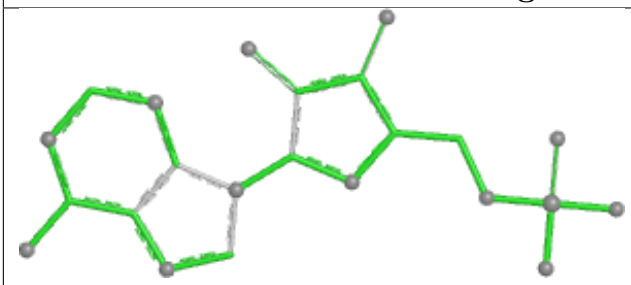


Rings

Ligand AMP G 302



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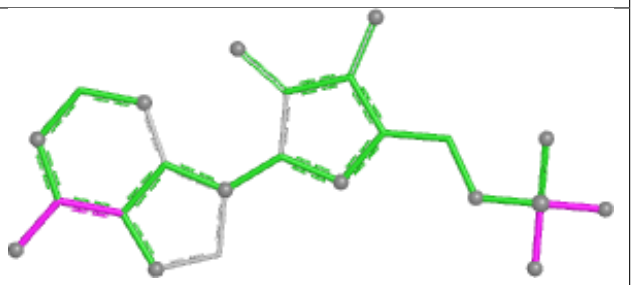

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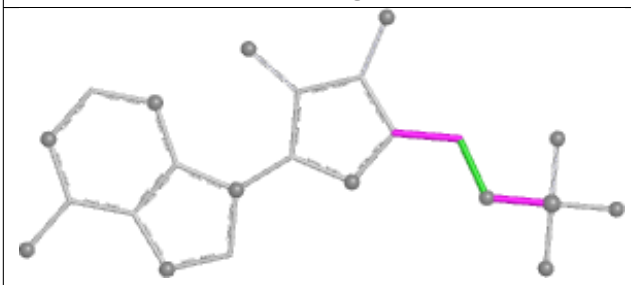

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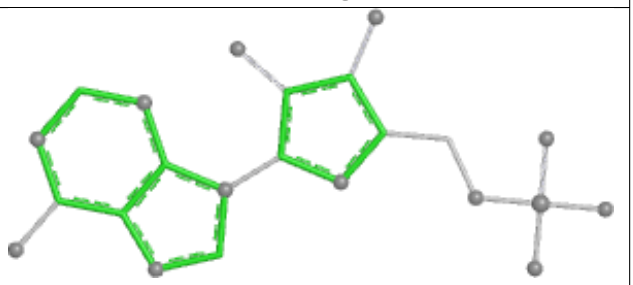
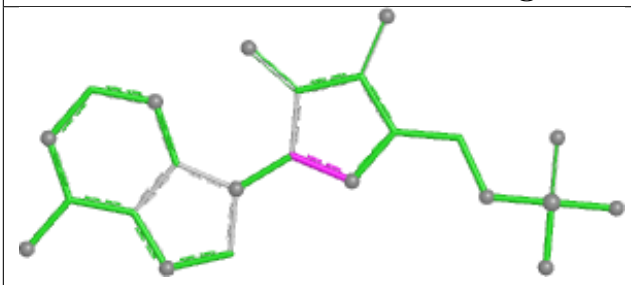


Rings

Ligand AMP D 302



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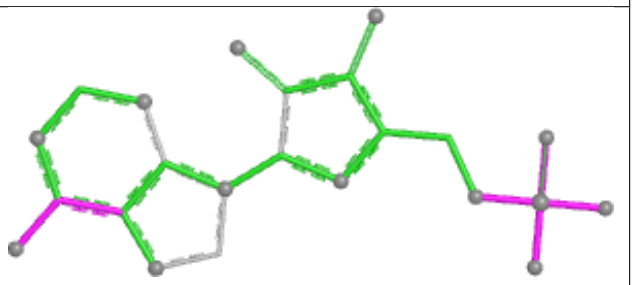

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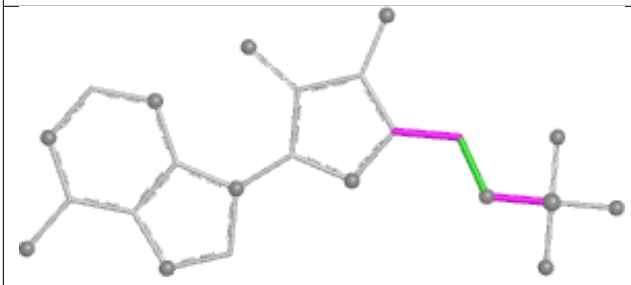

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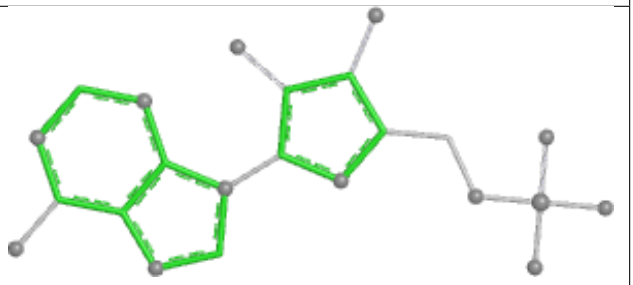
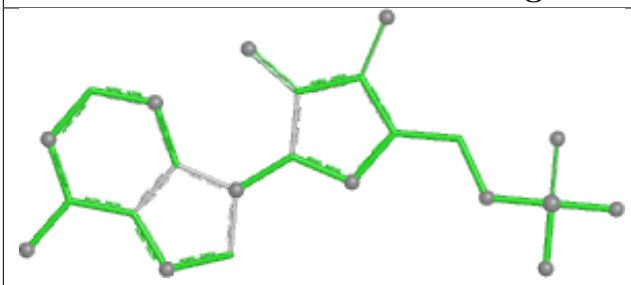


Rings

Ligand AMP I 302



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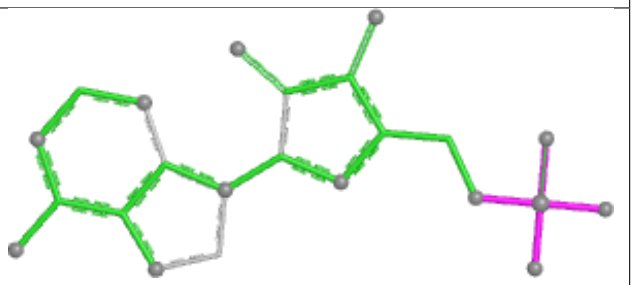

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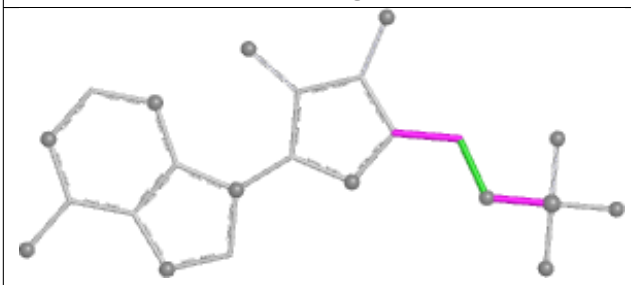

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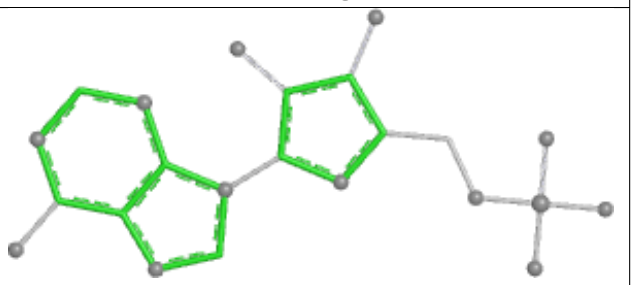
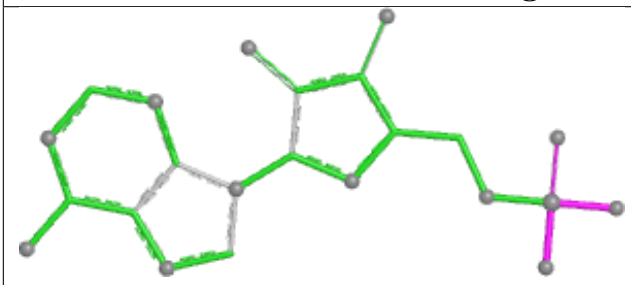


Rings

Ligand AMP L 301



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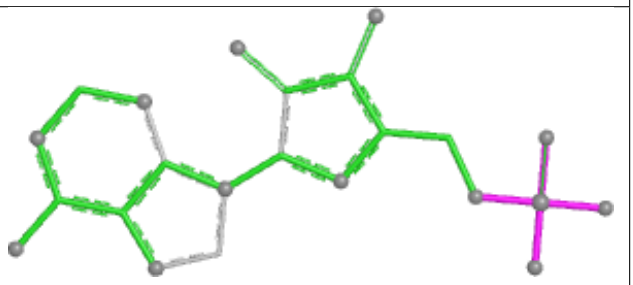

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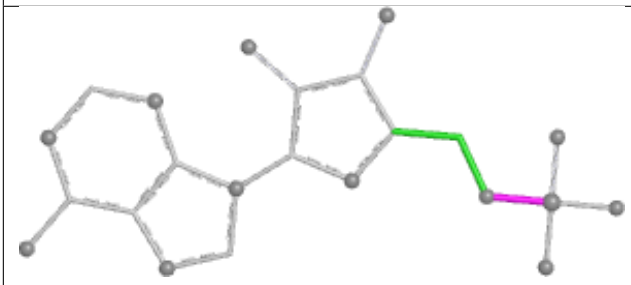

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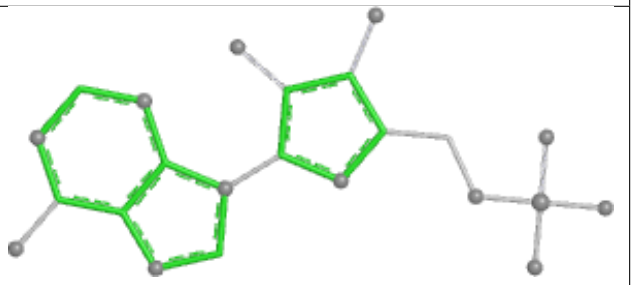
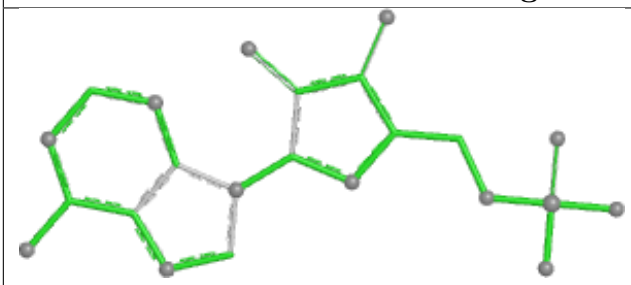


Rings

Ligand AMP F 301



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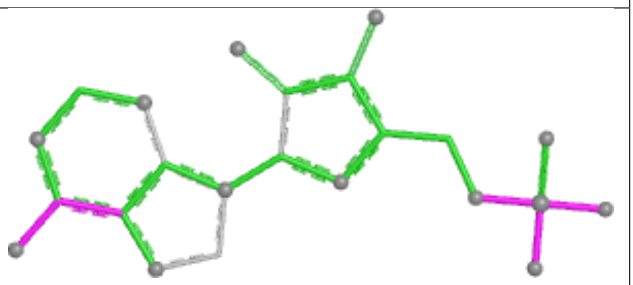

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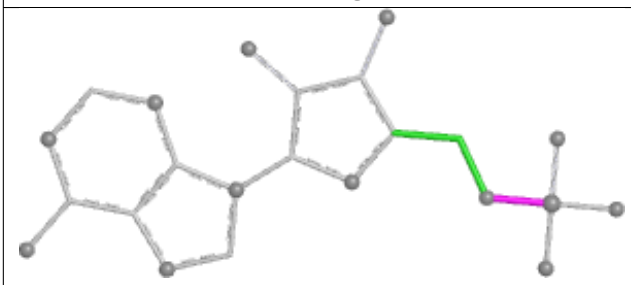

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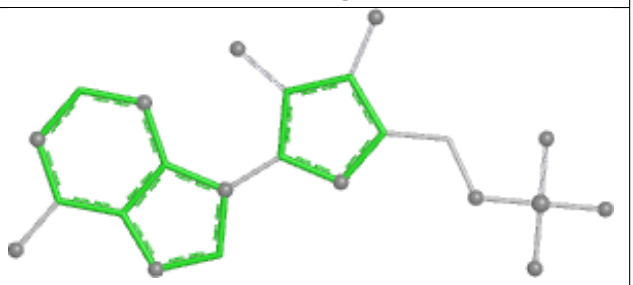
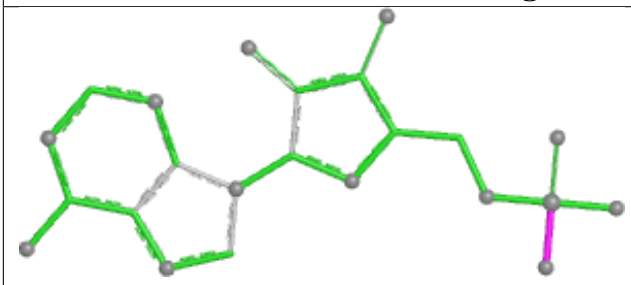


Rings

Ligand AMP L 302



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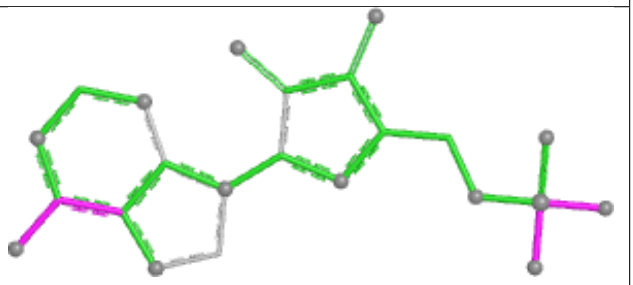

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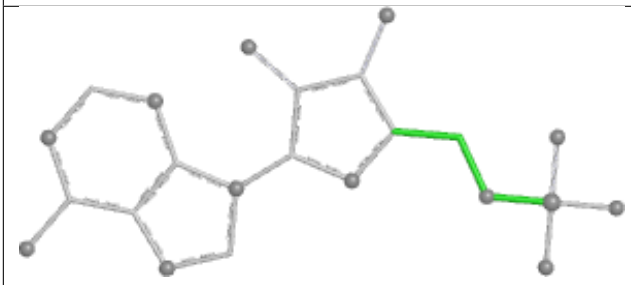

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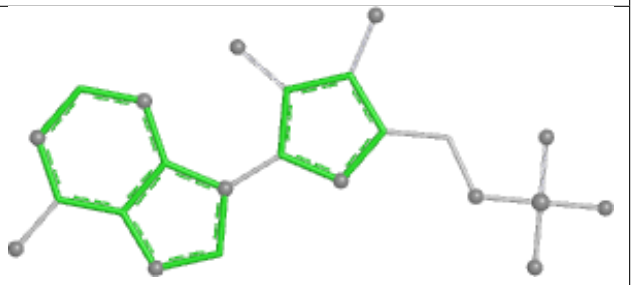
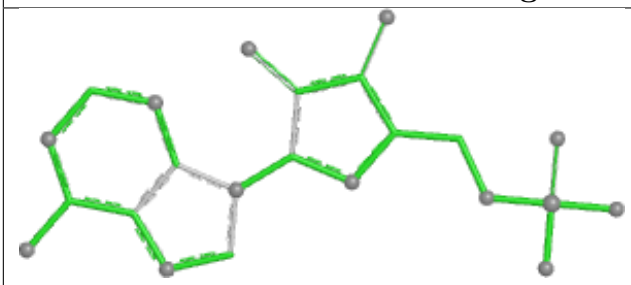


Rings

Ligand AMP E 301



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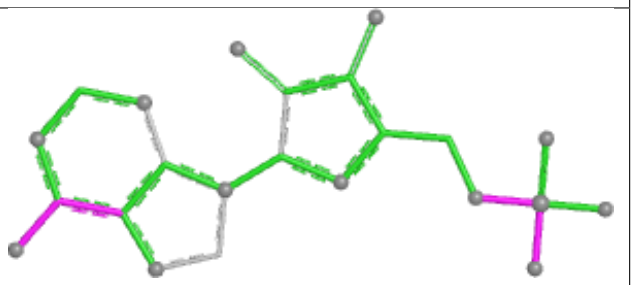

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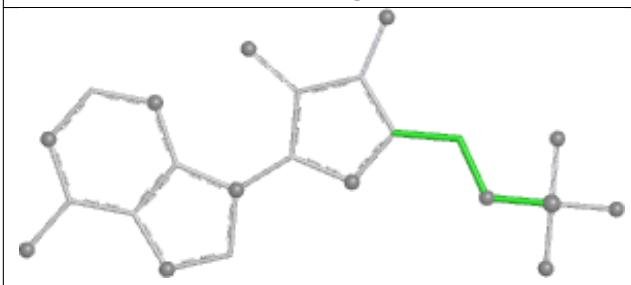

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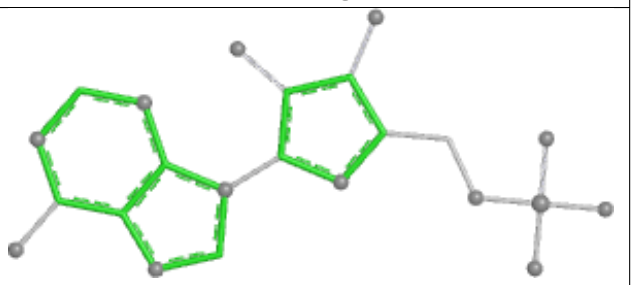
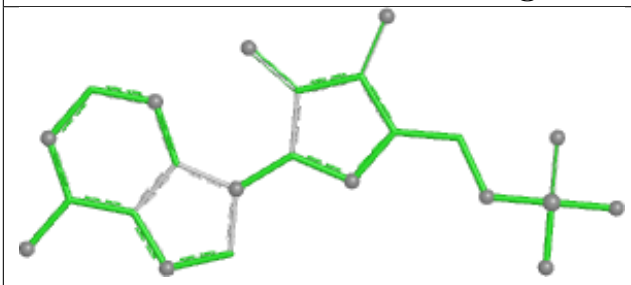


Rings

Ligand AMP C 301



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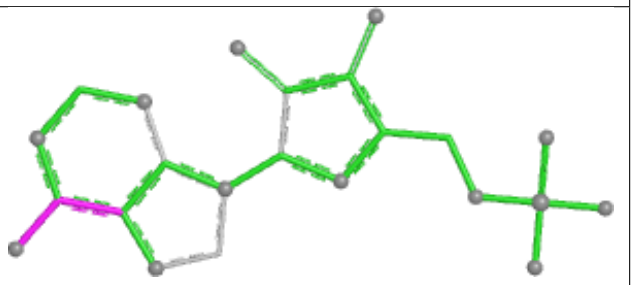
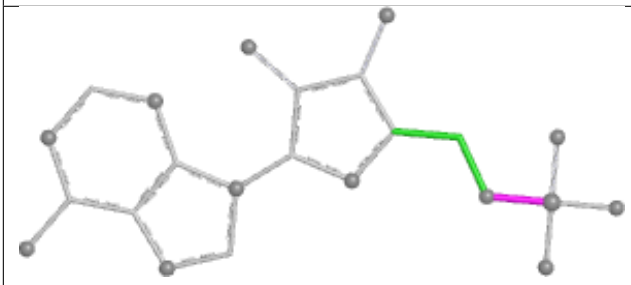


Bond angles



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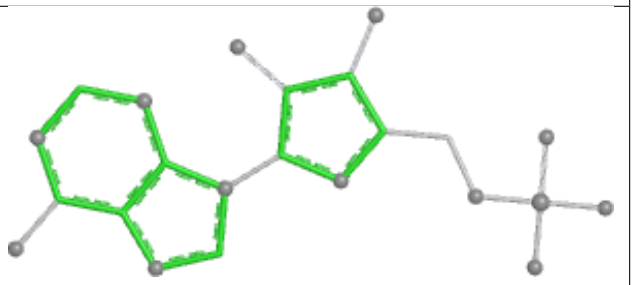
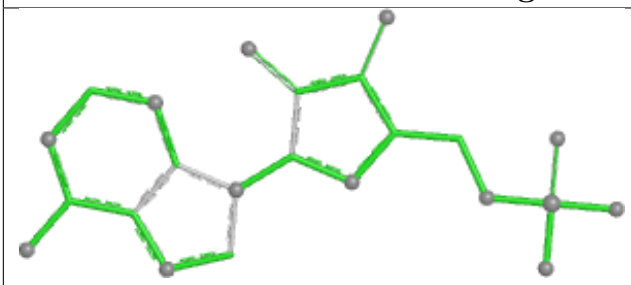


Rings

Ligand AMP H 301



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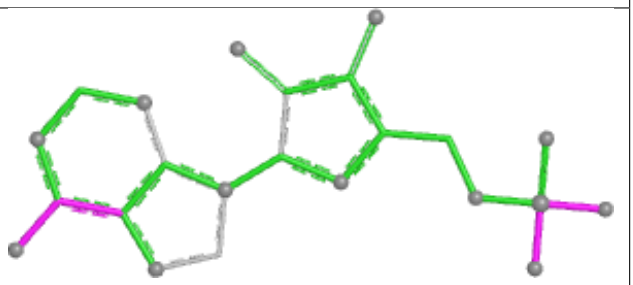
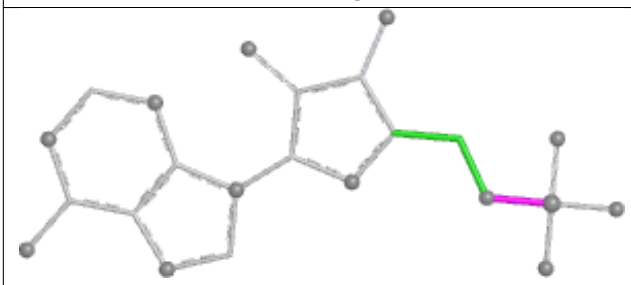


Bond angles



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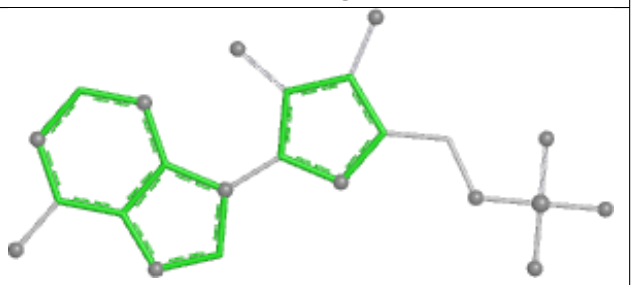

Rings

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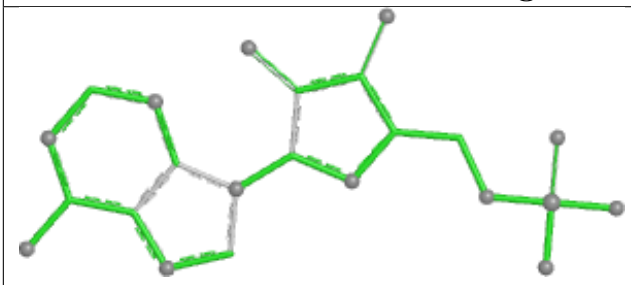
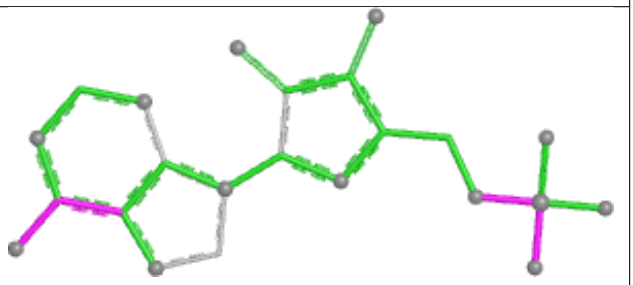
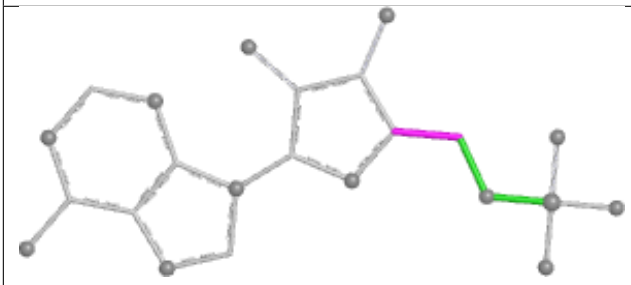


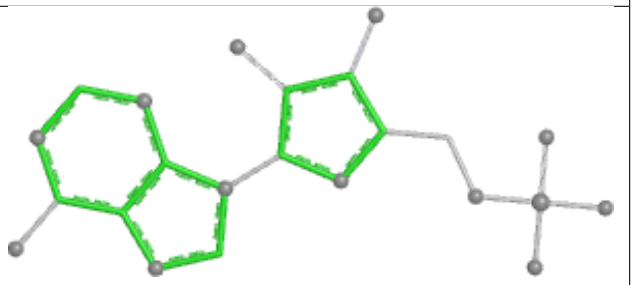
Bond lengths



Bond angles

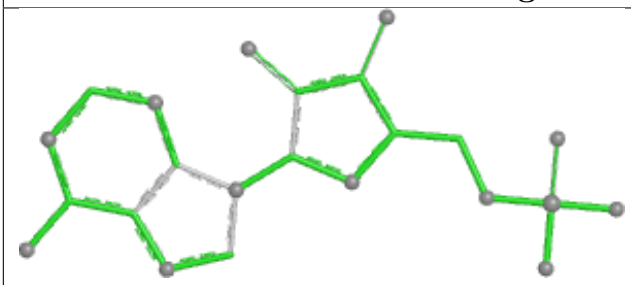


Torsions

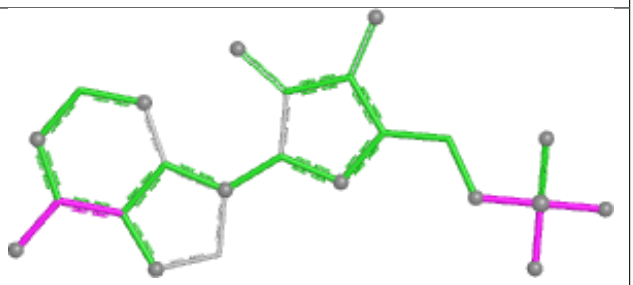


Rings

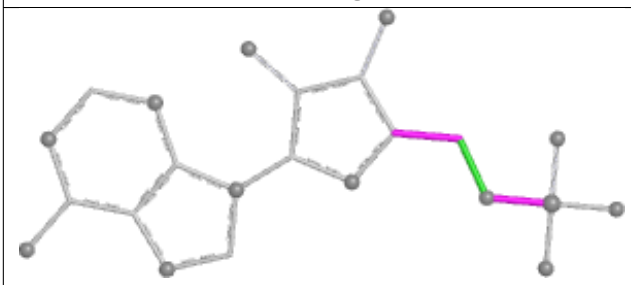
Ligand AMP A 302



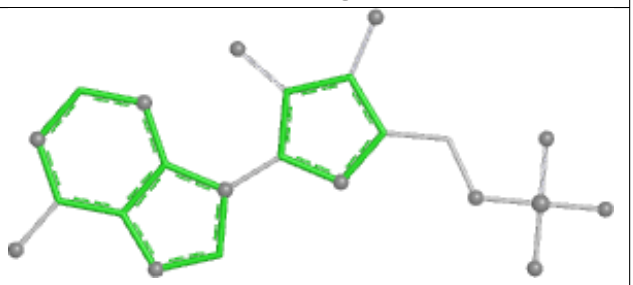
Bond lengths



Bond angles

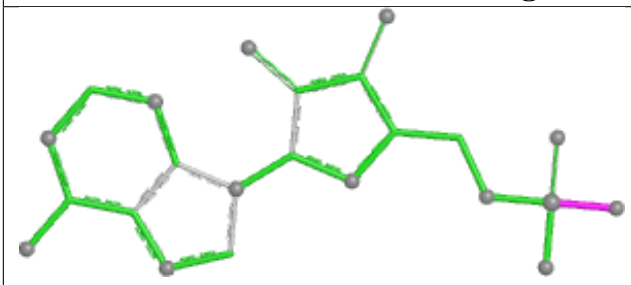


Torsions

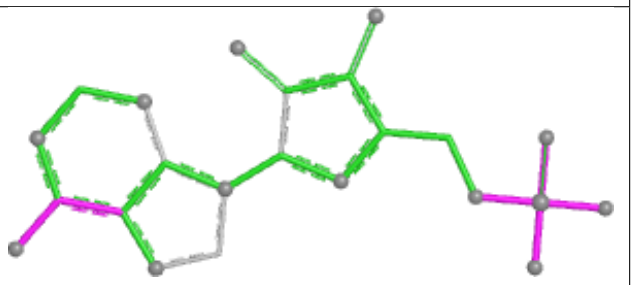


Rings

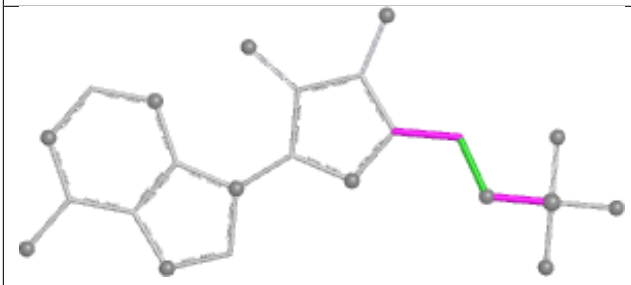
Ligand AMP F 302



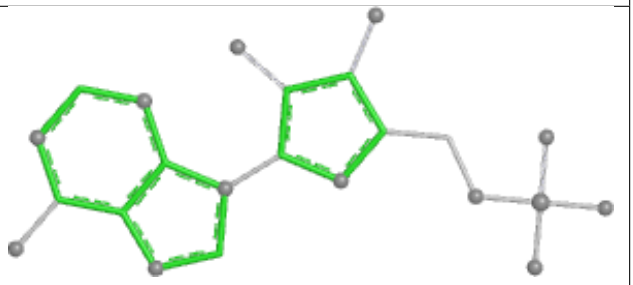
Bond lengths



Bond angles

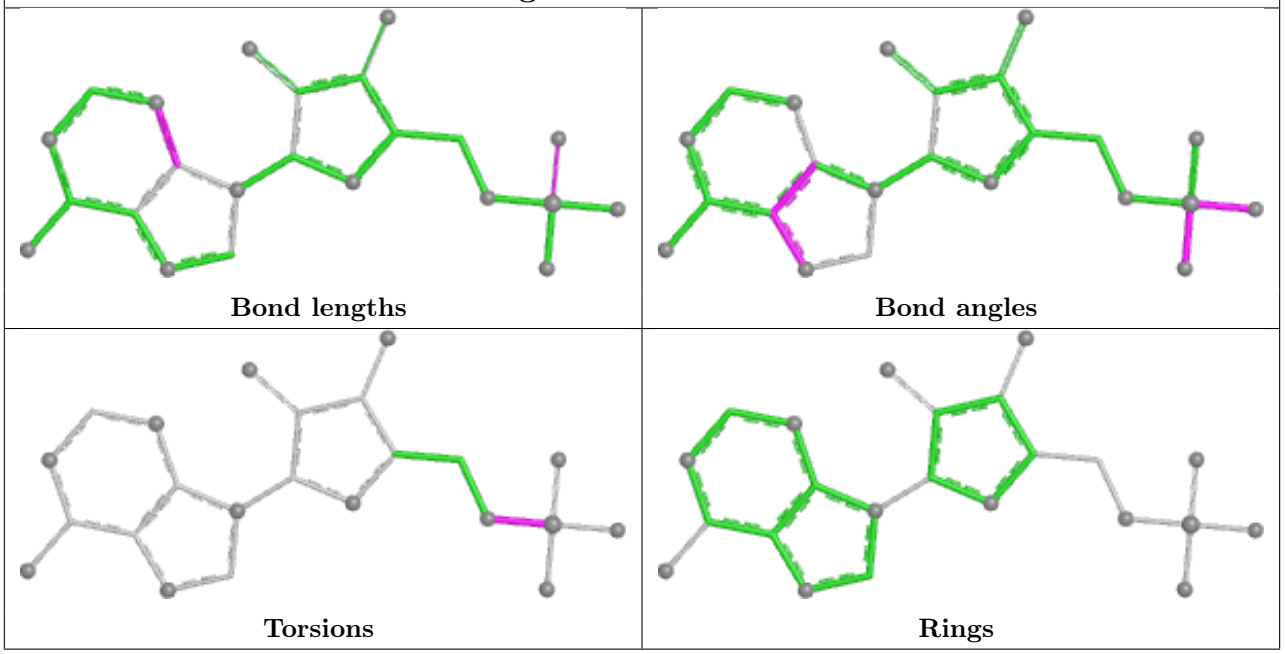


Torsions

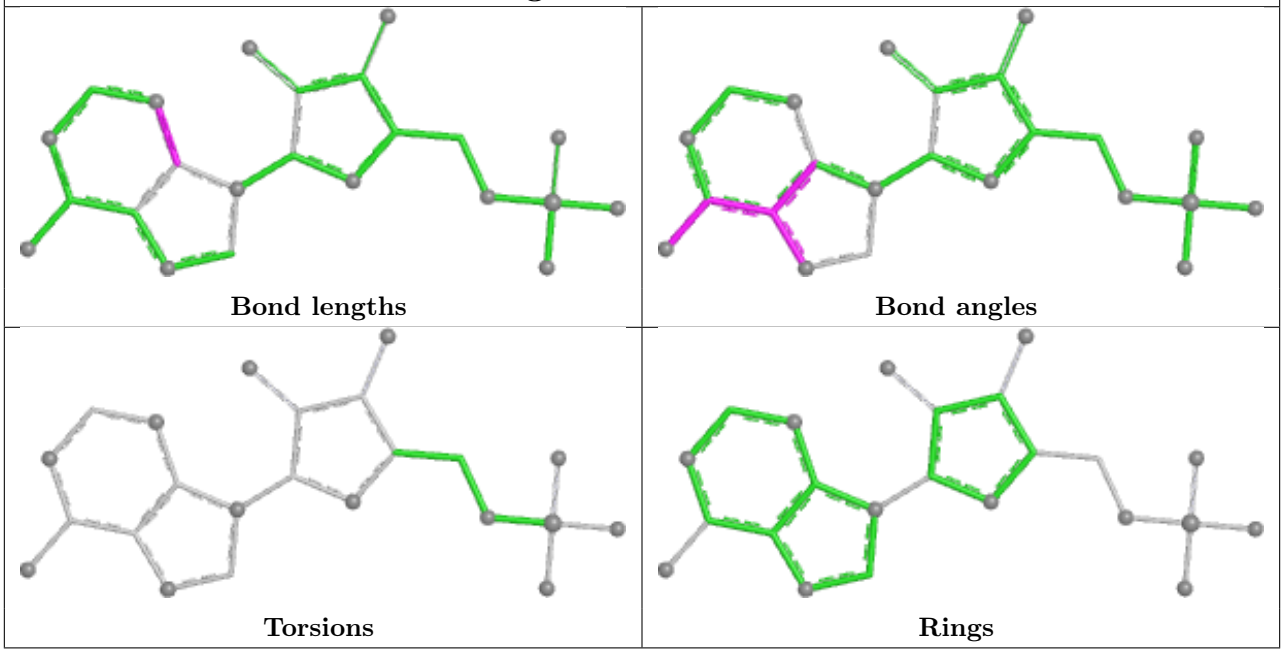


Rings

Ligand AMP D 301



Ligand AMP I 301



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	191/200 (95%)	0.68	16 (8%) 11 10	40, 67, 93, 104	0
1	B	191/200 (95%)	0.25	3 (1%) 72 70	34, 52, 71, 81	0
1	C	191/200 (95%)	0.79	17 (8%) 9 9	38, 59, 94, 116	0
1	D	191/200 (95%)	0.37	5 (2%) 56 54	39, 58, 75, 85	0
1	E	191/200 (95%)	0.32	3 (1%) 72 70	38, 57, 80, 90	0
1	F	191/200 (95%)	0.69	15 (7%) 12 11	39, 59, 88, 96	0
1	G	191/200 (95%)	0.84	25 (13%) 3 3	51, 80, 106, 121	0
1	H	191/200 (95%)	0.66	12 (6%) 20 18	49, 72, 94, 105	0
1	I	191/200 (95%)	0.72	19 (9%) 7 6	52, 73, 95, 103	0
1	J	191/200 (95%)	0.73	18 (9%) 8 7	44, 67, 99, 108	0
1	K	191/200 (95%)	0.75	23 (12%) 4 3	44, 79, 112, 127	0
1	L	191/200 (95%)	0.69	18 (9%) 8 7	42, 65, 88, 93	0
All	All	2292/2400 (95%)	0.62	174 (7%) 13 12	34, 65, 96, 127	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	52	LEU	9.2
1	C	136	ALA	7.6
1	H	137	THR	7.0
1	A	140	ARG	6.7
1	F	141	ASP	6.5

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

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

6.3 Carbohydrates (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	I	303	1/1	0.77	0.12	88,88,88,88	0
3	MG	H	303	1/1	0.86	0.11	72,72,72,72	0
3	MG	E	303	1/1	0.88	0.13	55,55,55,55	0
3	MG	K	303	1/1	0.88	0.10	81,81,81,81	0
3	MG	C	303	1/1	0.91	0.11	54,54,54,54	0
3	MG	L	303	1/1	0.93	0.13	71,71,71,71	0
2	AMP	I	301	23/23	0.94	0.17	53,66,78,83	0
2	AMP	I	302	23/23	0.94	0.14	53,69,78,80	0
3	MG	A	303	1/1	0.95	0.09	70,70,70,70	0
2	AMP	A	302	23/23	0.95	0.15	53,67,72,74	0
3	MG	J	303	1/1	0.95	0.10	55,55,55,55	0
2	AMP	K	301	23/23	0.95	0.16	53,70,78,83	0
3	MG	G	303	1/1	0.95	0.04	70,70,70,70	0
2	AMP	H	302	23/23	0.96	0.14	53,68,76,80	0
2	AMP	C	302	23/23	0.96	0.18	48,53,56,60	0
2	AMP	D	302	23/23	0.96	0.17	52,54,60,63	0
2	AMP	J	302	23/23	0.96	0.14	53,56,59,62	0
2	AMP	E	302	23/23	0.96	0.15	52,54,60,62	0
2	AMP	K	302	23/23	0.96	0.15	53,74,81,84	0
2	AMP	L	302	23/23	0.96	0.15	53,62,71,75	0
2	AMP	G	301	23/23	0.96	0.14	53,69,74,75	0
2	AMP	F	302	23/23	0.97	0.18	51,53,56,57	0
2	AMP	J	301	23/23	0.97	0.16	53,61,67,70	0
3	MG	F	303	1/1	0.97	0.07	49,49,49,49	0
2	AMP	C	301	23/23	0.97	0.16	53,55,62,64	0
2	AMP	G	302	23/23	0.97	0.14	53,72,79,83	0
2	AMP	H	301	23/23	0.97	0.14	53,64,69,72	0
2	AMP	A	301	23/23	0.97	0.16	53,56,62,62	0
2	AMP	F	301	23/23	0.97	0.16	51,53,57,58	0
3	MG	B	303	1/1	0.97	0.14	49,49,49,49	0
2	AMP	B	302	23/23	0.98	0.13	44,52,53,54	0
2	AMP	E	301	23/23	0.98	0.15	46,51,53,53	0

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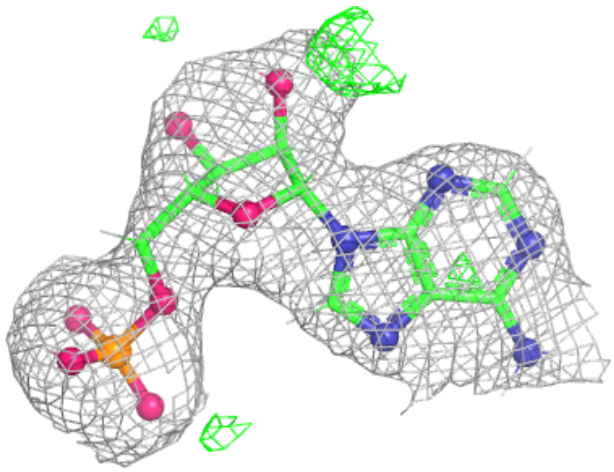
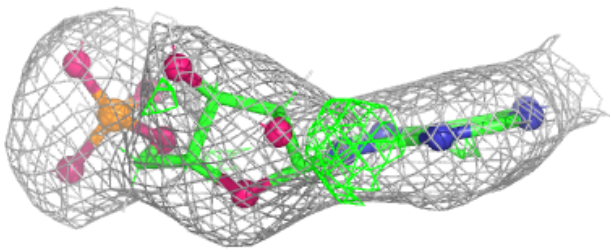
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AMP	D	301	23/23	0.98	0.14	45,53,54,58	0
2	AMP	L	301	23/23	0.98	0.16	49,53,62,70	0
2	AMP	B	301	23/23	0.99	0.16	41,46,53,53	0
3	MG	D	303	1/1	0.99	0.06	57,57,57,57	0

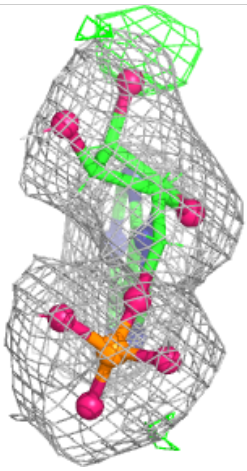
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP I 301:

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

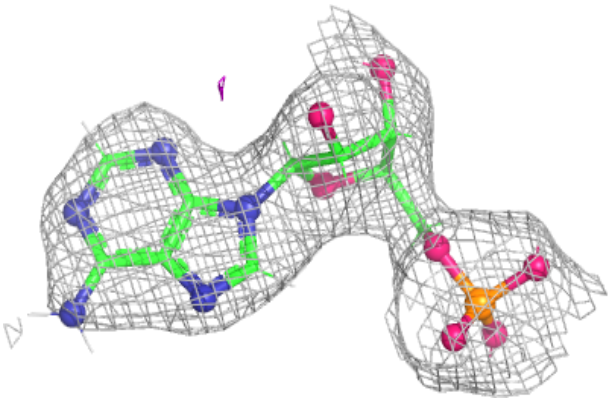


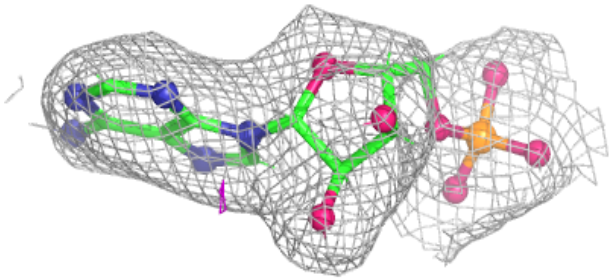


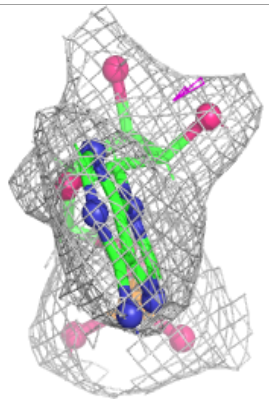


Electron density around AMP I 302:

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

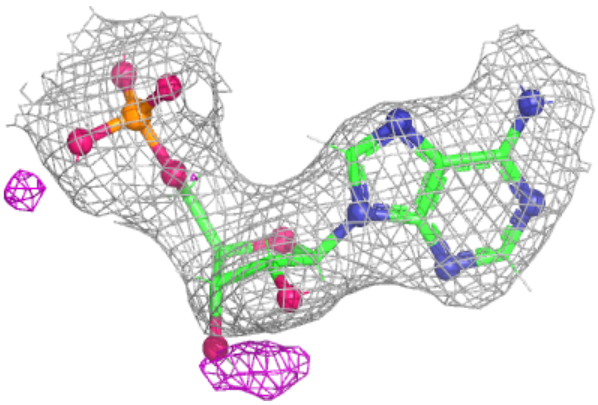


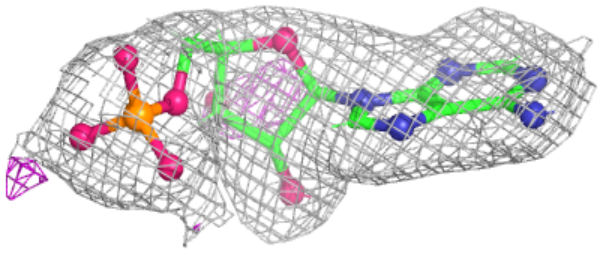


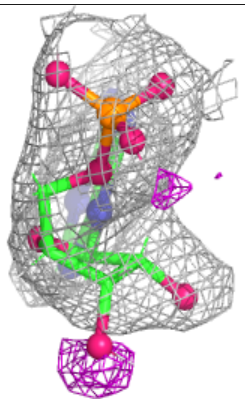


Electron density around AMP A 302:

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

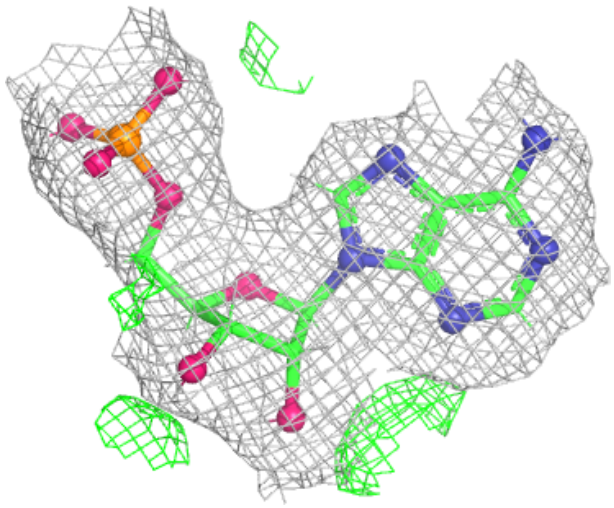


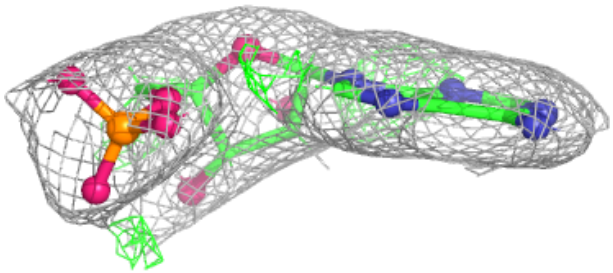


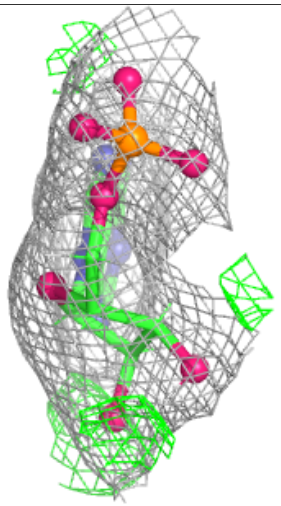


Electron density around AMP K 301:

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

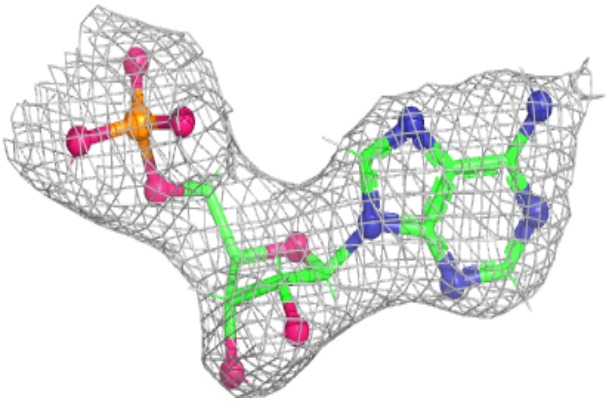


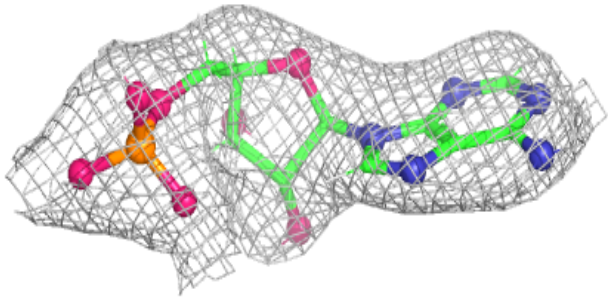


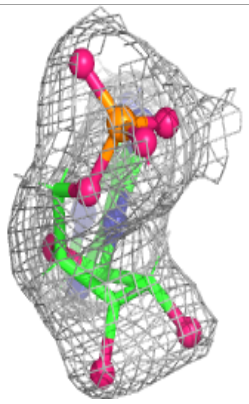


Electron density around AMP H 302:

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

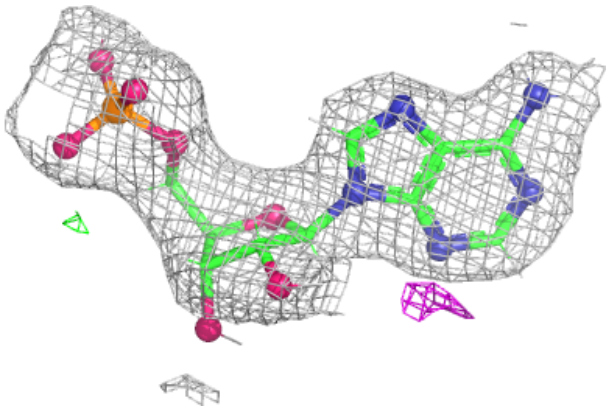


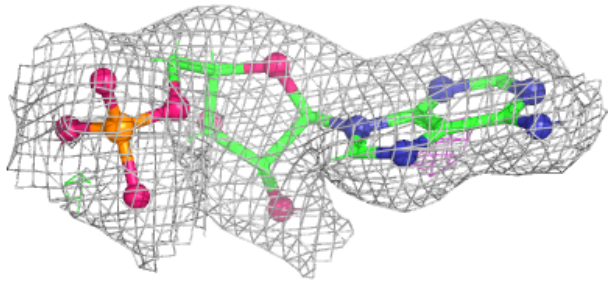


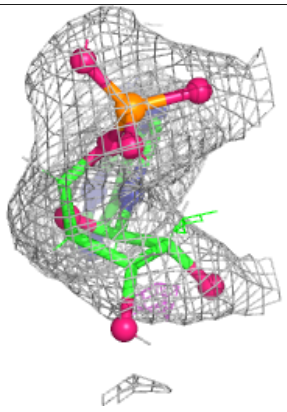


Electron density around AMP C 302:

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

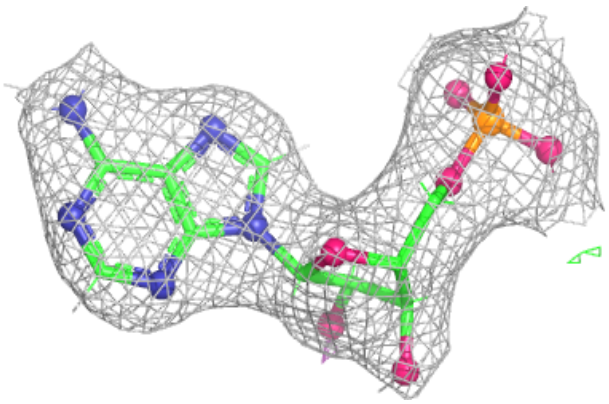


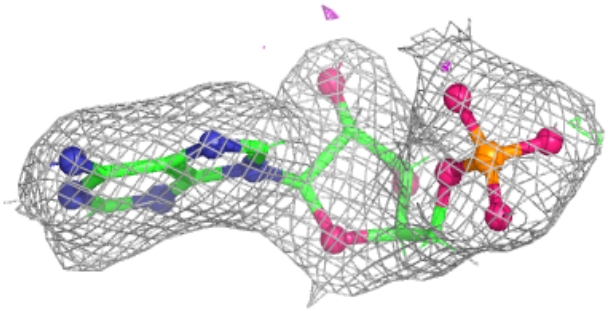


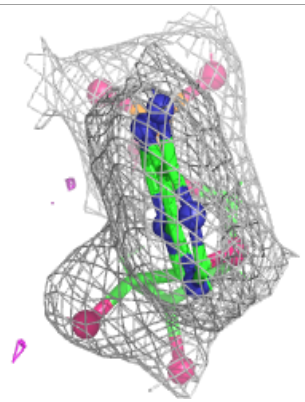


Electron density around AMP D 302:

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

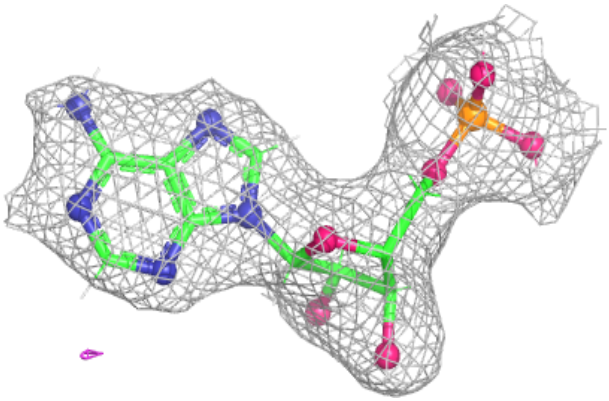


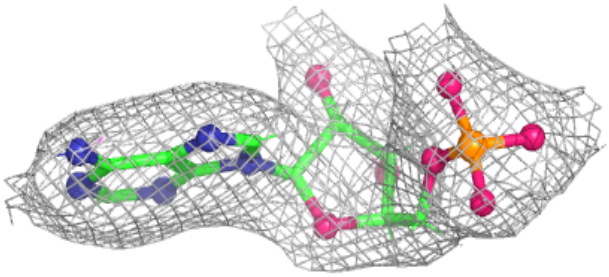


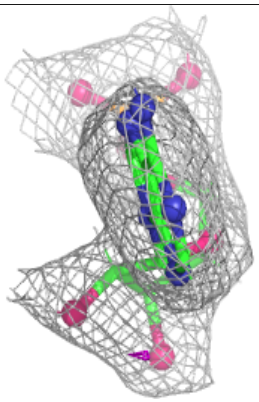


Electron density around AMP J 302:

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

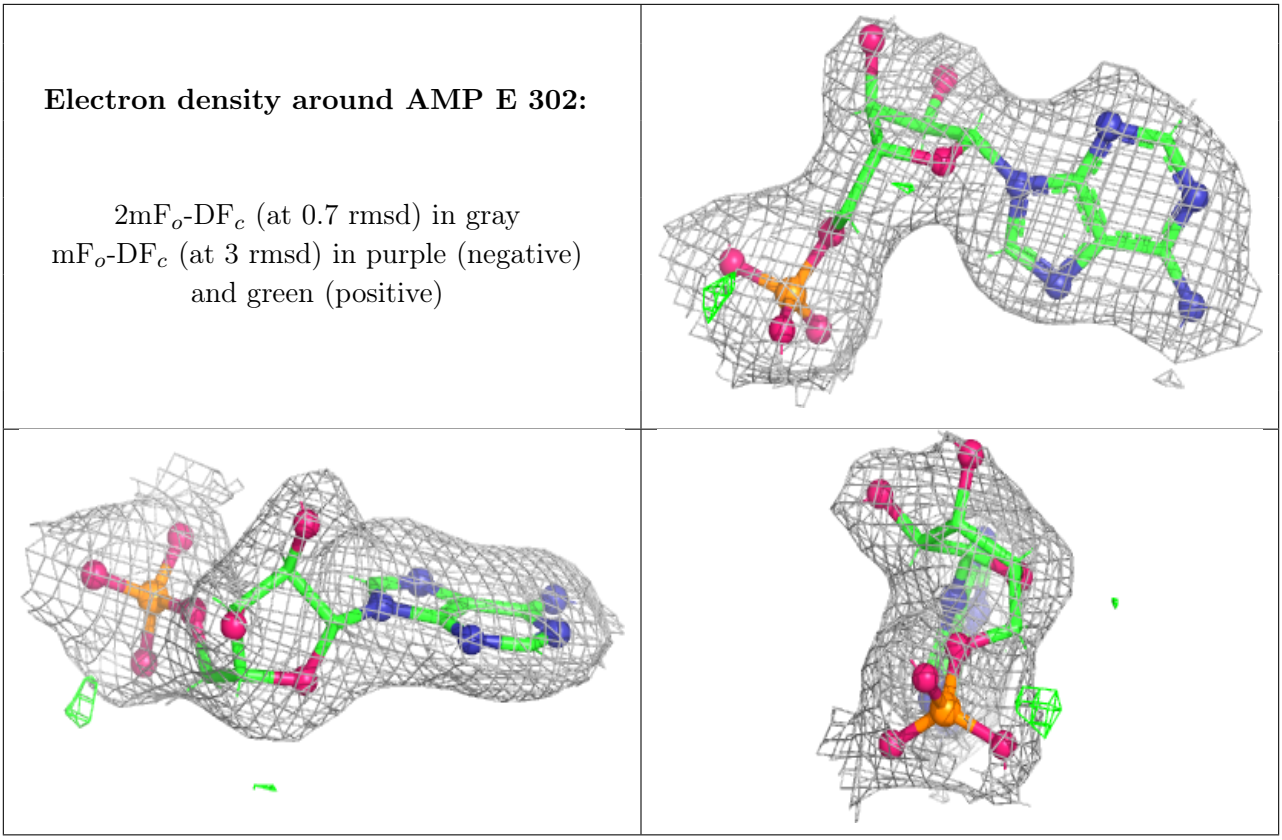






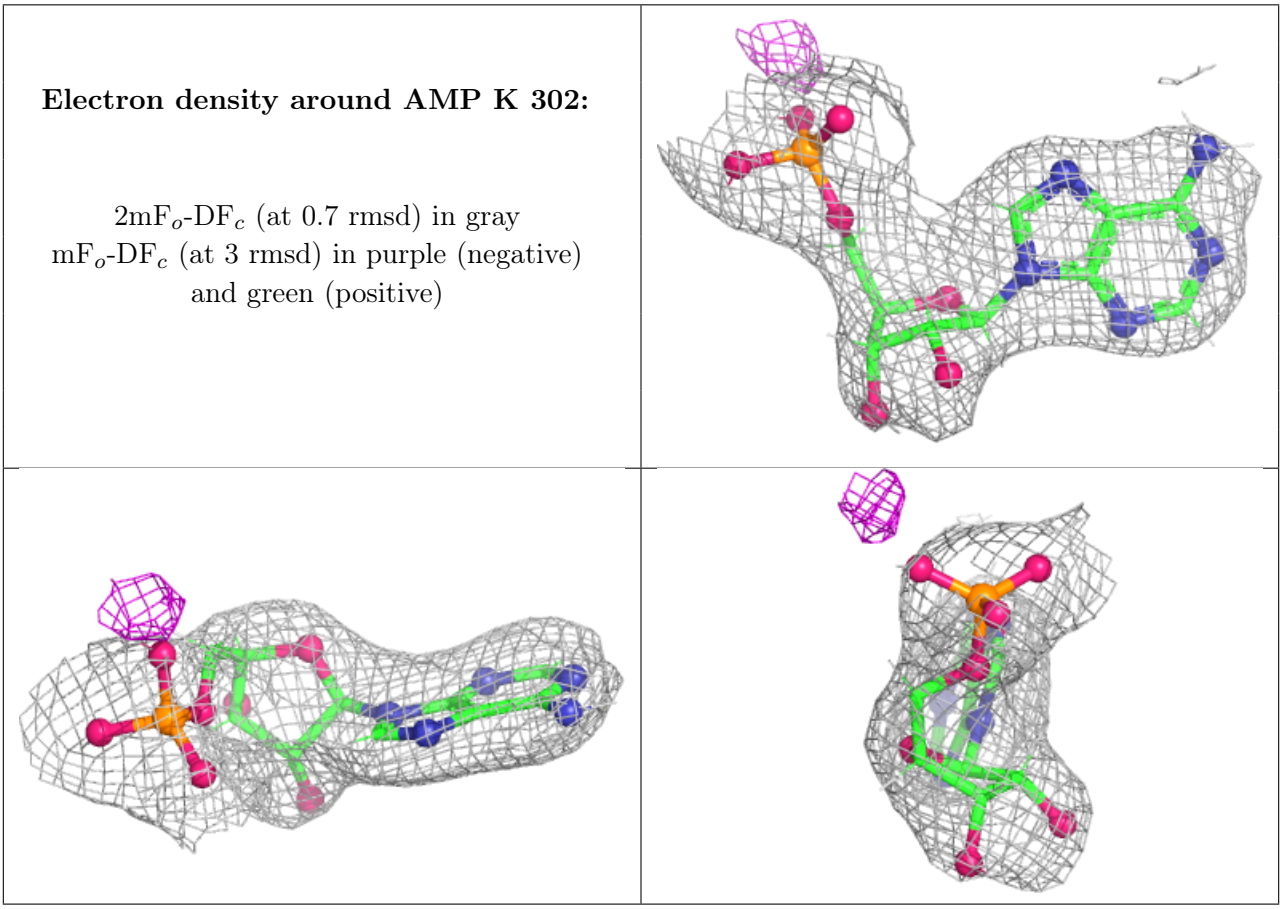
Electron density around AMP E 302:

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



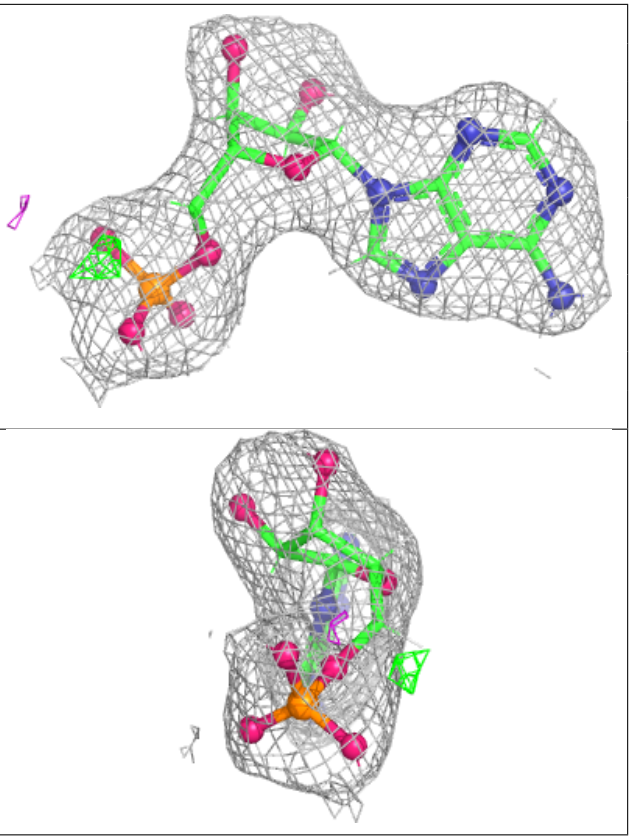
Electron density around AMP K 302:

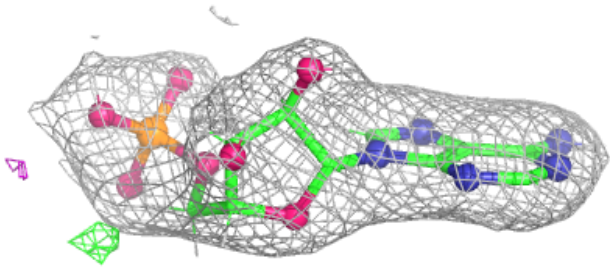
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around AMP L 302:

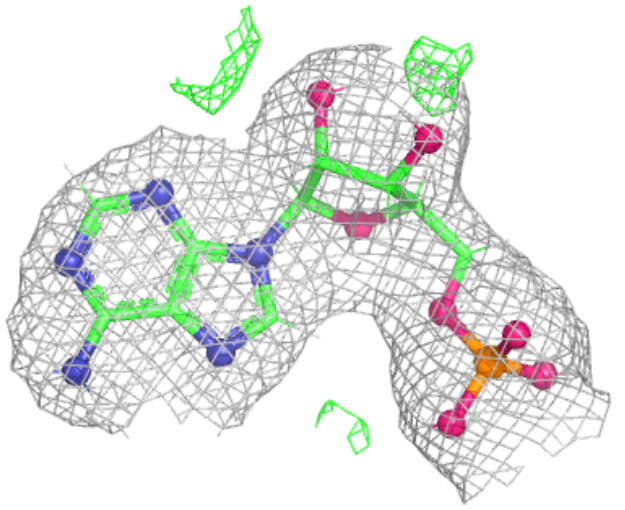
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

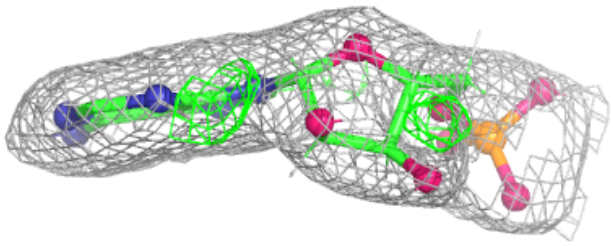


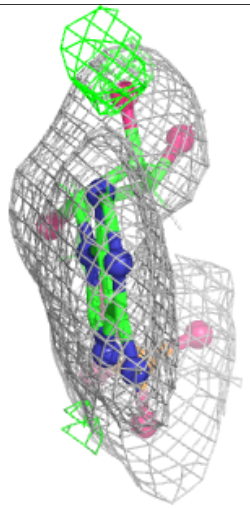


Electron density around AMP G 301:

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

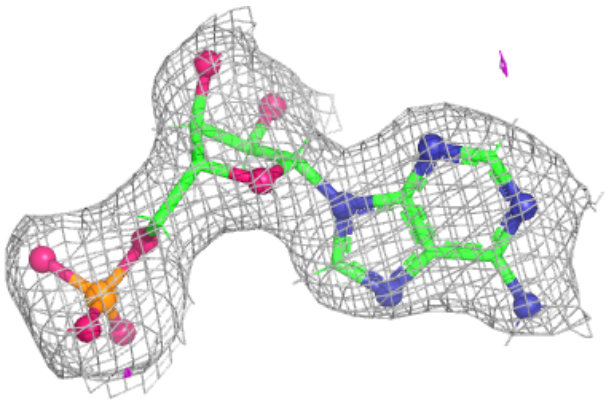


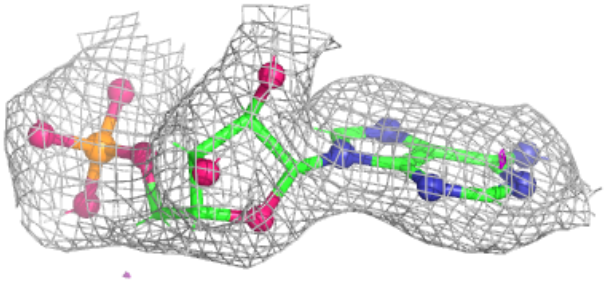


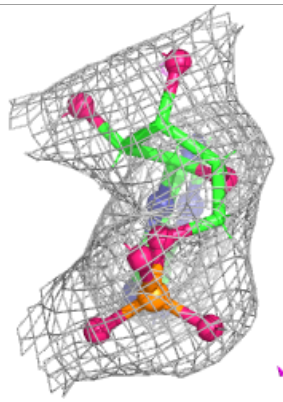


Electron density around AMP F 302:

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

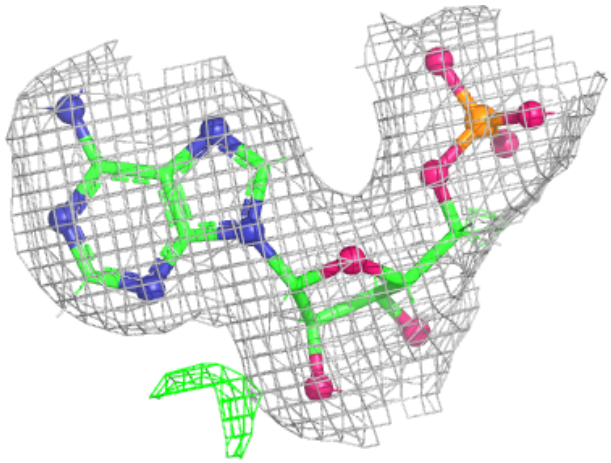


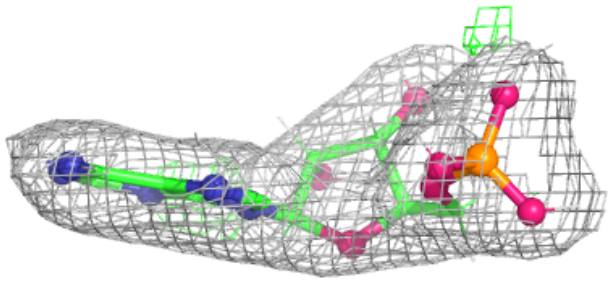


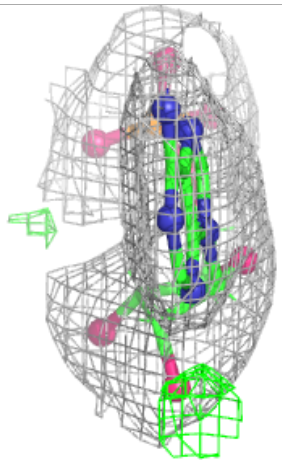


Electron density around AMP J 301:

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

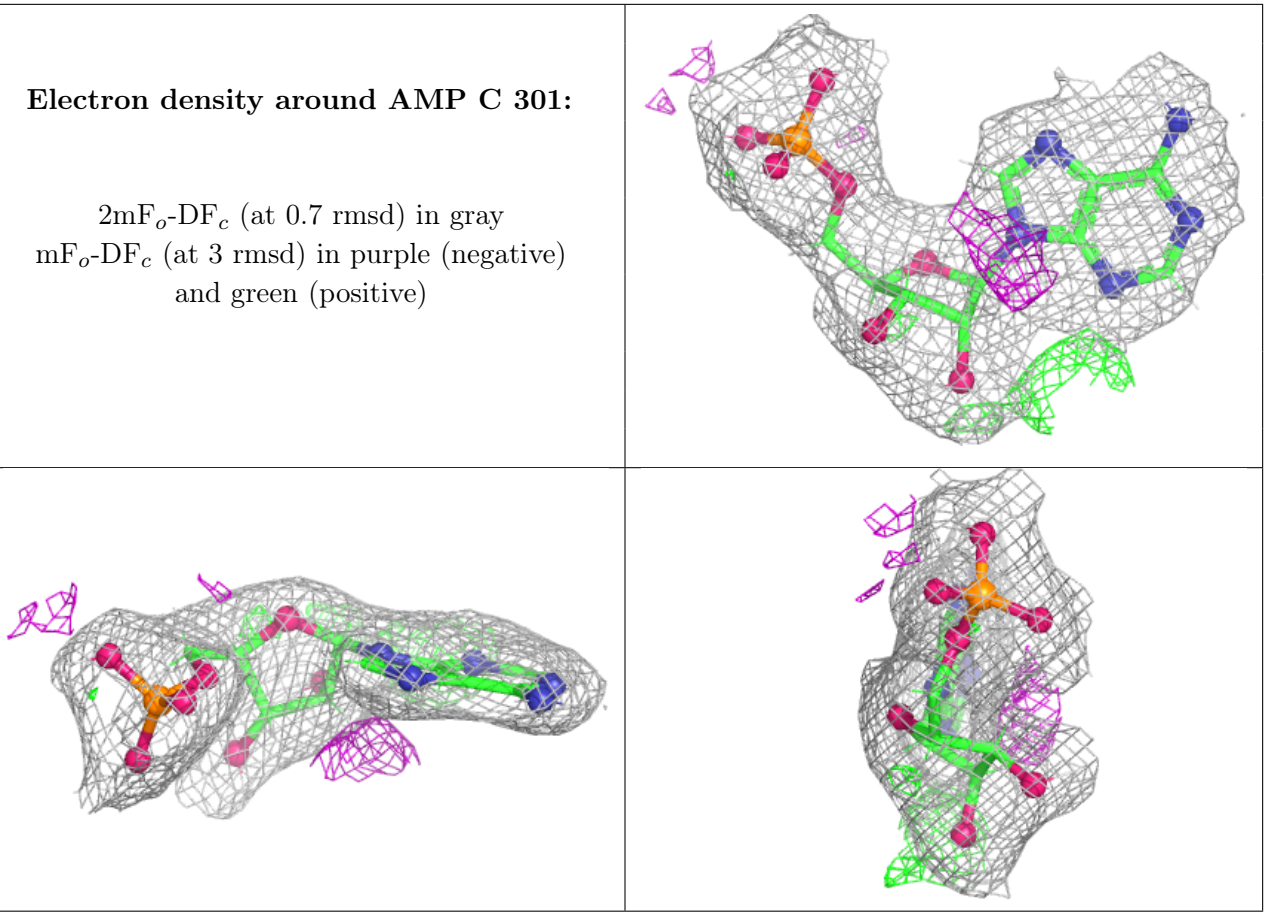






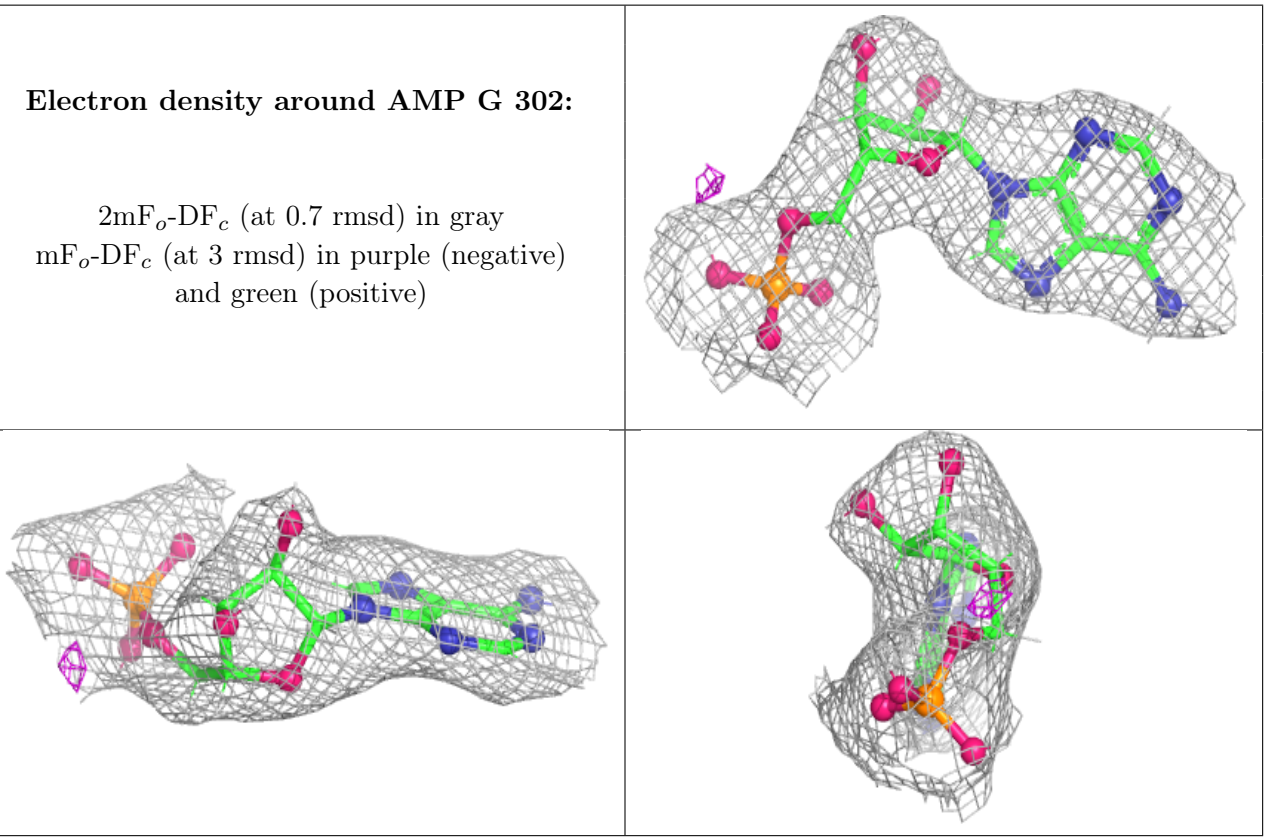
Electron density around AMP C 301:

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



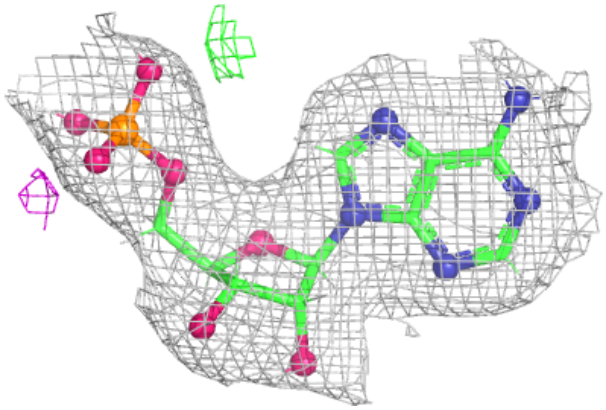
Electron density around AMP G 302:

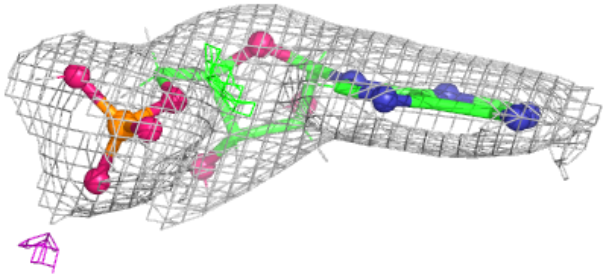
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

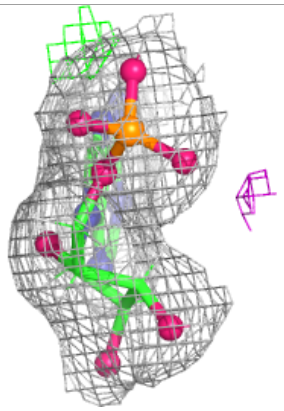


Electron density around AMP H 301:

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

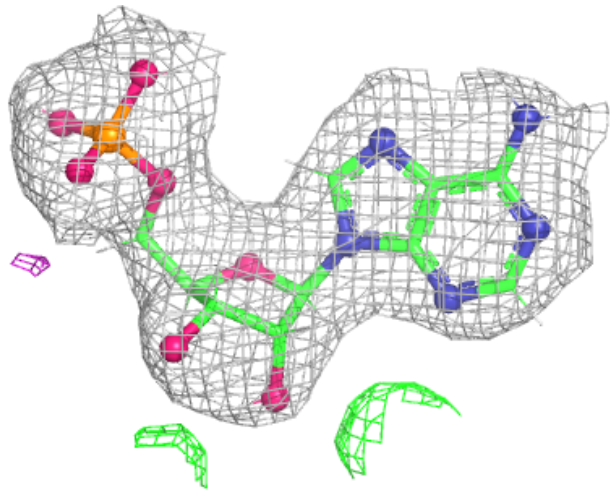


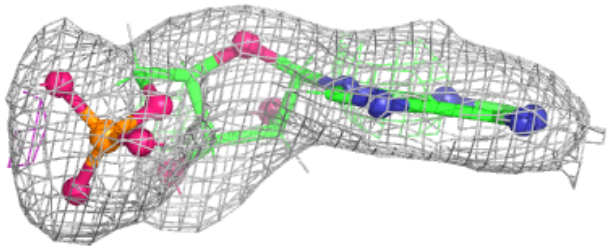


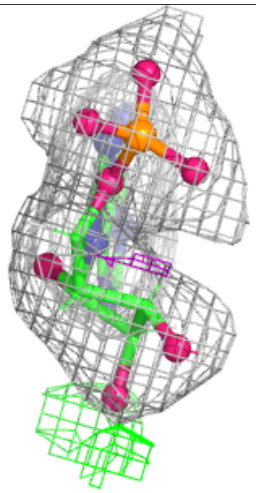


Electron density around AMP A 301:

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

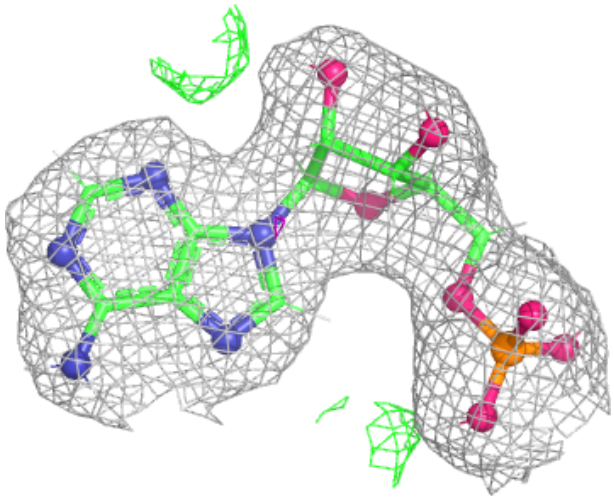


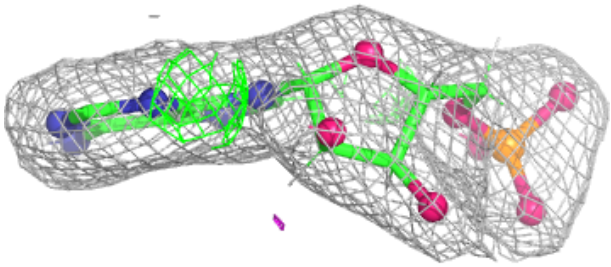


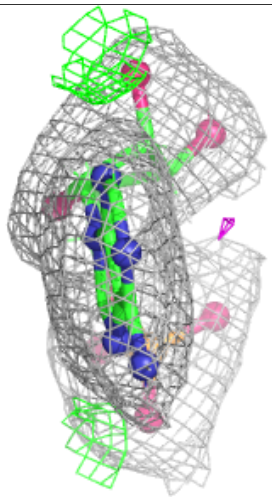


Electron density around AMP F 301:

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

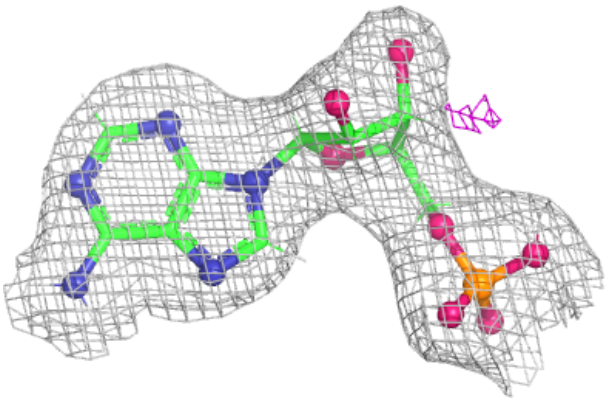


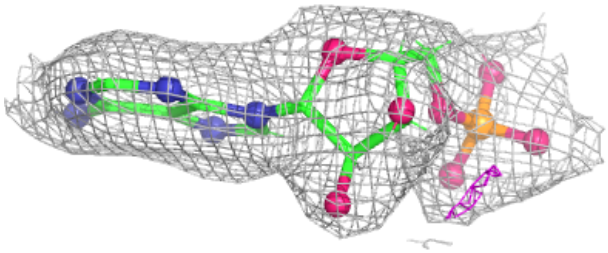


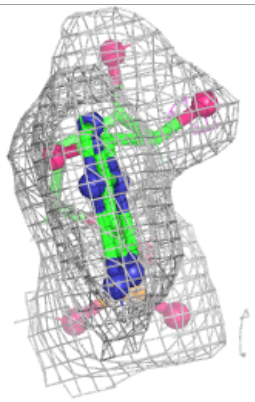


Electron density around AMP B 302:

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

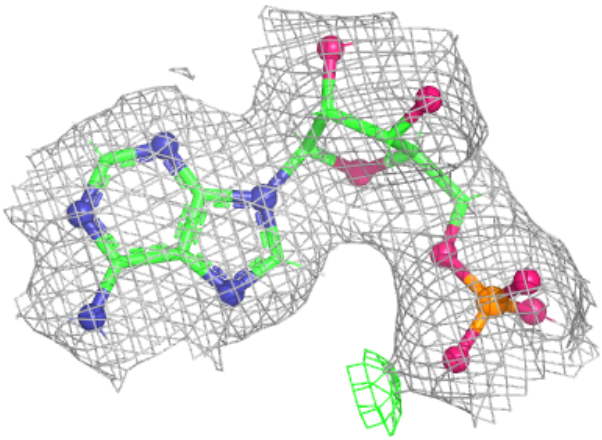


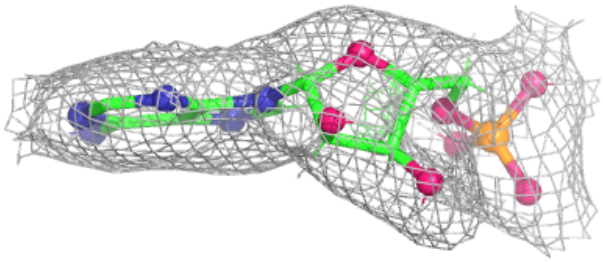


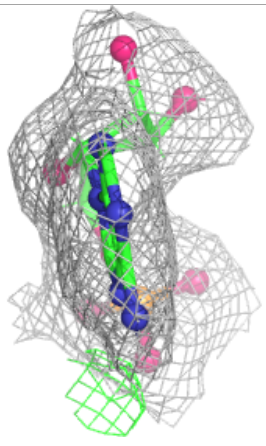


Electron density around AMP E 301:

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

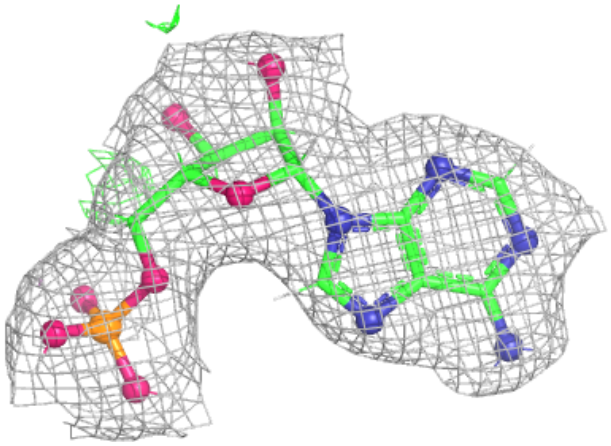


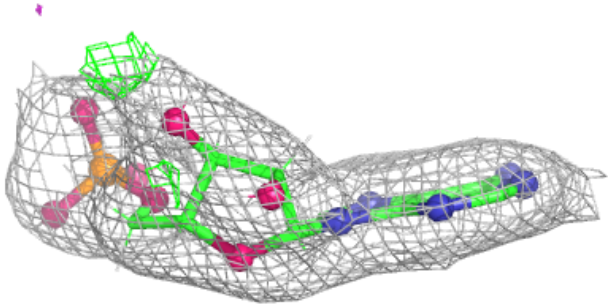


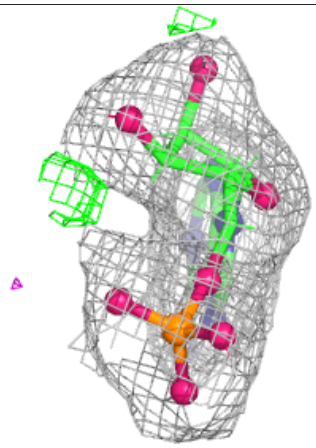


Electron density around AMP D 301:

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

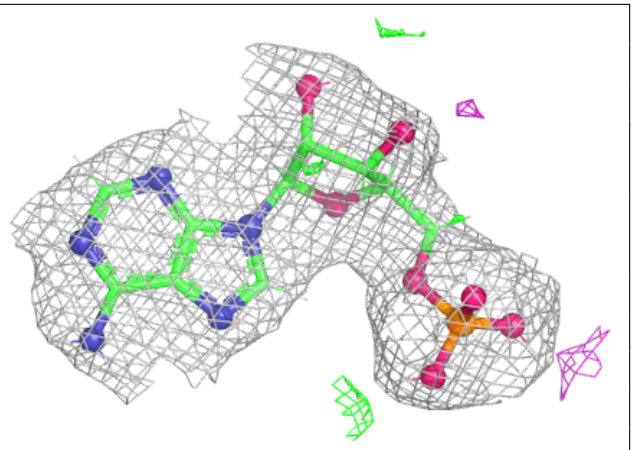


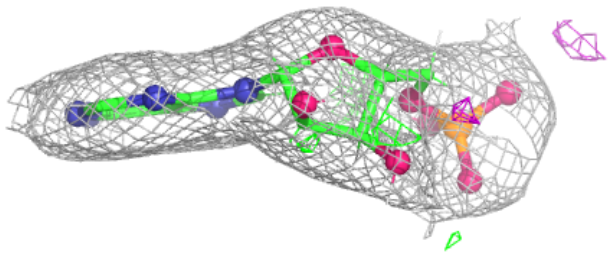


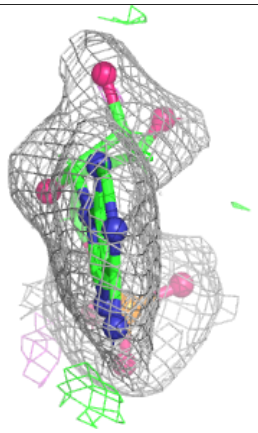


Electron density around AMP L 301:

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

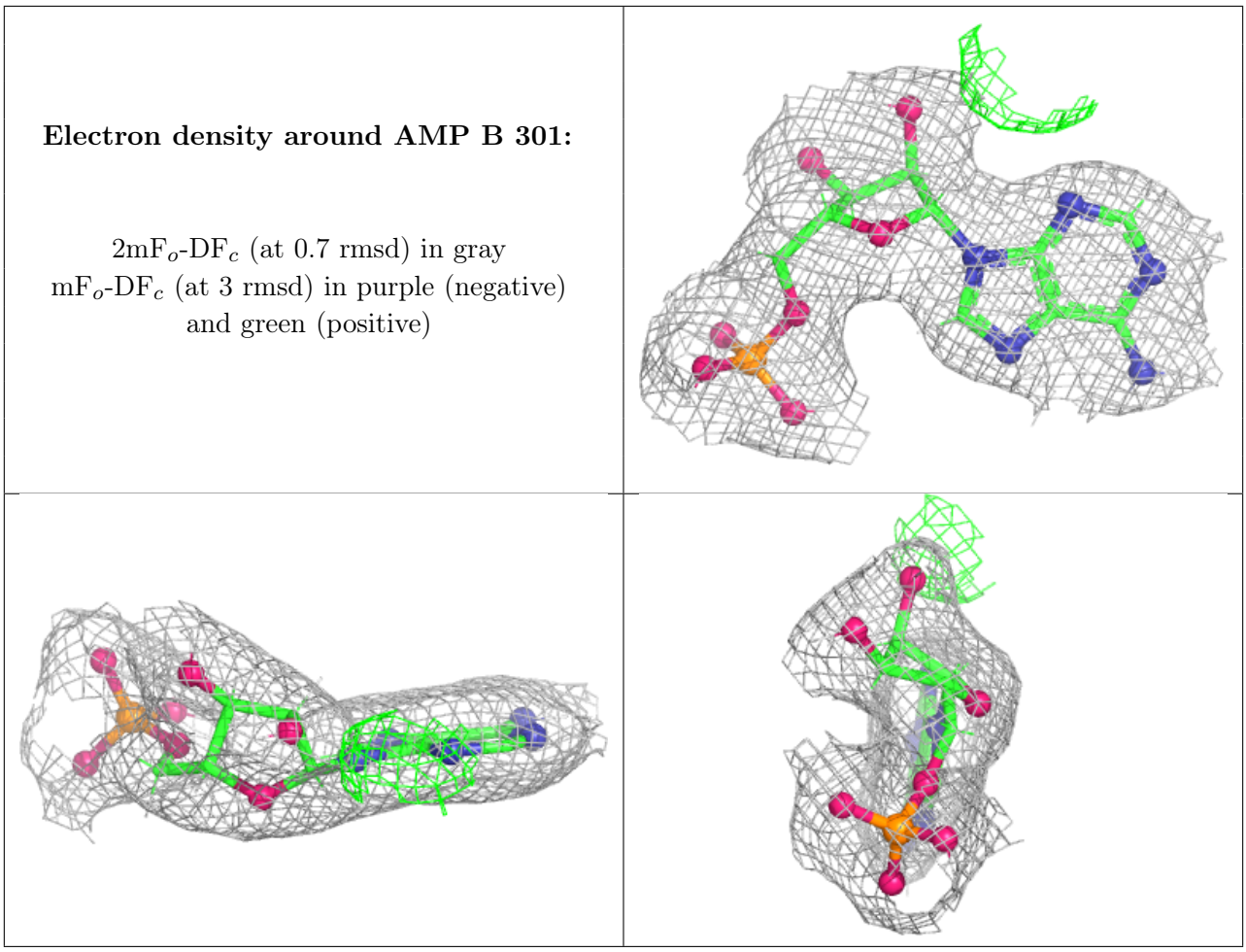






Electron density around AMP B 301:

$2mF_o$-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

There are no such residues in this entry.