



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:38 AM UTC

PDB ID : 9HG1 / pdb_00009hg1
Title : Crystal structure of M. smegmatis GMP reductase in complex with GMP and ATP.
Authors : Dolezal, M.; Klima, M.; Pichova, I.
Deposited on : 2024-11-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

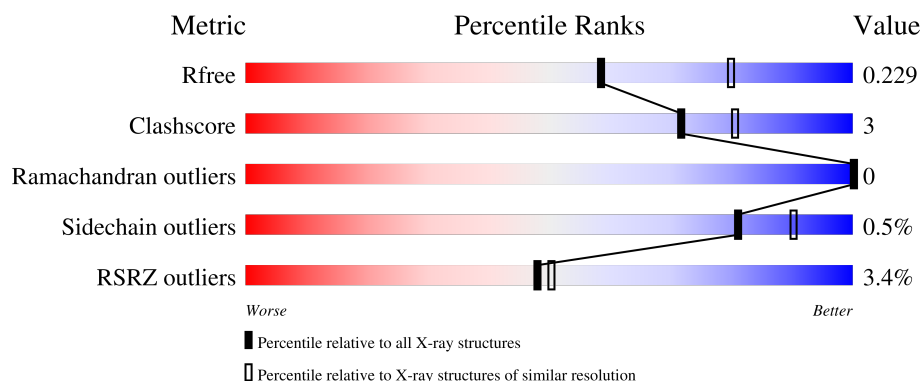
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	 2% 88% 7% 5%
1	B	496	 2% 89% 7% 5%
1	C	496	 3% 86% 9% 5%
1	D	496	 4% 85% 10% 5%
1	E	496	 4% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	496	
1	G	496	
1	H	496	
1	I	496	
1	J	496	
1	K	496	
1	L	496	
1	M	496	
1	N	496	
1	O	496	
1	P	496	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57130 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 GMP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	B	473	Total	C	N	O	S	0	1	0
			3423	2136	606	667	14			
1	C	473	Total	C	N	O	S	0	1	0
			3423	2136	606	667	14			
1	D	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	E	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	F	473	Total	C	N	O	S	0	1	0
			3424	2137	606	667	14			
1	G	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	H	473	Total	C	N	O	S	0	1	0
			3423	2136	606	667	14			
1	I	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	J	473	Total	C	N	O	S	0	1	0
			3424	2137	606	667	14			
1	K	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	L	473	Total	C	N	O	S	0	1	0
			3425	2138	606	667	14			
1	M	473	Total	C	N	O	S	0	1	0
			3423	2136	606	667	14			
1	N	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			
1	O	473	Total	C	N	O	S	0	1	0
			3423	2136	606	667	14			
1	P	473	Total	C	N	O	S	0	1	0
			3429	2139	609	667	14			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP A0QYE8
A	480	THR	-	expression tag	UNP A0QYE8
A	481	ALA	-	expression tag	UNP A0QYE8
A	482	ALA	-	expression tag	UNP A0QYE8
A	483	ALA	-	expression tag	UNP A0QYE8
A	484	LYS	-	expression tag	UNP A0QYE8
A	485	GLU	-	expression tag	UNP A0QYE8
A	486	ASP	-	expression tag	UNP A0QYE8
A	487	LEU	-	expression tag	UNP A0QYE8
A	488	GLU	-	expression tag	UNP A0QYE8
A	489	HIS	-	expression tag	UNP A0QYE8
A	490	HIS	-	expression tag	UNP A0QYE8
A	491	HIS	-	expression tag	UNP A0QYE8
A	492	HIS	-	expression tag	UNP A0QYE8
A	493	HIS	-	expression tag	UNP A0QYE8
A	494	HIS	-	expression tag	UNP A0QYE8
A	495	HIS	-	expression tag	UNP A0QYE8
A	496	HIS	-	expression tag	UNP A0QYE8
B	2	VAL	-	insertion	UNP A0QYE8
B	480	THR	-	expression tag	UNP A0QYE8
B	481	ALA	-	expression tag	UNP A0QYE8
B	482	ALA	-	expression tag	UNP A0QYE8
B	483	ALA	-	expression tag	UNP A0QYE8
B	484	LYS	-	expression tag	UNP A0QYE8
B	485	GLU	-	expression tag	UNP A0QYE8
B	486	ASP	-	expression tag	UNP A0QYE8
B	487	LEU	-	expression tag	UNP A0QYE8
B	488	GLU	-	expression tag	UNP A0QYE8
B	489	HIS	-	expression tag	UNP A0QYE8
B	490	HIS	-	expression tag	UNP A0QYE8
B	491	HIS	-	expression tag	UNP A0QYE8
B	492	HIS	-	expression tag	UNP A0QYE8
B	493	HIS	-	expression tag	UNP A0QYE8
B	494	HIS	-	expression tag	UNP A0QYE8
B	495	HIS	-	expression tag	UNP A0QYE8
B	496	HIS	-	expression tag	UNP A0QYE8
C	2	VAL	-	insertion	UNP A0QYE8
C	480	THR	-	expression tag	UNP A0QYE8
C	481	ALA	-	expression tag	UNP A0QYE8
C	482	ALA	-	expression tag	UNP A0QYE8
C	483	ALA	-	expression tag	UNP A0QYE8
C	484	LYS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	485	GLU	-	expression tag	UNP A0QYE8
C	486	ASP	-	expression tag	UNP A0QYE8
C	487	LEU	-	expression tag	UNP A0QYE8
C	488	GLU	-	expression tag	UNP A0QYE8
C	489	HIS	-	expression tag	UNP A0QYE8
C	490	HIS	-	expression tag	UNP A0QYE8
C	491	HIS	-	expression tag	UNP A0QYE8
C	492	HIS	-	expression tag	UNP A0QYE8
C	493	HIS	-	expression tag	UNP A0QYE8
C	494	HIS	-	expression tag	UNP A0QYE8
C	495	HIS	-	expression tag	UNP A0QYE8
C	496	HIS	-	expression tag	UNP A0QYE8
D	2	VAL	-	insertion	UNP A0QYE8
D	480	THR	-	expression tag	UNP A0QYE8
D	481	ALA	-	expression tag	UNP A0QYE8
D	482	ALA	-	expression tag	UNP A0QYE8
D	483	ALA	-	expression tag	UNP A0QYE8
D	484	LYS	-	expression tag	UNP A0QYE8
D	485	GLU	-	expression tag	UNP A0QYE8
D	486	ASP	-	expression tag	UNP A0QYE8
D	487	LEU	-	expression tag	UNP A0QYE8
D	488	GLU	-	expression tag	UNP A0QYE8
D	489	HIS	-	expression tag	UNP A0QYE8
D	490	HIS	-	expression tag	UNP A0QYE8
D	491	HIS	-	expression tag	UNP A0QYE8
D	492	HIS	-	expression tag	UNP A0QYE8
D	493	HIS	-	expression tag	UNP A0QYE8
D	494	HIS	-	expression tag	UNP A0QYE8
D	495	HIS	-	expression tag	UNP A0QYE8
D	496	HIS	-	expression tag	UNP A0QYE8
E	2	VAL	-	insertion	UNP A0QYE8
E	480	THR	-	expression tag	UNP A0QYE8
E	481	ALA	-	expression tag	UNP A0QYE8
E	482	ALA	-	expression tag	UNP A0QYE8
E	483	ALA	-	expression tag	UNP A0QYE8
E	484	LYS	-	expression tag	UNP A0QYE8
E	485	GLU	-	expression tag	UNP A0QYE8
E	486	ASP	-	expression tag	UNP A0QYE8
E	487	LEU	-	expression tag	UNP A0QYE8
E	488	GLU	-	expression tag	UNP A0QYE8
E	489	HIS	-	expression tag	UNP A0QYE8
E	490	HIS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	491	HIS	-	expression tag	UNP A0QYE8
E	492	HIS	-	expression tag	UNP A0QYE8
E	493	HIS	-	expression tag	UNP A0QYE8
E	494	HIS	-	expression tag	UNP A0QYE8
E	495	HIS	-	expression tag	UNP A0QYE8
E	496	HIS	-	expression tag	UNP A0QYE8
F	2	VAL	-	insertion	UNP A0QYE8
F	480	THR	-	expression tag	UNP A0QYE8
F	481	ALA	-	expression tag	UNP A0QYE8
F	482	ALA	-	expression tag	UNP A0QYE8
F	483	ALA	-	expression tag	UNP A0QYE8
F	484	LYS	-	expression tag	UNP A0QYE8
F	485	GLU	-	expression tag	UNP A0QYE8
F	486	ASP	-	expression tag	UNP A0QYE8
F	487	LEU	-	expression tag	UNP A0QYE8
F	488	GLU	-	expression tag	UNP A0QYE8
F	489	HIS	-	expression tag	UNP A0QYE8
F	490	HIS	-	expression tag	UNP A0QYE8
F	491	HIS	-	expression tag	UNP A0QYE8
F	492	HIS	-	expression tag	UNP A0QYE8
F	493	HIS	-	expression tag	UNP A0QYE8
F	494	HIS	-	expression tag	UNP A0QYE8
F	495	HIS	-	expression tag	UNP A0QYE8
F	496	HIS	-	expression tag	UNP A0QYE8
G	2	VAL	-	insertion	UNP A0QYE8
G	480	THR	-	expression tag	UNP A0QYE8
G	481	ALA	-	expression tag	UNP A0QYE8
G	482	ALA	-	expression tag	UNP A0QYE8
G	483	ALA	-	expression tag	UNP A0QYE8
G	484	LYS	-	expression tag	UNP A0QYE8
G	485	GLU	-	expression tag	UNP A0QYE8
G	486	ASP	-	expression tag	UNP A0QYE8
G	487	LEU	-	expression tag	UNP A0QYE8
G	488	GLU	-	expression tag	UNP A0QYE8
G	489	HIS	-	expression tag	UNP A0QYE8
G	490	HIS	-	expression tag	UNP A0QYE8
G	491	HIS	-	expression tag	UNP A0QYE8
G	492	HIS	-	expression tag	UNP A0QYE8
G	493	HIS	-	expression tag	UNP A0QYE8
G	494	HIS	-	expression tag	UNP A0QYE8
G	495	HIS	-	expression tag	UNP A0QYE8
G	496	HIS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	2	VAL	-	insertion	UNP A0QYE8
H	480	THR	-	expression tag	UNP A0QYE8
H	481	ALA	-	expression tag	UNP A0QYE8
H	482	ALA	-	expression tag	UNP A0QYE8
H	483	ALA	-	expression tag	UNP A0QYE8
H	484	LYS	-	expression tag	UNP A0QYE8
H	485	GLU	-	expression tag	UNP A0QYE8
H	486	ASP	-	expression tag	UNP A0QYE8
H	487	LEU	-	expression tag	UNP A0QYE8
H	488	GLU	-	expression tag	UNP A0QYE8
H	489	HIS	-	expression tag	UNP A0QYE8
H	490	HIS	-	expression tag	UNP A0QYE8
H	491	HIS	-	expression tag	UNP A0QYE8
H	492	HIS	-	expression tag	UNP A0QYE8
H	493	HIS	-	expression tag	UNP A0QYE8
H	494	HIS	-	expression tag	UNP A0QYE8
H	495	HIS	-	expression tag	UNP A0QYE8
H	496	HIS	-	expression tag	UNP A0QYE8
I	2	VAL	-	insertion	UNP A0QYE8
I	480	THR	-	expression tag	UNP A0QYE8
I	481	ALA	-	expression tag	UNP A0QYE8
I	482	ALA	-	expression tag	UNP A0QYE8
I	483	ALA	-	expression tag	UNP A0QYE8
I	484	LYS	-	expression tag	UNP A0QYE8
I	485	GLU	-	expression tag	UNP A0QYE8
I	486	ASP	-	expression tag	UNP A0QYE8
I	487	LEU	-	expression tag	UNP A0QYE8
I	488	GLU	-	expression tag	UNP A0QYE8
I	489	HIS	-	expression tag	UNP A0QYE8
I	490	HIS	-	expression tag	UNP A0QYE8
I	491	HIS	-	expression tag	UNP A0QYE8
I	492	HIS	-	expression tag	UNP A0QYE8
I	493	HIS	-	expression tag	UNP A0QYE8
I	494	HIS	-	expression tag	UNP A0QYE8
I	495	HIS	-	expression tag	UNP A0QYE8
I	496	HIS	-	expression tag	UNP A0QYE8
J	2	VAL	-	insertion	UNP A0QYE8
J	480	THR	-	expression tag	UNP A0QYE8
J	481	ALA	-	expression tag	UNP A0QYE8
J	482	ALA	-	expression tag	UNP A0QYE8
J	483	ALA	-	expression tag	UNP A0QYE8
J	484	LYS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	485	GLU	-	expression tag	UNP A0QYE8
J	486	ASP	-	expression tag	UNP A0QYE8
J	487	LEU	-	expression tag	UNP A0QYE8
J	488	GLU	-	expression tag	UNP A0QYE8
J	489	HIS	-	expression tag	UNP A0QYE8
J	490	HIS	-	expression tag	UNP A0QYE8
J	491	HIS	-	expression tag	UNP A0QYE8
J	492	HIS	-	expression tag	UNP A0QYE8
J	493	HIS	-	expression tag	UNP A0QYE8
J	494	HIS	-	expression tag	UNP A0QYE8
J	495	HIS	-	expression tag	UNP A0QYE8
J	496	HIS	-	expression tag	UNP A0QYE8
K	2	VAL	-	insertion	UNP A0QYE8
K	480	THR	-	expression tag	UNP A0QYE8
K	481	ALA	-	expression tag	UNP A0QYE8
K	482	ALA	-	expression tag	UNP A0QYE8
K	483	ALA	-	expression tag	UNP A0QYE8
K	484	LYS	-	expression tag	UNP A0QYE8
K	485	GLU	-	expression tag	UNP A0QYE8
K	486	ASP	-	expression tag	UNP A0QYE8
K	487	LEU	-	expression tag	UNP A0QYE8
K	488	GLU	-	expression tag	UNP A0QYE8
K	489	HIS	-	expression tag	UNP A0QYE8
K	490	HIS	-	expression tag	UNP A0QYE8
K	491	HIS	-	expression tag	UNP A0QYE8
K	492	HIS	-	expression tag	UNP A0QYE8
K	493	HIS	-	expression tag	UNP A0QYE8
K	494	HIS	-	expression tag	UNP A0QYE8
K	495	HIS	-	expression tag	UNP A0QYE8
K	496	HIS	-	expression tag	UNP A0QYE8
L	2	VAL	-	insertion	UNP A0QYE8
L	480	THR	-	expression tag	UNP A0QYE8
L	481	ALA	-	expression tag	UNP A0QYE8
L	482	ALA	-	expression tag	UNP A0QYE8
L	483	ALA	-	expression tag	UNP A0QYE8
L	484	LYS	-	expression tag	UNP A0QYE8
L	485	GLU	-	expression tag	UNP A0QYE8
L	486	ASP	-	expression tag	UNP A0QYE8
L	487	LEU	-	expression tag	UNP A0QYE8
L	488	GLU	-	expression tag	UNP A0QYE8
L	489	HIS	-	expression tag	UNP A0QYE8
L	490	HIS	-	expression tag	UNP A0QYE8

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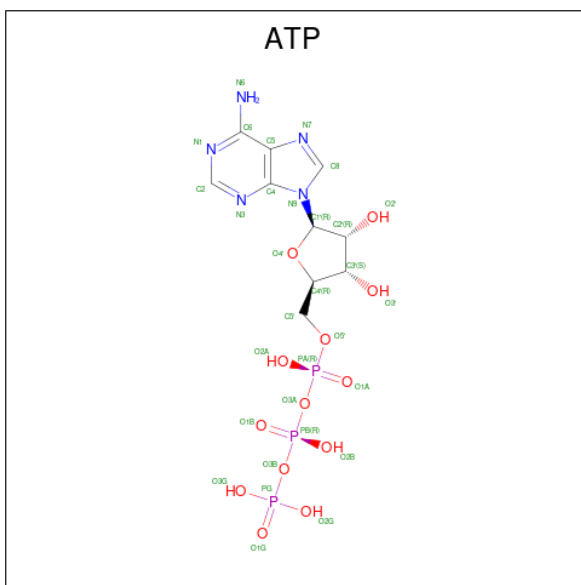
Chain	Residue	Modelled	Actual	Comment	Reference
L	491	HIS	-	expression tag	UNP A0QYE8
L	492	HIS	-	expression tag	UNP A0QYE8
L	493	HIS	-	expression tag	UNP A0QYE8
L	494	HIS	-	expression tag	UNP A0QYE8
L	495	HIS	-	expression tag	UNP A0QYE8
L	496	HIS	-	expression tag	UNP A0QYE8
M	2	VAL	-	insertion	UNP A0QYE8
M	480	THR	-	expression tag	UNP A0QYE8
M	481	ALA	-	expression tag	UNP A0QYE8
M	482	ALA	-	expression tag	UNP A0QYE8
M	483	ALA	-	expression tag	UNP A0QYE8
M	484	LYS	-	expression tag	UNP A0QYE8
M	485	GLU	-	expression tag	UNP A0QYE8
M	486	ASP	-	expression tag	UNP A0QYE8
M	487	LEU	-	expression tag	UNP A0QYE8
M	488	GLU	-	expression tag	UNP A0QYE8
M	489	HIS	-	expression tag	UNP A0QYE8
M	490	HIS	-	expression tag	UNP A0QYE8
M	491	HIS	-	expression tag	UNP A0QYE8
M	492	HIS	-	expression tag	UNP A0QYE8
M	493	HIS	-	expression tag	UNP A0QYE8
M	494	HIS	-	expression tag	UNP A0QYE8
M	495	HIS	-	expression tag	UNP A0QYE8
M	496	HIS	-	expression tag	UNP A0QYE8
N	2	VAL	-	insertion	UNP A0QYE8
N	480	THR	-	expression tag	UNP A0QYE8
N	481	ALA	-	expression tag	UNP A0QYE8
N	482	ALA	-	expression tag	UNP A0QYE8
N	483	ALA	-	expression tag	UNP A0QYE8
N	484	LYS	-	expression tag	UNP A0QYE8
N	485	GLU	-	expression tag	UNP A0QYE8
N	486	ASP	-	expression tag	UNP A0QYE8
N	487	LEU	-	expression tag	UNP A0QYE8
N	488	GLU	-	expression tag	UNP A0QYE8
N	489	HIS	-	expression tag	UNP A0QYE8
N	490	HIS	-	expression tag	UNP A0QYE8
N	491	HIS	-	expression tag	UNP A0QYE8
N	492	HIS	-	expression tag	UNP A0QYE8
N	493	HIS	-	expression tag	UNP A0QYE8
N	494	HIS	-	expression tag	UNP A0QYE8
N	495	HIS	-	expression tag	UNP A0QYE8
N	496	HIS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	2	VAL	-	insertion	UNP A0QYE8
O	480	THR	-	expression tag	UNP A0QYE8
O	481	ALA	-	expression tag	UNP A0QYE8
O	482	ALA	-	expression tag	UNP A0QYE8
O	483	ALA	-	expression tag	UNP A0QYE8
O	484	LYS	-	expression tag	UNP A0QYE8
O	485	GLU	-	expression tag	UNP A0QYE8
O	486	ASP	-	expression tag	UNP A0QYE8
O	487	LEU	-	expression tag	UNP A0QYE8
O	488	GLU	-	expression tag	UNP A0QYE8
O	489	HIS	-	expression tag	UNP A0QYE8
O	490	HIS	-	expression tag	UNP A0QYE8
O	491	HIS	-	expression tag	UNP A0QYE8
O	492	HIS	-	expression tag	UNP A0QYE8
O	493	HIS	-	expression tag	UNP A0QYE8
O	494	HIS	-	expression tag	UNP A0QYE8
O	495	HIS	-	expression tag	UNP A0QYE8
O	496	HIS	-	expression tag	UNP A0QYE8
P	2	VAL	-	insertion	UNP A0QYE8
P	480	THR	-	expression tag	UNP A0QYE8
P	481	ALA	-	expression tag	UNP A0QYE8
P	482	ALA	-	expression tag	UNP A0QYE8
P	483	ALA	-	expression tag	UNP A0QYE8
P	484	LYS	-	expression tag	UNP A0QYE8
P	485	GLU	-	expression tag	UNP A0QYE8
P	486	ASP	-	expression tag	UNP A0QYE8
P	487	LEU	-	expression tag	UNP A0QYE8
P	488	GLU	-	expression tag	UNP A0QYE8
P	489	HIS	-	expression tag	UNP A0QYE8
P	490	HIS	-	expression tag	UNP A0QYE8
P	491	HIS	-	expression tag	UNP A0QYE8
P	492	HIS	-	expression tag	UNP A0QYE8
P	493	HIS	-	expression tag	UNP A0QYE8
P	494	HIS	-	expression tag	UNP A0QYE8
P	495	HIS	-	expression tag	UNP A0QYE8
P	496	HIS	-	expression tag	UNP A0QYE8

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



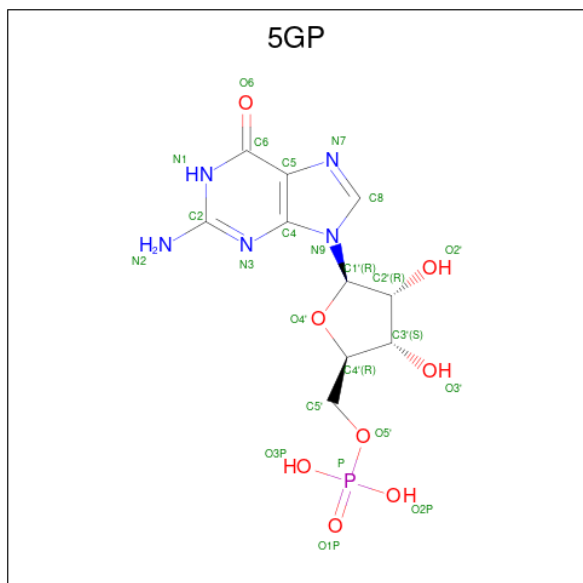
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	B	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	C	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	D	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	E	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	F	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	G	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	H	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	I	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	J	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	K	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	L	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	M	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	N	1	Total 62	C 20	N 10	O 26	P 6	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
2	P	1	Total	C	N	O	P	0	1
			62	20	10	26	6		

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	F	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	G	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	H	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	I	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	K	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	L	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	M	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	N	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	O	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	P	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	65	Total	O	0	0
			65	65		
4	C	38	Total	O	0	0
			38	38		
4	D	35	Total	O	0	0
			35	35		
4	E	78	Total	O	0	0
			78	78		
4	F	82	Total	O	0	0
			82	82		
4	G	81	Total	O	0	0
			81	81		
4	H	87	Total	O	0	0
			87	87		
4	I	66	Total	O	0	0
			66	66		
4	J	43	Total	O	0	0
			43	43		
4	K	78	Total	O	0	0
			78	78		
4	L	74	Total	O	0	0
			74	74		

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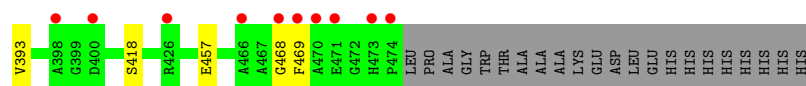
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	39	Total 39	O 39	0	0
4	N	30	Total 30	O 30	0	0
4	O	34	Total 34	O 34	0	0
4	P	34	Total 34	O 34	0	0

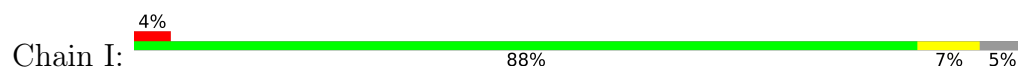
- Molecule 1: GMP reductase



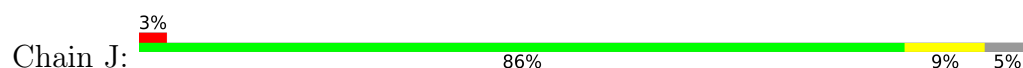




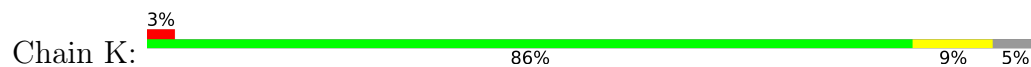
- Molecule 1: GMP reductase



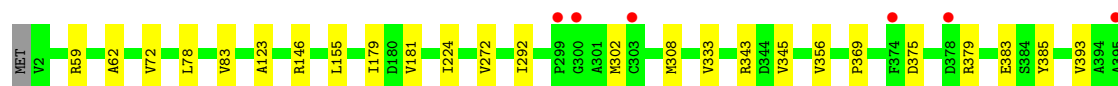
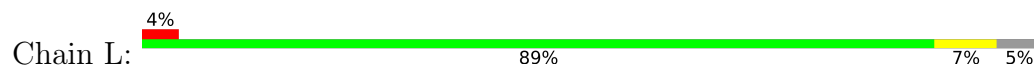
- Molecule 1: GMP reductase



- Molecule 1: GMP reductase

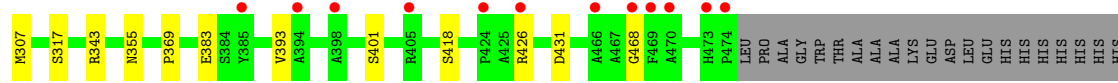
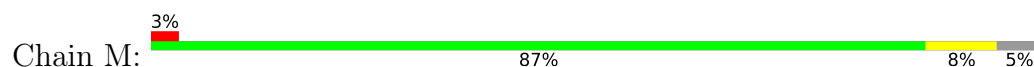


- Molecule 1: GMP reductase



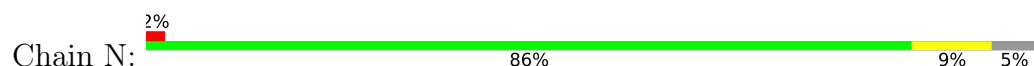


• Molecule 1: GMP reductase



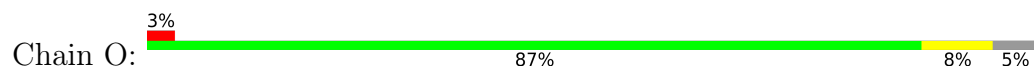
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• Molecule 1: GMP reductase



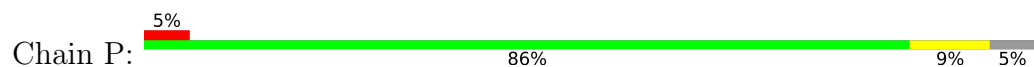
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HIS

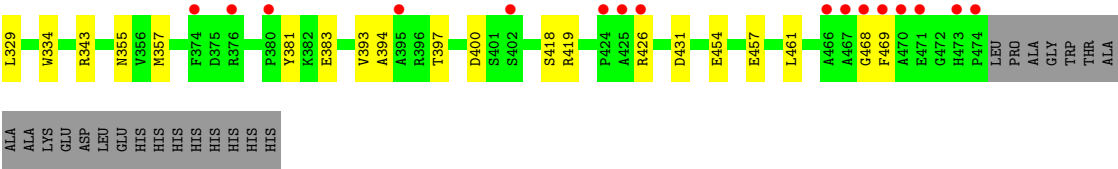
• Molecule 1: GMP reductase



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HIS

• Molecule 1: GMP reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.57Å 113.60Å 178.06Å 82.70° 77.24° 66.75°	Depositor
Resolution (Å)	49.33 – 2.30 49.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.33-2.30) 96.7 (49.33-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21_5204	Depositor
R, R_{free}	0.200 , 0.230 0.200 , 0.229	Depositor DCC
R_{free} test set	16984 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	57130	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 5GP

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	0.17	0/3489	0.33	0/4753
1	B	0.15	0/3483	0.31	0/4746
1	C	0.17	0/3483	0.33	0/4746
1	D	0.18	0/3489	0.32	0/4753
1	E	0.18	0/3489	0.36	0/4753
1	F	0.17	0/3484	0.34	0/4747
1	G	0.17	0/3489	0.34	0/4753
1	H	0.17	0/3483	0.33	0/4746
1	I	0.16	0/3489	0.33	0/4753
1	J	0.16	0/3484	0.32	0/4747
1	K	0.18	0/3489	0.36	0/4753
1	L	0.19	0/3485	0.36	0/4748
1	M	0.17	0/3483	0.32	0/4746
1	N	0.16	0/3489	0.31	0/4753
1	O	0.15	0/3483	0.31	0/4746
1	P	0.17	0/3489	0.33	0/4753
All	All	0.17	0/55780	0.33	0/75996

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3429	0	3407	24	0
1	B	3423	0	3396	21	0
1	C	3423	0	3396	29	0
1	D	3429	0	3407	30	0
1	E	3429	0	3407	22	0
1	F	3424	0	3398	22	0
1	G	3429	0	3407	17	0
1	H	3423	0	3396	23	0
1	I	3429	0	3407	21	0
1	J	3424	0	3398	35	0
1	K	3429	0	3407	28	0
1	L	3425	0	3400	23	0
1	M	3423	0	3396	27	0
1	N	3429	0	3407	28	0
1	O	3423	0	3396	28	0
1	P	3429	0	3407	31	0
2	A	62	0	24	1	0
2	B	62	0	24	0	0
2	C	62	0	24	3	0
2	D	62	0	24	0	0
2	E	62	0	24	1	0
2	F	62	0	24	3	0
2	G	62	0	24	2	0
2	H	62	0	24	5	0
2	I	62	0	24	1	0
2	J	62	0	24	2	0
2	K	62	0	24	2	0
2	L	62	0	24	4	0
2	M	62	0	24	2	0
2	N	62	0	24	0	0
2	O	62	0	24	1	0
2	P	62	0	24	0	0
3	A	24	0	12	1	0
3	B	24	0	12	0	0
3	C	24	0	12	1	0
3	D	24	0	12	0	0
3	E	24	0	12	0	0
3	F	24	0	12	1	0
3	G	24	0	12	0	0
3	H	24	0	12	1	0
3	I	24	0	12	1	0
3	J	24	0	12	0	0
3	K	24	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	24	0	12	0	0
3	M	24	0	12	1	0
3	N	24	0	12	0	0
3	O	24	0	12	1	0
3	P	24	0	12	0	0
4	A	70	0	0	1	0
4	B	65	0	0	0	0
4	C	38	0	0	0	0
4	D	35	0	0	0	0
4	E	78	0	0	0	0
4	F	82	0	0	0	0
4	G	81	0	0	0	0
4	H	87	0	0	0	0
4	I	66	0	0	0	0
4	J	43	0	0	0	0
4	K	78	0	0	0	0
4	L	74	0	0	0	0
4	M	39	0	0	0	0
4	N	30	0	0	0	0
4	O	34	0	0	1	0
4	P	34	0	0	0	0
All	All	57130	0	55008	367	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 3.

All (367) 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:D:383:GLU:HB2	1:E:146:ARG:HH12	1.45	0.79
1:B:302:MET:HE1	1:B:418:SER:HB3	1.72	0.71
1:H:377:ASP:HB2	1:H:379:ARG:HD3	1.73	0.71
1:F:59:ARG:NH1	2:F:501[B]:ATP:O2G	2.25	0.70
1:M:401:SER:HB3	1:P:168:ARG:HH22	1.57	0.69
1:E:113:ASN:HA	1:E:116:LEU:HD12	1.72	0.69
1:O:283:ARG:HG2	1:O:329:LEU:HD11	1.76	0.68
1:C:302:MET:HE1	1:C:418:SER:HB3	1.76	0.67
1:H:302:MET:HE1	1:H:418:SER:HB3	1.76	0.67
1:J:302:MET:HE1	1:J:418:SER:HB2	1.76	0.66
1:O:113:ASN:HA	1:O:116:LEU:HD12	1.75	0.66
1:L:302:MET:HE2	1:L:385:TYR:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:HE2	1:A:385:TYR:HA	1.78	0.65
1:A:59:ARG:NH2	2:A:501[B]:ATP:O2G	2.30	0.65
1:A:106:GLU:OE2	1:A:151:ARG:NH2	2.24	0.64
1:M:302:MET:HE1	1:M:418:SER:HB2	1.78	0.64
1:H:128:PHE:HB2	1:H:133:ILE:HD13	1.79	0.64
1:M:17:ASN:OD1	1:M:343:ARG:NH2	2.29	0.64
1:P:302:MET:HE1	1:P:418:SER:HB2	1.79	0.64
1:B:146:ARG:HH12	1:G:383:GLU:HB2	1.62	0.63
1:G:106:GLU:OE2	1:G:151:ARG:NH1	2.27	0.63
1:P:454:GLU:HA	1:P:457[B]:GLU:HG2	1.81	0.63
1:P:306:ARG:HD3	1:P:312:GLY:HA3	1.81	0.63
1:L:59:ARG:HG2	2:L:502[B]:ATP:O1B	1.99	0.62
1:O:464:GLN:OE1	1:P:306:ARG:NH2	2.32	0.62
1:D:302:MET:HE2	1:D:385:TYR:HA	1.80	0.62
1:I:59:ARG:NH2	2:I:501[A]:ATP:O3G	2.31	0.62
1:P:283:ARG:HG3	1:P:329:LEU:HD11	1.81	0.61
1:C:342:PRO:HB3	1:C:436:ILE:HA	1.83	0.61
1:F:302:MET:HE1	1:F:418:SER:HB2	1.83	0.60
1:E:168:ARG:HH21	1:F:401:SER:HB3	1.67	0.60
1:J:343:ARG:NH1	1:J:344:ASP:OD1	2.35	0.60
1:I:302:MET:HE1	1:I:418:SER:HB2	1.83	0.60
1:J:97:VAL:HG22	1:J:184:MET:HG3	1.84	0.60
1:K:303:CYS:SG	3:K:502:5GP:N2	2.75	0.60
1:J:343:ARG:HH21	1:J:469:PHE:HZ	1.48	0.59
1:B:224:ILE:HD11	1:B:393:VAL:HG22	1.82	0.59
1:C:59:ARG:NH2	2:C:501[B]:ATP:O2G	2.36	0.59
1:J:426:ARG:HD2	1:J:426:ARG:O	2.03	0.58
1:K:17:ASN:OD1	1:K:343:ARG:NH2	2.36	0.58
1:C:59:ARG:NH2	2:C:501[A]:ATP:O3G	2.36	0.58
1:F:249:HIS:HB3	1:F:252:GLN:HE21	1.69	0.58
1:O:343:ARG:NH1	1:O:344:ASP:OD1	2.37	0.58
1:J:106:GLU:OE1	1:J:151:ARG:NH2	2.33	0.58
1:J:272:VAL:HG22	1:J:292:ILE:HB	1.86	0.58
1:C:131:ARG:NH2	1:C:188:ASP:O	2.38	0.57
1:J:17:ASN:OD1	1:J:343:ARG:NH2	2.37	0.57
1:I:375:ASP:OD1	1:I:379:ARG:HG2	2.05	0.56
1:B:106:GLU:OE2	1:B:151:ARG:NH2	2.32	0.56
1:N:468:GLY:HA2	1:O:15:THR:HG21	1.87	0.56
1:L:146:ARG:HH12	1:M:383:GLU:HB2	1.70	0.56
1:J:179:ILE:HG22	1:J:181:VAL:H	1.71	0.56
1:D:170:VAL:HA	1:D:173:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:ILE:HD11	1:I:393:VAL:HG22	1.87	0.56
1:K:106:GLU:OE1	1:K:151:ARG:NH2	2.39	0.56
1:D:228:VAL:HG11	1:D:258:ALA:HB1	1.88	0.56
1:J:188:ASP:OD1	1:J:190:THR:HG23	2.06	0.55
1:D:283:ARG:HG3	1:D:329:LEU:HD21	1.87	0.55
1:P:110:SER:HB2	1:P:146:ARG:HG3	1.88	0.55
1:K:302:MET:HE2	1:K:385:TYR:HA	1.87	0.55
1:A:383:GLU:HB2	1:H:146:ARG:HH12	1.71	0.55
1:E:106:GLU:OE1	1:E:151:ARG:NH2	2.40	0.55
1:J:224:ILE:HD11	1:J:393:VAL:HG22	1.87	0.55
1:J:246:ASP:OD2	1:J:391:ARG:HD2	2.07	0.55
1:L:457[B]:GLU:HG2	1:L:458:LYS:HG3	1.87	0.55
1:O:246:ASP:OD2	1:O:391:ARG:HD2	2.06	0.55
1:O:252:GLN:HE22	1:O:393:VAL:HG21	1.72	0.55
1:H:360:SER:OG	3:H:502:5GP:O3P	2.25	0.54
1:I:468:GLY:HA2	1:J:15:THR:HG21	1.90	0.54
1:M:303:CYS:SG	3:M:501:5GP:N2	2.80	0.54
1:L:62:ALA:HA	1:L:72:VAL:HG21	1.89	0.54
1:D:315:GLN:O	1:D:319:VAL:HG23	2.07	0.54
1:H:29:ALA:HB3	1:H:33:ASP:OD2	2.08	0.54
1:C:303:CYS:SG	3:C:502:5GP:N2	2.80	0.54
1:D:246:ASP:OD2	1:D:391:ARG:HD2	2.07	0.54
1:H:369:PRO:HB3	2:H:501[B]:ATP:H5'2	1.90	0.54
1:N:166:ASP:OD2	1:N:168:ARG:HB2	2.07	0.53
1:O:10:PRO:HG3	1:O:14:LEU:HD21	1.91	0.53
1:A:106:GLU:CD	1:A:151:ARG:HH22	2.17	0.53
1:O:468:GLY:HA2	1:P:15:THR:HG21	1.90	0.53
1:D:123:ALA:HB3	1:D:181:VAL:HG21	1.89	0.53
1:D:36:LEU:HD11	1:D:441:ARG:HG3	1.91	0.53
1:J:174:LEU:HD21	1:J:182:ALA:HB2	1.91	0.53
1:P:224:ILE:HD11	1:P:393:VAL:HG22	1.91	0.53
1:M:287:GLU:HA	1:M:287:GLU:OE1	2.08	0.52
1:E:302:MET:HE1	1:E:418:SER:CB	2.39	0.52
1:J:146:ARG:HH12	1:O:383:GLU:HB2	1.74	0.52
1:L:375:ASP:OD1	1:L:379:ARG:N	2.42	0.52
1:A:224:ILE:HD11	1:A:393:VAL:HG22	1.91	0.52
1:J:97:VAL:HG21	1:J:163:VAL:HG23	1.91	0.52
1:N:31:ARG:HB3	1:N:441:ARG:HB3	1.91	0.52
1:A:272:VAL:HG22	1:A:292:ILE:HB	1.91	0.52
1:D:381:TYR:CE2	1:D:419:ARG:HD3	2.44	0.52
1:F:59:ARG:NH1	2:F:501[A]:ATP:O2G	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ASN:OD1	1:G:343:ARG:NH2	2.41	0.52
1:H:123:ALA:HB3	1:H:181:VAL:HG21	1.92	0.52
1:K:400:ASP:OD2	1:K:408:LYS:NZ	2.32	0.52
1:I:62:ALA:HA	1:I:72:VAL:HG21	1.91	0.52
1:M:62:ALA:HA	1:M:72:VAL:HG21	1.92	0.52
1:M:97:VAL:HG21	1:M:163:VAL:HG23	1.90	0.51
1:I:302:MET:HE1	1:I:418:SER:CB	2.40	0.51
1:B:50:VAL:HB	1:B:72:VAL:HG22	1.92	0.51
1:E:15:THR:HG21	1:H:468:GLY:HA2	1.91	0.51
1:N:272:VAL:HG22	1:N:292:ILE:HB	1.92	0.51
1:P:31:ARG:HB2	1:P:31:ARG:HH11	1.75	0.51
1:J:369:PRO:HB3	2:J:501[B]:ATP:H5'2	1.92	0.51
1:H:59:ARG:HH12	2:H:501[A]:ATP:PG	2.33	0.51
1:N:105:PRO:HG3	1:N:133:ILE:HD11	1.91	0.51
1:O:106:GLU:OE1	1:O:151:ARG:NH2	2.43	0.51
1:E:302:MET:HE1	1:E:418:SER:HB3	1.92	0.51
1:H:369:PRO:HB3	2:H:501[A]:ATP:H5'2	1.92	0.51
1:L:369:PRO:HB3	2:L:502[B]:ATP:H5'2	1.92	0.51
1:J:62:ALA:HA	1:J:72:VAL:HG21	1.91	0.51
1:C:106:GLU:OE2	1:C:151:ARG:NH2	2.44	0.51
1:P:62:ALA:HA	1:P:72:VAL:HG21	1.93	0.51
1:E:123:ALA:HB3	1:E:181:VAL:HG21	1.92	0.50
1:I:100:PRO:HD3	1:I:193:GLY:HA2	1.94	0.50
1:N:97:VAL:HG21	1:N:163:VAL:HG23	1.92	0.50
1:J:16:TYR:HB3	1:J:343:ARG:NH1	2.27	0.50
1:E:58:GLY:HA3	1:E:369:PRO:HG3	1.92	0.50
1:G:328:GLN:CD	1:J:3:ARG:HD3	2.37	0.50
1:F:16:TYR:O	1:F:343:ARG:NH2	2.38	0.50
1:O:50:VAL:HB	1:O:72:VAL:HG22	1.94	0.50
1:O:233:GLN:O	1:O:237:GLU:HG2	2.12	0.50
1:A:105:PRO:HG3	1:A:133:ILE:HD11	1.92	0.50
1:E:62:ALA:HA	1:E:72:VAL:HG21	1.94	0.50
1:A:303:CYS:SG	3:A:502:5GP:N2	2.85	0.49
1:K:175:GLU:HG2	1:K:176:HIS:CE1	2.47	0.49
1:N:423:ASP:HB3	1:N:426:ARG:O	2.11	0.49
1:N:17:ASN:HA	1:N:343:ARG:HH21	1.78	0.49
1:A:435:HIS:NE2	1:B:308:MET:SD	2.86	0.49
1:C:369:PRO:HB3	2:C:501[B]:ATP:H5'2	1.94	0.49
1:A:168:ARG:NH2	1:B:401:SER:OG	2.45	0.49
1:C:383:GLU:HB2	1:F:146:ARG:HH12	1.78	0.49
1:K:109:VAL:HG22	1:K:153:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:224:ILE:HD11	1:N:393:VAL:HG22	1.95	0.49
1:B:246:ASP:OD2	1:B:391:ARG:HD2	2.13	0.49
1:A:15:THR:HG21	1:D:468:GLY:HA2	1.95	0.49
1:H:62:ALA:HA	1:H:72:VAL:HG21	1.94	0.48
1:J:369:PRO:HB3	2:J:501[A]:ATP:H5'2	1.94	0.48
1:O:435:HIS:NE2	1:P:308:MET:SD	2.86	0.48
1:J:468:GLY:HA2	1:K:15:THR:HG21	1.95	0.48
1:M:224:ILE:HD11	1:M:393:VAL:HG22	1.94	0.48
1:H:59:ARG:HH12	2:H:501[B]:ATP:PG	2.36	0.48
1:N:128:PHE:HB2	1:N:133:ILE:HD13	1.94	0.48
1:P:109:VAL:HG22	1:P:153:ILE:HD13	1.96	0.48
1:C:78:LEU:HD23	1:C:83:VAL:HG22	1.95	0.48
1:L:272:VAL:HG22	1:L:292:ILE:HB	1.96	0.48
1:E:155:LEU:HD12	1:E:179:ILE:HD11	1.94	0.48
1:E:468:GLY:HA2	1:F:15:THR:HG21	1.96	0.48
1:H:60:ARG:NE	2:H:501[A]:ATP:O3G	2.44	0.48
1:C:446:TYR:HA	1:D:249:HIS:CD2	2.48	0.48
1:I:15:THR:HG21	1:L:468:GLY:HA2	1.96	0.48
1:L:78:LEU:HD23	1:L:83:VAL:HG22	1.96	0.48
1:C:131:ARG:NH2	1:C:189:GLY:HA3	2.29	0.48
1:O:369:PRO:HB3	2:O:502[B]:ATP:H5'2	1.96	0.48
1:H:106:GLU:OE2	1:H:151:ARG:NH2	2.39	0.48
1:P:128:PHE:HB2	1:P:133:ILE:HD13	1.95	0.48
1:G:62:ALA:HA	1:G:72:VAL:HG21	1.96	0.47
1:A:2:VAL:HG13	1:A:456:HIS:CE1	2.49	0.47
1:C:162:PRO:O	1:C:165:THR:OG1	2.24	0.47
1:C:228:VAL:HG11	1:C:258:ALA:HB1	1.96	0.47
1:M:59:ARG:NH2	2:M:502[B]:ATP:O2G	2.46	0.47
1:C:224:ILE:HD11	1:C:393:VAL:HG22	1.95	0.47
1:E:407:ARG:HG2	1:E:407:ARG:HH11	1.78	0.47
1:H:343:ARG:NH1	1:H:469:PHE:CE1	2.82	0.47
1:J:16:TYR:HB3	1:J:343:ARG:HH12	1.78	0.47
1:O:303:CYS:SG	3:O:501:5GP:N2	2.87	0.47
1:P:16:TYR:C	1:P:343:ARG:HH21	2.23	0.47
1:A:426:ARG:HB3	1:A:431:ASP:CG	2.40	0.47
1:D:186:ALA:HB1	1:D:187:PRO:HD2	1.96	0.47
1:D:316:PHE:HZ	1:D:461:LEU:HD13	1.78	0.47
1:F:369:PRO:HB3	2:F:501[B]:ATP:H5'2	1.95	0.47
1:K:50:VAL:HB	1:K:72:VAL:HG22	1.96	0.47
1:K:369:PRO:HB3	2:K:501[B]:ATP:H5'2	1.97	0.46
1:M:307:MET:HE1	1:P:469:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:224:ILE:O	1:P:254:LYS:HE2	2.14	0.46
1:N:20:PHE:CZ	1:N:462:GLY:HA3	2.49	0.46
1:N:169:GLU:O	1:N:173:LEU:HG	2.14	0.46
1:C:343:ARG:NH1	1:C:469:PHE:CE1	2.83	0.46
1:I:262:VAL:HG11	1:I:271:LEU:HD21	1.96	0.46
1:K:401:SER:N	1:K:404:ASP:OD2	2.41	0.46
1:N:50:VAL:HB	1:N:72:VAL:HG22	1.97	0.46
1:D:334:TRP:CD1	1:D:355:ASN:HB2	2.50	0.46
1:L:155:LEU:HD13	1:L:179:ILE:HD11	1.96	0.46
1:M:244:VAL:HG22	1:M:272:VAL:HB	1.98	0.46
1:N:377:ASP:OD1	1:N:377:ASP:N	2.48	0.46
1:P:272:VAL:HG22	1:P:292:ILE:HB	1.98	0.46
1:D:51:ALA:HA	1:D:357:MET:HE2	1.98	0.46
1:L:146:ARG:NH1	1:M:383:GLU:HB2	2.30	0.46
1:D:105:PRO:HG3	1:D:133:ILE:HD11	1.97	0.46
1:F:468:GLY:HA2	1:G:15:THR:HG21	1.98	0.46
1:B:277:VAL:O	1:B:313:ARG:NH1	2.41	0.46
1:F:62:ALA:HA	1:F:72:VAL:HG21	1.97	0.46
1:I:113:ASN:HA	1:I:116:LEU:HB2	1.97	0.46
1:K:128:PHE:O	1:K:131:ARG:HB3	2.16	0.46
1:M:15:THR:HG21	1:P:468:GLY:HA2	1.98	0.46
1:J:262:VAL:HG11	1:J:271:LEU:HD21	1.97	0.45
1:L:123:ALA:HB3	1:L:181:VAL:HG21	1.96	0.45
1:B:78:LEU:HD23	1:B:83:VAL:HG22	1.98	0.45
1:K:327:ARG:HB2	1:K:327:ARG:CZ	2.45	0.45
1:A:17:ASN:OD1	1:A:343:ARG:NH2	2.50	0.45
1:I:107:ASP:O	1:I:150:VAL:HG23	2.16	0.45
1:I:151:ARG:HG3	1:I:152:ASP:OD1	2.16	0.45
1:N:87:VAL:HG22	1:N:218:ILE:HG21	1.99	0.45
1:P:109:VAL:HG23	1:P:148:ALA:O	2.16	0.45
1:I:310:GLY:HA2	1:L:343:ARG:NH1	2.32	0.45
1:K:245:ILE:HG22	1:K:255:MET:HE1	1.98	0.45
1:M:262:VAL:HG11	1:M:271:LEU:HD21	1.99	0.45
1:P:225:ASN:CG	1:P:394:ALA:H	2.22	0.45
1:A:246:ASP:OD2	1:A:391:ARG:HD2	2.17	0.45
1:C:113:ASN:HA	1:C:116:LEU:HD12	1.99	0.45
1:C:272:VAL:HG22	1:C:292:ILE:HB	1.98	0.45
1:N:316:PHE:HZ	1:N:461:LEU:HD13	1.82	0.45
1:B:381:TYR:CE2	1:B:419:ARG:HG2	2.51	0.45
1:C:342:PRO:HD3	1:C:361:TRP:HH2	1.82	0.45
1:M:197:ARG:O	1:M:201:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:ILE:HG22	1:O:181:VAL:H	1.82	0.45
1:G:29:ALA:HB3	1:G:33:ASP:OD2	2.17	0.45
1:K:464:GLN:HB2	1:K:468:GLY:HA3	1.98	0.45
1:A:137:THR:H	1:A:140:ASN:HD22	1.64	0.45
1:B:62:ALA:HA	1:B:72:VAL:HG21	1.99	0.45
1:M:49:VAL:HG22	1:M:71:ILE:HG22	1.98	0.45
1:F:423:ASP:HB3	1:F:426:ARG:O	2.17	0.44
1:K:31:ARG:HE	1:K:442:SER:HB2	1.82	0.44
1:P:426:ARG:HB3	1:P:431:ASP:CG	2.42	0.44
1:A:110:SER:HB2	1:A:146:ARG:HG2	1.99	0.44
1:D:423:ASP:HB3	1:D:426:ARG:O	2.17	0.44
1:B:302:MET:HE1	1:B:418:SER:CB	2.43	0.44
1:D:378:ASP:OD1	1:D:378:ASP:O	2.35	0.44
1:E:78:LEU:HD23	1:E:83:VAL:HG22	1.99	0.44
1:M:369:PRO:HB3	2:M:502[B]:ATP:H5'2	1.99	0.44
1:B:457[B]:GLU:HG2	1:B:458:LYS:HG3	1.98	0.44
1:F:256:LEU:O	1:F:260:LYS:HE3	2.18	0.44
1:F:426:ARG:HB3	1:F:431:ASP:CG	2.42	0.44
1:I:272:VAL:HG22	1:I:292:ILE:HB	1.99	0.44
1:M:272:VAL:HG22	1:M:292:ILE:HB	1.99	0.44
1:D:146:ARG:HE	1:D:146:ARG:HB2	1.63	0.44
1:D:272:VAL:HG22	1:D:292:ILE:HB	1.98	0.44
1:E:272:VAL:HG22	1:E:292:ILE:HB	1.99	0.44
1:F:323:ALA:O	1:F:327:ARG:HG3	2.17	0.44
1:K:59:ARG:HG2	2:K:501[B]:ATP:O3A	2.18	0.44
1:B:272:VAL:HG22	1:B:292:ILE:HB	1.98	0.44
1:B:468:GLY:HA2	1:C:15:THR:HG21	2.00	0.44
1:O:62:ALA:HA	1:O:72:VAL:HG21	2.00	0.44
1:H:97:VAL:HG21	1:H:163:VAL:HG23	1.98	0.43
1:L:423:ASP:HB3	1:L:426:ARG:O	2.18	0.43
1:D:110:SER:HB2	1:D:146:ARG:HG2	1.99	0.43
1:E:224:ILE:HD11	1:E:393:VAL:HG22	1.99	0.43
1:E:464:GLN:OE1	1:F:306:ARG:NH1	2.50	0.43
1:F:123:ALA:HB3	1:F:181:VAL:HG21	1.99	0.43
1:M:10:PRO:HG3	1:M:14:LEU:HD21	2.00	0.43
1:M:426:ARG:HB3	1:M:431:ASP:CG	2.43	0.43
1:E:59:ARG:HE	1:E:59:ARG:HB2	1.45	0.43
1:E:369:PRO:HB3	2:E:501[B]:ATP:H5'2	2.00	0.43
1:F:303:CYS:SG	3:F:502:5GP:N2	2.91	0.43
1:G:369:PRO:HB3	2:G:501[B]:ATP:H5'2	2.00	0.43
1:J:423:ASP:HB3	1:J:426:ARG:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:ILE:HD11	1:K:393:VAL:HG22	1.99	0.43
1:P:334:TRP:CD1	1:P:355:ASN:HB2	2.52	0.43
1:B:385:TYR:CE1	1:G:146:ARG:HD2	2.54	0.43
1:C:316:PHE:HZ	1:C:461:LEU:HD13	1.84	0.43
1:M:155:LEU:HD13	1:M:179:ILE:HD11	2.01	0.43
1:J:426:ARG:HD3	1:J:431:ASP:HB3	2.01	0.43
1:L:400:ASP:HB3	1:L:404:ASP:HB3	2.01	0.43
1:P:51:ALA:HA	1:P:357:MET:HE2	2.00	0.43
1:A:52:ASN:HA	1:A:73:VAL:O	2.19	0.43
1:C:468:GLY:HA2	1:D:15:THR:HG21	2.00	0.43
1:J:61:MET:HE2	1:J:61:MET:HB2	1.93	0.43
1:N:174:LEU:HD21	1:N:182:ALA:HB2	2.00	0.43
1:N:400:ASP:HB3	1:N:404:ASP:HB2	2.00	0.43
1:O:423:ASP:OD2	1:O:426:ARG:HB2	2.18	0.43
1:C:246:ASP:OD2	1:C:391:ARG:HD2	2.19	0.43
1:G:50:VAL:HB	1:G:72:VAL:HG22	2.00	0.43
1:K:383:GLU:HB2	1:N:146:ARG:HH12	1.83	0.43
1:K:454:GLU:HA	1:K:457[B]:GLU:HG2	2.00	0.43
1:O:409:GLY:HA2	1:O:412:GLU:HB2	2.00	0.43
1:B:197:ARG:O	1:B:201:ILE:HG12	2.19	0.43
1:K:435:HIS:NE2	1:L:308:MET:SD	2.92	0.43
1:L:426:ARG:HB3	1:L:431:ASP:CG	2.44	0.42
1:F:153:ILE:H	1:F:153:ILE:HG13	1.56	0.42
1:H:224:ILE:HD11	1:H:393:VAL:HG22	2.00	0.42
1:I:246:ASP:OD2	1:I:391:ARG:HD2	2.19	0.42
1:K:127:VAL:HG13	1:K:131:ARG:H	1.84	0.42
1:L:345:VAL:HG13	1:L:356:VAL:HG21	2.01	0.42
1:O:379:ARG:HE	1:O:379:ARG:HA	1.83	0.42
1:B:49:VAL:O	1:B:357:MET:HA	2.19	0.42
1:C:283:ARG:HG2	1:C:329:LEU:HD11	2.00	0.42
1:G:49:VAL:HG22	1:G:71:ILE:HG22	2.01	0.42
1:H:49:VAL:HG11	1:H:334:TRP:CZ3	2.54	0.42
1:H:302:MET:HE1	1:H:418:SER:CB	2.46	0.42
1:L:224:ILE:HD11	1:L:393:VAL:HG22	2.01	0.42
1:N:136:VAL:HG21	1:N:150:VAL:HG13	2.02	0.42
1:E:91:LYS:NZ	1:E:241:ASP:OD2	2.51	0.42
1:H:301:ALA:C	1:H:302:MET:HE2	2.45	0.42
1:J:271:LEU:HD23	1:J:271:LEU:HA	1.86	0.42
1:M:468:GLY:HA2	1:N:15:THR:HG21	2.00	0.42
1:D:127:VAL:CG1	1:D:191:LEU:HD12	2.50	0.42
1:D:224:ILE:HD11	1:D:393:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:343:ARG:NH2	1:J:469:PHE:CZ	2.88	0.42
1:K:274:GLY:HA3	1:K:294:LYS:HB3	2.00	0.42
1:N:377:ASP:HB2	1:N:379:ARG:HD2	2.00	0.42
1:O:17:ASN:OD1	1:O:343:ARG:NH2	2.52	0.42
1:P:50:VAL:HB	1:P:72:VAL:HG22	2.02	0.42
1:A:25:ARG:NH1	1:B:284:ASP:OD2	2.52	0.42
1:I:3:ARG:HB2	1:I:3:ARG:HH11	1.84	0.42
1:I:274:GLY:HA3	1:I:294:LYS:HB3	2.01	0.42
1:A:166:ASP:OD2	1:A:168:ARG:HB2	2.19	0.42
1:C:131:ARG:HH22	1:C:189:GLY:HA3	1.84	0.42
1:P:334:TRP:NE1	1:P:355:ASN:HB2	2.35	0.42
1:C:343:ARG:HG3	1:D:310:GLY:HA2	2.01	0.42
1:F:454:GLU:HA	1:F:457[B]:GLU:HG2	2.02	0.42
1:G:435:HIS:NE2	1:H:308:MET:SD	2.93	0.42
1:L:59:ARG:HG2	2:L:502[B]:ATP:PB	2.60	0.42
1:M:14:LEU:H	1:M:317:SER:HG	1.64	0.42
1:G:377:ASP:HB2	1:G:379:ARG:HG2	2.02	0.41
1:G:423:ASP:HB3	1:G:426:ARG:O	2.20	0.41
1:O:249:HIS:HD2	4:O:629:HOH:O	2.03	0.41
1:A:249:HIS:HD2	4:A:644:HOH:O	2.02	0.41
1:J:469:PHE:CE1	1:K:307:MET:HE1	2.54	0.41
1:M:228:VAL:HG11	1:M:258:ALA:HB1	2.02	0.41
1:O:381:TYR:HA	1:O:421:SER:HA	2.02	0.41
1:D:174:LEU:HD21	1:D:182:ALA:HB2	2.01	0.41
1:J:136:VAL:HG21	1:J:150:VAL:HG13	2.02	0.41
1:N:78:LEU:HD12	1:N:79:PRO:HD2	2.02	0.41
1:C:93:ARG:HB2	1:C:216:LEU:HD12	2.03	0.41
1:G:113:ASN:HA	1:G:116:LEU:HB2	2.02	0.41
1:G:369:PRO:HB3	2:G:501[A]:ATP:H5'2	2.02	0.41
1:I:146:ARG:HH12	1:P:383:GLU:HB2	1.86	0.41
1:J:206:TYR:OH	1:J:434:ASP:OD1	2.33	0.41
1:O:252:GLN:NE2	1:O:393:VAL:HG21	2.35	0.41
1:A:62:ALA:HA	1:A:72:VAL:HG21	2.02	0.41
1:L:369:PRO:HB3	2:L:502[A]:ATP:H5'2	2.02	0.41
1:L:383:GLU:HB2	1:M:146:ARG:HH12	1.84	0.41
1:P:381:TYR:CE2	1:P:419:ARG:HG2	2.55	0.41
1:B:426:ARG:HB3	1:B:431:ASP:CG	2.45	0.41
1:D:426:ARG:HB3	1:D:431:ASP:CG	2.45	0.41
1:E:423:ASP:HB3	1:E:426:ARG:O	2.20	0.41
1:H:244:VAL:HG22	1:H:272:VAL:HB	2.01	0.41
1:J:146:ARG:HE	1:J:146:ARG:HB2	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:59:ARG:HG3	1:O:60:ARG:N	2.36	0.41
1:D:50:VAL:HB	1:D:72:VAL:HG22	2.02	0.41
1:K:62:ALA:HA	1:K:72:VAL:HG21	2.02	0.41
1:K:128:PHE:CD1	1:K:129:GLU:HG3	2.55	0.41
1:M:47:PRO:HA	1:M:355:ASN:OD1	2.21	0.41
1:O:272:VAL:HG22	1:O:292:ILE:HB	2.03	0.41
1:C:50:VAL:HB	1:C:72:VAL:HG22	2.03	0.41
1:C:146:ARG:NH1	1:F:383:GLU:OE1	2.50	0.41
1:E:153:ILE:H	1:E:153:ILE:HG13	1.61	0.41
1:G:244:VAL:HG22	1:G:272:VAL:HB	2.02	0.41
1:K:381:TYR:CE2	1:K:419:ARG:HG2	2.55	0.41
1:K:423:ASP:HB3	1:K:426:ARG:O	2.21	0.41
1:N:302:MET:HE1	1:N:418:SER:CB	2.50	0.41
1:N:364:GLY:O	1:N:422:LEU:HG	2.21	0.41
1:P:316:PHE:HZ	1:P:461:LEU:HD13	1.85	0.41
1:P:397:THR:HA	1:P:400:ASP:OD2	2.21	0.41
1:N:473:HIS:HB3	1:O:304:THR:HG22	2.02	0.41
1:P:47:PRO:HA	1:P:355:ASN:OD1	2.20	0.41
1:J:31:ARG:HE	1:J:442:SER:HB2	1.86	0.40
1:N:302:MET:HE1	1:N:418:SER:HB3	2.02	0.40
1:I:303:CYS:SG	3:I:502:5GP:N2	2.94	0.40
1:A:49:VAL:O	1:A:357:MET:HA	2.21	0.40
1:I:10:PRO:HG3	1:I:14:LEU:HD21	2.03	0.40
1:J:50:VAL:HB	1:J:72:VAL:HG22	2.04	0.40
1:D:179:ILE:HG22	1:D:181:VAL:H	1.86	0.40
1:F:105:PRO:HG3	1:F:133:ILE:HD11	2.03	0.40
1:N:170:VAL:HG11	1:N:195:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/496 (95%)	462 (98%)	10 (2%)	0	100	100
1	B	472/496 (95%)	463 (98%)	9 (2%)	0	100	100
1	C	472/496 (95%)	463 (98%)	9 (2%)	0	100	100
1	D	472/496 (95%)	459 (97%)	13 (3%)	0	100	100
1	E	472/496 (95%)	462 (98%)	10 (2%)	0	100	100
1	F	472/496 (95%)	461 (98%)	11 (2%)	0	100	100
1	G	472/496 (95%)	460 (98%)	12 (2%)	0	100	100
1	H	472/496 (95%)	465 (98%)	7 (2%)	0	100	100
1	I	472/496 (95%)	461 (98%)	11 (2%)	0	100	100
1	J	472/496 (95%)	463 (98%)	9 (2%)	0	100	100
1	K	472/496 (95%)	462 (98%)	10 (2%)	0	100	100
1	L	472/496 (95%)	464 (98%)	8 (2%)	0	100	100
1	M	472/496 (95%)	466 (99%)	6 (1%)	0	100	100
1	N	472/496 (95%)	461 (98%)	11 (2%)	0	100	100
1	O	472/496 (95%)	461 (98%)	11 (2%)	0	100	100
1	P	472/496 (95%)	464 (98%)	8 (2%)	0	100	100
All	All	7552/7936 (95%)	7397 (98%)	155 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/372 (94%)	349 (99%)	2 (1%)	78	89
1	B	350/372 (94%)	349 (100%)	1 (0%)	86	93
1	C	350/372 (94%)	348 (99%)	2 (1%)	78	89
1	D	351/372 (94%)	350 (100%)	1 (0%)	86	93
1	E	351/372 (94%)	348 (99%)	3 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	350/372 (94%)	348 (99%)	2 (1%)	78	89
1	G	351/372 (94%)	348 (99%)	3 (1%)	70	84
1	H	350/372 (94%)	346 (99%)	4 (1%)	65	81
1	I	351/372 (94%)	348 (99%)	3 (1%)	70	84
1	J	350/372 (94%)	349 (100%)	1 (0%)	86	93
1	K	351/372 (94%)	349 (99%)	2 (1%)	78	89
1	L	350/372 (94%)	349 (100%)	1 (0%)	86	93
1	M	350/372 (94%)	350 (100%)	0	100	100
1	N	351/372 (94%)	350 (100%)	1 (0%)	86	93
1	O	350/372 (94%)	349 (100%)	1 (0%)	86	93
1	P	351/372 (94%)	351 (100%)	0	100	100
All	All	5608/5952 (94%)	5581 (100%)	27 (0%)	81	90

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	417	THR
1	B	397	THR
1	C	6	ASP
1	C	115	LEU
1	D	150	VAL
1	E	333	VAL
1	E	355	ASN
1	E	417	THR
1	F	333	VAL
1	F	355	ASN
1	G	6	ASP
1	G	378	ASP
1	G	417	THR
1	H	333	VAL
1	H	360	SER
1	H	457[A]	GLU
1	H	457[B]	GLU
1	I	6	ASP
1	I	138	GLU
1	I	333	VAL
1	J	56	VAL

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Mol	Chain	Res	Type
1	K	333	VAL
1	K	401	SER
1	L	333	VAL
1	N	377	ASP
1	O	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	328	GLN
1	B	249	HIS
1	B	341	HIS
1	C	328	GLN
1	D	113	ASN
1	D	140	ASN
1	D	252	GLN
1	E	473	HIS
1	F	249	HIS
1	H	117	HIS
1	H	176	HIS
1	H	341	HIS
1	I	117	HIS
1	J	117	HIS
1	J	341	HIS
1	K	473	HIS
1	M	341	HIS
1	M	456	HIS
1	N	332	HIS
1	N	456	HIS
1	O	117	HIS
1	O	176	HIS
1	P	140	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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	ATP	H	501[B]	-	32,33,33	0.56	0	48,52,52	0.51	0
2	ATP	F	501[B]	-	32,33,33	0.57	0	48,52,52	0.55	0
2	ATP	N	502[A]	-	32,33,33	0.57	0	48,52,52	0.55	0
2	ATP	O	502[B]	-	32,33,33	0.56	0	48,52,52	0.53	0
3	5GP	M	501	-	26,26,26	0.41	0	39,40,40	0.56	0
2	ATP	C	501[A]	-	32,33,33	0.53	0	48,52,52	0.57	0
3	5GP	C	502	-	26,26,26	0.38	0	39,40,40	0.52	0
2	ATP	M	502[B]	-	32,33,33	0.58	0	48,52,52	0.53	0
2	ATP	P	502[B]	-	32,33,33	0.55	0	48,52,52	0.52	0
3	5GP	H	502	-	26,26,26	0.41	0	39,40,40	0.59	0
3	5GP	K	502	-	26,26,26	0.40	0	39,40,40	0.51	0
3	5GP	E	502	-	26,26,26	0.39	0	39,40,40	0.53	0
2	ATP	D	501[A]	-	32,33,33	0.56	0	48,52,52	0.55	0
2	ATP	J	501[A]	-	32,33,33	0.57	0	48,52,52	0.55	0
2	ATP	H	501[A]	-	32,33,33	0.56	0	48,52,52	0.64	0
2	ATP	F	501[A]	-	32,33,33	0.56	0	48,52,52	0.56	0
2	ATP	E	501[B]	-	32,33,33	0.55	0	48,52,52	0.53	0
2	ATP	K	501[B]	-	32,33,33	0.56	0	48,52,52	0.53	0
3	5GP	F	502	-	26,26,26	0.40	0	39,40,40	0.59	0
2	ATP	O	502[A]	-	32,33,33	0.57	0	48,52,52	0.55	0
3	5GP	I	502	-	26,26,26	0.42	0	39,40,40	0.52	0
3	5GP	L	501	-	26,26,26	0.40	0	39,40,40	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	M	502[A]	-	32,33,33	0.56	0	48,52,52	0.52	0
2	ATP	P	502[A]	-	32,33,33	0.55	0	48,52,52	0.57	0
3	5GP	O	501	-	26,26,26	0.40	0	39,40,40	0.52	0
2	ATP	A	501[B]	-	32,33,33	0.56	0	48,52,52	0.54	0
2	ATP	B	501[B]	-	32,33,33	0.56	0	48,52,52	0.53	0
2	ATP	I	501[B]	-	32,33,33	0.55	0	48,52,52	0.51	0
2	ATP	L	502[B]	-	32,33,33	0.56	0	48,52,52	0.53	0
3	5GP	D	502	-	26,26,26	0.39	0	39,40,40	0.54	0
3	5GP	G	502	-	26,26,26	0.40	0	39,40,40	0.56	0
2	ATP	K	501[A]	-	32,33,33	0.55	0	48,52,52	0.56	0
2	ATP	G	501[B]	-	32,33,33	0.54	0	48,52,52	0.56	0
2	ATP	E	501[A]	-	32,33,33	0.56	0	48,52,52	0.54	0
2	ATP	J	501[B]	-	32,33,33	0.56	0	48,52,52	0.54	0
2	ATP	N	502[B]	-	32,33,33	0.55	0	48,52,52	0.53	0
3	5GP	J	502	-	26,26,26	0.39	0	39,40,40	0.56	0
2	ATP	C	501[B]	-	32,33,33	0.56	0	48,52,52	0.52	0
3	5GP	P	501	-	26,26,26	0.40	0	39,40,40	0.54	0
2	ATP	A	501[A]	-	32,33,33	0.55	0	48,52,52	0.56	0
2	ATP	B	501[A]	-	32,33,33	0.56	0	48,52,52	0.53	0
2	ATP	I	501[A]	-	32,33,33	0.55	0	48,52,52	0.56	0
2	ATP	L	502[A]	-	32,33,33	0.56	0	48,52,52	0.57	0
3	5GP	B	502	-	26,26,26	0.39	0	39,40,40	0.56	0
3	5GP	N	501	-	26,26,26	0.39	0	39,40,40	0.48	0
3	5GP	A	502	-	26,26,26	0.40	0	39,40,40	0.55	0
2	ATP	D	501[B]	-	32,33,33	0.57	0	48,52,52	0.52	0
2	ATP	G	501[A]	-	32,33,33	0.55	0	48,52,52	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	H	501[B]	-	-	2/22/38/38	0/3/3/3
2	ATP	F	501[B]	-	-	2/22/38/38	0/3/3/3
2	ATP	N	502[A]	-	-	4/22/38/38	0/3/3/3
2	ATP	O	502[B]	-	-	3/22/38/38	0/3/3/3
3	5GP	M	501	-	-	0/10/26/26	0/3/3/3
2	ATP	C	501[A]	-	-	1/22/38/38	0/3/3/3
3	5GP	C	502	-	-	0/10/26/26	0/3/3/3
2	ATP	M	502[B]	-	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	P	502[B]	-	-	6/22/38/38	0/3/3/3
3	5GP	H	502	-	-	0/10/26/26	0/3/3/3
3	5GP	K	502	-	-	0/10/26/26	0/3/3/3
3	5GP	E	502	-	-	0/10/26/26	0/3/3/3
2	ATP	D	501[A]	-	-	5/22/38/38	0/3/3/3
2	ATP	J	501[A]	-	-	2/22/38/38	0/3/3/3
2	ATP	H	501[A]	-	-	0/22/38/38	0/3/3/3
2	ATP	F	501[A]	-	-	0/22/38/38	0/3/3/3
2	ATP	E	501[B]	-	-	3/22/38/38	0/3/3/3
2	ATP	K	501[B]	-	-	9/22/38/38	0/3/3/3
3	5GP	F	502	-	-	0/10/26/26	0/3/3/3
2	ATP	O	502[A]	-	-	2/22/38/38	0/3/3/3
3	5GP	I	502	-	-	0/10/26/26	0/3/3/3
3	5GP	L	501	-	-	0/10/26/26	0/3/3/3
2	ATP	M	502[A]	-	-	5/22/38/38	0/3/3/3
2	ATP	P	502[A]	-	-	2/22/38/38	0/3/3/3
3	5GP	O	501	-	-	0/10/26/26	0/3/3/3
2	ATP	A	501[B]	-	-	4/22/38/38	0/3/3/3
2	ATP	B	501[B]	-	-	5/22/38/38	0/3/3/3
2	ATP	I	501[B]	-	-	9/22/38/38	0/3/3/3
2	ATP	L	502[B]	-	-	5/22/38/38	0/3/3/3
3	5GP	D	502	-	-	0/10/26/26	0/3/3/3
3	5GP	G	502	-	-	0/10/26/26	0/3/3/3
2	ATP	K	501[A]	-	-	4/22/38/38	0/3/3/3
2	ATP	G	501[B]	-	-	2/22/38/38	0/3/3/3
2	ATP	E	501[A]	-	-	7/22/38/38	0/3/3/3
2	ATP	J	501[B]	-	-	2/22/38/38	0/3/3/3
2	ATP	N	502[B]	-	-	8/22/38/38	0/3/3/3
3	5GP	J	502	-	-	0/10/26/26	0/3/3/3
2	ATP	C	501[B]	-	-	6/22/38/38	0/3/3/3
3	5GP	P	501	-	-	0/10/26/26	0/3/3/3
2	ATP	A	501[A]	-	-	1/22/38/38	0/3/3/3
2	ATP	B	501[A]	-	-	2/22/38/38	0/3/3/3
2	ATP	I	501[A]	-	-	2/22/38/38	0/3/3/3
2	ATP	L	502[A]	-	-	2/22/38/38	0/3/3/3
3	5GP	B	502	-	-	0/10/26/26	0/3/3/3
3	5GP	N	501	-	-	0/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5GP	A	502	-	-	0/10/26/26	0/3/3/3
2	ATP	D	501[B]	-	-	3/22/38/38	0/3/3/3
2	ATP	G	501[A]	-	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[B]	ATP	PB-O3B-PG-O2G
2	C	501[B]	ATP	C5'-O5'-PA-O2A
2	D	501[A]	ATP	C5'-O5'-PA-O2A
2	E	501[A]	ATP	C5'-O5'-PA-O1A
2	I	501[B]	ATP	C5'-O5'-PA-O2A
2	I	501[B]	ATP	C5'-O5'-PA-O3A
2	K	501[B]	ATP	C5'-O5'-PA-O2A
2	K	501[B]	ATP	C5'-O5'-PA-O3A
2	L	502[B]	ATP	PB-O3B-PG-O2G
2	L	502[B]	ATP	C5'-O5'-PA-O2A
2	M	502[A]	ATP	C5'-O5'-PA-O1A
2	M	502[A]	ATP	C5'-O5'-PA-O3A
2	M	502[B]	ATP	C5'-O5'-PA-O2A
2	M	502[B]	ATP	C5'-O5'-PA-O3A
2	N	502[B]	ATP	C5'-O5'-PA-O2A
2	N	502[B]	ATP	C5'-O5'-PA-O3A
2	P	502[B]	ATP	C5'-O5'-PA-O2A
2	D	501[B]	ATP	O4'-C4'-C5'-O5'
2	D	501[B]	ATP	C3'-C4'-C5'-O5'
2	N	502[B]	ATP	O4'-C4'-C5'-O5'
2	N	502[B]	ATP	C3'-C4'-C5'-O5'
2	I	501[B]	ATP	O4'-C4'-C5'-O5'
2	K	501[B]	ATP	O4'-C4'-C5'-O5'
2	M	502[B]	ATP	O4'-C4'-C5'-O5'
2	M	502[B]	ATP	C3'-C4'-C5'-O5'
2	P	502[B]	ATP	O4'-C4'-C5'-O5'
2	I	501[B]	ATP	C3'-C4'-C5'-O5'
2	K	501[B]	ATP	C3'-C4'-C5'-O5'
2	H	501[B]	ATP	PB-O3A-PA-O1A
2	J	501[B]	ATP	PB-O3A-PA-O1A
2	K	501[B]	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	K	501[B]	ATP	PA-O3A-PB-O1B
2	O	502[B]	ATP	PB-O3A-PA-O1A
2	D	501[B]	ATP	PB-O3A-PA-O5'
2	N	502[B]	ATP	PB-O3A-PA-O5'
2	E	501[A]	ATP	PB-O3B-PG-O1G
2	I	501[B]	ATP	PB-O3B-PG-O1G
2	P	502[B]	ATP	PB-O3B-PG-O2G
2	P	502[B]	ATP	C3'-C4'-C5'-O5'
2	A	501[B]	ATP	PB-O3A-PA-O2A
2	B	501[B]	ATP	PB-O3A-PA-O2A
2	C	501[B]	ATP	PG-O3B-PB-O2B
2	G	501[B]	ATP	PB-O3A-PA-O2A
2	J	501[A]	ATP	PA-O3A-PB-O2B
2	M	502[A]	ATP	PG-O3B-PB-O1B
2	M	502[B]	ATP	PG-O3B-PB-O2B
2	N	502[A]	ATP	PA-O3A-PB-O2B
2	O	502[A]	ATP	PA-O3A-PB-O2B
2	D	501[A]	ATP	O4'-C4'-C5'-O5'
2	D	501[A]	ATP	C5'-O5'-PA-O1A
2	D	501[A]	ATP	C5'-O5'-PA-O3A
2	E	501[A]	ATP	C5'-O5'-PA-O2A
2	E	501[A]	ATP	C5'-O5'-PA-O3A
2	I	501[A]	ATP	C5'-O5'-PA-O1A
2	I	501[B]	ATP	C5'-O5'-PA-O1A
2	K	501[B]	ATP	C5'-O5'-PA-O1A
2	L	502[B]	ATP	C5'-O5'-PA-O3A
2	M	502[A]	ATP	C5'-O5'-PA-O2A
2	M	502[B]	ATP	C5'-O5'-PA-O1A
2	N	502[B]	ATP	C5'-O5'-PA-O1A
2	C	501[B]	ATP	O4'-C4'-C5'-O5'
2	A	501[A]	ATP	PA-O3A-PB-O2B
2	E	501[B]	ATP	PB-O3A-PA-O2A
2	F	501[B]	ATP	PG-O3B-PB-O1B
2	F	501[B]	ATP	PG-O3B-PB-O2B
2	J	501[B]	ATP	PB-O3A-PA-O2A
2	K	501[A]	ATP	PA-O3A-PB-O1B
2	K	501[A]	ATP	PA-O3A-PB-O2B
2	K	501[B]	ATP	PG-O3B-PB-O2B
2	K	501[B]	ATP	PA-O3A-PB-O2B
2	N	502[A]	ATP	PB-O3A-PA-O1A
2	N	502[A]	ATP	PB-O3A-PA-O2A
2	N	502[B]	ATP	PA-O3A-PB-O2B

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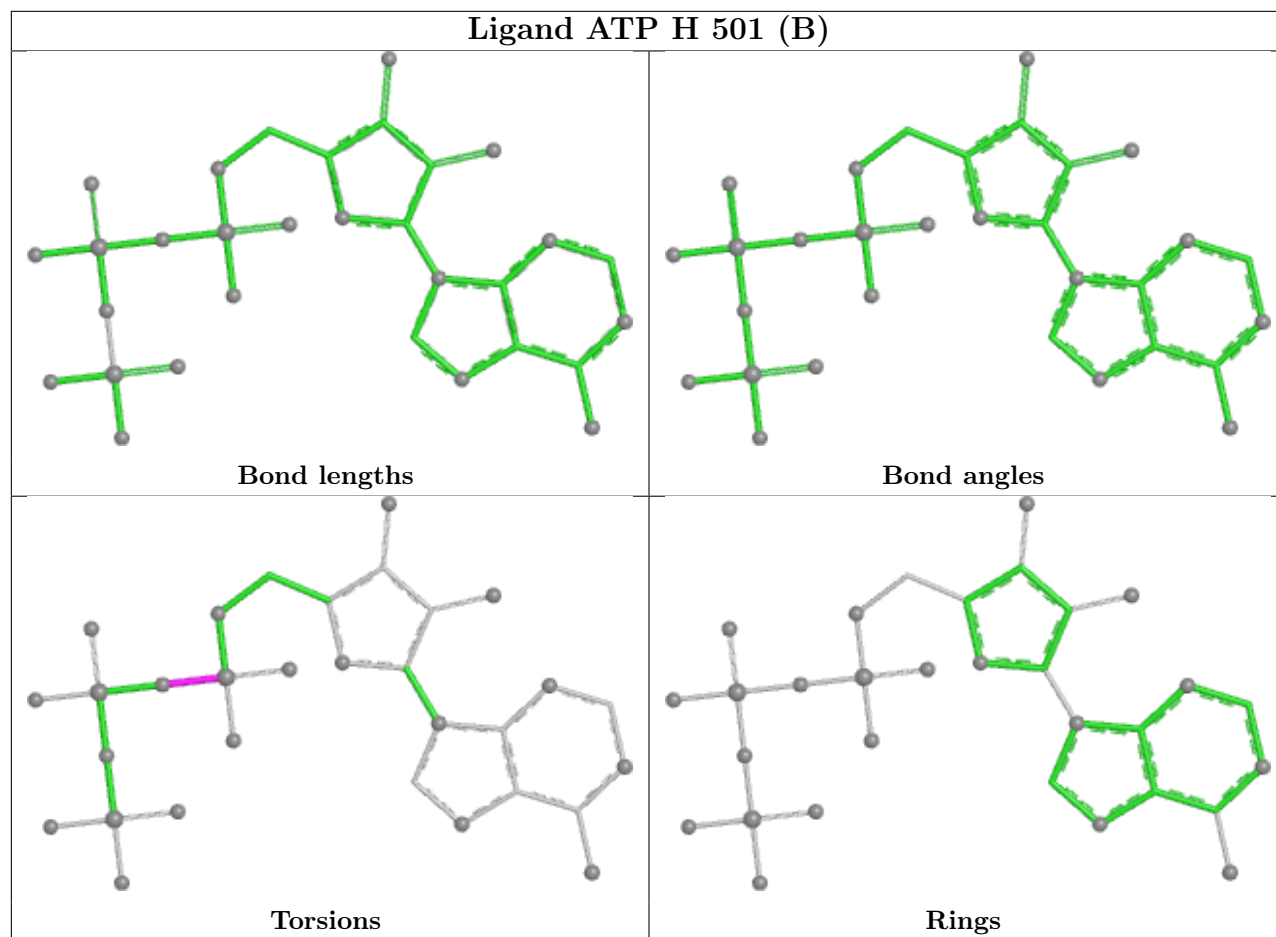
Mol	Chain	Res	Type	Atoms
2	B	501[B]	ATP	PB-O3B-PG-O1G
2	A	501[B]	ATP	PA-O3A-PB-O1B
2	G	501[B]	ATP	PB-O3A-PA-O1A
2	J	501[A]	ATP	PA-O3A-PB-O1B
2	P	502[A]	ATP	PA-O3A-PB-O2B
2	L	502[B]	ATP	PB-O3B-PG-O1G
2	B	501[B]	ATP	PB-O3B-PG-O2G
2	B	501[B]	ATP	PB-O3B-PG-O3G
2	C	501[B]	ATP	PB-O3B-PG-O2G
2	E	501[A]	ATP	PB-O3B-PG-O2G
2	E	501[A]	ATP	PB-O3B-PG-O3G
2	E	501[B]	ATP	PB-O3B-PG-O2G
2	I	501[B]	ATP	PB-O3B-PG-O2G
2	I	501[B]	ATP	PB-O3B-PG-O3G
2	D	501[A]	ATP	C3'-C4'-C5'-O5'
2	A	501[B]	ATP	PB-O3A-PA-O1A
2	B	501[A]	ATP	PA-O3A-PB-O2B
2	B	501[B]	ATP	PB-O3A-PA-O1A
2	C	501[A]	ATP	PA-O3A-PB-O2B
2	C	501[B]	ATP	PG-O3B-PB-O1B
2	E	501[B]	ATP	PB-O3A-PA-O1A
2	H	501[B]	ATP	PB-O3A-PA-O2A
2	I	501[B]	ATP	PG-O3B-PB-O2B
2	L	502[A]	ATP	PA-O3A-PB-O1B
2	M	502[A]	ATP	PG-O3B-PB-O2B
2	M	502[B]	ATP	PG-O3B-PB-O1B
2	N	502[A]	ATP	PA-O3A-PB-O1B
2	N	502[B]	ATP	PA-O3A-PB-O1B
2	O	502[B]	ATP	PG-O3B-PB-O2B
2	O	502[B]	ATP	PB-O3A-PA-O2A
2	P	502[A]	ATP	PA-O3A-PB-O1B
2	C	501[B]	ATP	C3'-C4'-C5'-O5'
2	L	502[B]	ATP	O4'-C4'-C5'-O5'
2	B	501[A]	ATP	PA-O3A-PB-O1B
2	E	501[A]	ATP	PA-O3A-PB-O1B
2	I	501[A]	ATP	PA-O3A-PB-O1B
2	K	501[A]	ATP	PB-O3A-PA-O1A
2	K	501[A]	ATP	PB-O3A-PA-O2A
2	L	502[A]	ATP	PA-O3A-PB-O2B
2	O	502[A]	ATP	PA-O3A-PB-O1B
2	P	502[B]	ATP	PG-O3B-PB-O1B
2	P	502[B]	ATP	PG-O3B-PB-O2B

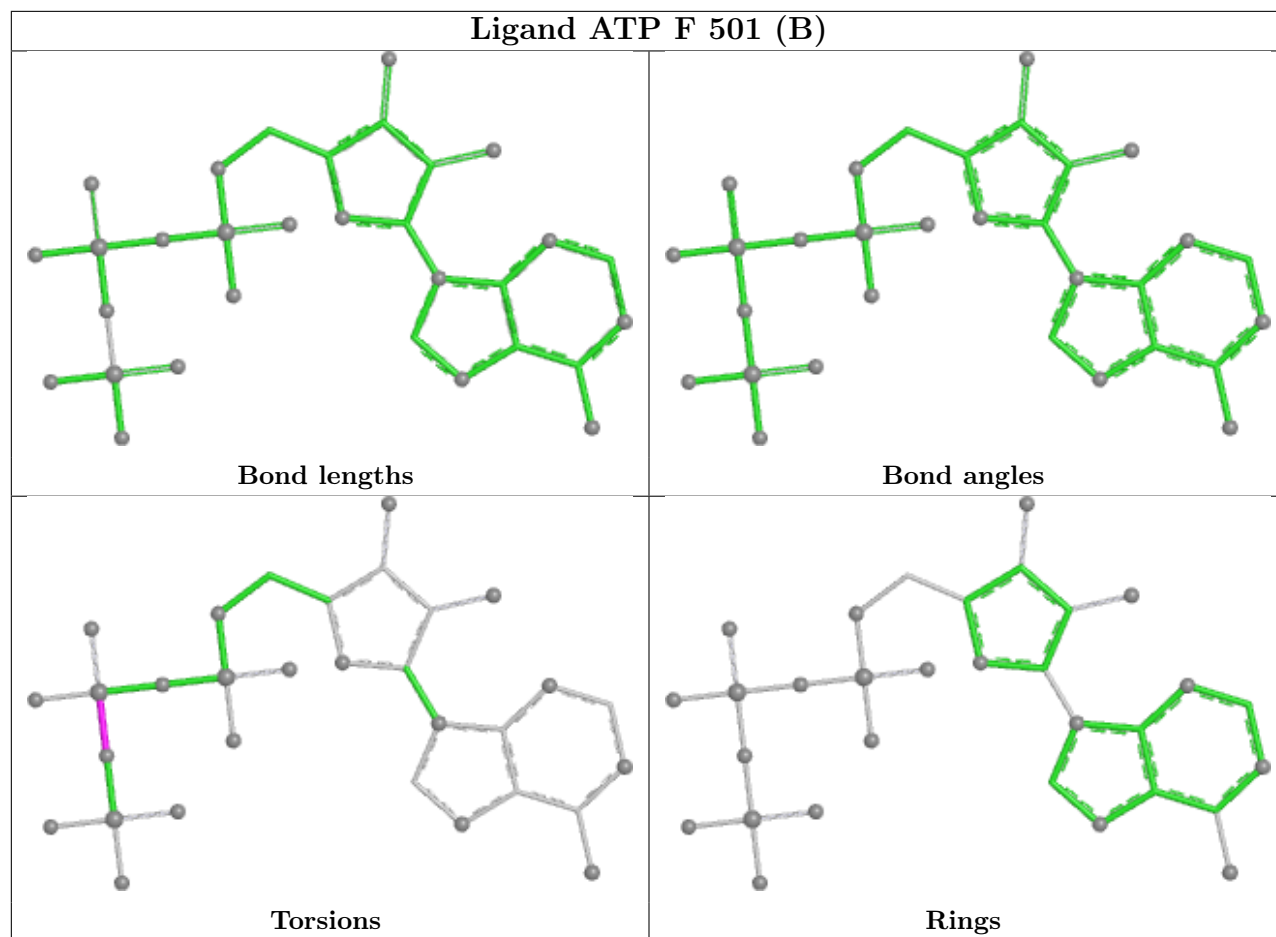
There are no ring outliers.

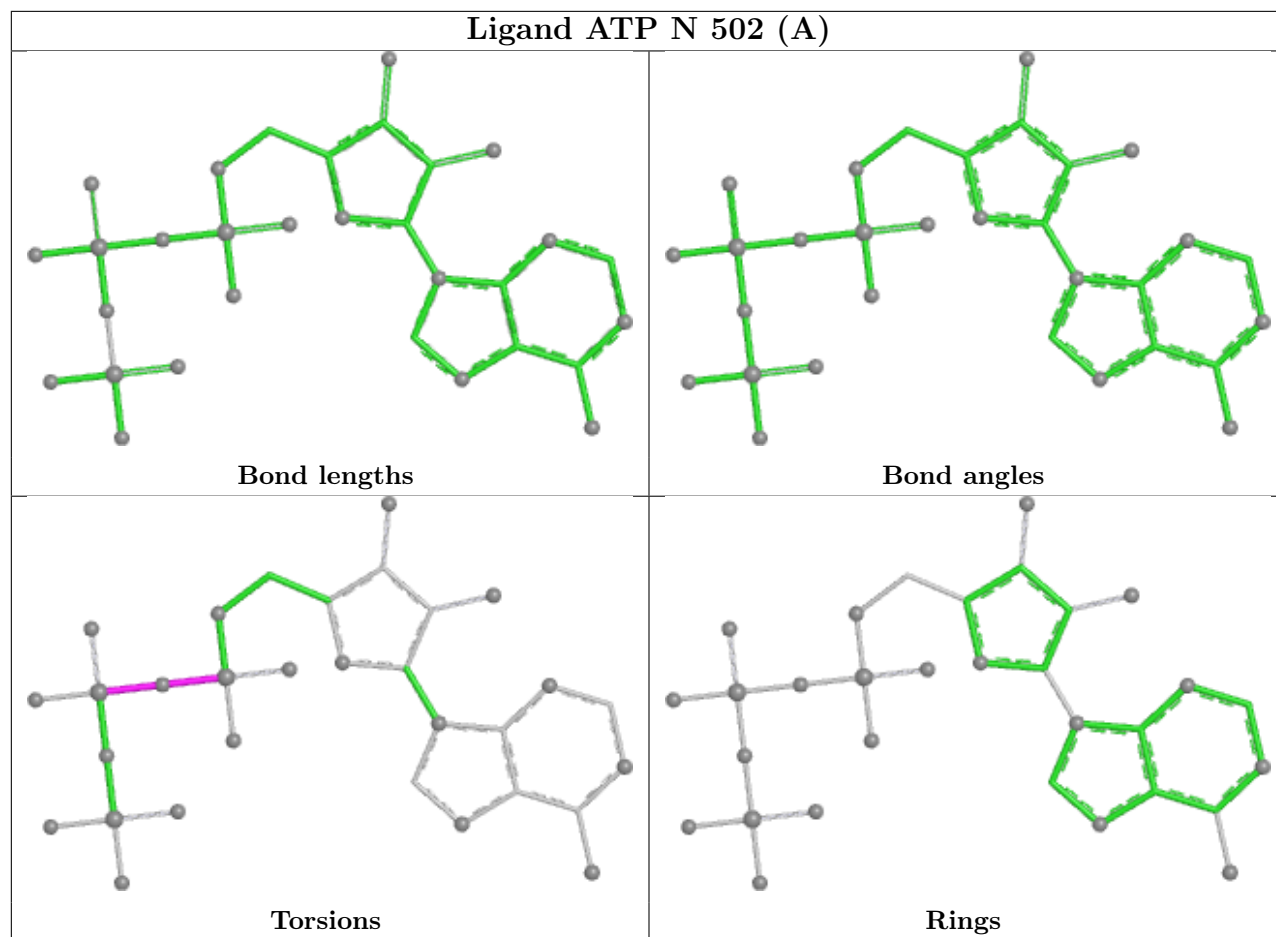
26 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501[B]	ATP	2	0
2	F	501[B]	ATP	2	0
2	O	502[B]	ATP	1	0
3	M	501	5GP	1	0
2	C	501[A]	ATP	1	0
3	C	502	5GP	1	0
2	M	502[B]	ATP	2	0
3	H	502	5GP	1	0
3	K	502	5GP	1	0
2	J	501[A]	ATP	1	0
2	H	501[A]	ATP	3	0
2	F	501[A]	ATP	1	0
2	E	501[B]	ATP	1	0
2	K	501[B]	ATP	2	0
3	F	502	5GP	1	0
3	I	502	5GP	1	0
3	O	501	5GP	1	0
2	A	501[B]	ATP	1	0
2	L	502[B]	ATP	3	0
2	G	501[B]	ATP	1	0
2	J	501[B]	ATP	1	0
2	C	501[B]	ATP	2	0
2	I	501[A]	ATP	1	0
2	L	502[A]	ATP	1	0
3	A	502	5GP	1	0
2	G	501[A]	ATP	1	0

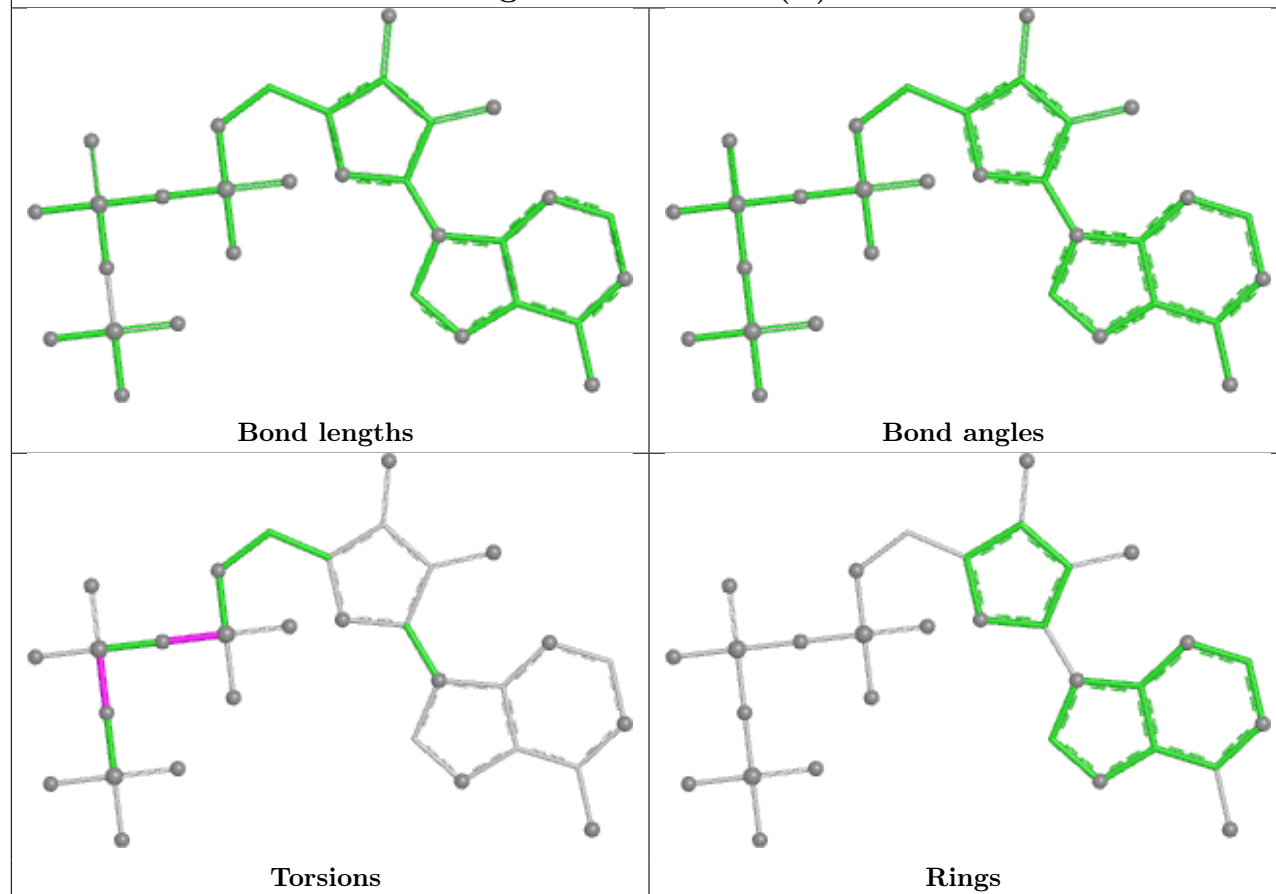
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



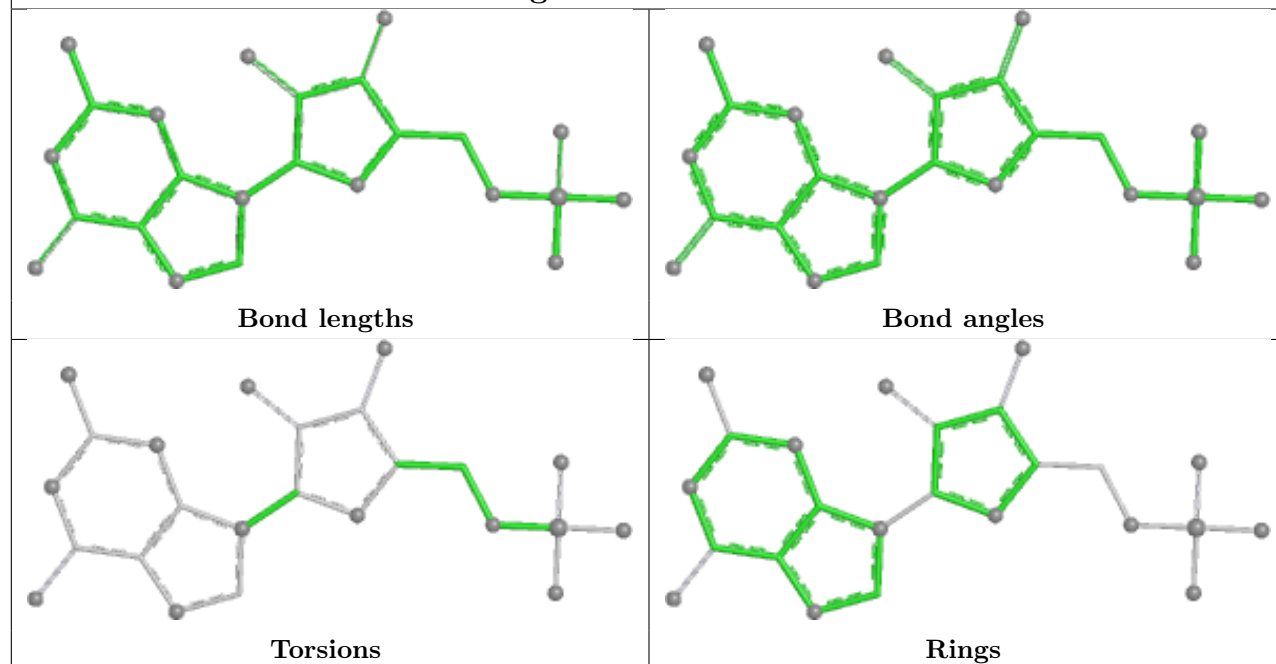




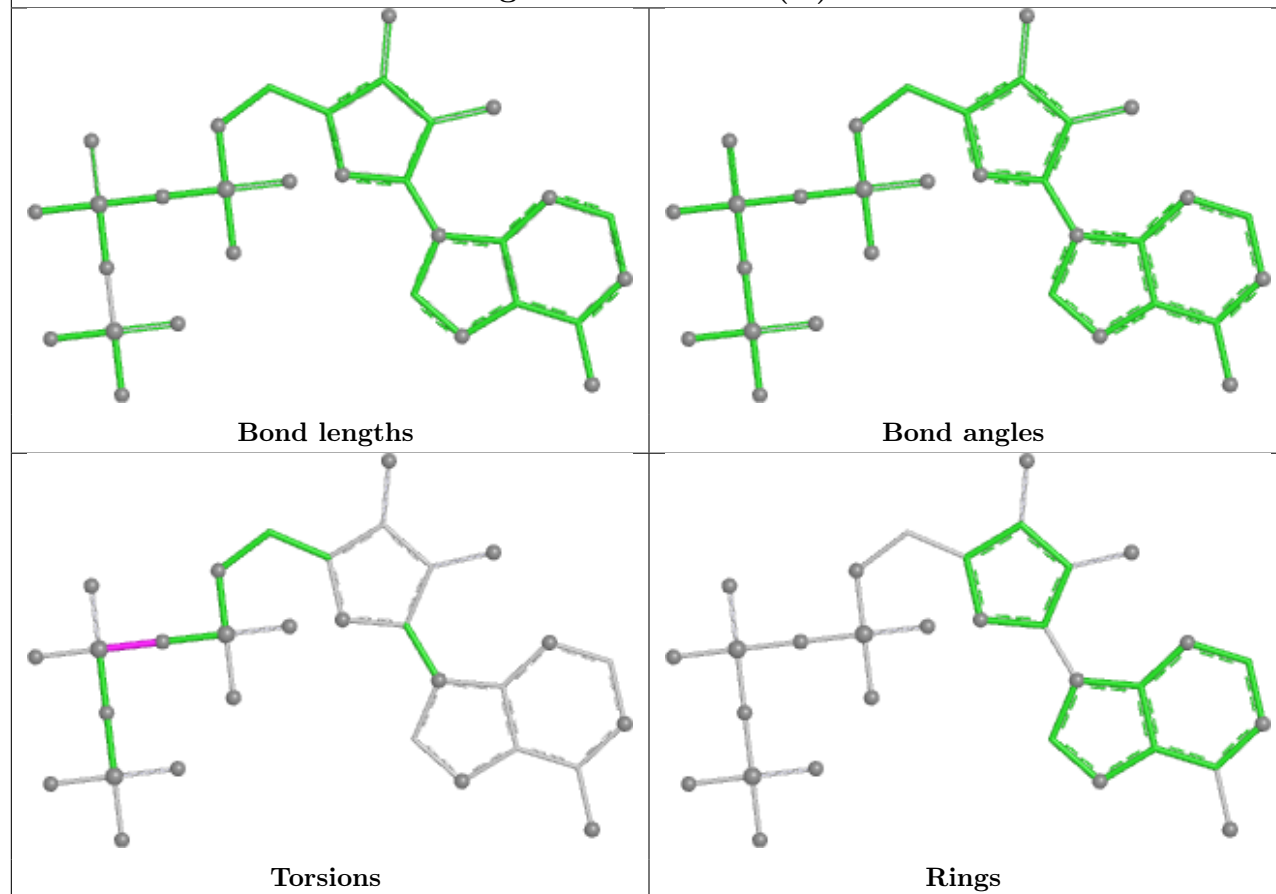
Ligand ATP O 502 (B)



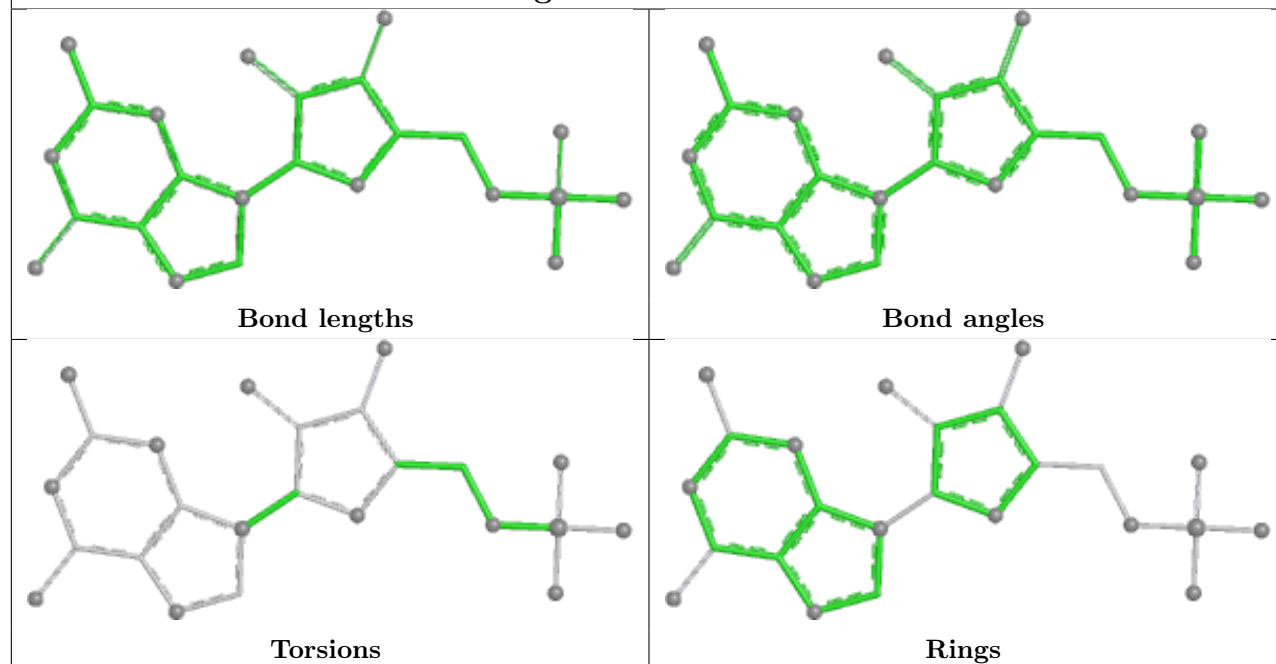
Ligand 5GP M 501

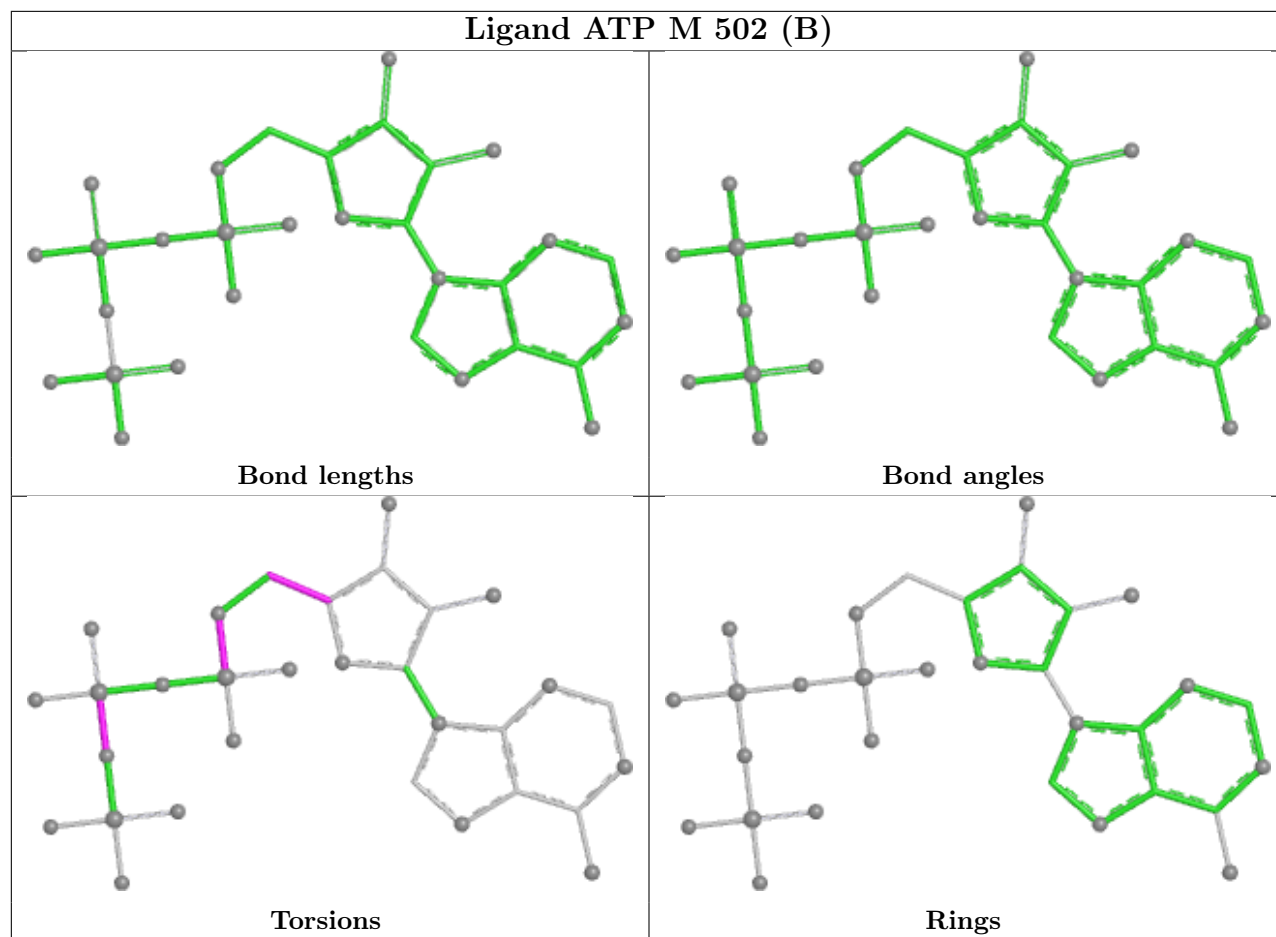


Ligand ATP C 501 (A)

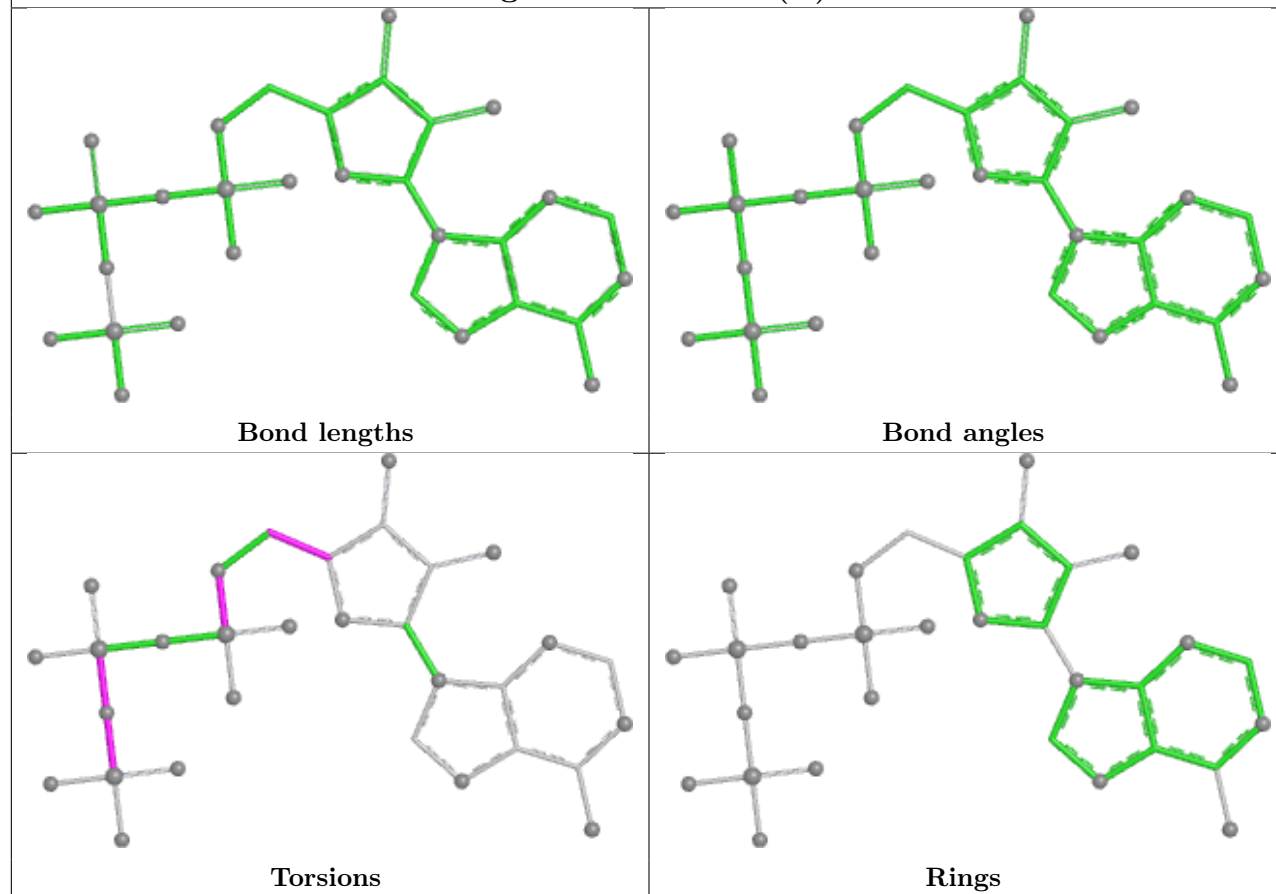


Ligand 5GP C 502

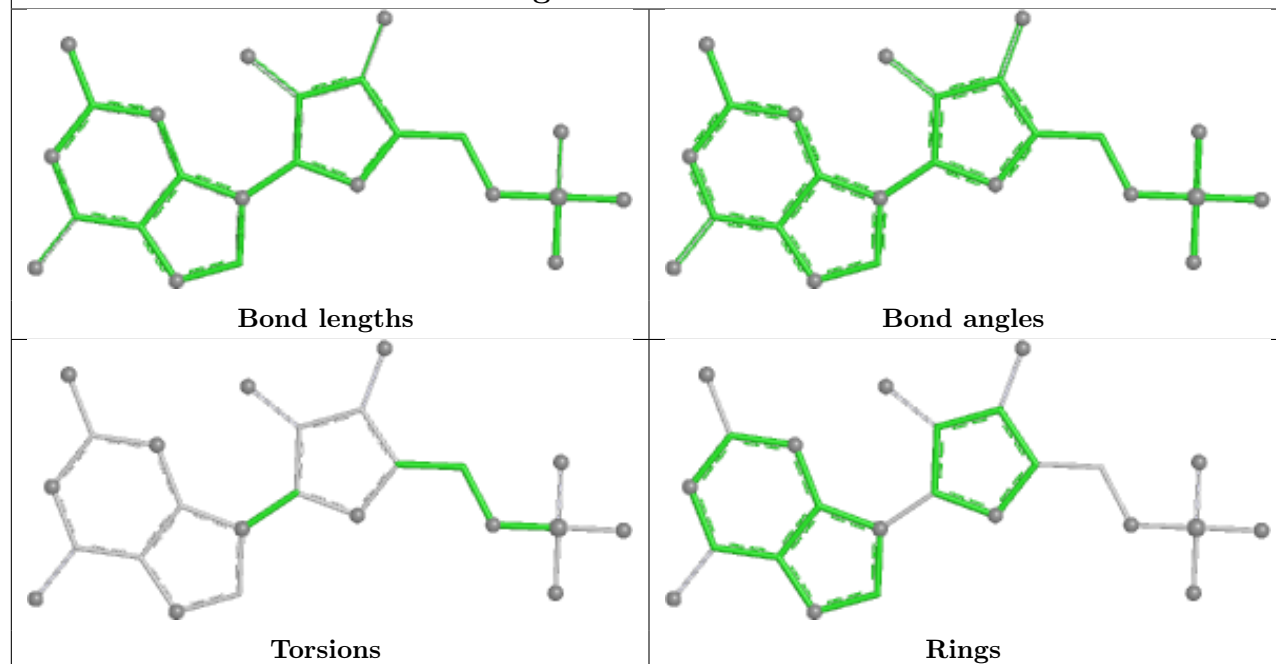




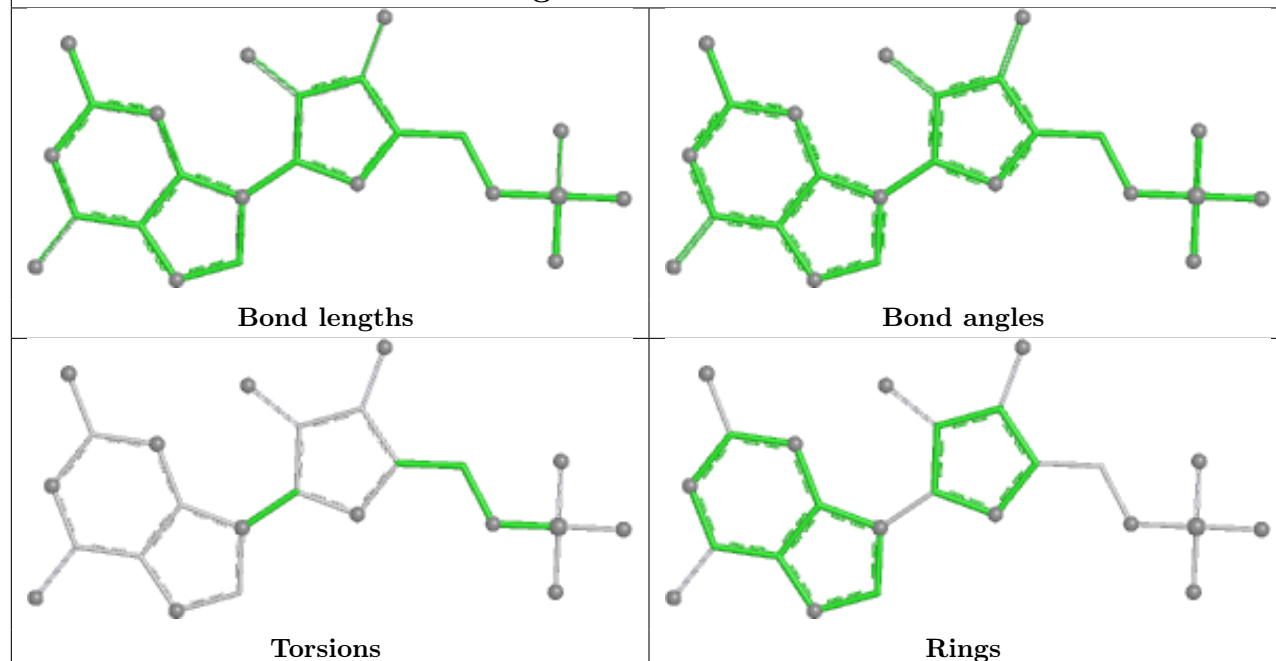
Ligand ATP P 502 (B)



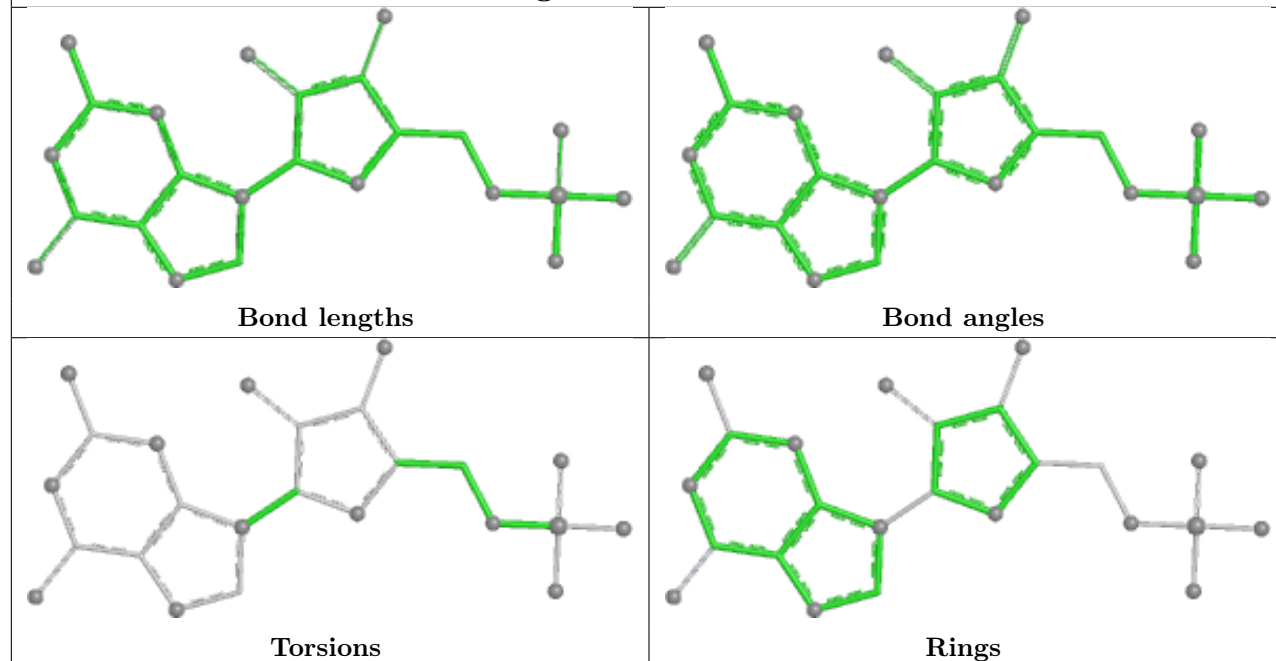
Ligand 5GP H 502

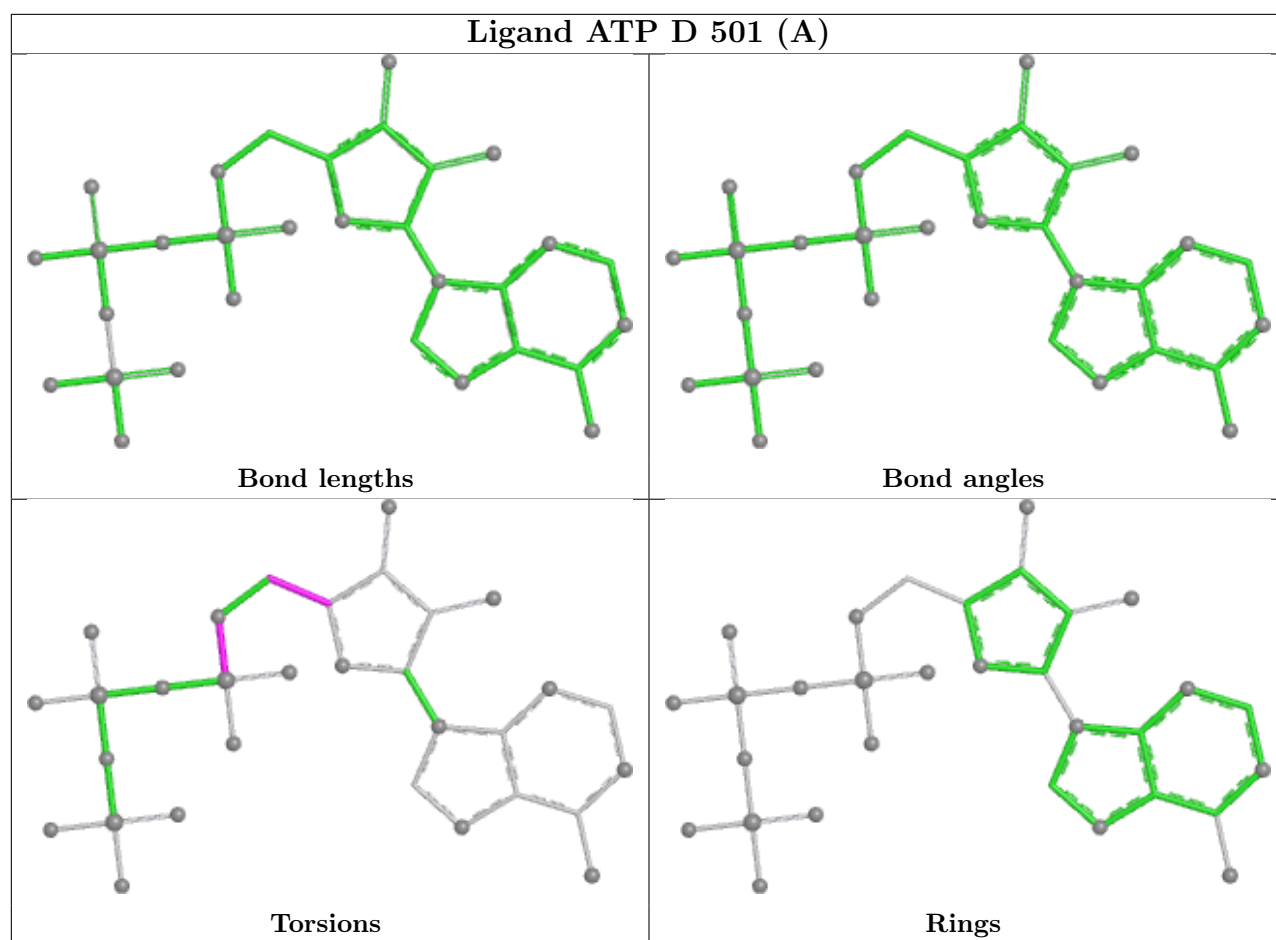


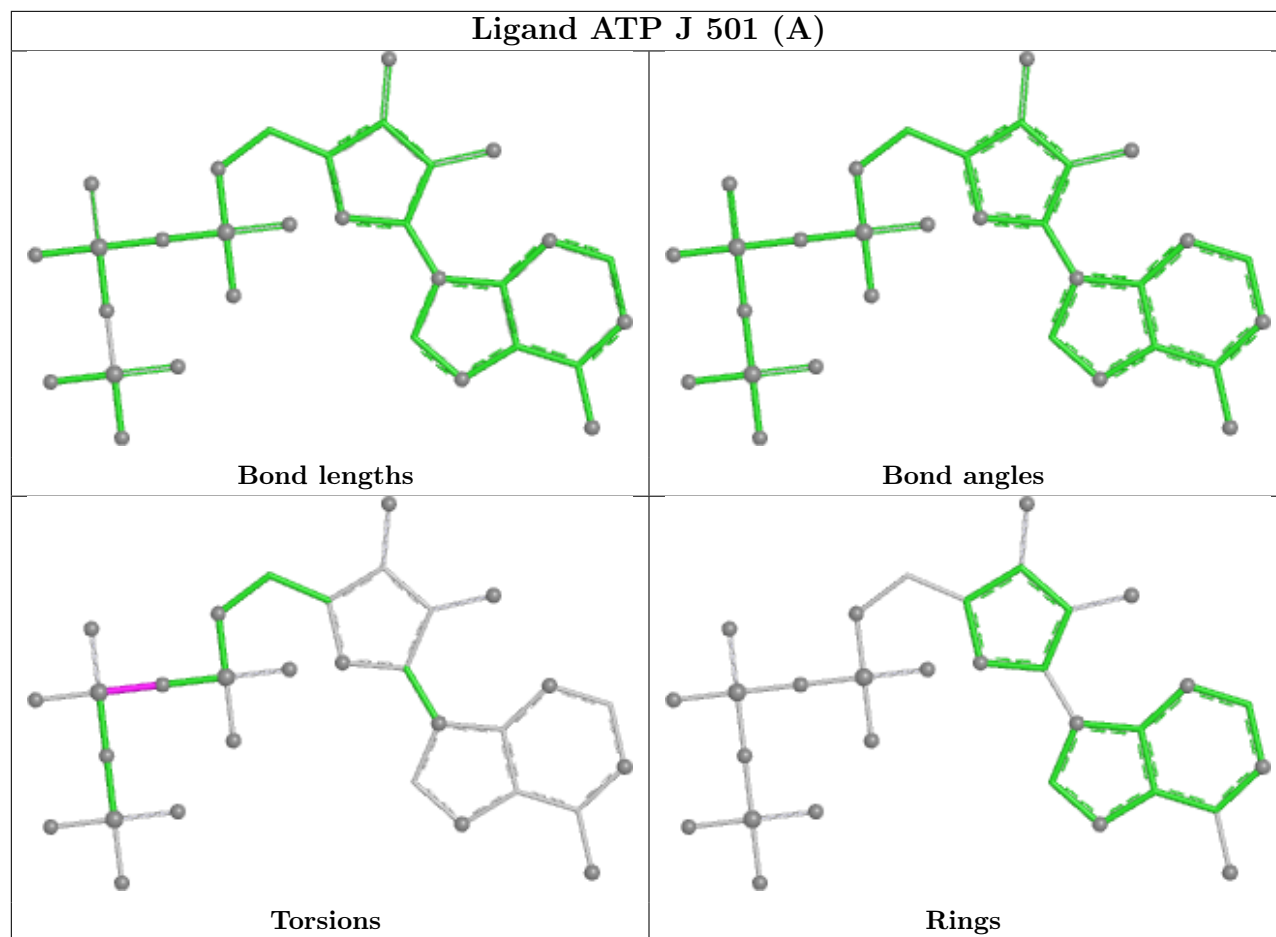
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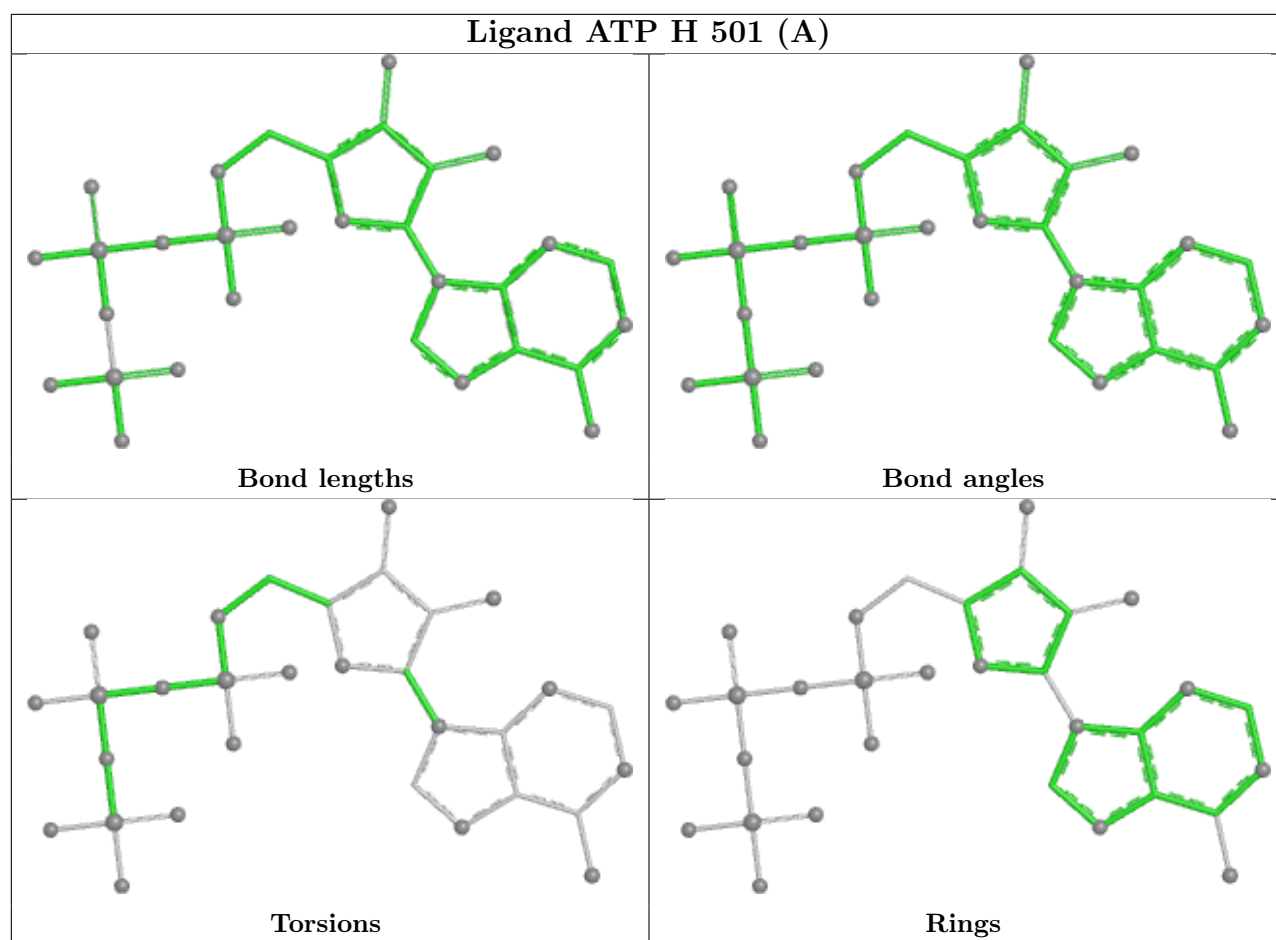


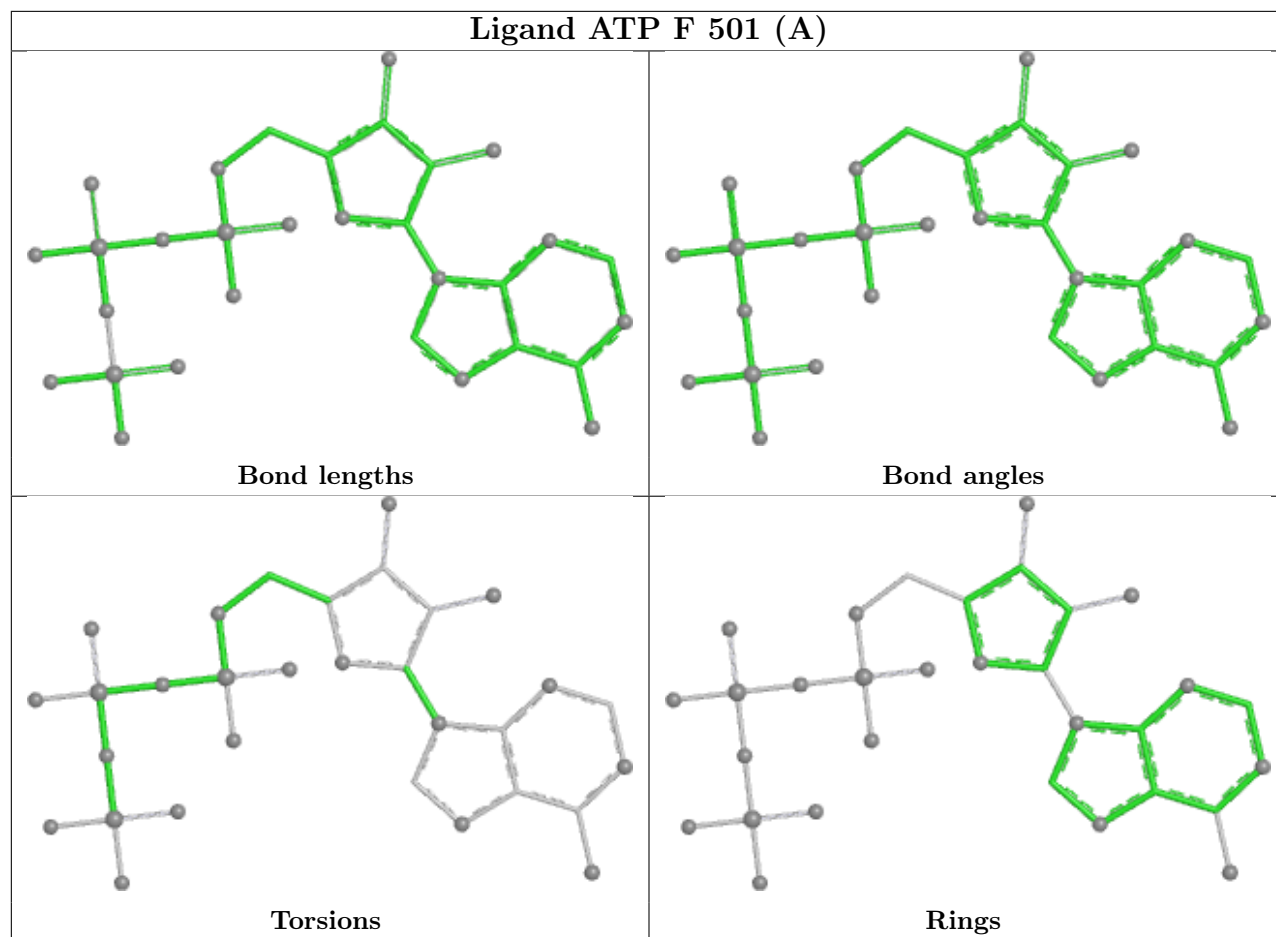
Ligand 5GP E 502

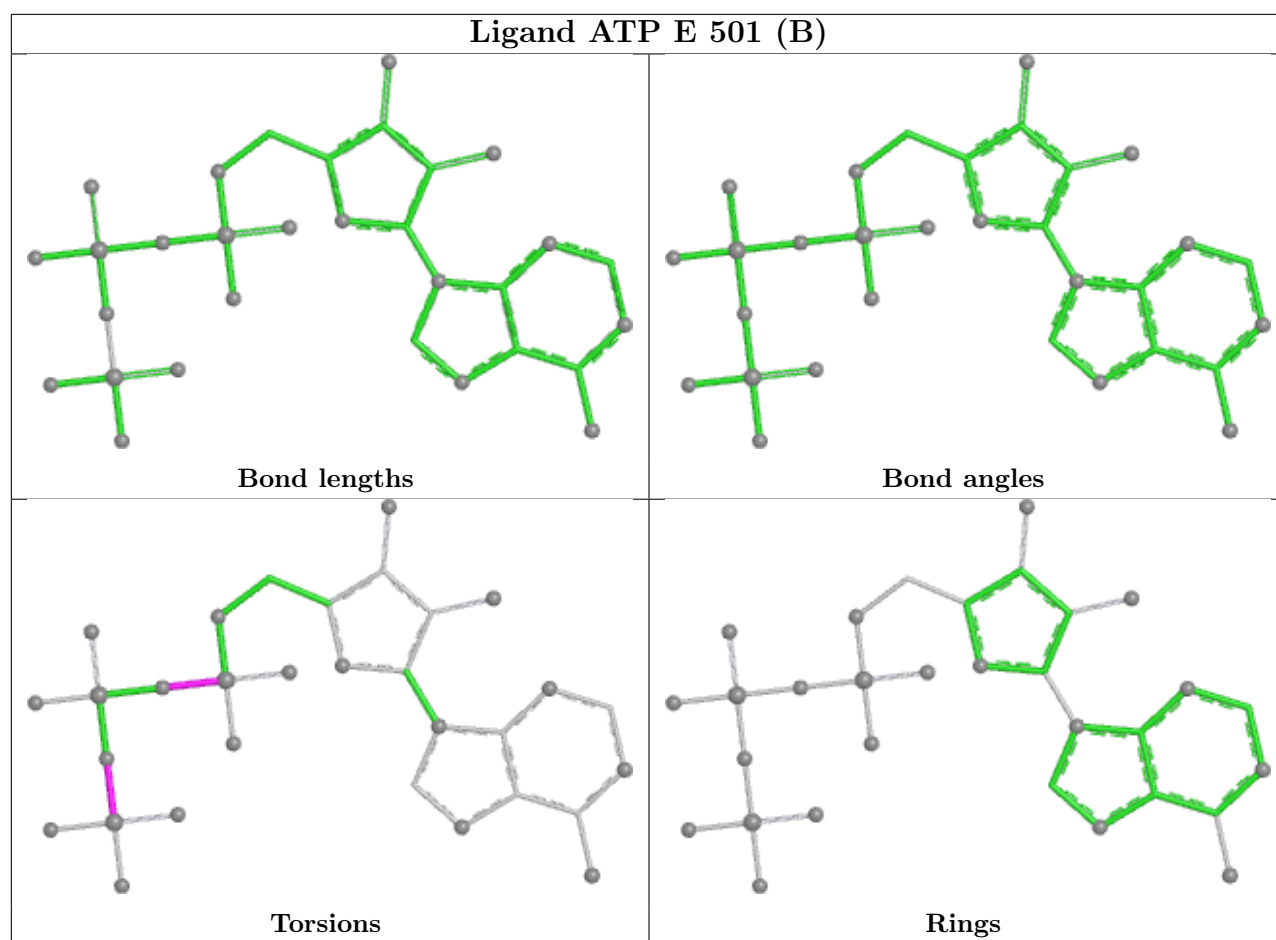




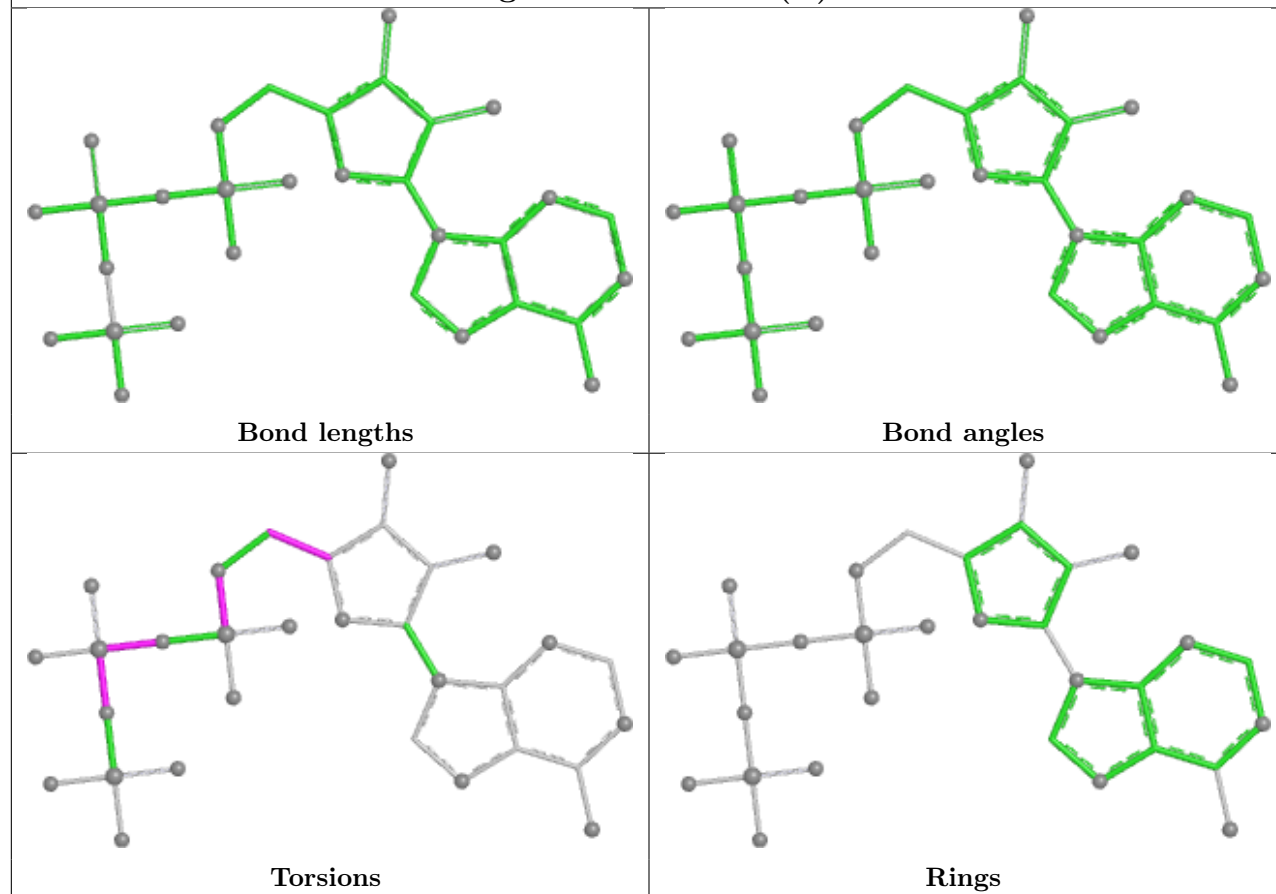




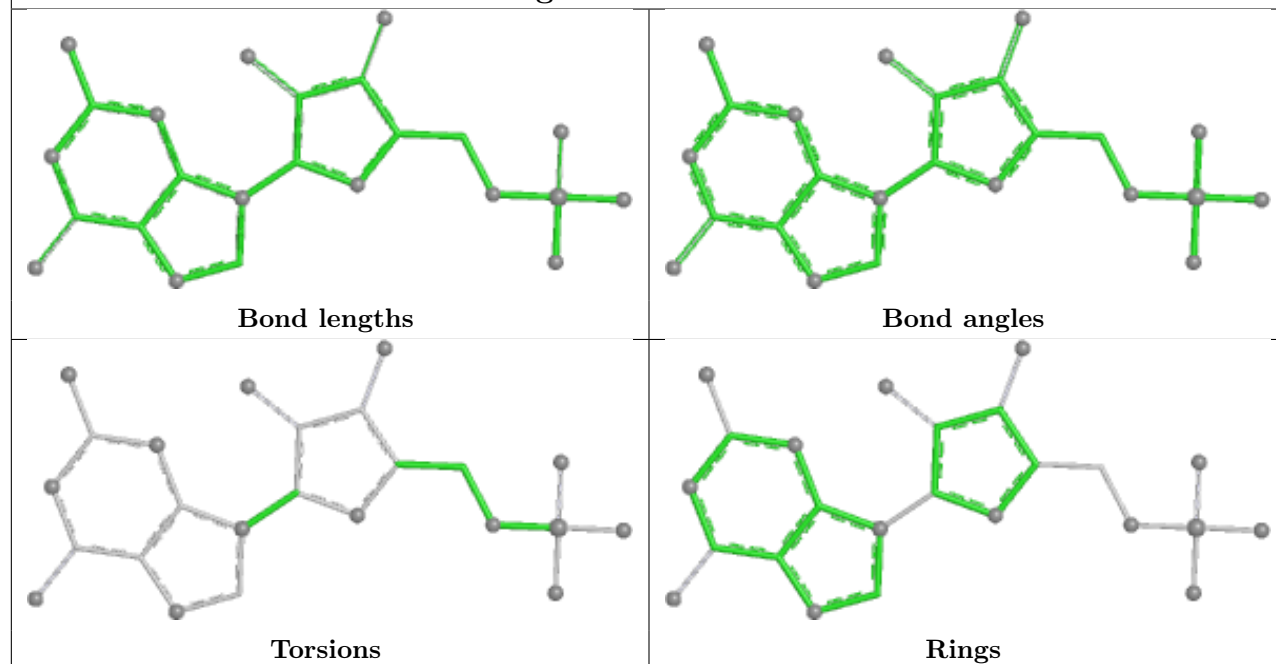




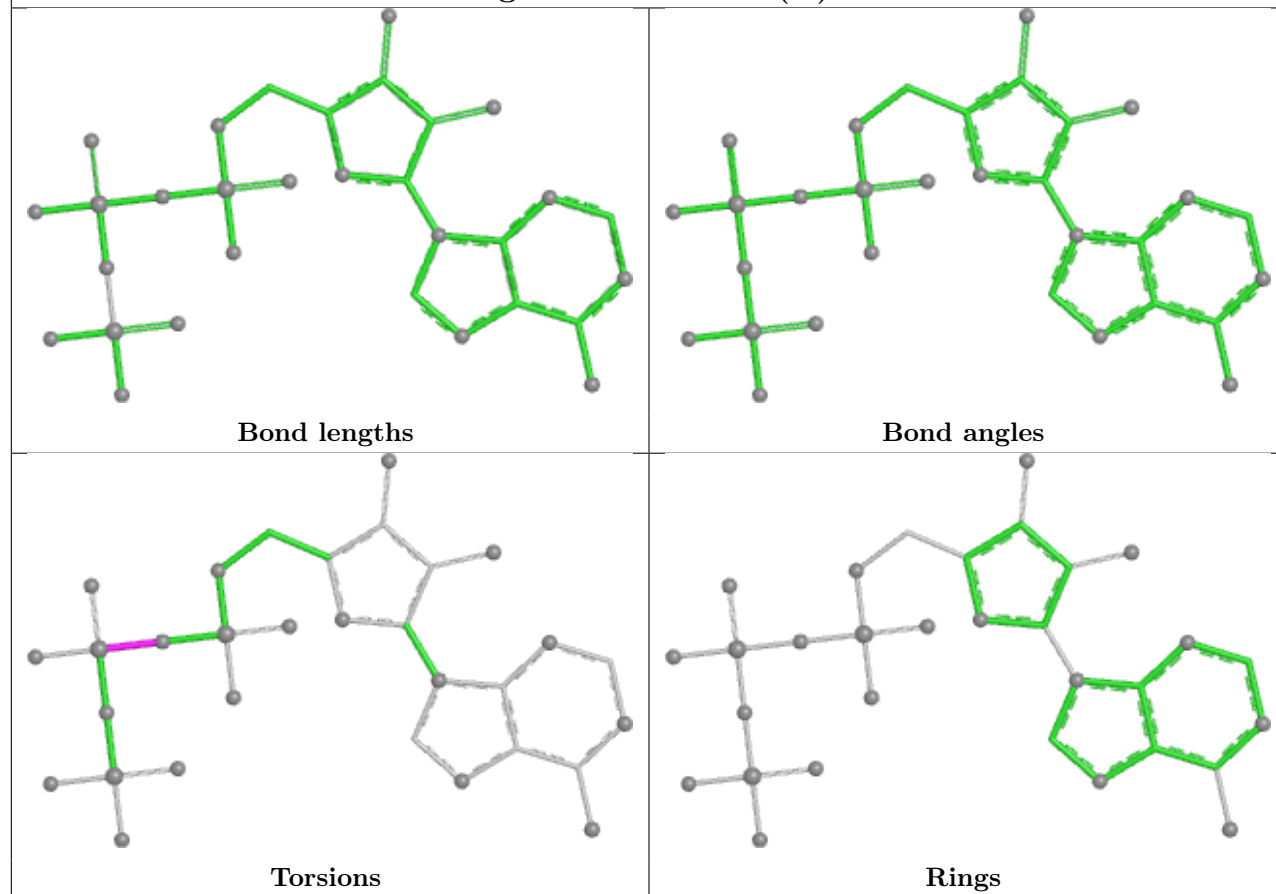
Ligand ATP K 501 (B)



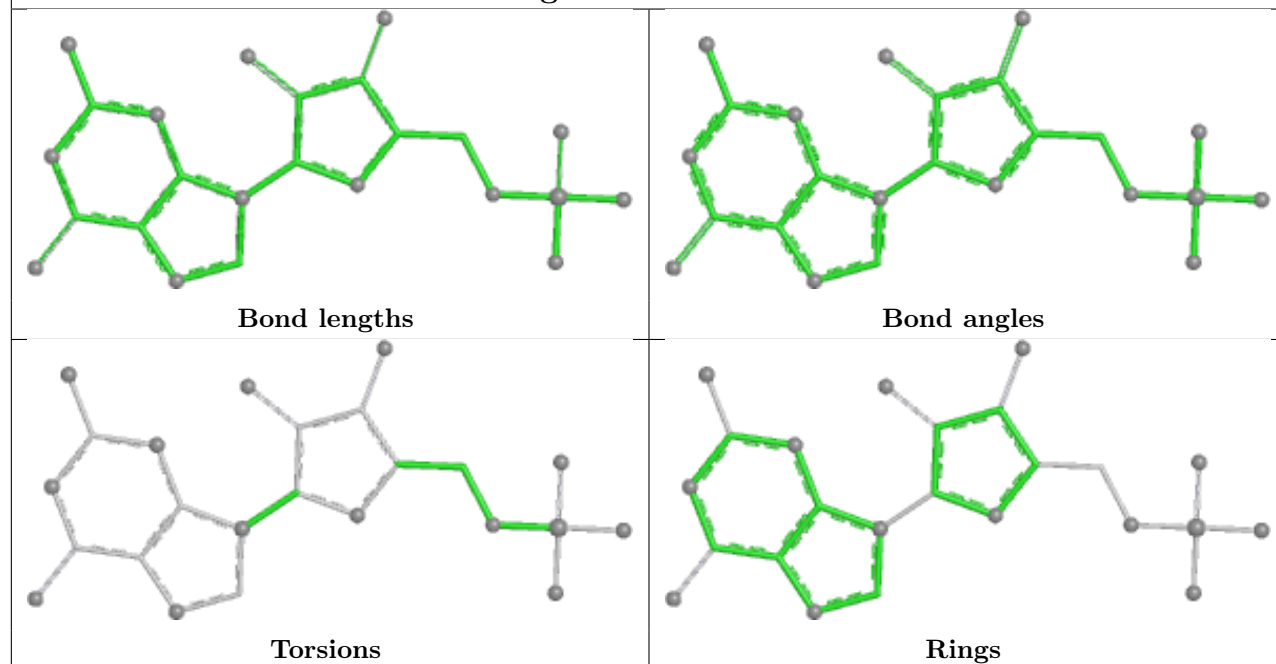
Ligand 5GP F 502



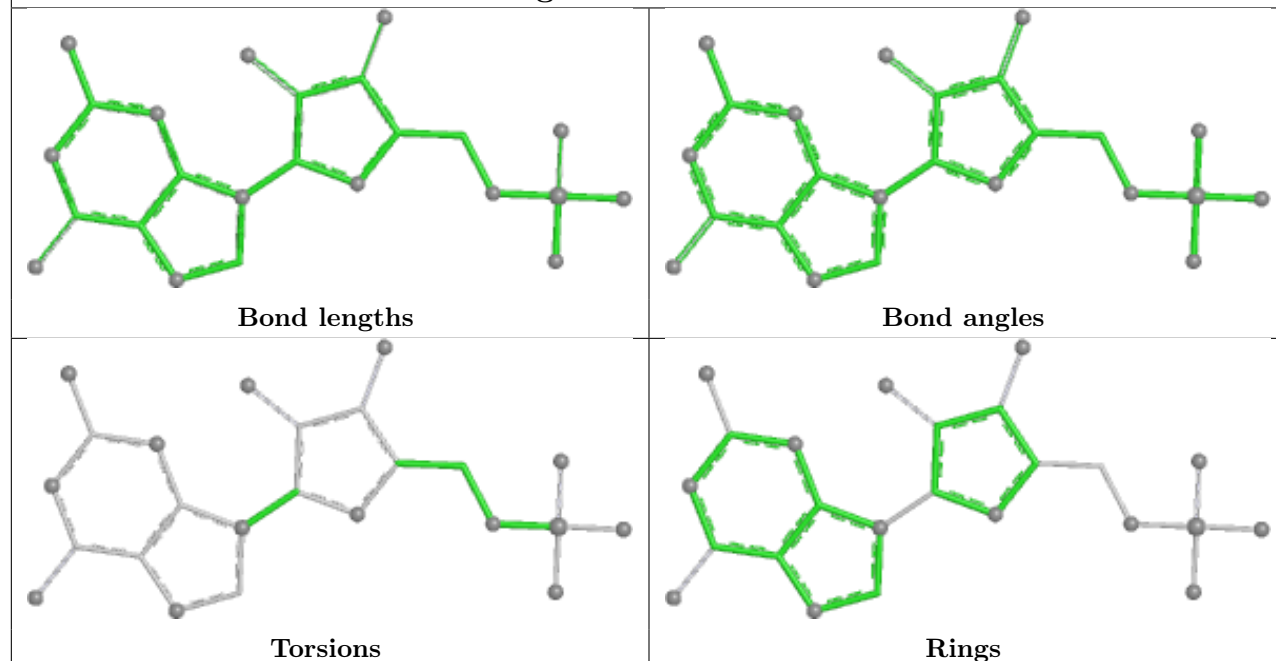
Ligand ATP O 502 (A)



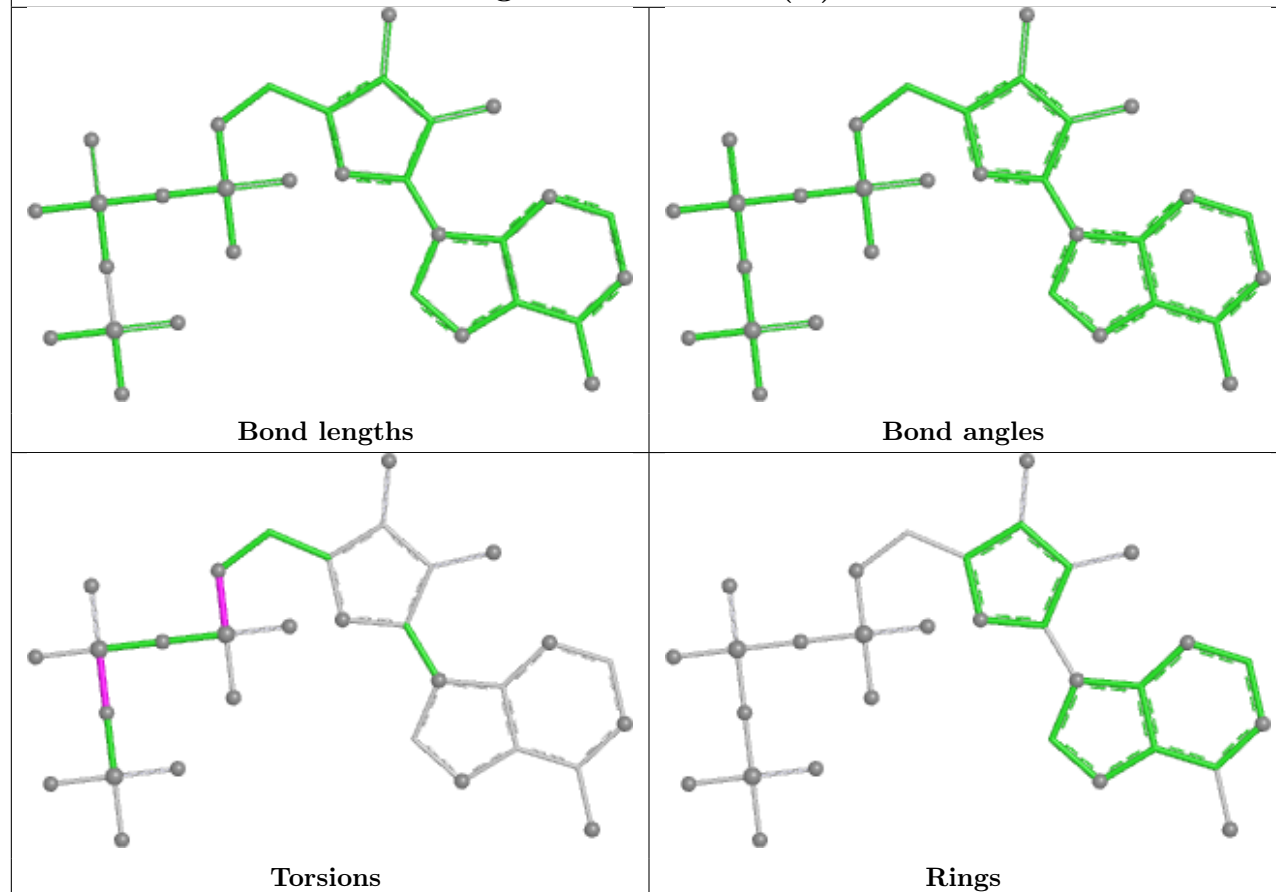
Ligand 5GP I 502



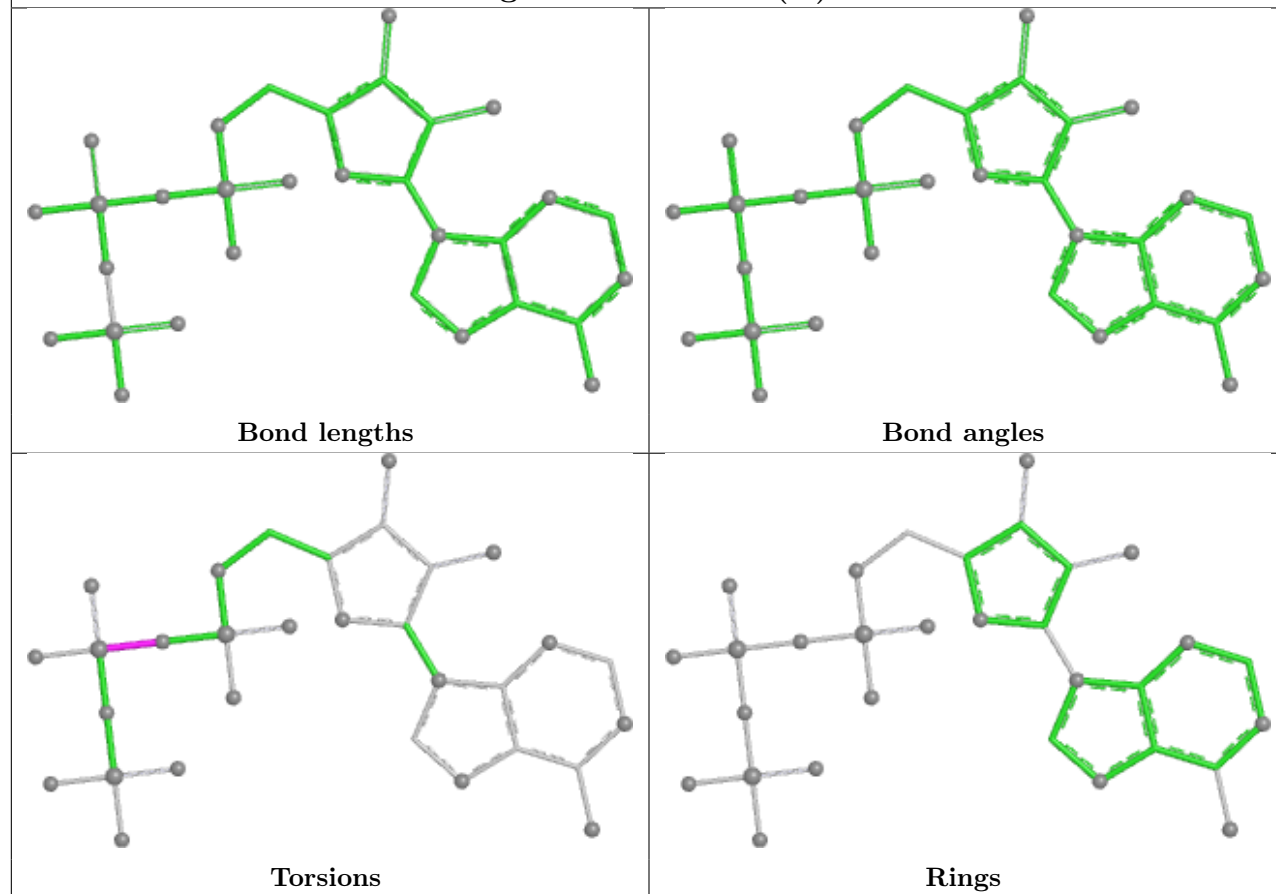
Ligand 5GP L 501



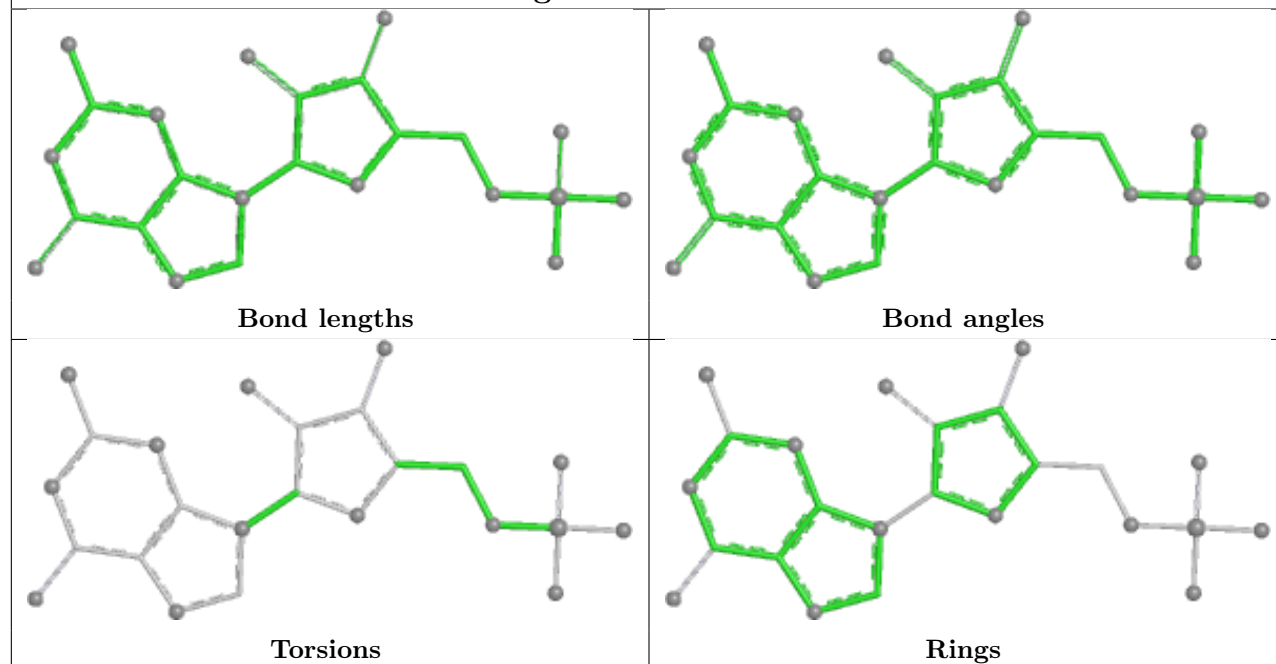
Ligand ATP M 502 (A)

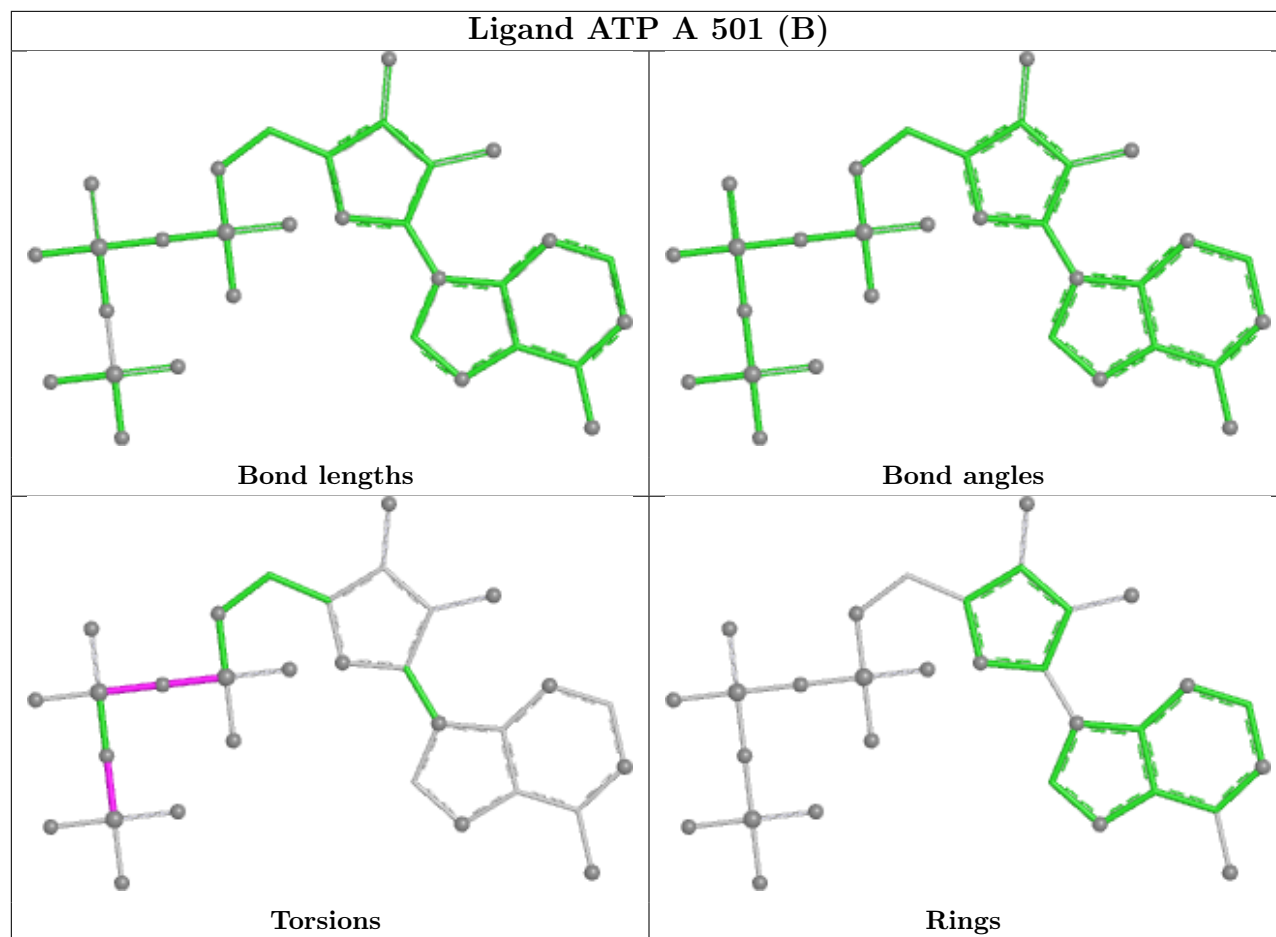


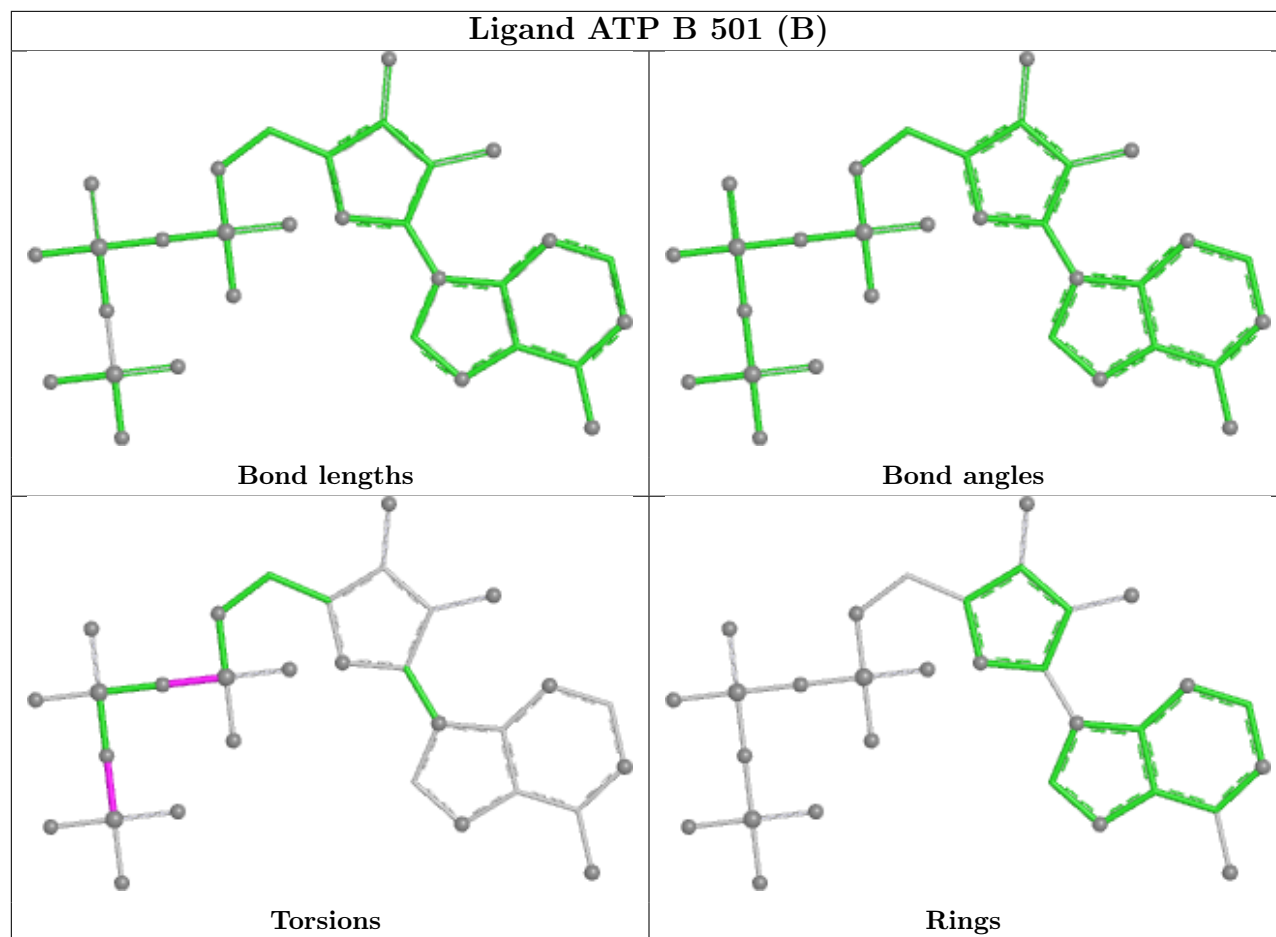
Ligand ATP P 502 (A)



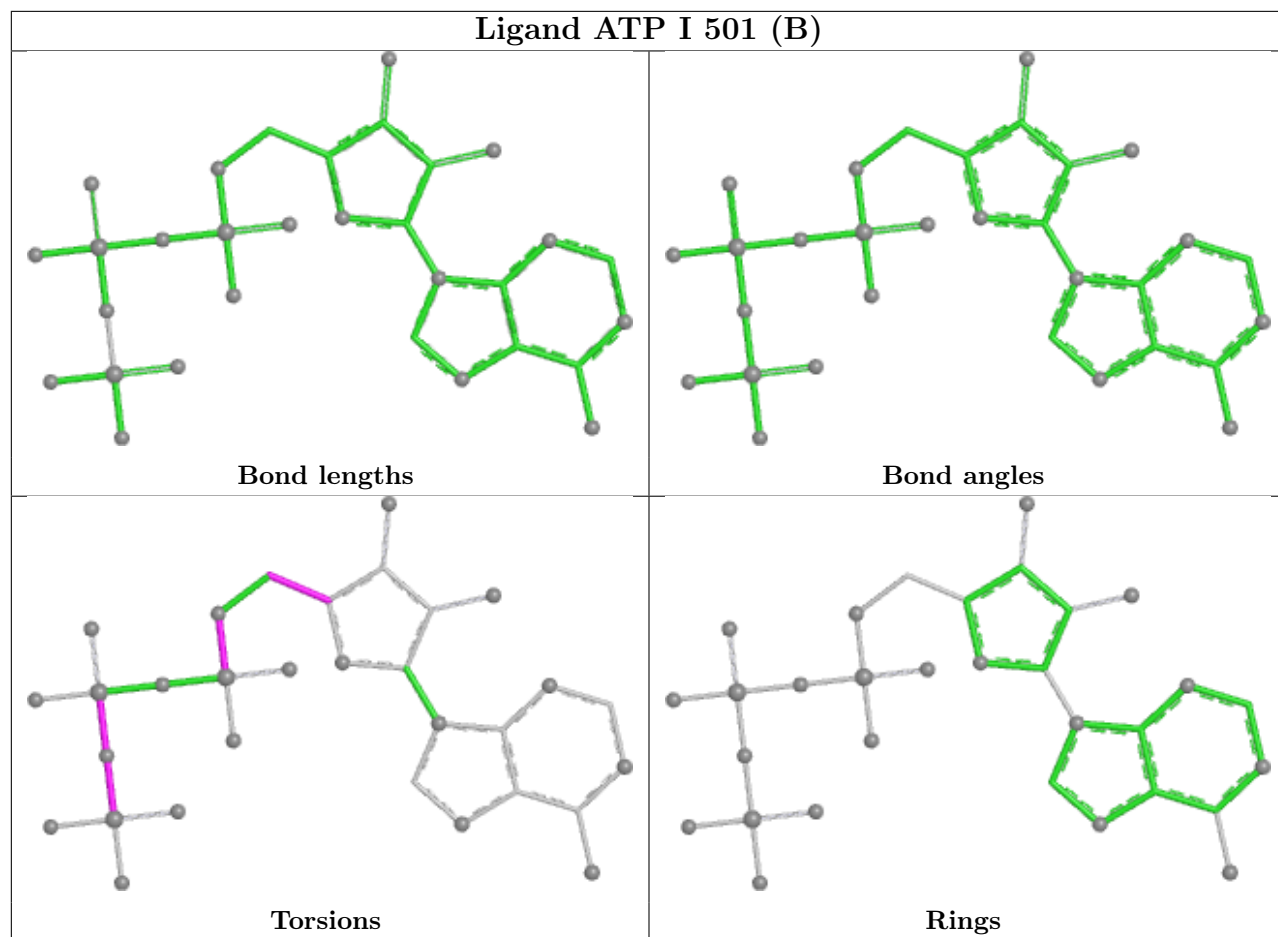
Ligand 5GP O 501



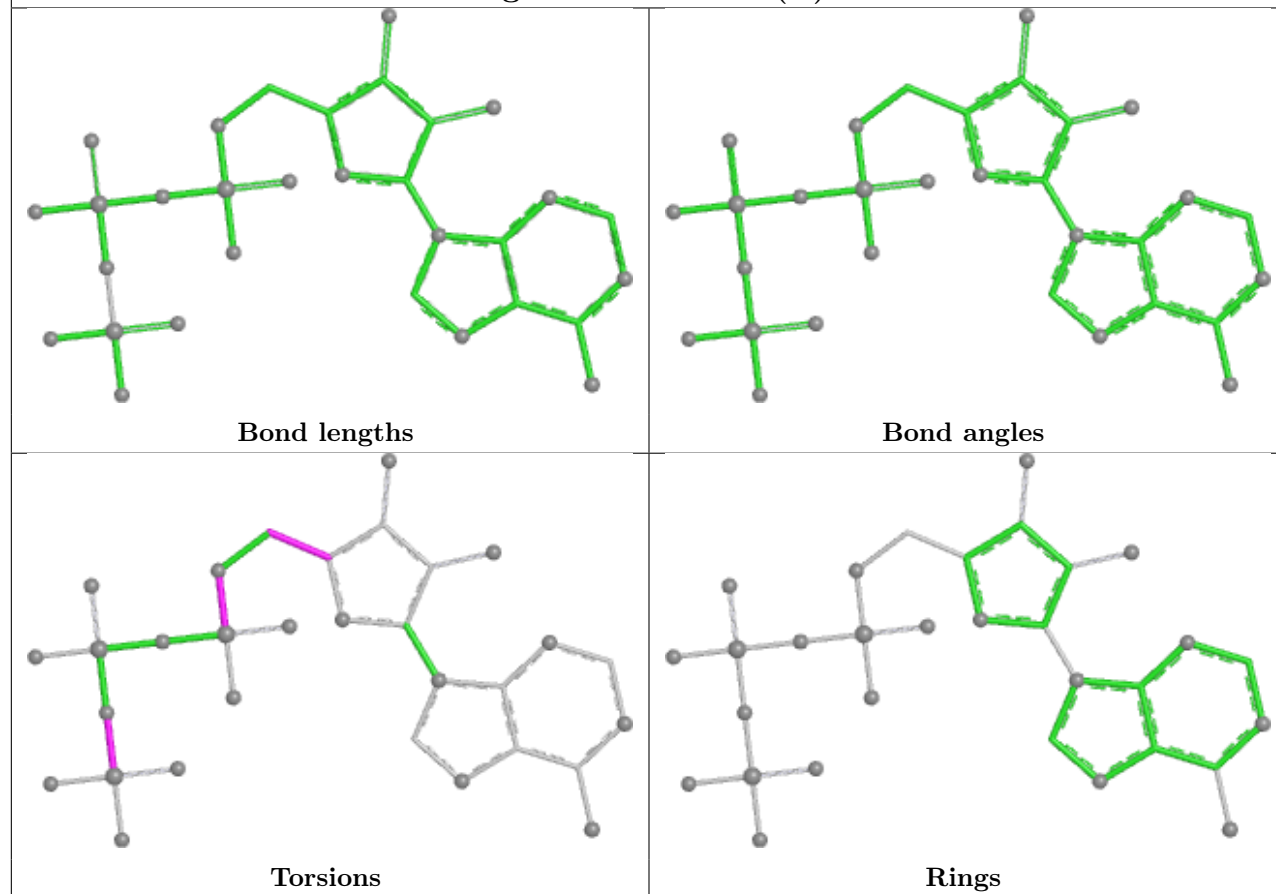




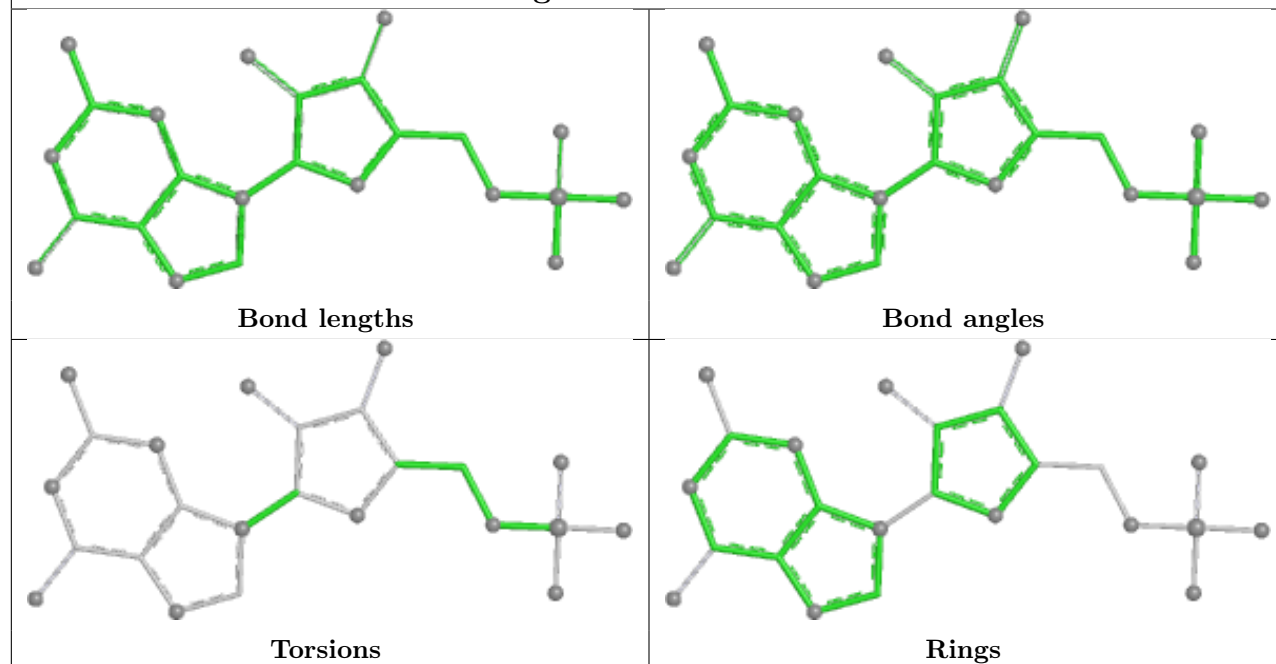
Ligand ATP I 501 (B)



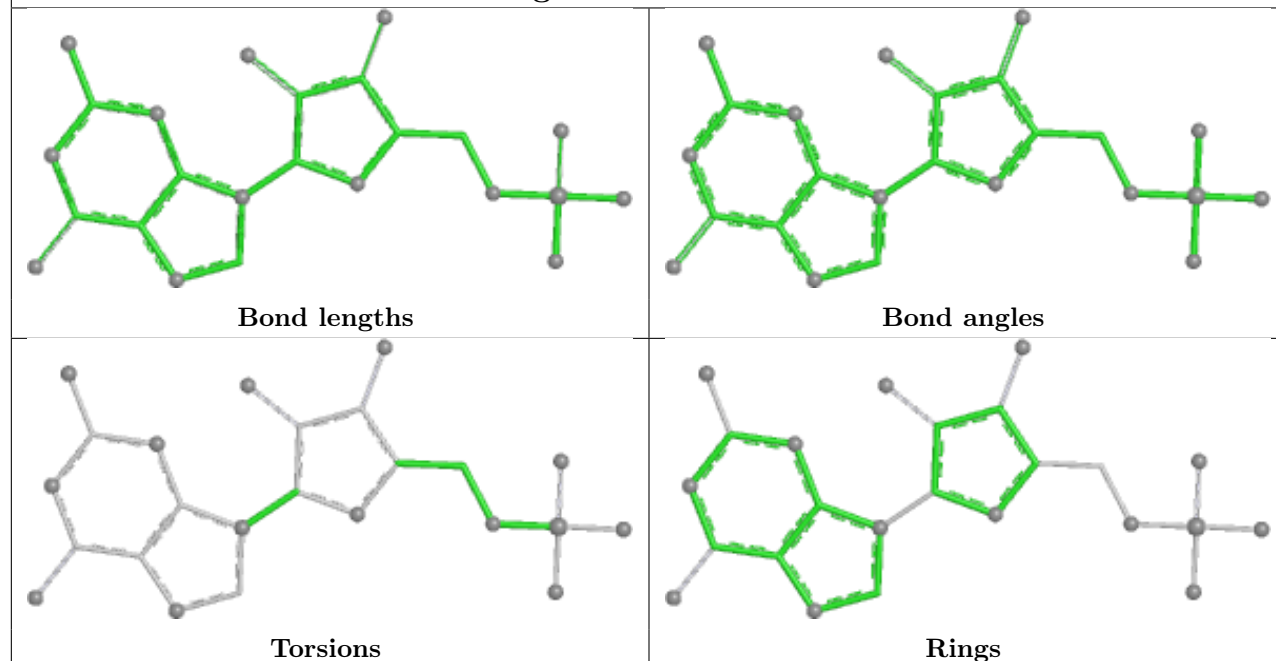
Ligand ATP L 502 (B)



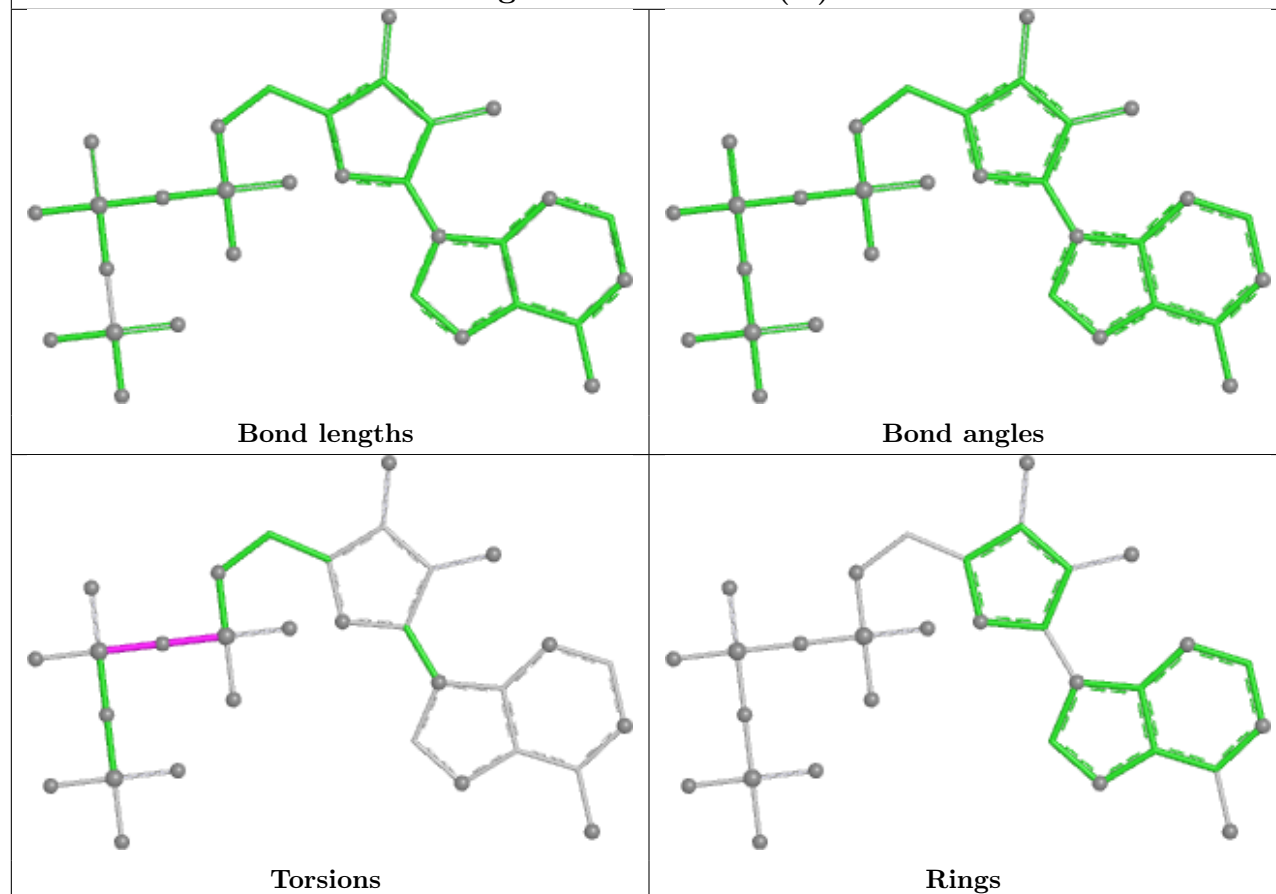
Ligand 5GP D 502

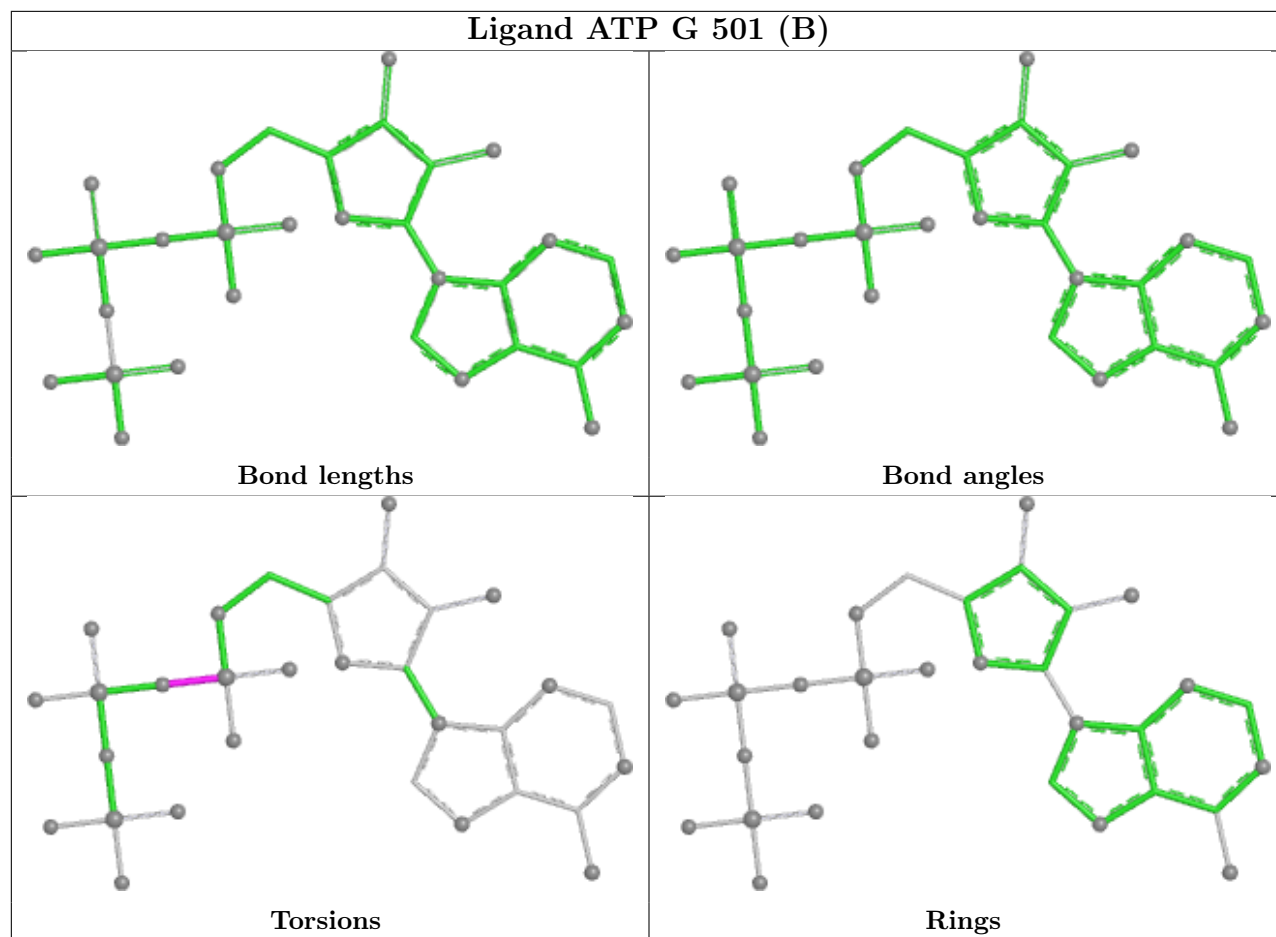


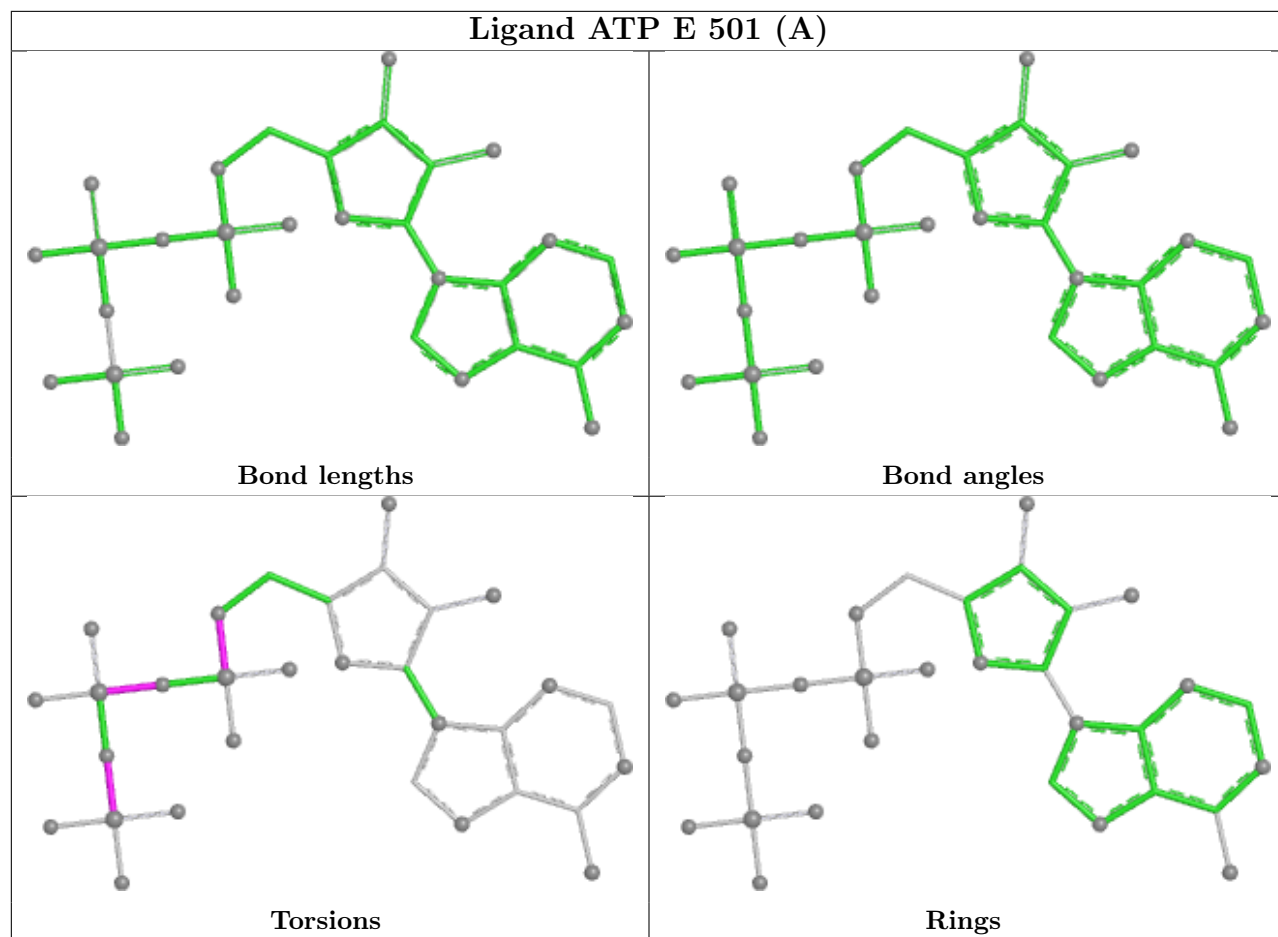
Ligand 5GP G 502



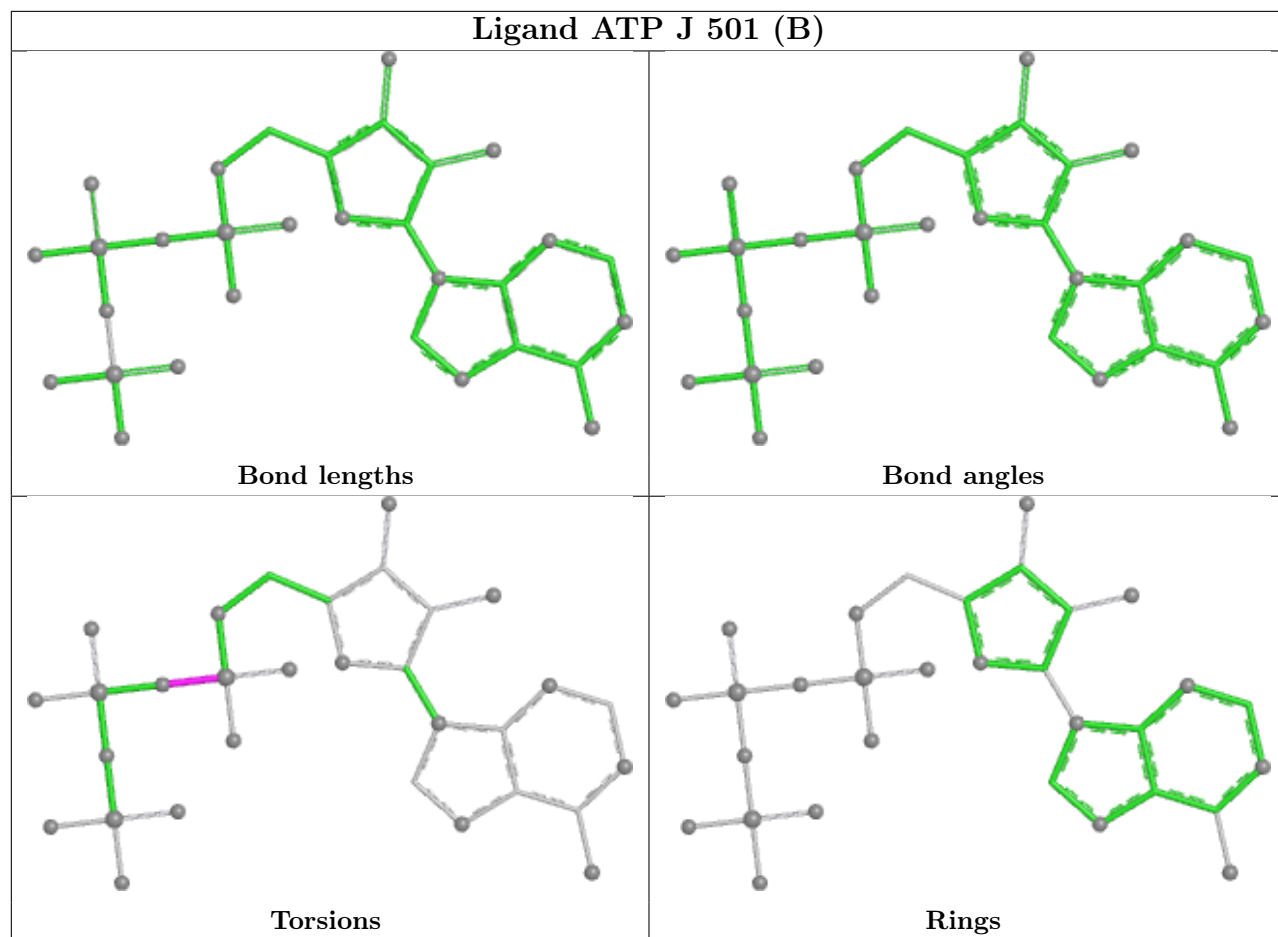
Ligand ATP K 501 (A)



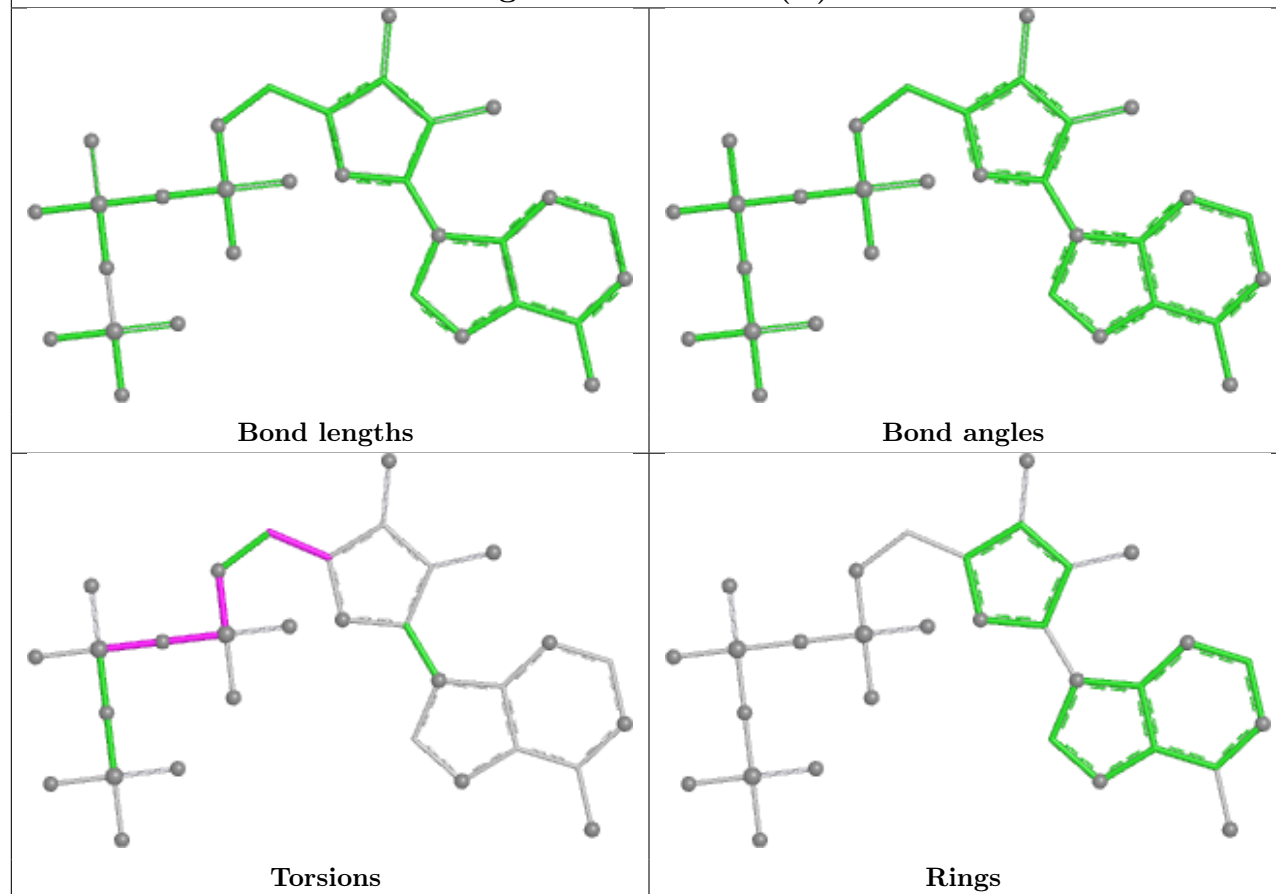




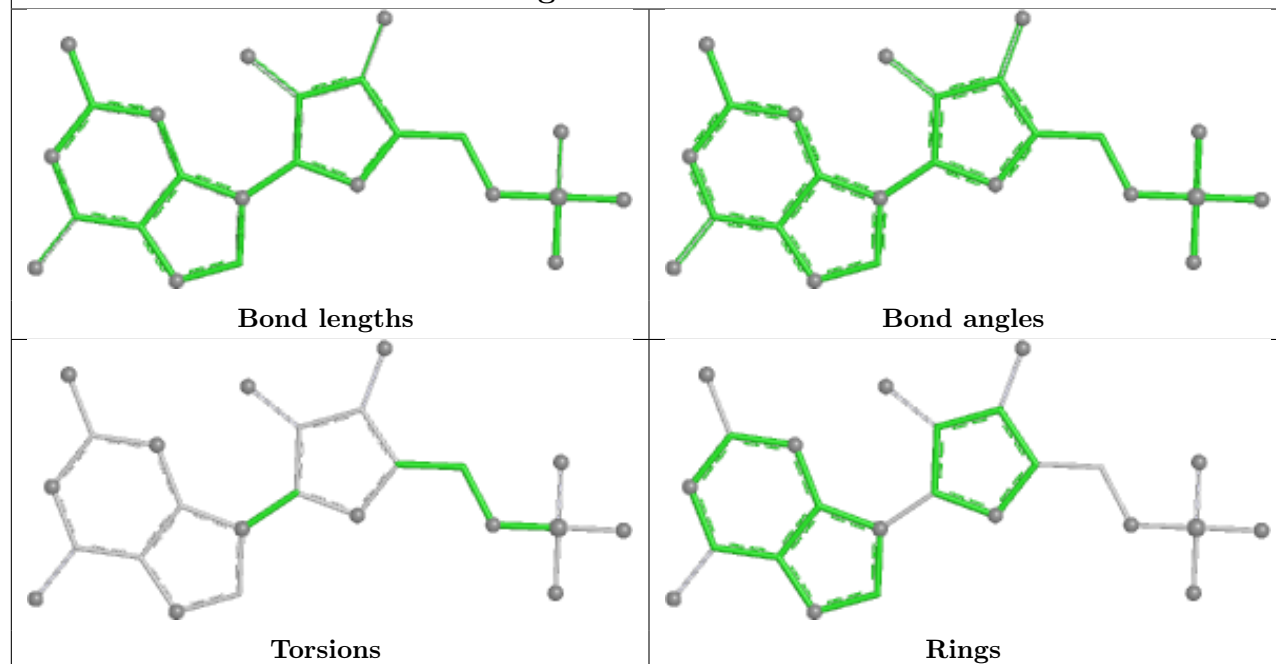
Ligand ATP J 501 (B)



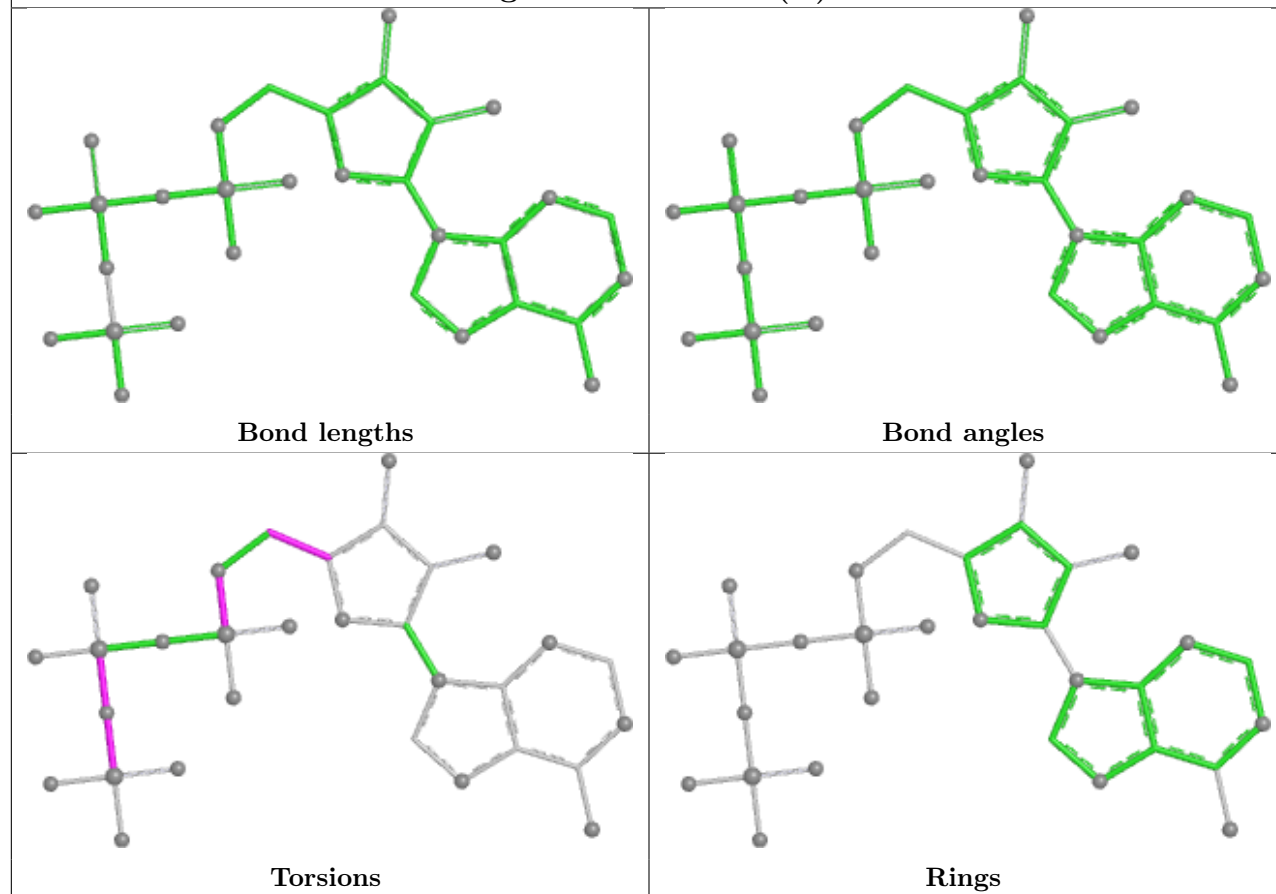
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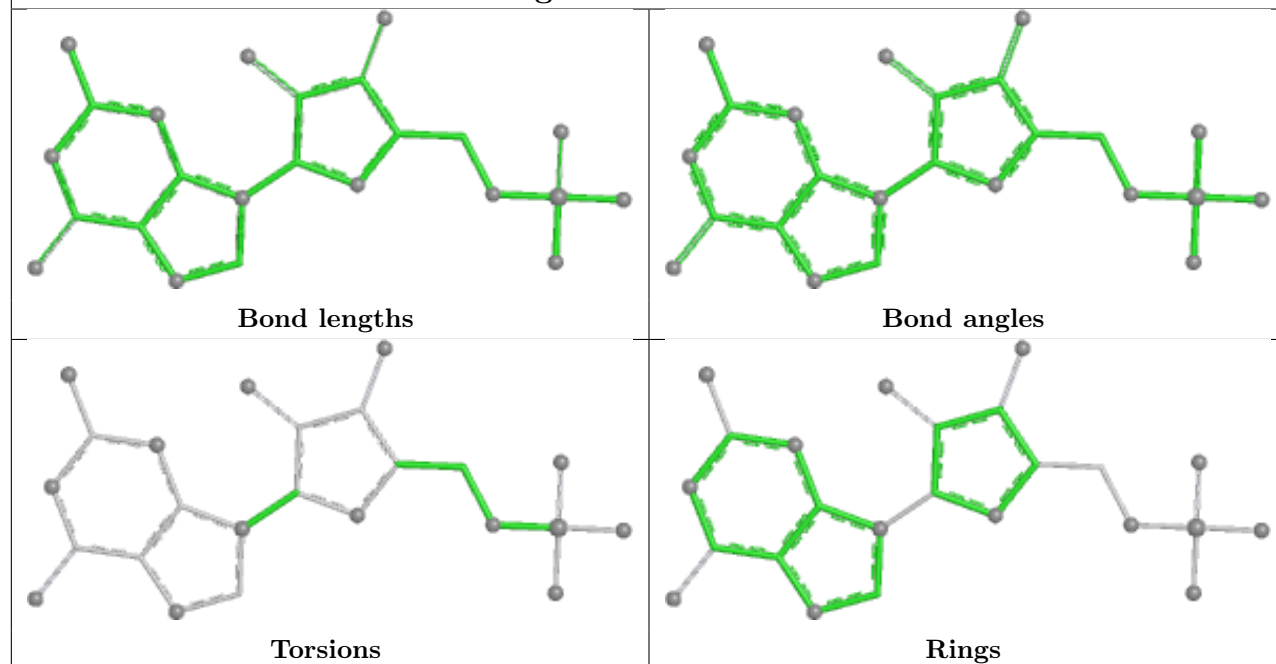
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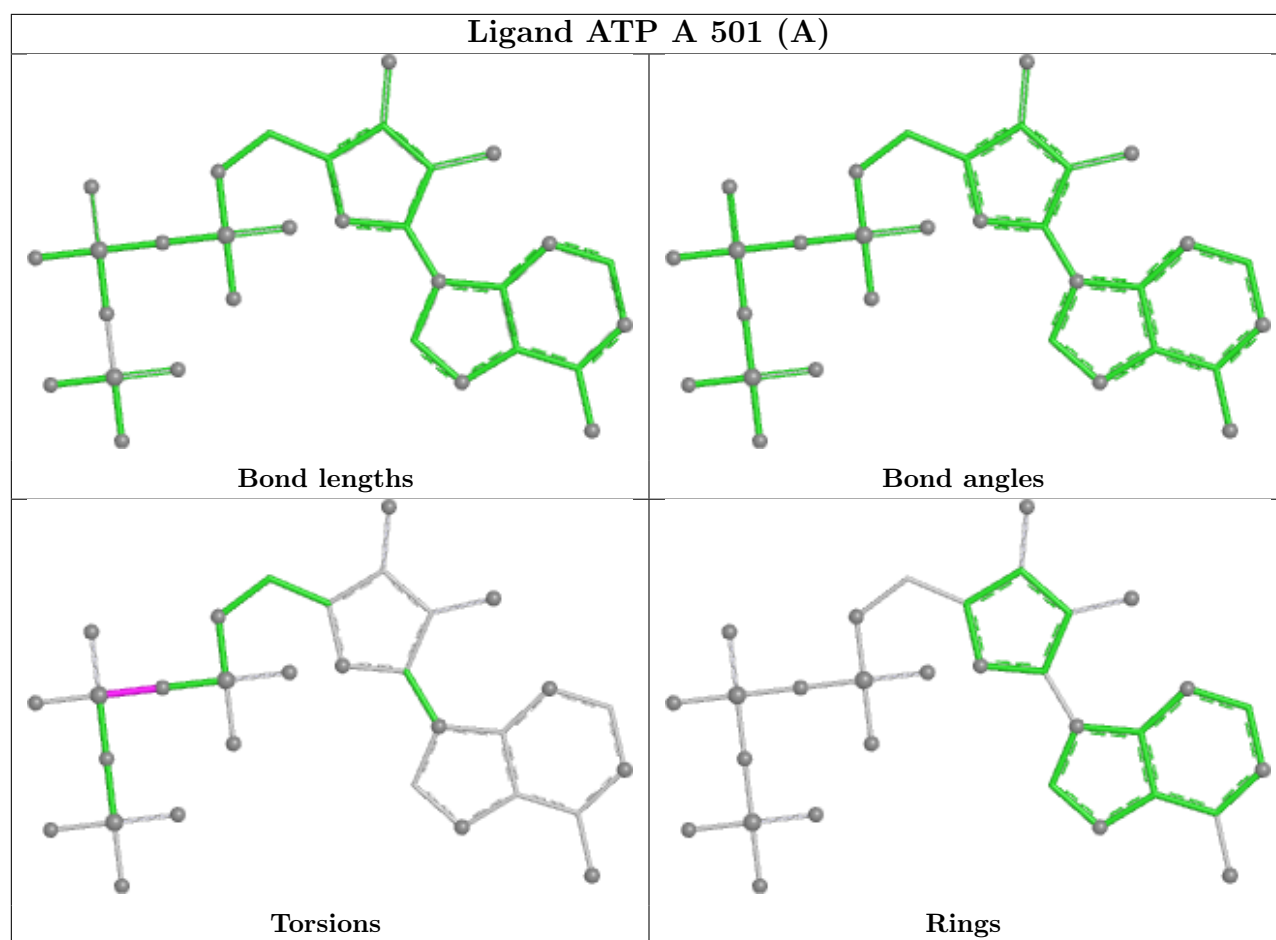


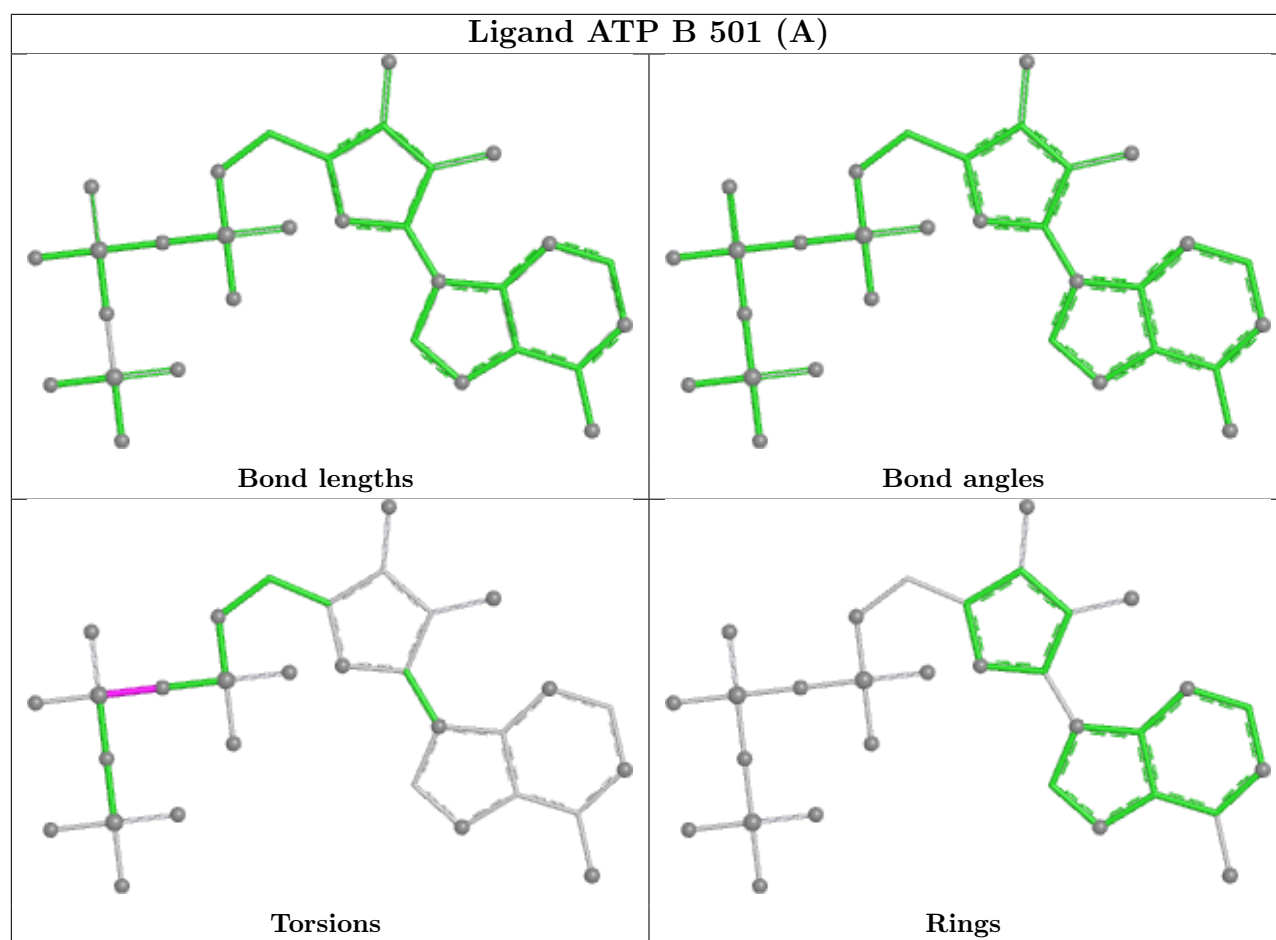
Ligand ATP C 501 (B)

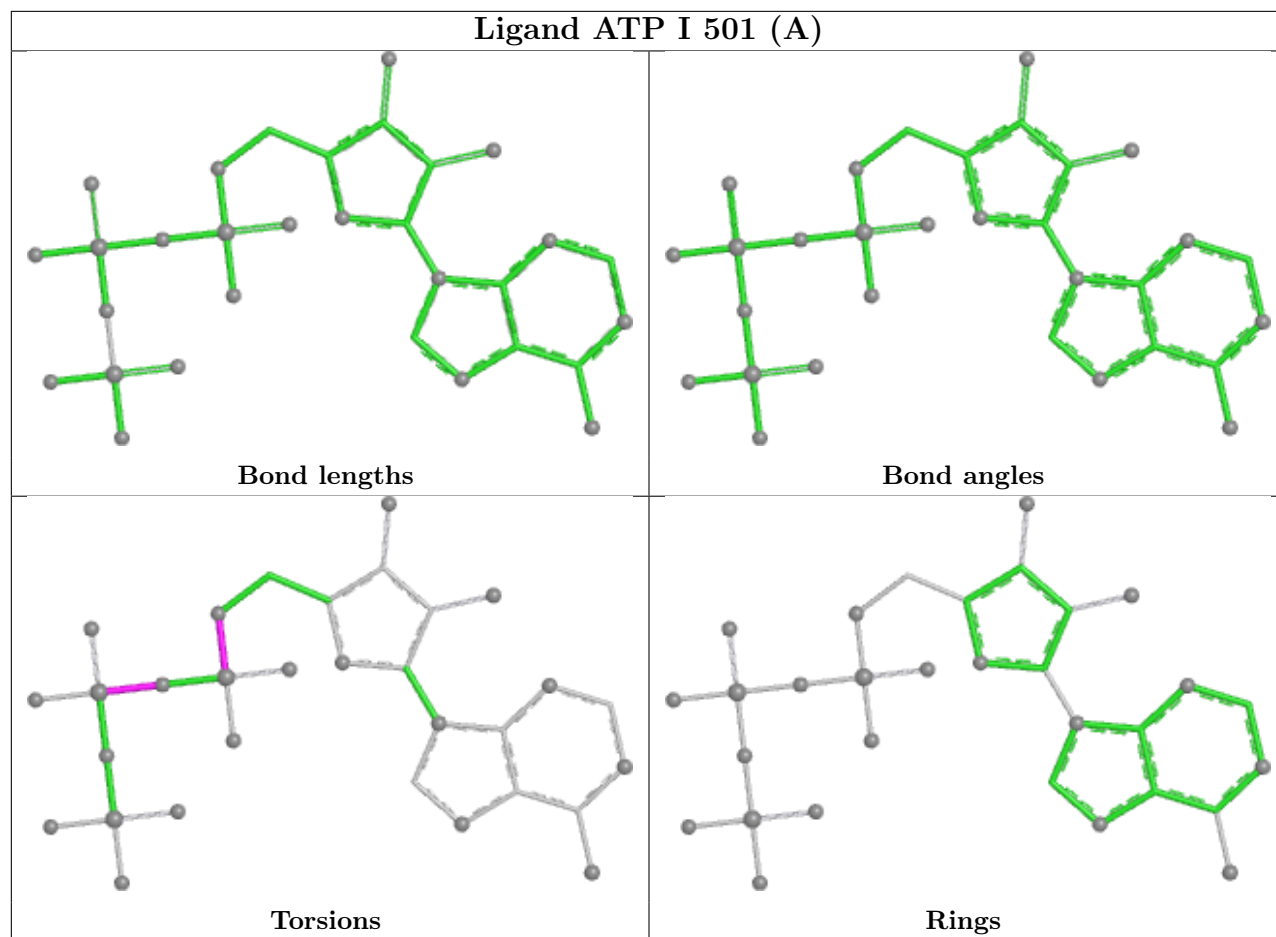


Ligand 5GP P 501

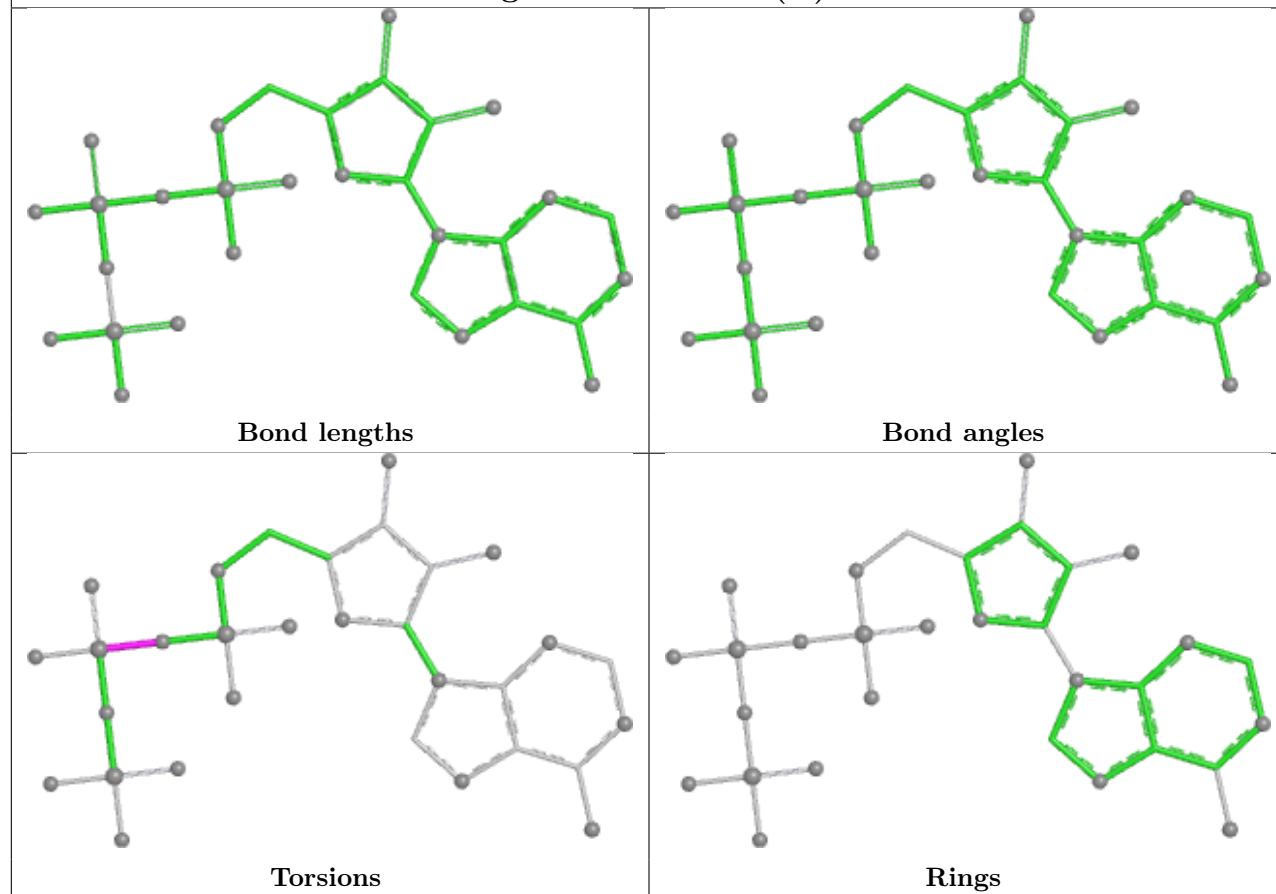




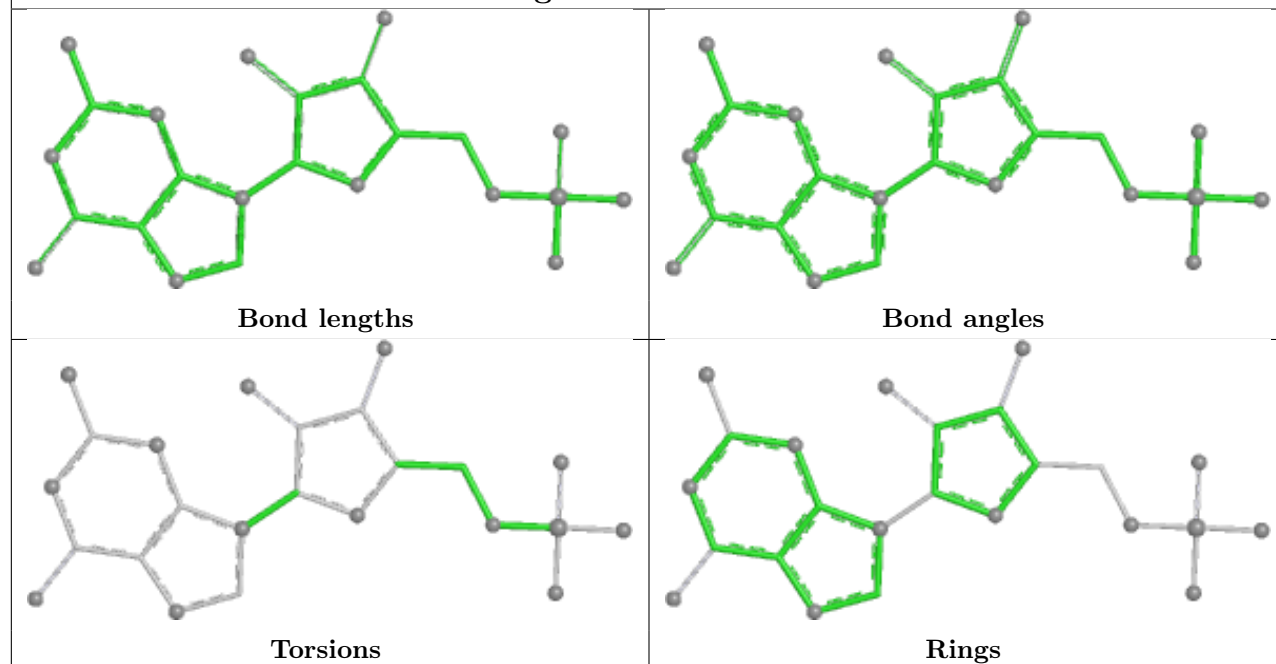




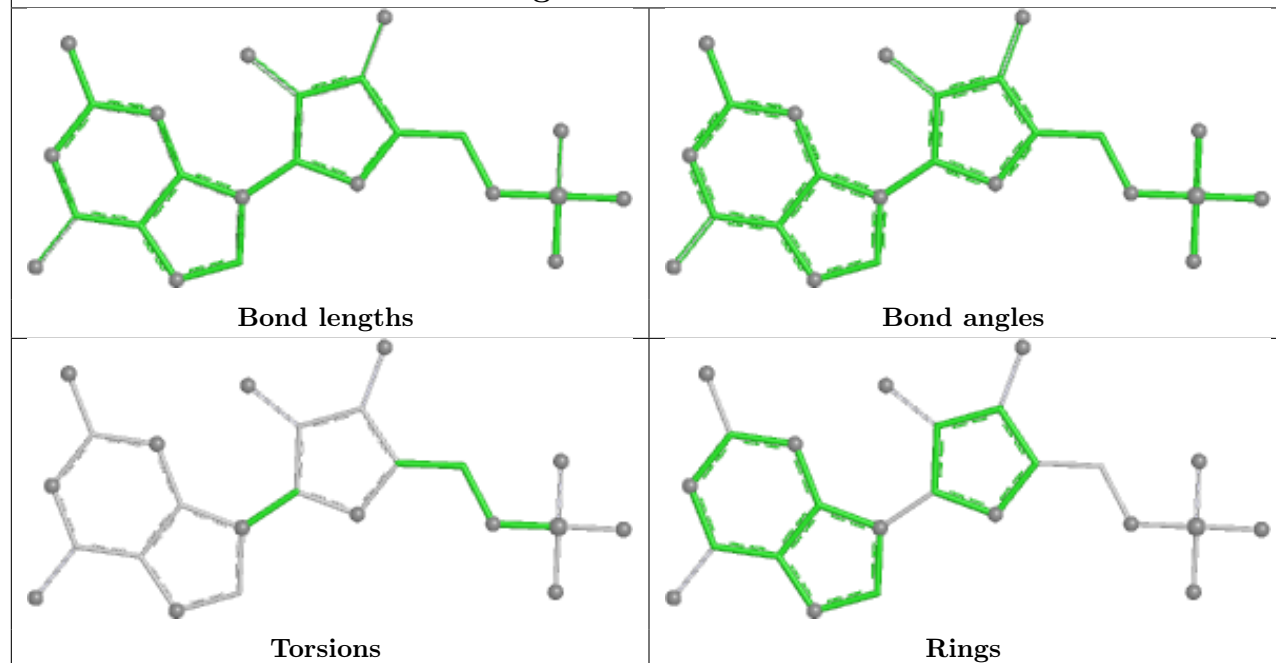
Ligand ATP L 502 (A)



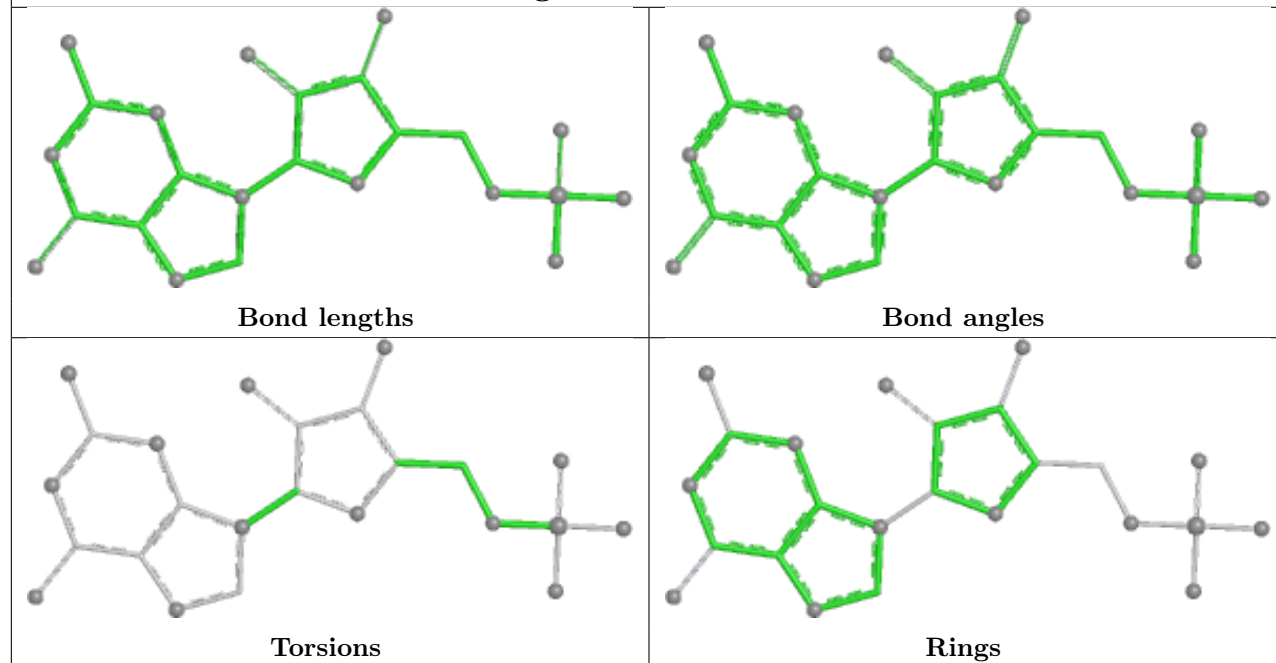
Ligand 5GP B 502

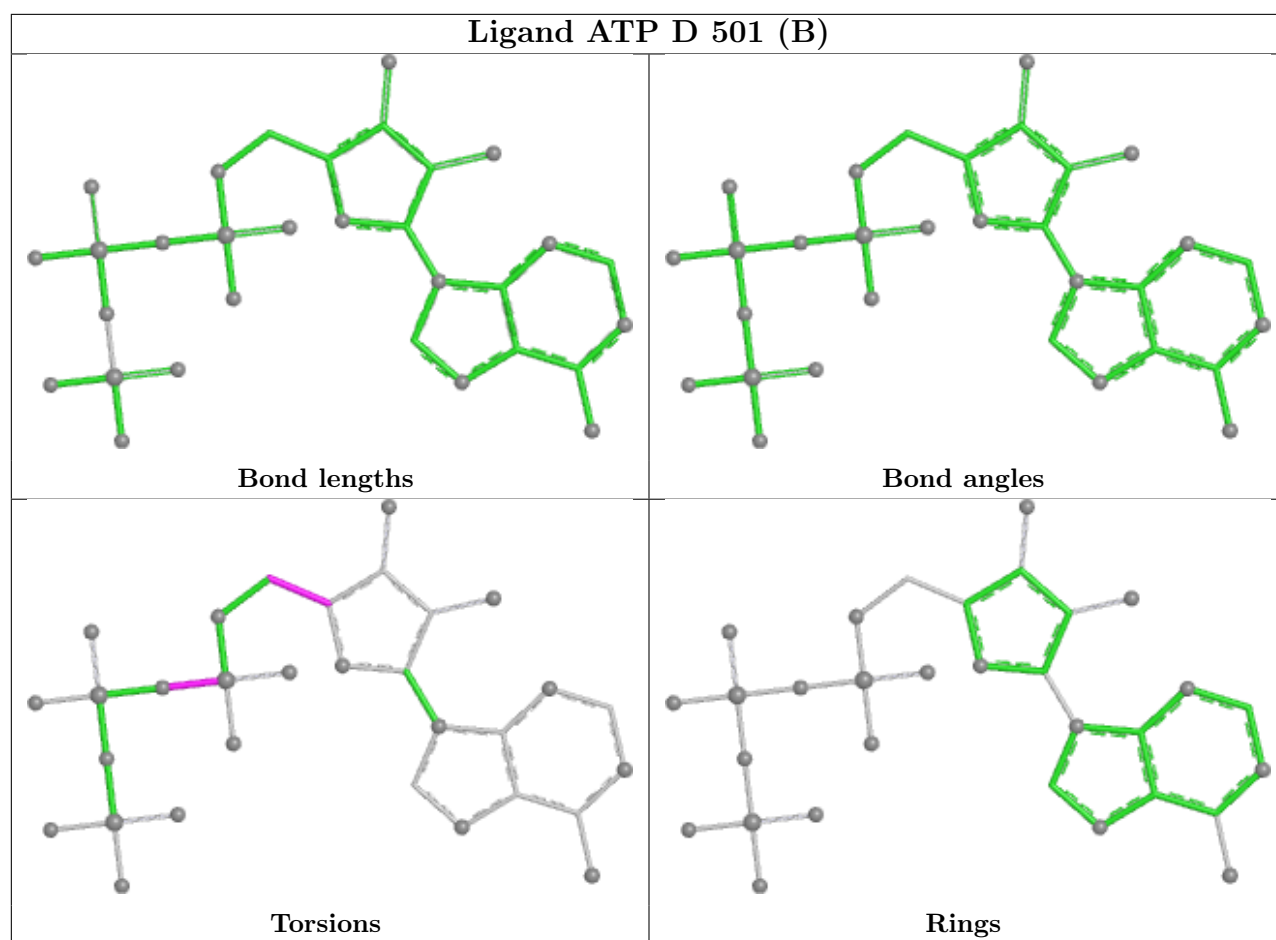


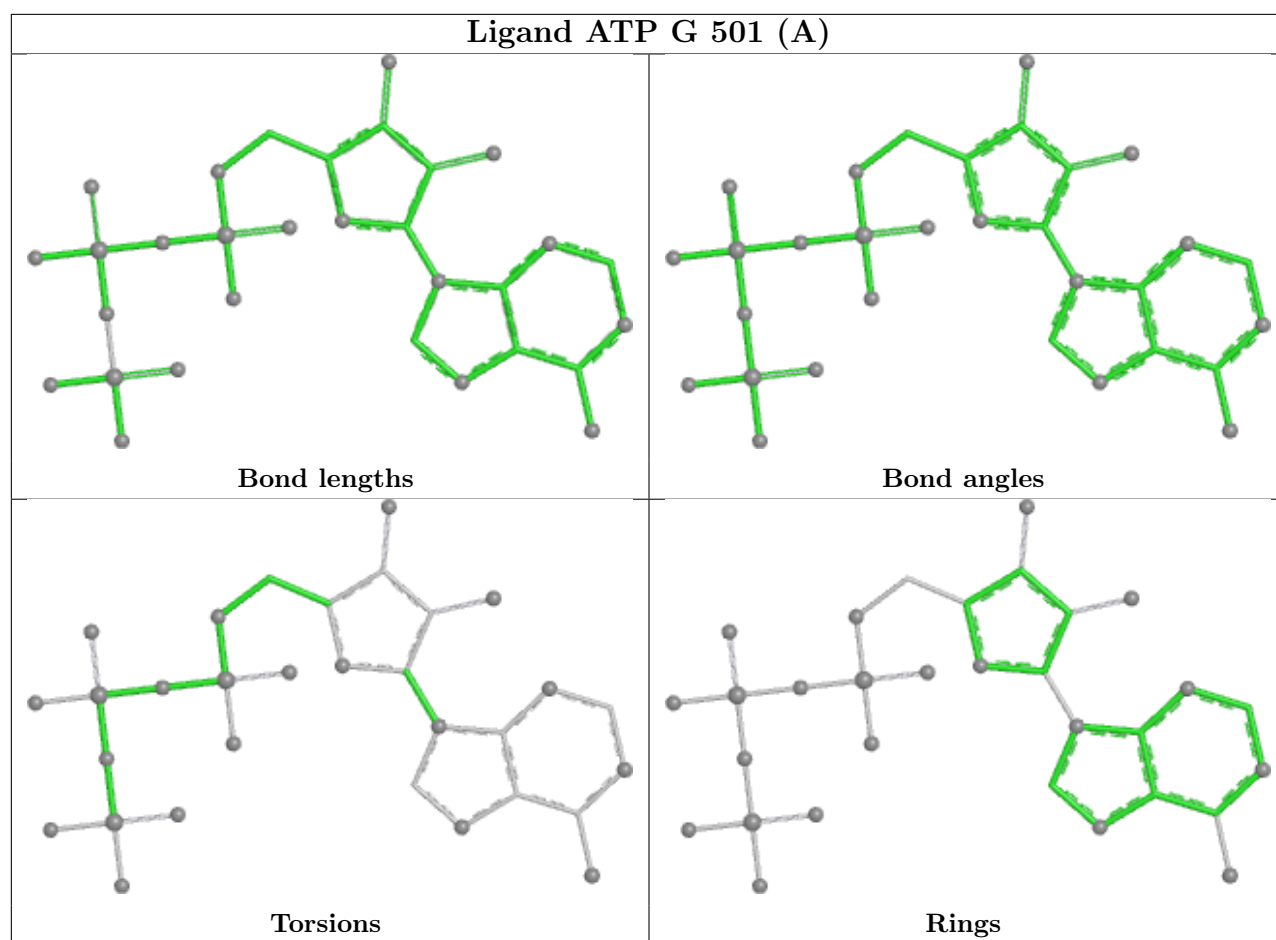
Ligand 5GP N 501



Ligand 5GP A 502







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, 95th 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	473/496 (95%)	0.12	12 (2%)	58	60	28, 43, 62, 82	1 (0%)
1	B	473/496 (95%)	0.18	12 (2%)	58	60	28, 46, 65, 94	1 (0%)
1	C	473/496 (95%)	0.31	17 (3%)	46	48	30, 49, 73, 95	1 (0%)
1	D	473/496 (95%)	0.41	21 (4%)	39	41	27, 51, 72, 105	1 (0%)
1	E	473/496 (95%)	0.12	19 (4%)	42	44	25, 43, 68, 100	1 (0%)
1	F	473/496 (95%)	0.06	15 (3%)	50	52	25, 42, 64, 104	1 (0%)
1	G	473/496 (95%)	0.10	12 (2%)	58	60	26, 41, 66, 91	1 (0%)
1	H	473/496 (95%)	0.10	13 (2%)	56	58	25, 41, 65, 96	1 (0%)
1	I	473/496 (95%)	0.19	18 (3%)	44	46	27, 45, 67, 96	1 (0%)
1	J	473/496 (95%)	0.29	17 (3%)	46	48	28, 48, 71, 103	1 (0%)
1	K	473/496 (95%)	0.14	16 (3%)	48	50	25, 43, 69, 106	1 (0%)
1	L	473/496 (95%)	0.11	19 (4%)	42	44	27, 41, 65, 101	1 (0%)
1	M	473/496 (95%)	0.34	17 (3%)	46	48	32, 50, 70, 107	1 (0%)
1	N	473/496 (95%)	0.33	12 (2%)	58	60	30, 51, 72, 101	1 (0%)
1	O	473/496 (95%)	0.42	17 (3%)	46	48	31, 52, 75, 106	1 (0%)
1	P	473/496 (95%)	0.44	23 (4%)	35	36	30, 52, 73, 99	1 (0%)
All	All	7568/7936 (95%)	0.23	260 (3%)	48	50	25, 47, 70, 107	16 (0%)

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	468	GLY	5.9
1	K	469	PHE	5.9
1	C	469	PHE	5.8
1	D	469	PHE	5.4
1	J	469	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	N	469	PHE	5.1
1	B	469	PHE	4.9
1	H	469	PHE	4.8
1	P	469	PHE	4.8
1	L	474	PRO	4.6
1	E	398	ALA	4.3
1	B	399	GLY	4.3
1	O	469	PHE	4.3
1	N	470	ALA	4.3
1	L	299	PRO	4.2
1	L	469	PHE	4.2
1	H	470	ALA	4.2
1	O	470	ALA	4.2
1	O	468	GLY	4.1
1	M	469	PHE	4.1
1	F	398	ALA	4.0
1	K	398	ALA	4.0
1	J	470	ALA	4.0
1	A	469	PHE	4.0
1	H	426	ARG	3.9
1	O	474	PRO	3.9
1	D	468	GLY	3.9
1	I	398	ALA	3.9
1	K	474	PRO	3.8
1	P	474	PRO	3.8
1	P	468	GLY	3.8
1	E	395	ALA	3.8
1	J	113	ASN	3.8
1	L	468	GLY	3.8
1	D	398	ALA	3.7
1	K	470	ALA	3.7
1	D	426	ARG	3.7
1	M	299	PRO	3.7
1	E	469	PHE	3.7
1	D	187	PRO	3.6
1	J	474	PRO	3.6
1	K	299	PRO	3.6
1	D	470	ALA	3.6
1	P	2	VAL	3.5
1	J	468	GLY	3.5
1	N	474	PRO	3.5
1	M	474	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	470	ALA	3.4
1	F	469	PHE	3.4
1	I	469	PHE	3.4
1	D	299	PRO	3.4
1	M	398	ALA	3.4
1	A	468	GLY	3.4
1	C	474	PRO	3.4
1	F	468	GLY	3.4
1	P	299	PRO	3.4
1	B	426	ARG	3.4
1	A	300	GLY	3.4
1	M	300	GLY	3.3
1	D	300	GLY	3.3
1	E	399	GLY	3.3
1	G	128	PHE	3.3
1	I	468	GLY	3.3
1	M	468	GLY	3.3
1	M	113	ASN	3.3
1	P	470	ALA	3.2
1	I	300	GLY	3.2
1	P	376	ARG	3.2
1	C	470	ALA	3.2
1	B	113	ASN	3.2
1	H	473	HIS	3.2
1	B	398	ALA	3.2
1	N	399	GLY	3.2
1	G	468	GLY	3.1
1	K	395	ALA	3.1
1	N	398	ALA	3.1
1	B	474	PRO	3.1
1	B	470	ALA	3.1
1	G	395	ALA	3.1
1	O	301	ALA	3.1
1	B	468	GLY	3.1
1	F	113	ASN	3.1
1	L	470	ALA	3.1
1	E	303	CYS	3.0
1	N	395	ALA	3.0
1	I	474	PRO	3.0
1	E	468	GLY	3.0
1	J	398	ALA	2.9
1	D	395	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	395	ALA	2.9
1	C	468	GLY	2.9
1	A	474	PRO	2.9
1	P	426	ARG	2.9
1	G	469	PHE	2.9
1	M	470	ALA	2.9
1	I	113	ASN	2.8
1	H	474	PRO	2.8
1	G	129	GLU	2.8
1	I	303	CYS	2.8
1	A	470	ALA	2.8
1	O	399	GLY	2.7
1	J	471	GLU	2.7
1	O	466	ALA	2.7
1	P	466	ALA	2.7
1	O	113	ASN	2.7
1	D	474	PRO	2.7
1	F	299	PRO	2.7
1	C	467	ALA	2.7
1	H	128	PHE	2.7
1	D	303	CYS	2.7
1	D	467	ALA	2.6
1	E	301	ALA	2.6
1	J	303	CYS	2.6
1	P	29	ALA	2.6
1	N	300	GLY	2.6
1	C	466	ALA	2.6
1	I	470	ALA	2.6
1	E	426	ARG	2.6
1	J	426	ARG	2.6
1	J	401	SER	2.6
1	D	405	ARG	2.6
1	A	425	ALA	2.6
1	D	402	SER	2.6
1	J	473	HIS	2.6
1	A	426	ARG	2.5
1	K	301	ALA	2.5
1	A	299	PRO	2.5
1	N	143	GLY	2.5
1	P	473	HIS	2.5
1	C	471	GLU	2.5
1	K	426	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	425	ALA	2.5
1	L	425	ALA	2.5
1	C	187	PRO	2.5
1	I	299	PRO	2.5
1	A	466	ALA	2.5
1	D	425	ALA	2.5
1	J	29	ALA	2.5
1	L	404	ASP	2.5
1	L	467	ALA	2.5
1	P	425	ALA	2.5
1	E	474	PRO	2.5
1	G	474	PRO	2.5
1	F	376	ARG	2.5
1	G	396	ARG	2.5
1	E	470	ALA	2.5
1	O	221	ALA	2.5
1	O	473	HIS	2.5
1	J	299	PRO	2.5
1	H	471	GLU	2.4
1	I	397	THR	2.4
1	I	395	ALA	2.4
1	J	376	ARG	2.4
1	L	426	ARG	2.4
1	F	303	CYS	2.4
1	C	128	PHE	2.4
1	D	2	VAL	2.4
1	H	400	ASP	2.4
1	N	187	PRO	2.4
1	O	467	ALA	2.4
1	P	300	GLY	2.4
1	E	473	HIS	2.4
1	B	376	ARG	2.4
1	L	374	PHE	2.4
1	I	396	ARG	2.4
1	K	473	HIS	2.4
1	K	113	ASN	2.3
1	E	299	PRO	2.3
1	H	29	ALA	2.3
1	H	466	ALA	2.3
1	H	468	GLY	2.3
1	E	425	ALA	2.3
1	O	29	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	426	ARG	2.3
1	L	424	PRO	2.3
1	I	399	GLY	2.3
1	H	398	ALA	2.3
1	N	426	ARG	2.3
1	P	402	SER	2.3
1	P	128	PHE	2.3
1	M	303	CYS	2.3
1	F	474	PRO	2.3
1	M	426	ARG	2.3
1	N	467	ALA	2.3
1	C	143	GLY	2.2
1	E	379	ARG	2.2
1	J	467	ALA	2.2
1	K	467	ALA	2.2
1	L	395	ALA	2.2
1	G	426	ARG	2.2
1	L	303	CYS	2.2
1	C	300	GLY	2.2
1	I	466	ALA	2.2
1	F	426	ARG	2.2
1	B	312	GLY	2.2
1	J	472	GLY	2.2
1	K	117	HIS	2.2
1	F	397	THR	2.2
1	F	401	SER	2.2
1	E	113	ASN	2.2
1	P	424	PRO	2.2
1	I	298	GLY	2.2
1	O	143	GLY	2.2
1	P	467	ALA	2.2
1	B	3	ARG	2.1
1	M	385	TYR	2.1
1	E	378	ASP	2.1
1	L	378	ASP	2.1
1	N	113	ASN	2.1
1	D	471	GLU	2.1
1	P	374	PHE	2.1
1	C	473	HIS	2.1
1	K	399	GLY	2.1
1	D	301	ALA	2.1
1	D	466	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	470	ALA	2.1
1	C	426	ARG	2.1
1	G	152	ASP	2.1
1	O	457[A]	GLU	2.1
1	D	397	THR	2.1
1	F	29	ALA	2.1
1	L	418	SER	2.1
1	M	301	ALA	2.1
1	O	378	ASP	2.1
1	A	473	HIS	2.1
1	L	473	HIS	2.1
1	D	424	PRO	2.1
1	P	130	GLY	2.1
1	E	376	ARG	2.1
1	I	405	ARG	2.1
1	B	397	THR	2.1
1	C	303	CYS	2.1
1	K	303	CYS	2.1
1	L	402	SER	2.1
1	A	398	ALA	2.1
1	C	29	ALA	2.1
1	E	29	ALA	2.1
1	M	394	ALA	2.1
1	M	466	ALA	2.1
1	P	301	ALA	2.1
1	P	471	GLU	2.1
1	G	155	LEU	2.1
1	M	473	HIS	2.1
1	M	424	PRO	2.1
1	P	380	PRO	2.1
1	F	2	VAL	2.1
1	C	164	GLY	2.1
1	I	128	PHE	2.1
1	O	300	GLY	2.1
1	A	467	ALA	2.0
1	P	395	ALA	2.0
1	K	405	ARG	2.0
1	M	405	ARG	2.0
1	G	330	GLY	2.0
1	J	399	GLY	2.0
1	L	300	GLY	2.0
1	F	425	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	113	ASN	2.0
1	E	396	ARG	2.0
1	L	408	LYS	2.0

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 oligosaccharides 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, 95th 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
2	ATP	D	501[A]	31/31	0.78	0.11	48,49,54,56	31
2	ATP	D	501[B]	31/31	0.78	0.11	48,49,55,58	31
2	ATP	E	501[A]	31/31	0.84	0.11	42,45,50,54	31
2	ATP	E	501[B]	31/31	0.84	0.11	42,44,49,51	31
2	ATP	K	501[A]	31/31	0.85	0.11	43,46,50,51	31
2	ATP	K	501[B]	31/31	0.85	0.11	44,46,50,51	31
2	ATP	O	502[A]	31/31	0.87	0.11	52,54,60,61	31
2	ATP	O	502[B]	31/31	0.87	0.11	52,54,60,61	31
2	ATP	B	501[A]	31/31	0.89	0.10	45,47,53,54	31
2	ATP	B	501[B]	31/31	0.89	0.10	45,47,53,55	31
2	ATP	L	502[A]	31/31	0.89	0.10	43,45,48,52	31
2	ATP	L	502[B]	31/31	0.89	0.10	43,45,48,50	31
2	ATP	G	501[A]	31/31	0.89	0.10	42,43,48,50	31
2	ATP	G	501[B]	31/31	0.89	0.10	42,43,48,49	31
2	ATP	P	502[A]	31/31	0.89	0.09	50,52,56,59	31
2	ATP	P	502[B]	31/31	0.89	0.09	50,52,57,59	31
2	ATP	M	502[A]	31/31	0.90	0.09	43,45,54,55	31
2	ATP	M	502[B]	31/31	0.90	0.09	43,45,54,55	31
2	ATP	J	501[A]	31/31	0.91	0.09	46,49,55,59	31
2	ATP	J	501[B]	31/31	0.91	0.09	46,49,56,57	31

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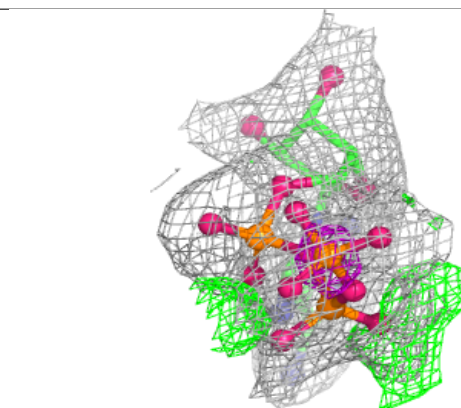
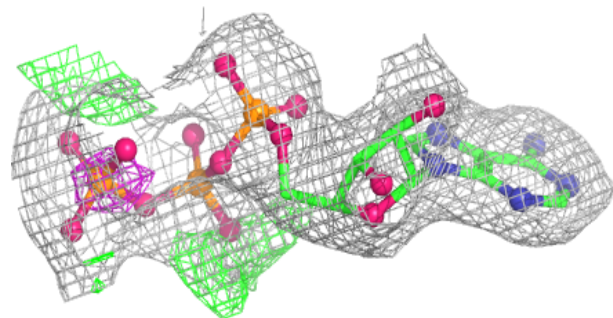
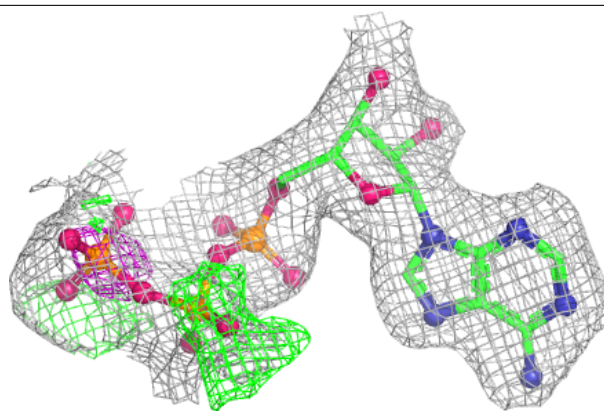
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	N	502[A]	31/31	0.91	0.09	44,45,54,54	31
2	ATP	N	502[B]	31/31	0.91	0.09	44,45,53,54	31
2	ATP	A	501[A]	31/31	0.91	0.09	41,43,51,52	31
2	ATP	A	501[B]	31/31	0.91	0.09	41,43,51,53	31
2	ATP	I	501[A]	31/31	0.91	0.08	46,49,54,54	31
2	ATP	I	501[B]	31/31	0.91	0.08	46,49,54,55	31
2	ATP	H	501[A]	31/31	0.92	0.10	40,43,50,55	31
2	ATP	H	501[B]	31/31	0.92	0.10	40,43,50,53	31
2	ATP	F	501[A]	31/31	0.92	0.09	43,47,50,50	31
2	ATP	F	501[B]	31/31	0.92	0.09	43,47,50,50	31
2	ATP	C	501[A]	31/31	0.92	0.08	43,45,52,54	31
2	ATP	C	501[B]	31/31	0.92	0.08	44,45,52,55	31
3	5GP	P	501	24/24	0.95	0.07	50,54,60,62	0
3	5GP	F	502	24/24	0.96	0.06	35,41,48,49	0
3	5GP	I	502	24/24	0.96	0.07	37,42,51,52	0
3	5GP	J	502	24/24	0.96	0.07	41,46,50,53	0
3	5GP	K	502	24/24	0.96	0.07	37,42,53,54	0
3	5GP	L	501	24/24	0.96	0.07	34,43,51,55	0
3	5GP	M	501	24/24	0.96	0.06	40,48,53,57	0
3	5GP	N	501	24/24	0.96	0.07	43,47,53,56	0
3	5GP	O	501	24/24	0.96	0.06	47,52,57,58	0
3	5GP	D	502	24/24	0.96	0.07	44,51,58,63	0
3	5GP	G	502	24/24	0.97	0.06	32,38,40,41	0
3	5GP	H	502	24/24	0.97	0.06	34,38,44,46	0
3	5GP	A	502	24/24	0.97	0.06	37,42,48,51	0
3	5GP	E	502	24/24	0.97	0.06	34,40,48,48	0
3	5GP	C	502	24/24	0.97	0.06	40,45,51,51	0
3	5GP	B	502	24/24	0.98	0.05	39,43,51,52	0

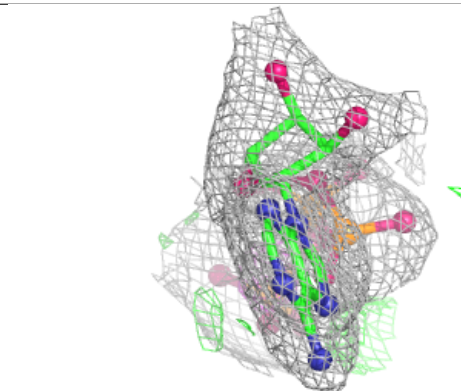
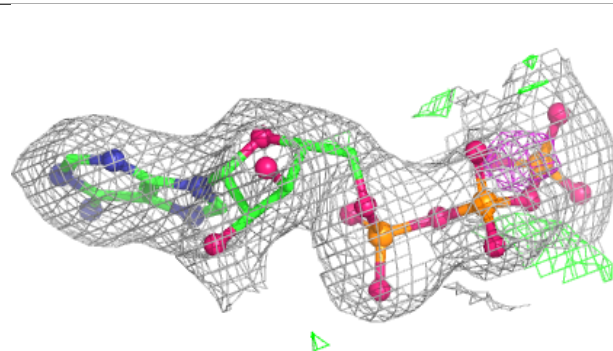
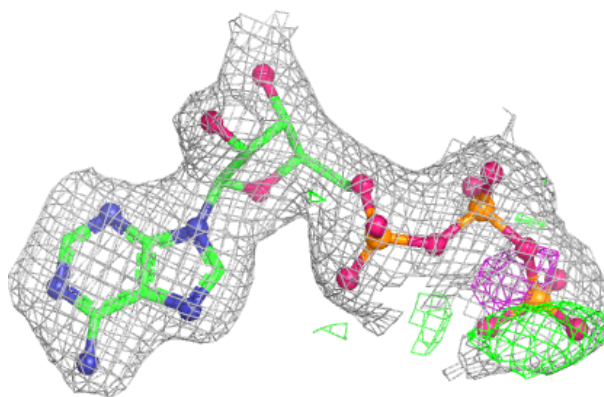
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 501 (A):

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

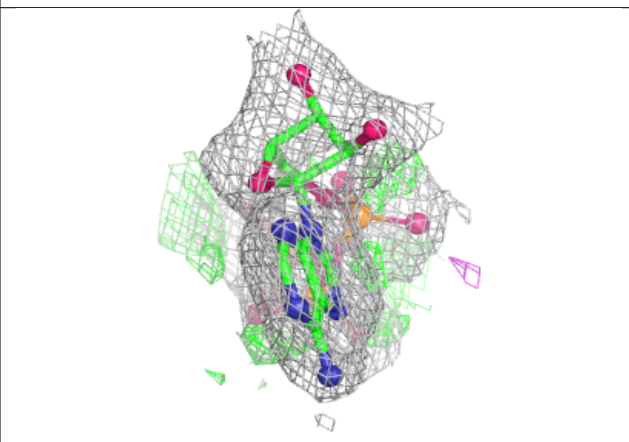
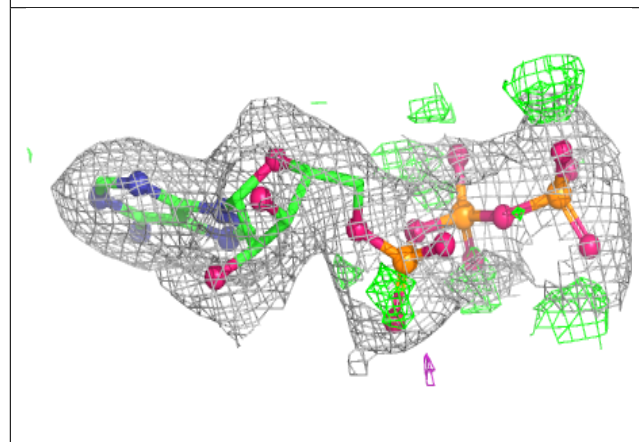
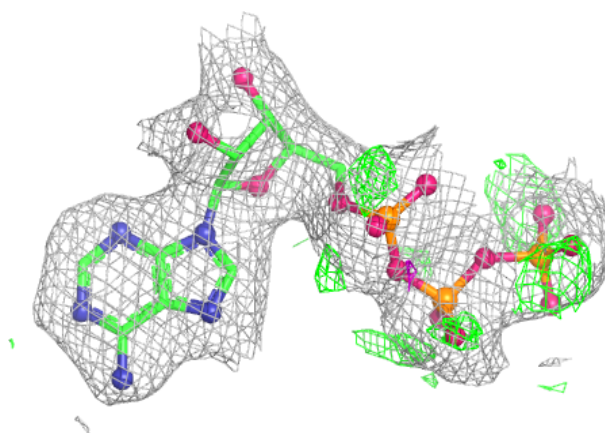
**Electron density around ATP D 501 (B):**

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

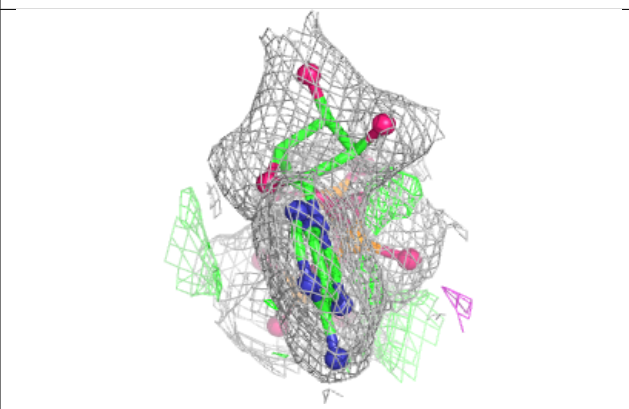
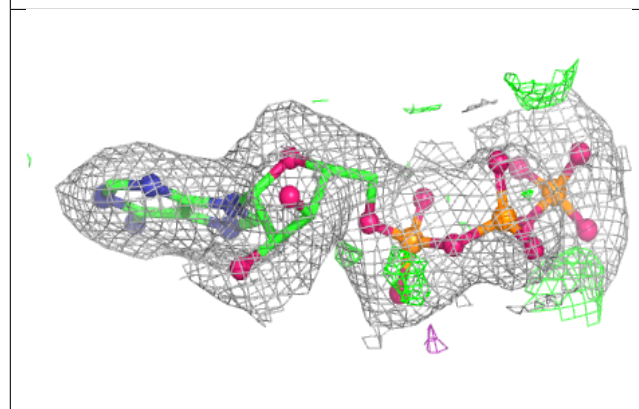
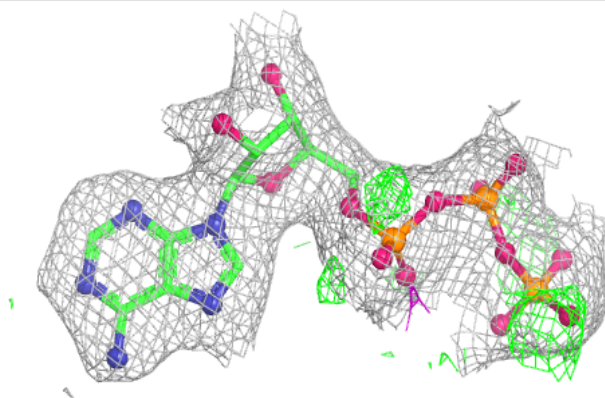


Electron density around ATP E 501 (A):

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

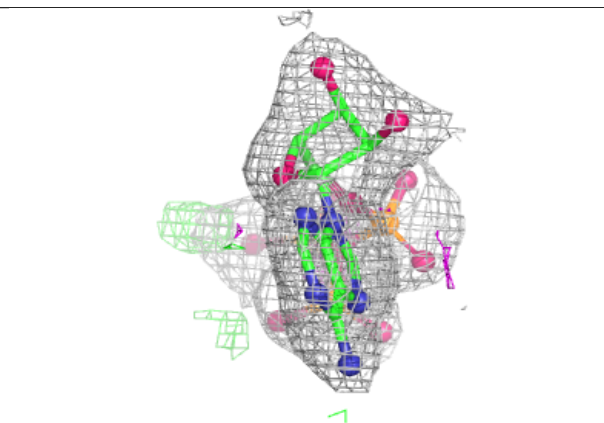
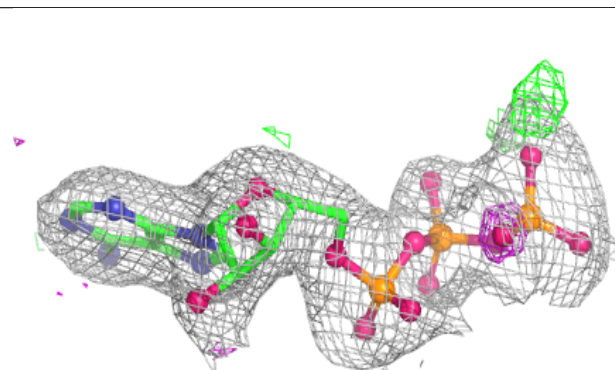
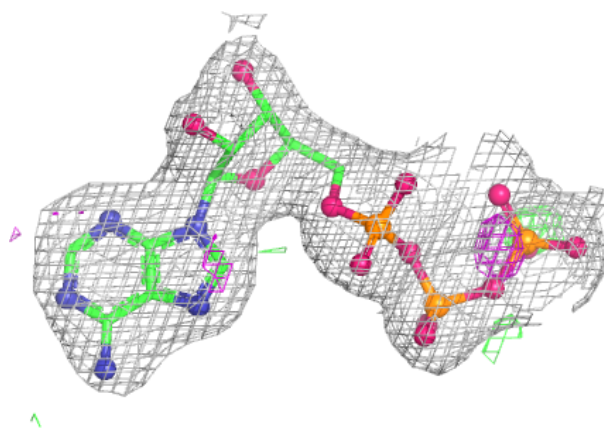
**Electron density around ATP E 501 (B):**

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



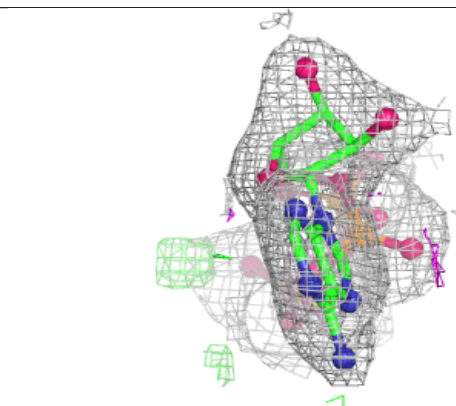
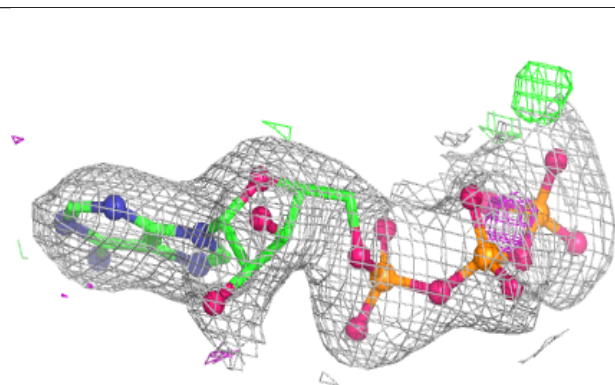
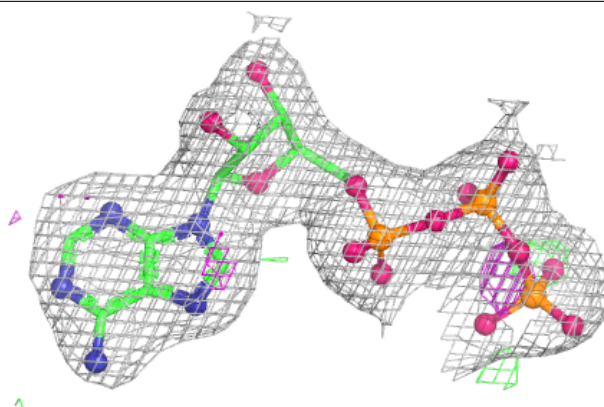
Electron density around ATP K 501 (A):

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



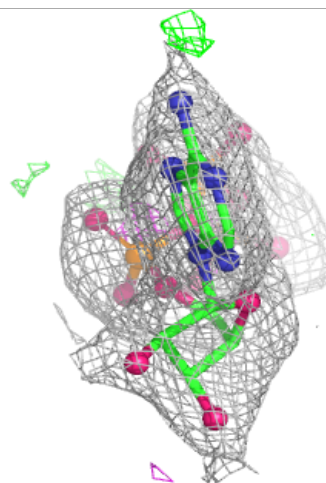
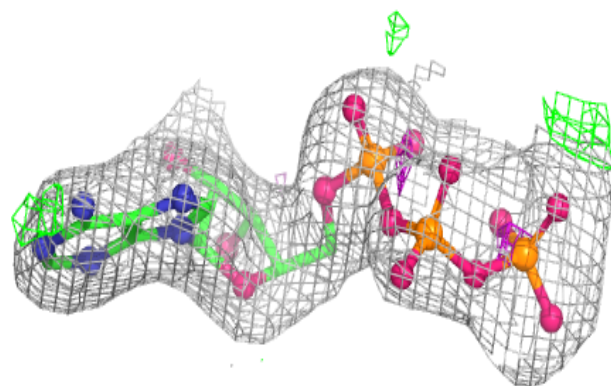
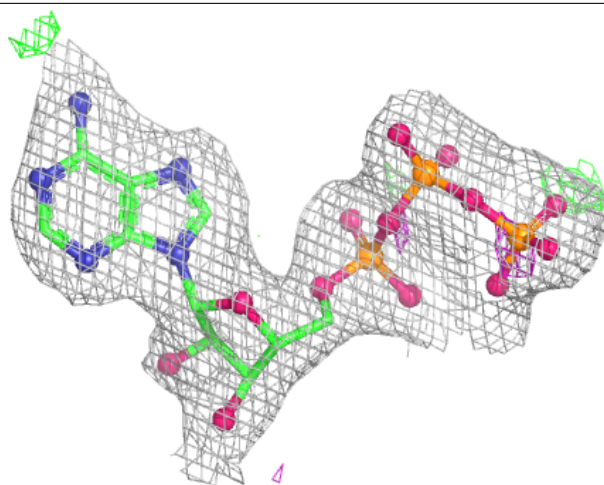
Electron density around ATP K 501 (B):

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



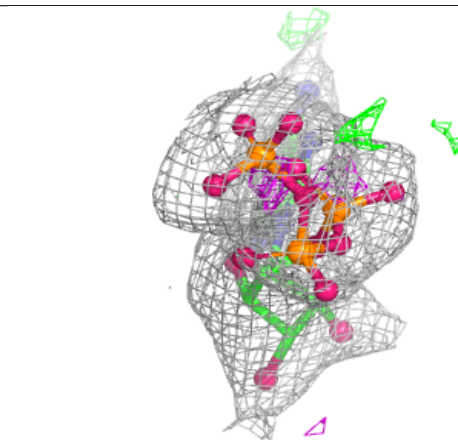
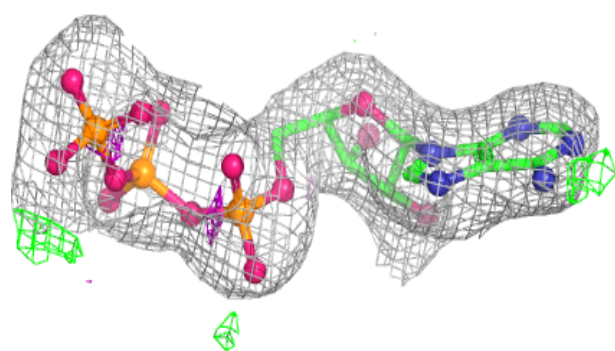
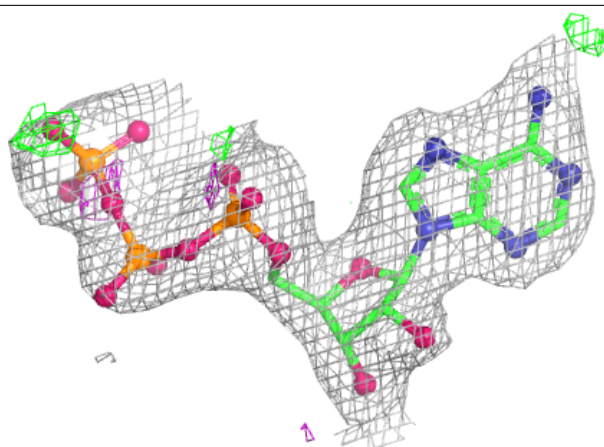
Electron density around ATP O 502 (A):

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

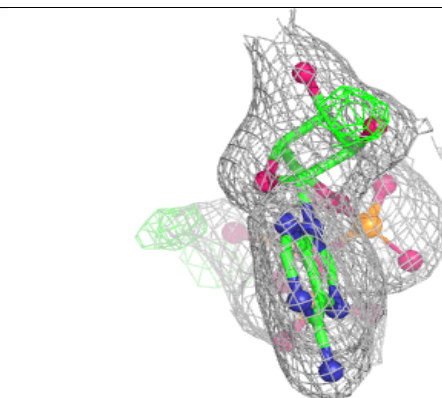
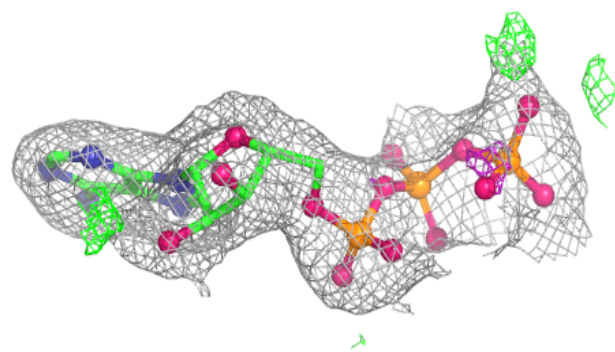
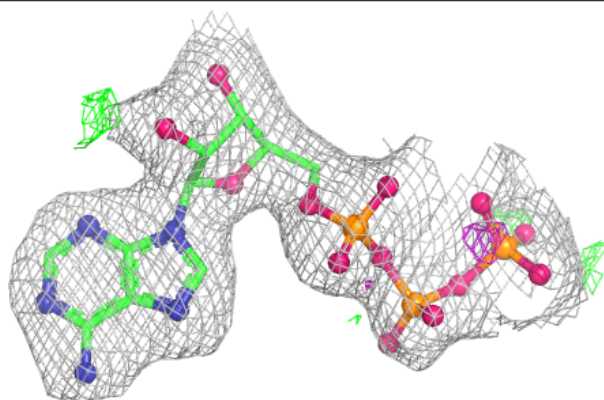


Electron density around ATP O 502 (B):

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

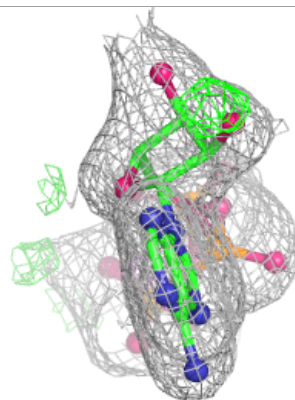
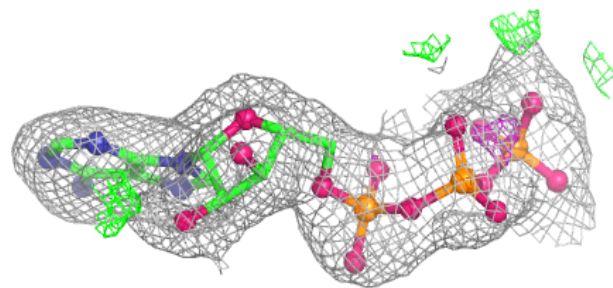
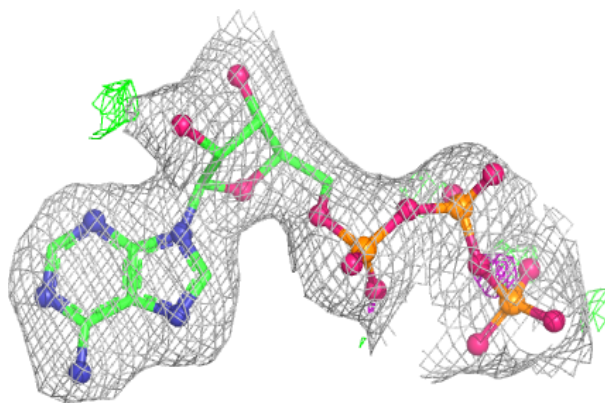
**Electron density around ATP B 501 (A):**

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



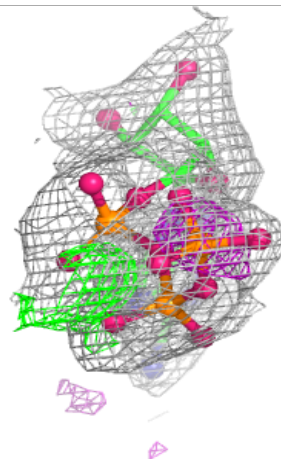
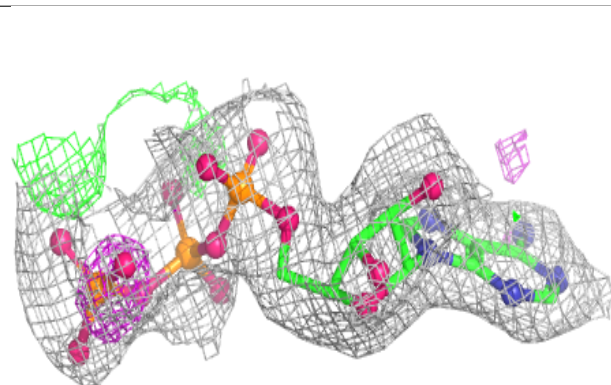
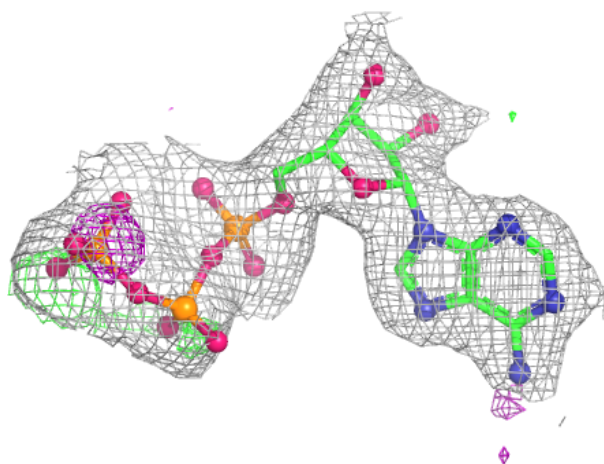
Electron density around ATP B 501 (B):

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



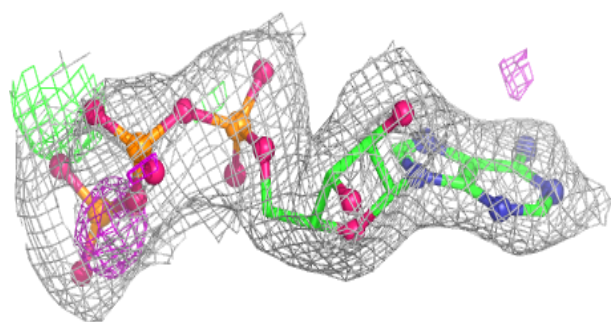
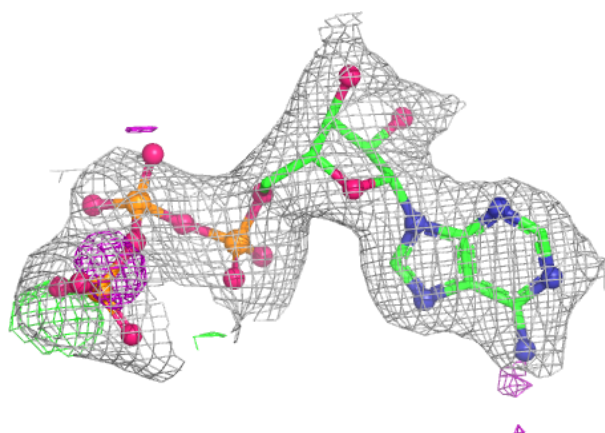
Electron density around ATP L 502 (A):

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

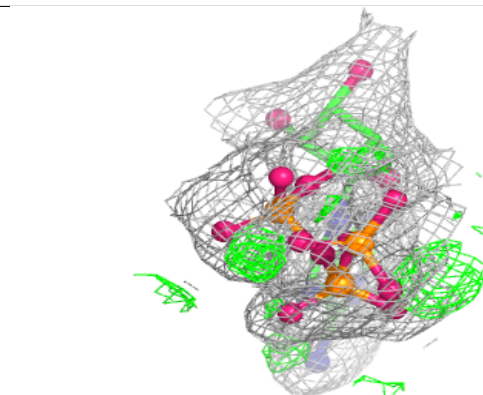
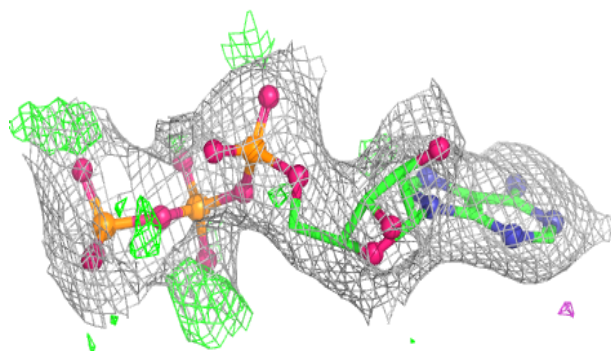
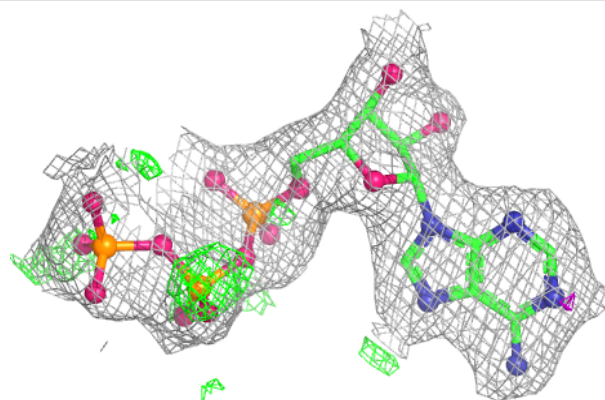


Electron density around ATP L 502 (B):

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

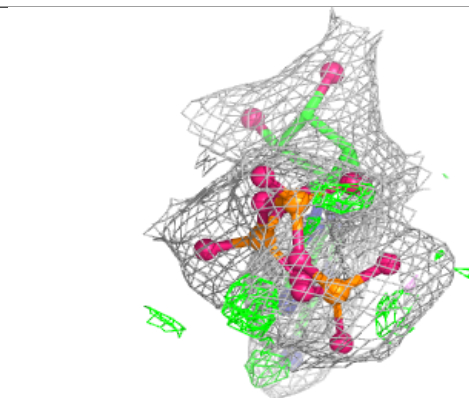
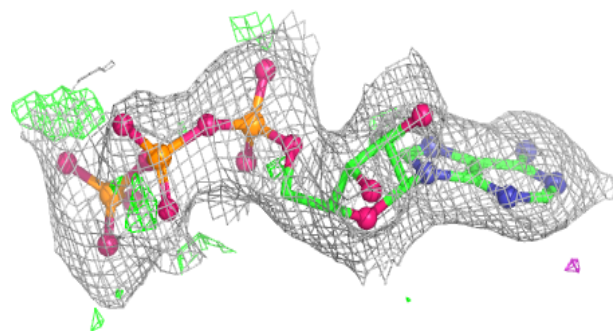
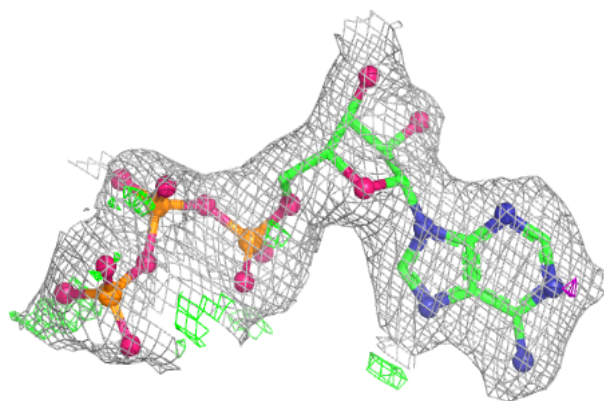
**Electron density around ATP G 501 (A):**

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

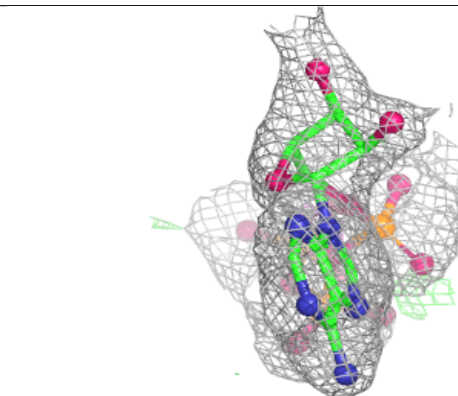
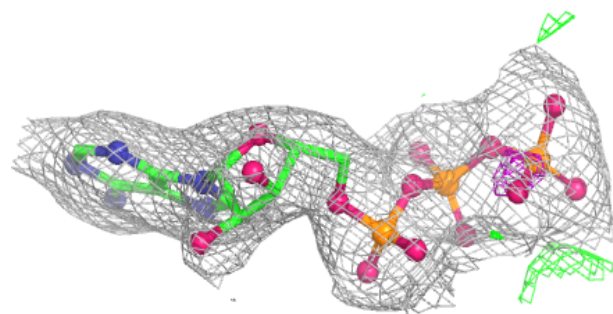
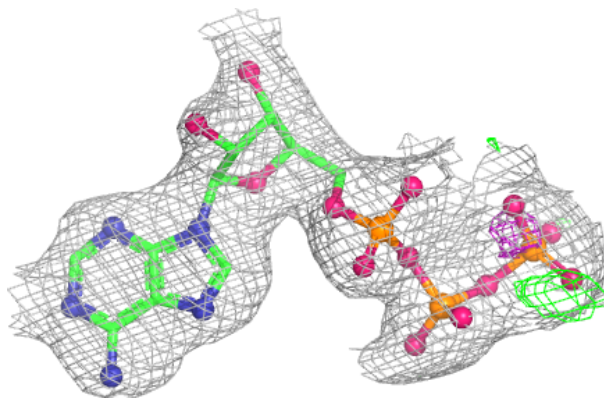


Electron density around ATP G 501 (B):

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

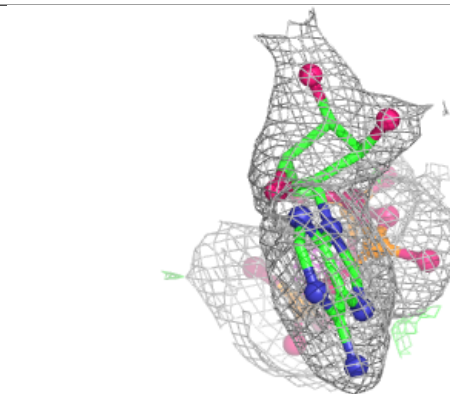
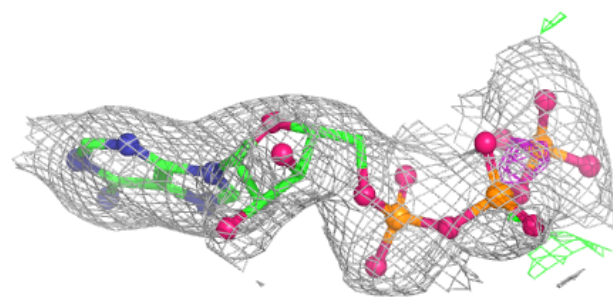
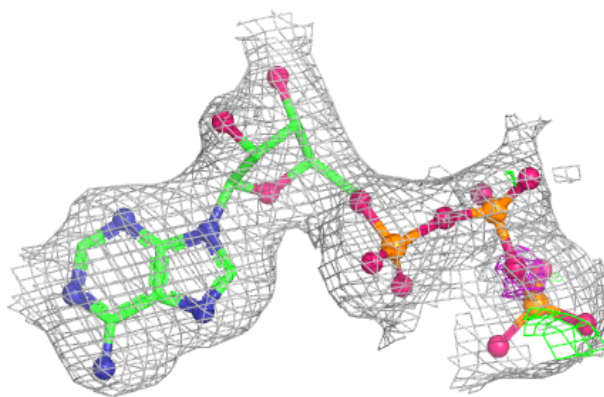
**Electron density around ATP P 502 (A):**

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

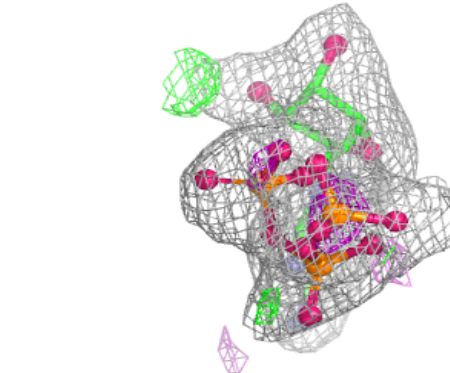
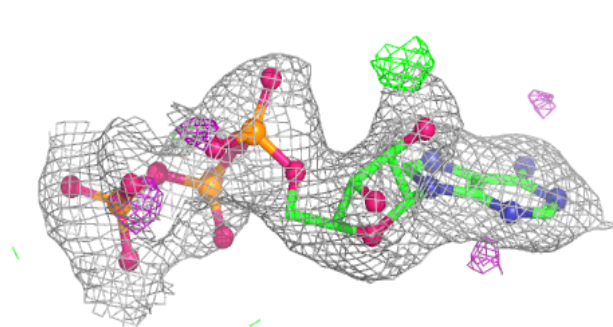
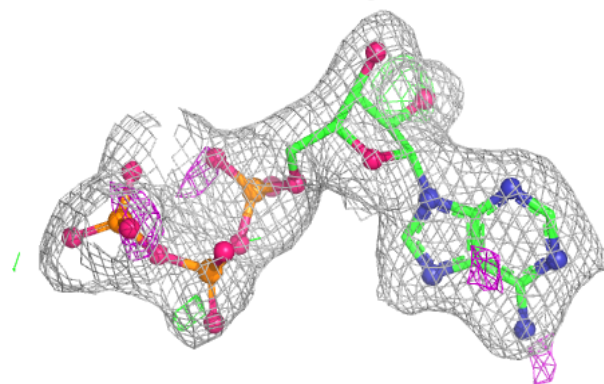


Electron density around ATP P 502 (B):

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

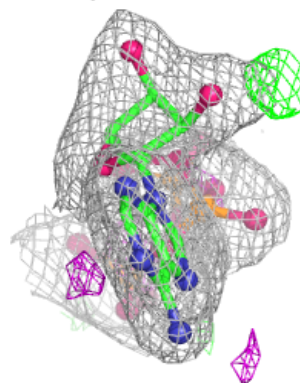
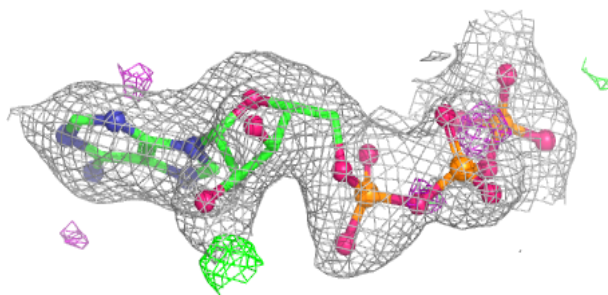
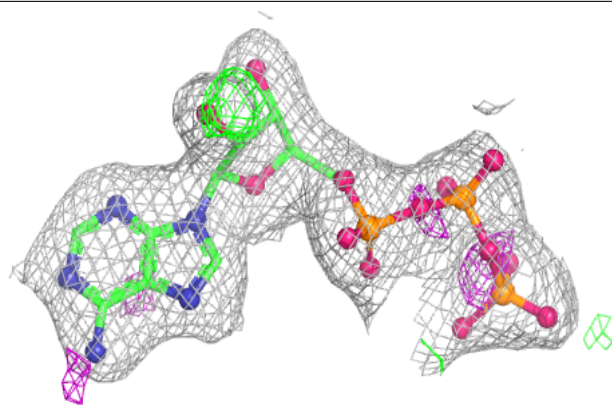
**Electron density around ATP M 502 (A):**

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

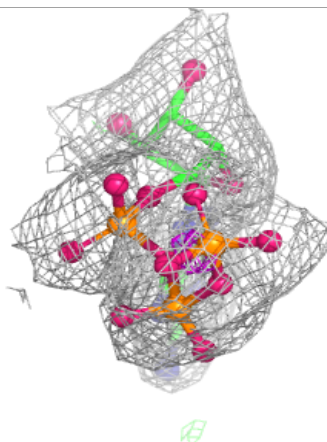
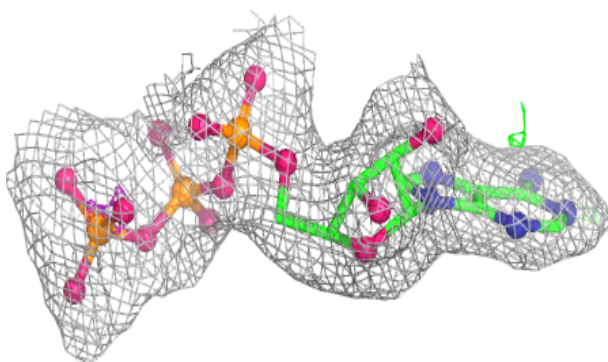
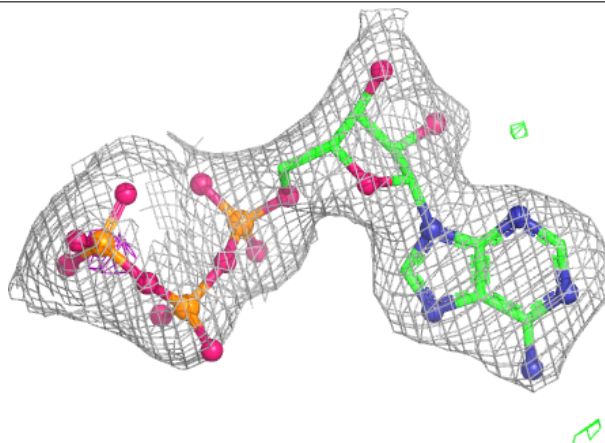


Electron density around ATP M 502 (B):

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

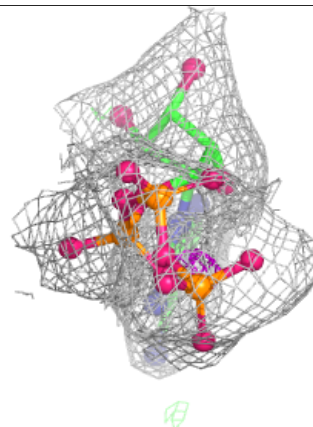
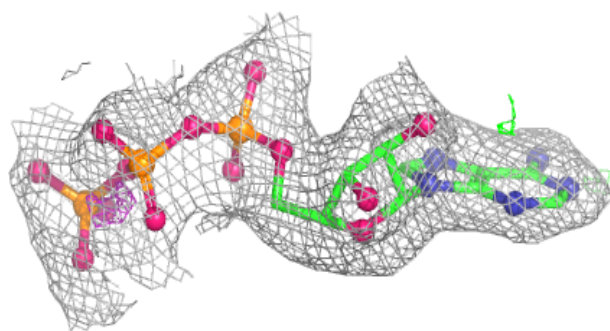
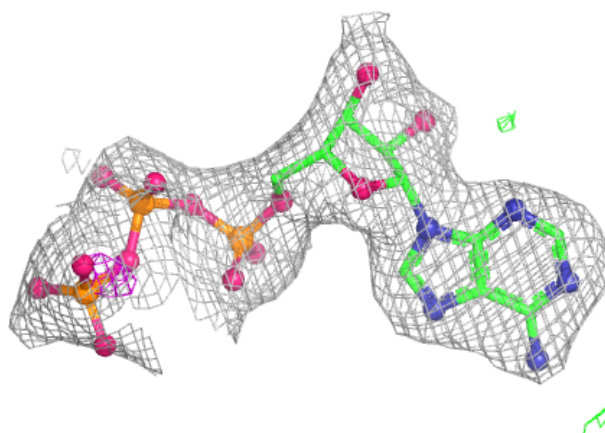
**Electron density around ATP J 501 (A):**

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



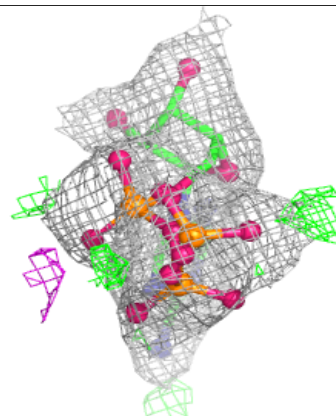
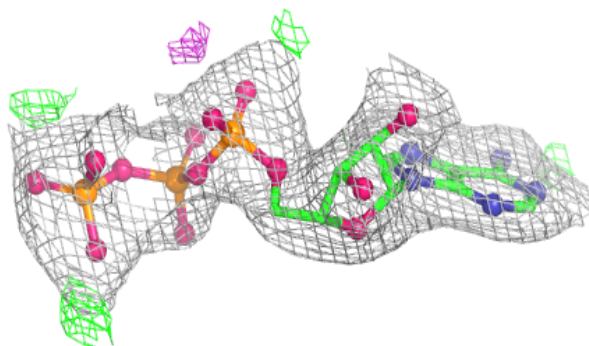
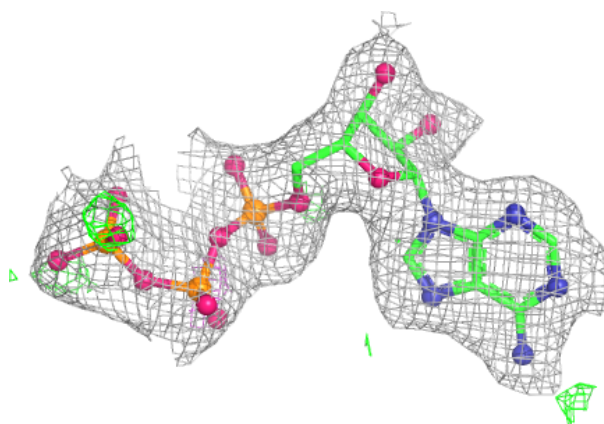
Electron density around ATP J 501 (B):

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

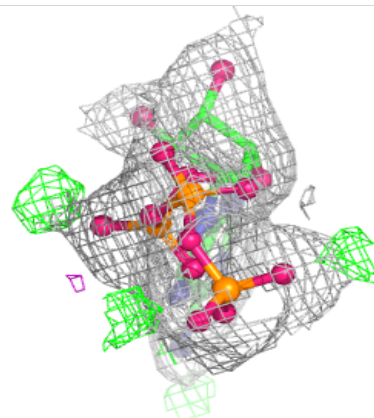
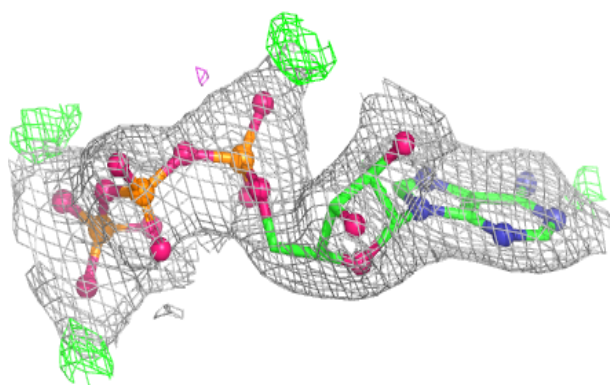
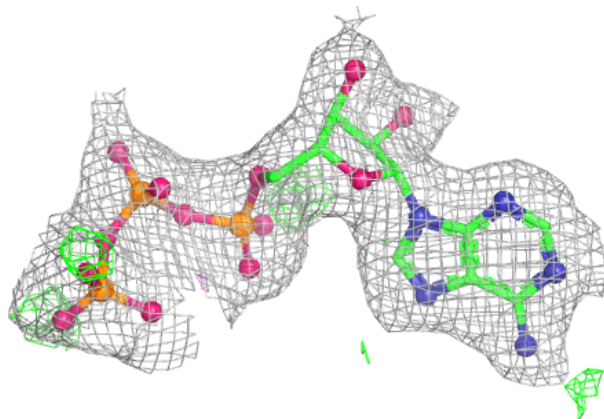


Electron density around ATP N 502 (A):

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

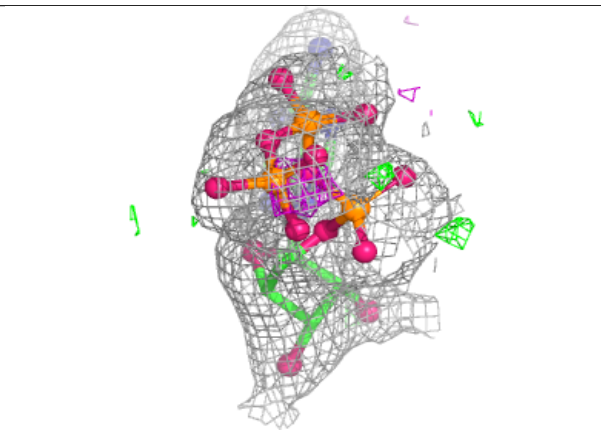
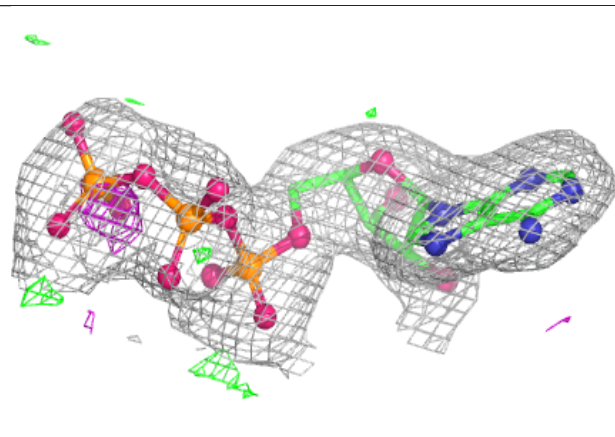
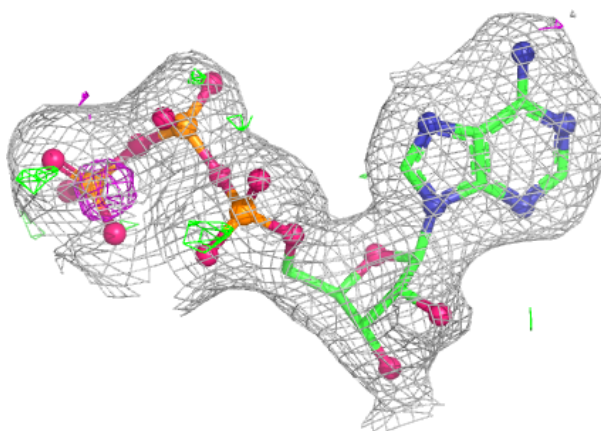
**Electron density around ATP N 502 (B):**

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

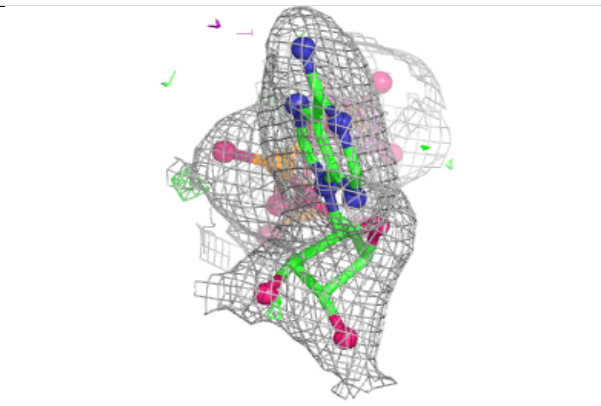
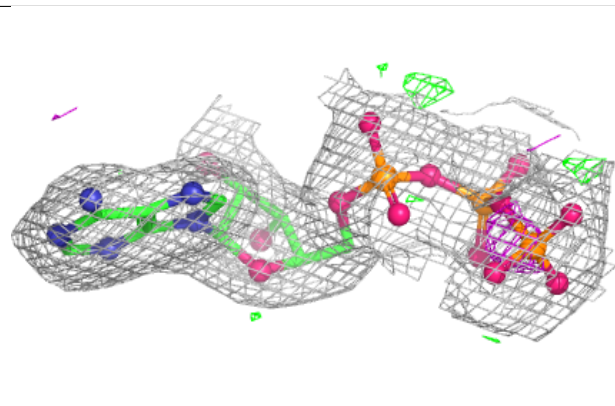
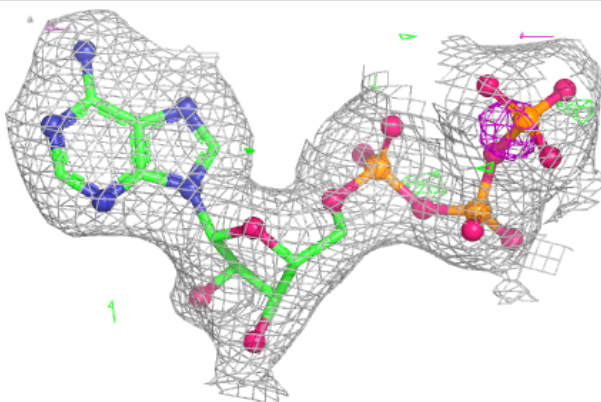


Electron density around ATP A 501 (A):

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

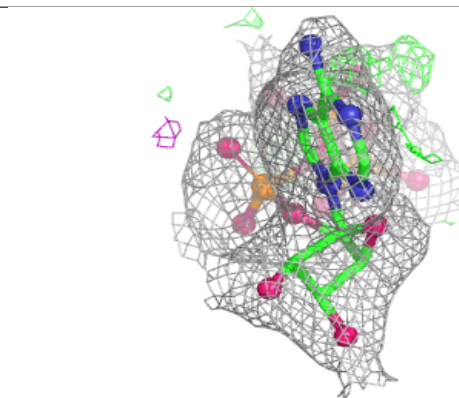
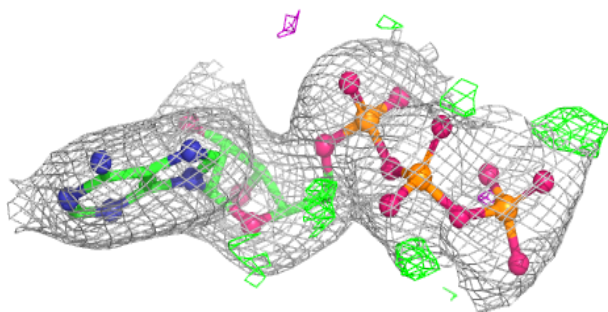
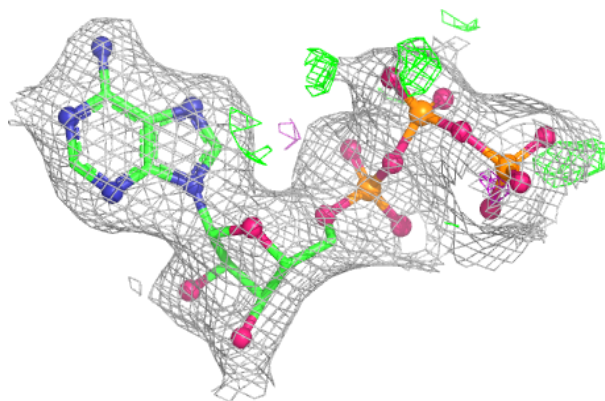
**Electron density around ATP A 501 (B):**

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

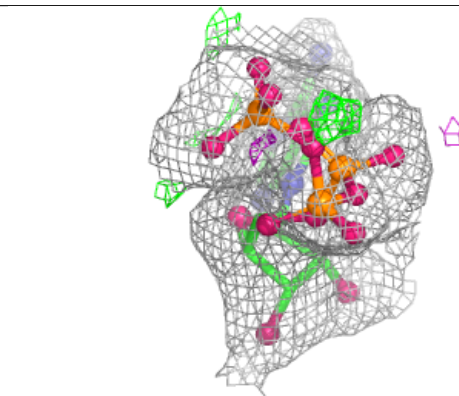
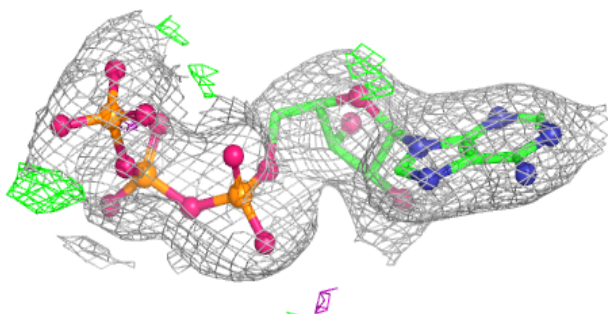
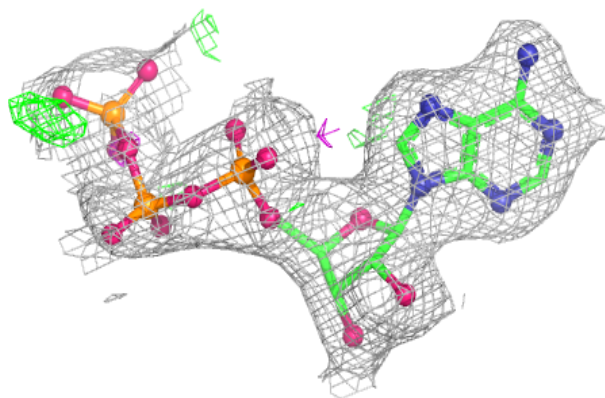


Electron density around ATP I 501 (A):

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

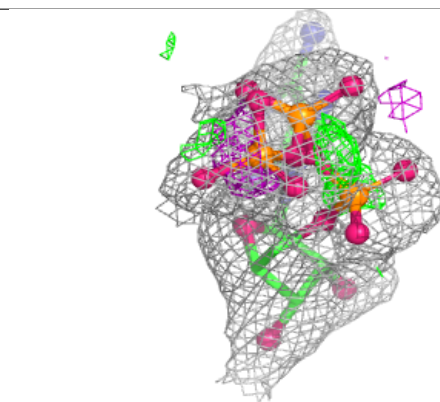
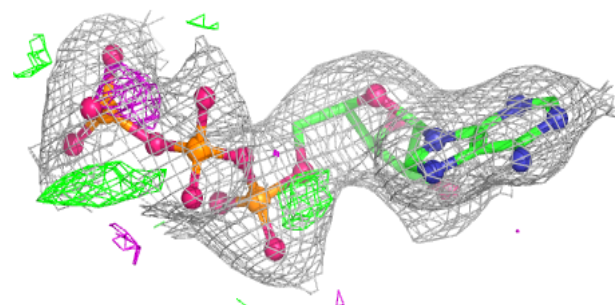
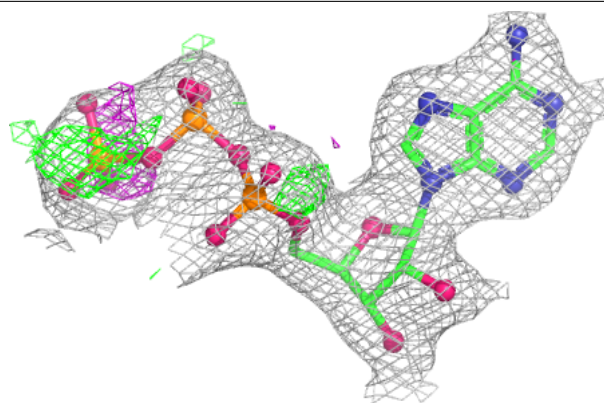
**Electron density around ATP I 501 (B):**

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

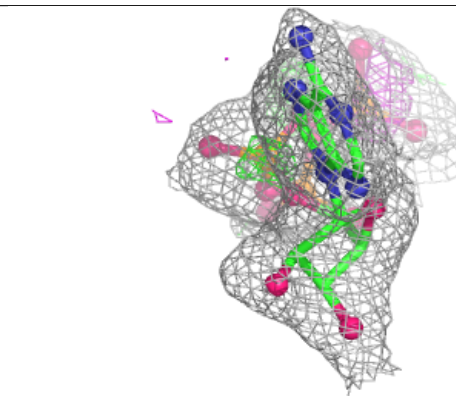
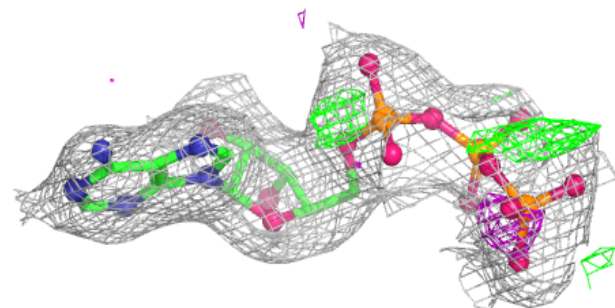
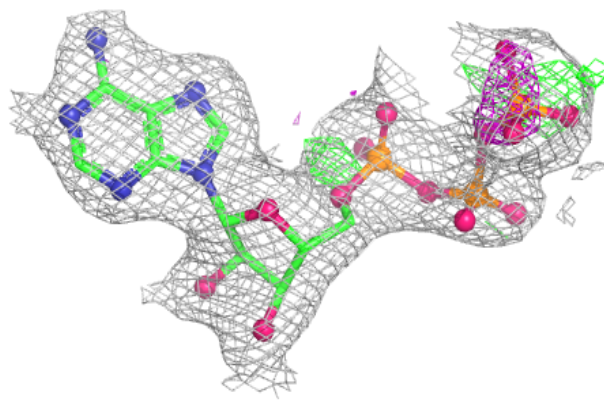


Electron density around ATP H 501 (A):

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

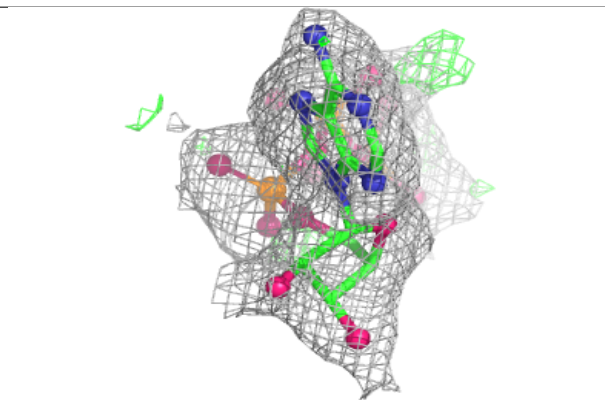
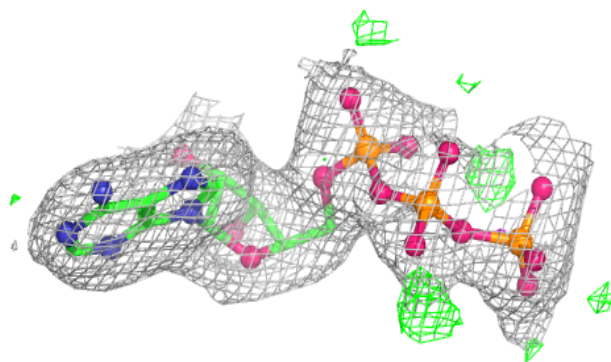
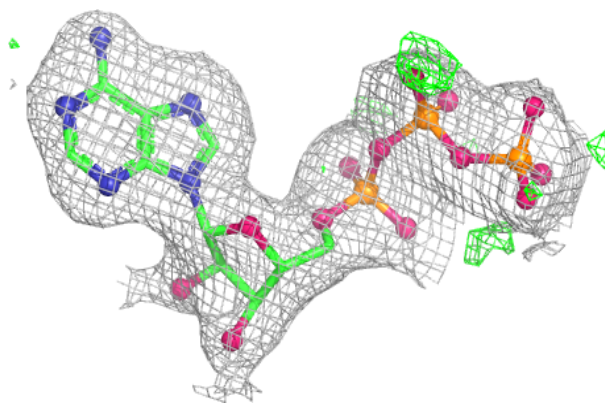
**Electron density around ATP H 501 (B):**

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

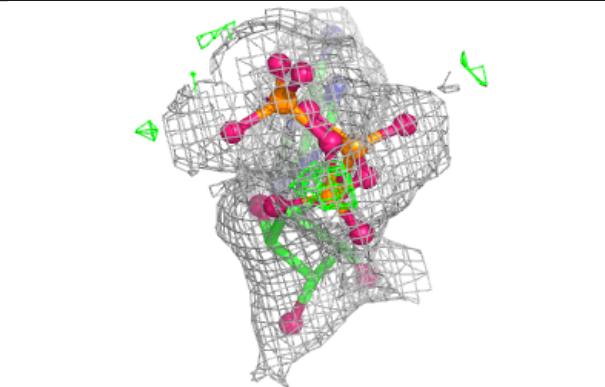
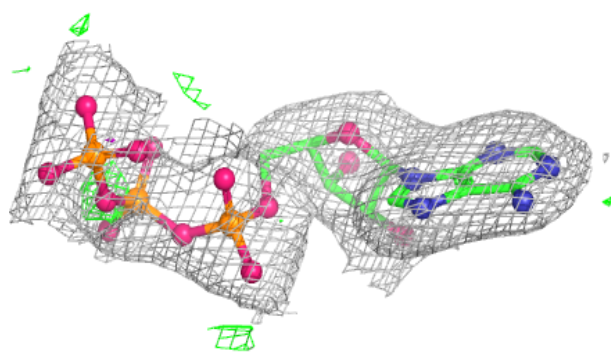
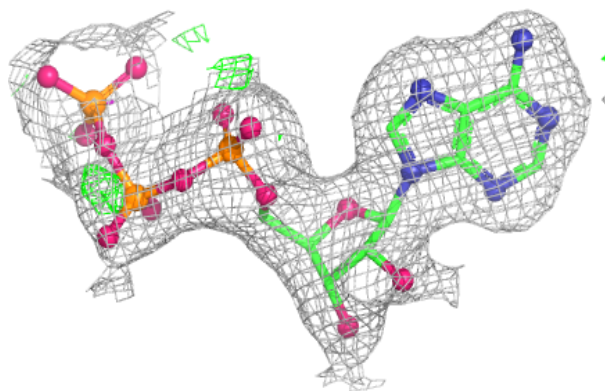


Electron density around ATP F 501 (A):

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

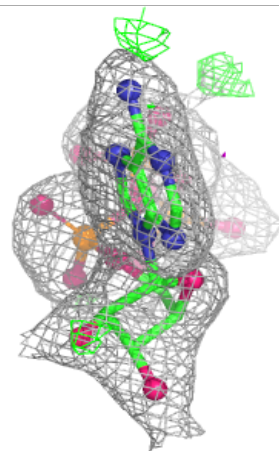
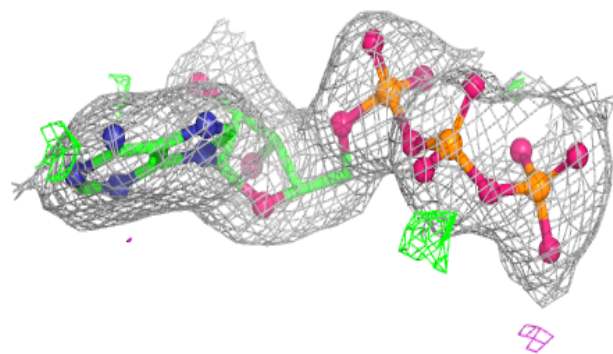
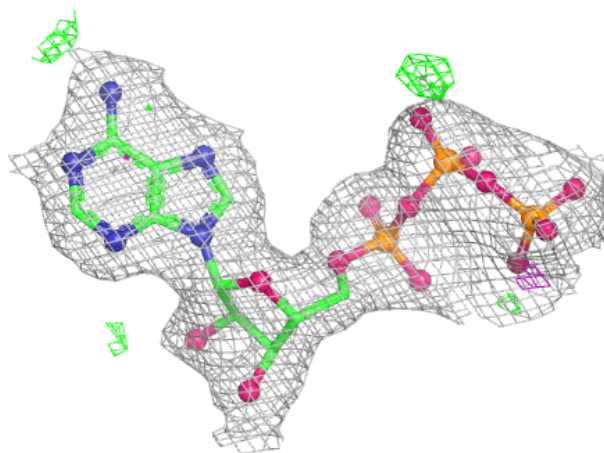
**Electron density around ATP F 501 (B):**

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



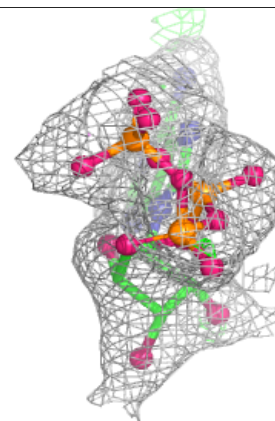
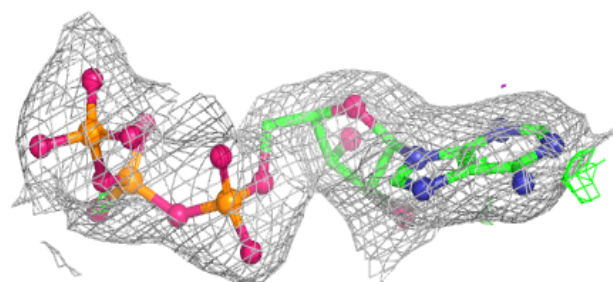
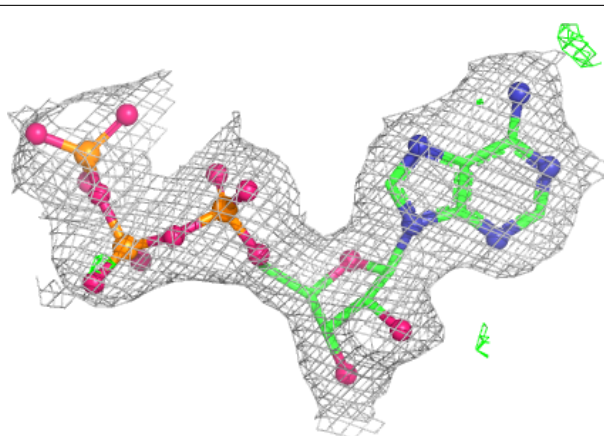
Electron density around ATP C 501 (A):

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

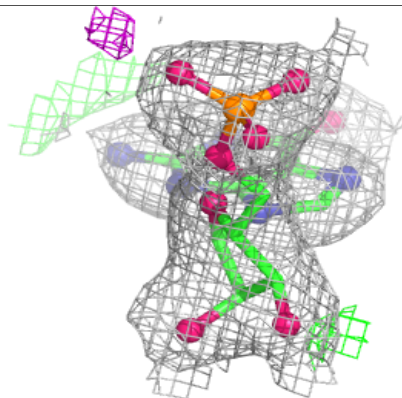
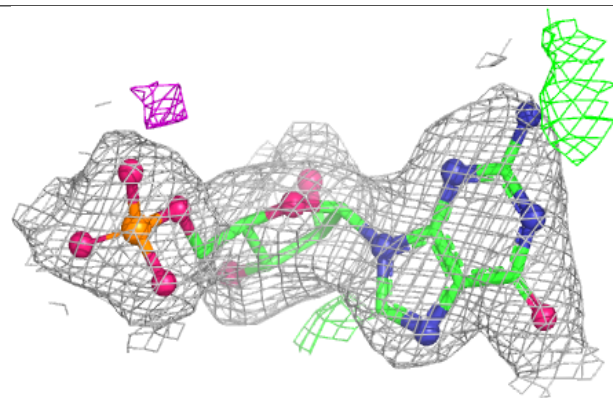
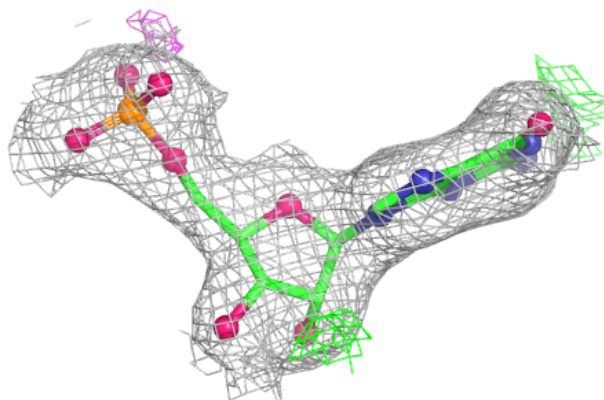


Electron density around ATP C 501 (B):

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

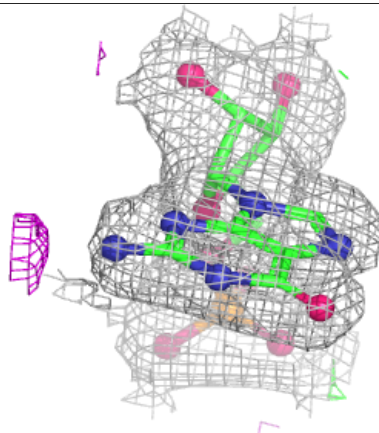
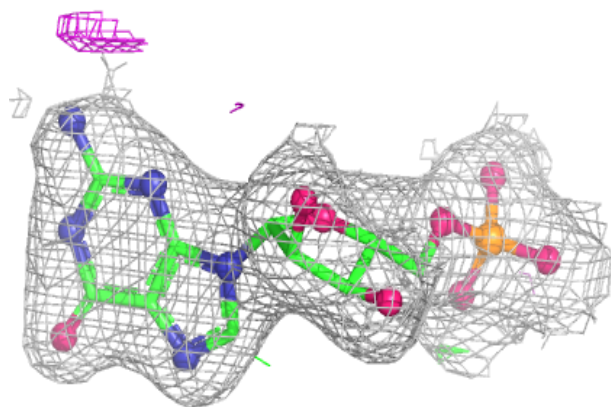
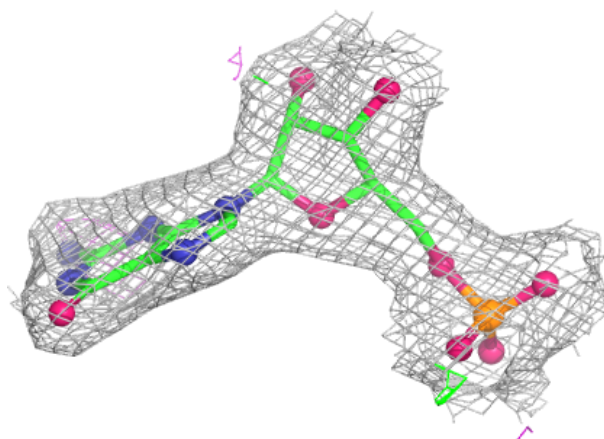
**Electron density around 5GP P 501:**

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

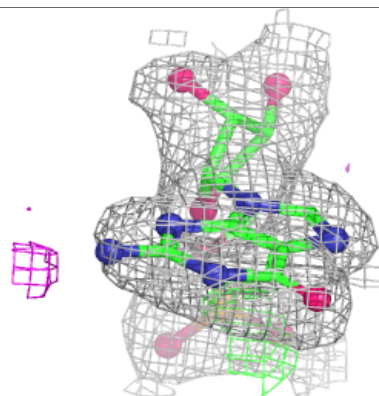
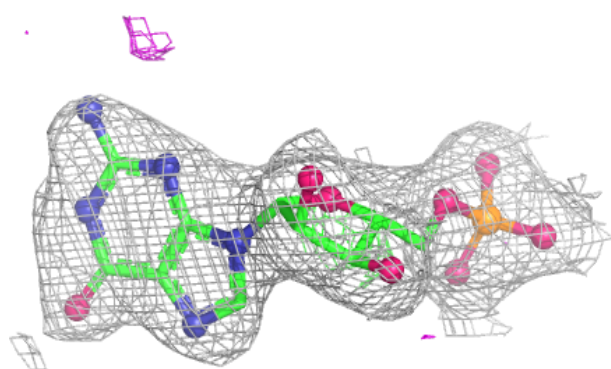
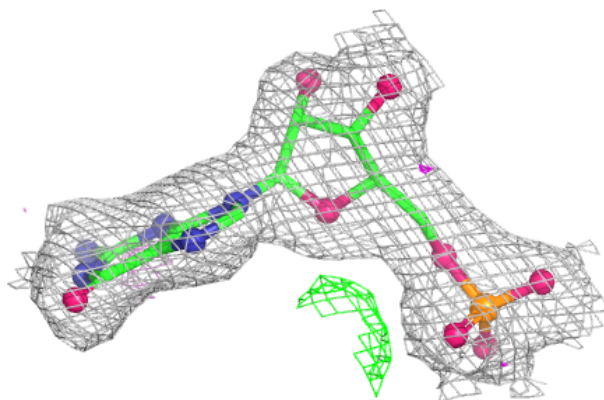


Electron density around 5GP F 502:

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

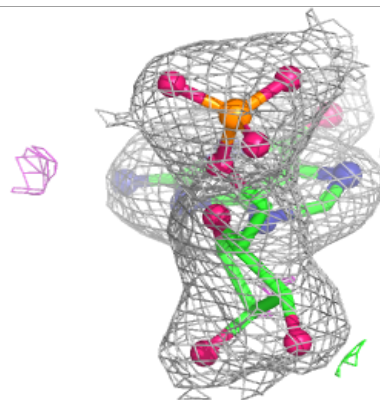
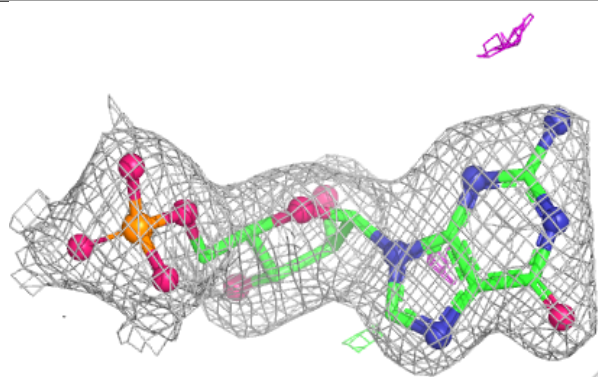
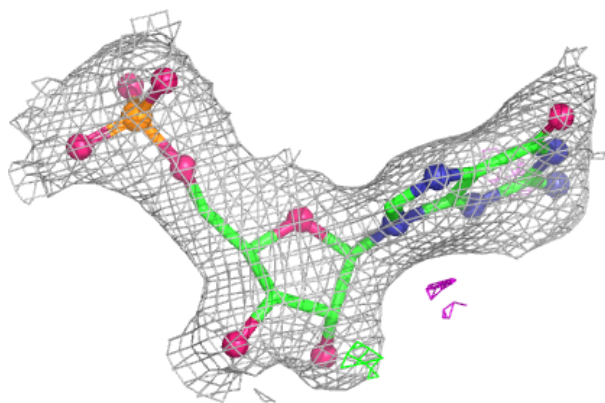
**Electron density around 5GP I 502:**

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

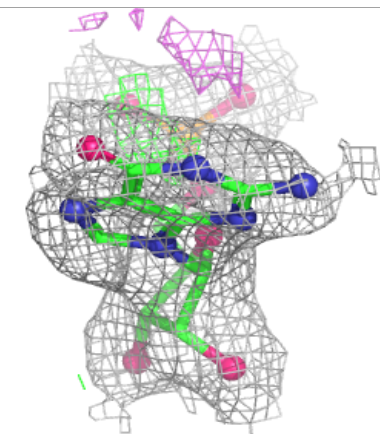
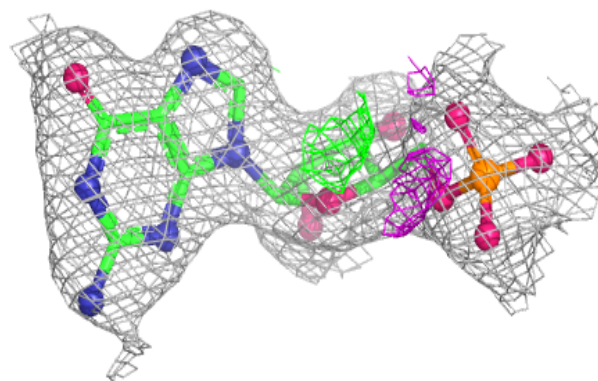
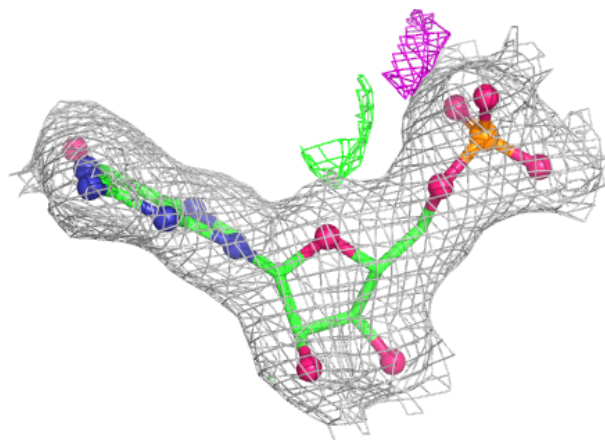


Electron density around 5GP J 502:

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

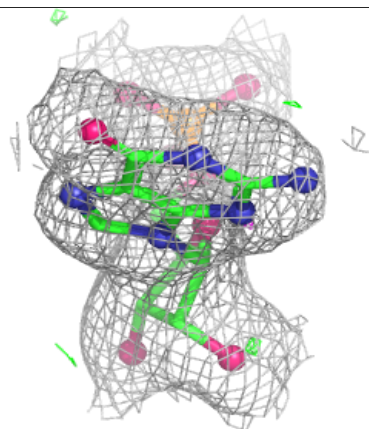
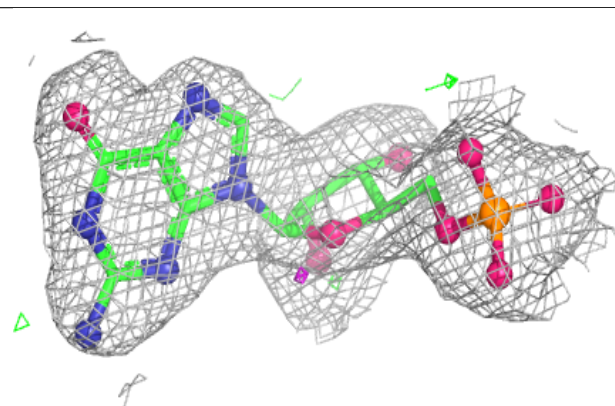
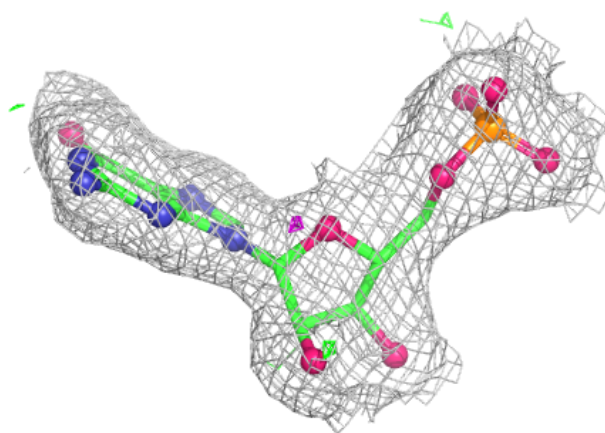
**Electron density around 5GP K 502:**

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



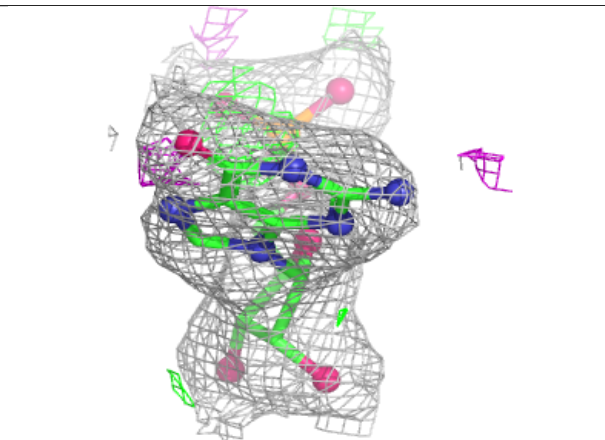
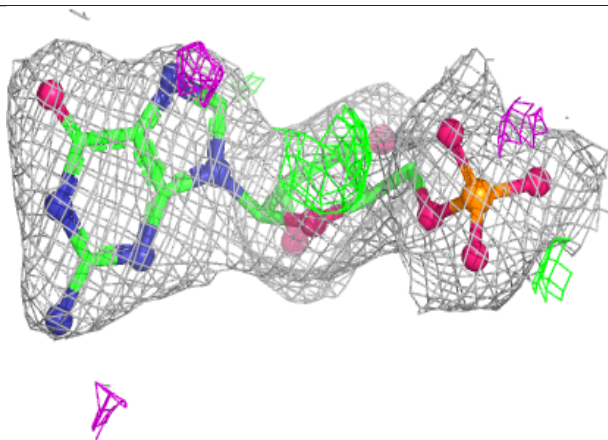
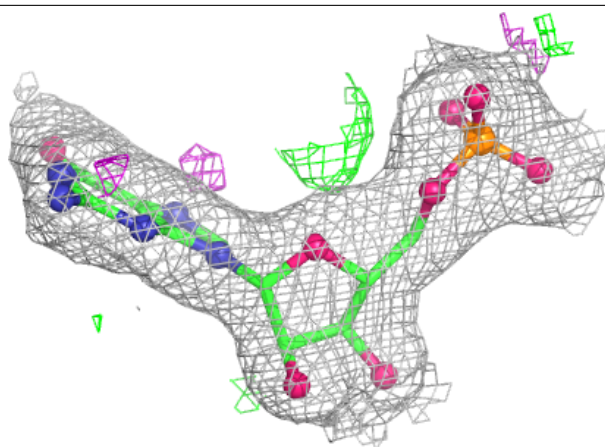
Electron density around 5GP L 501:

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

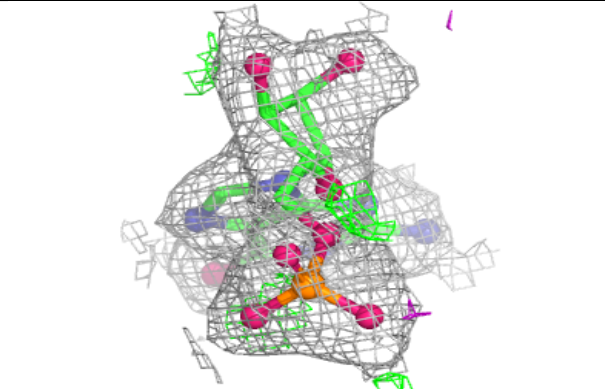
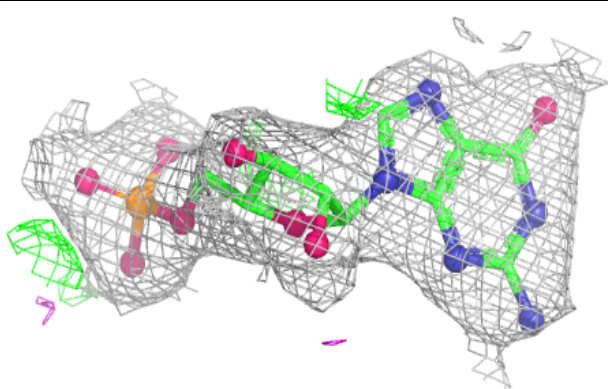
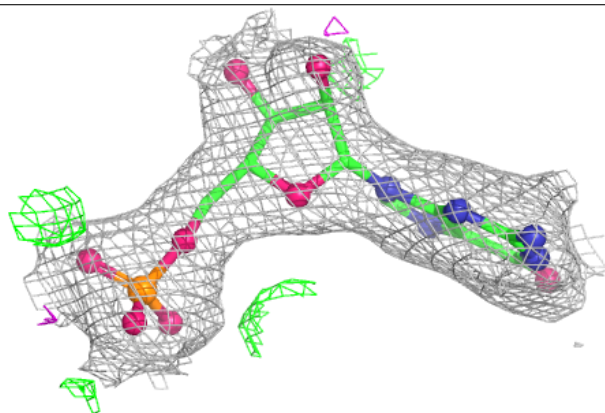


Electron density around 5GP M 501:

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

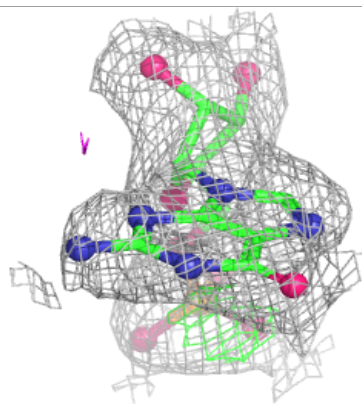
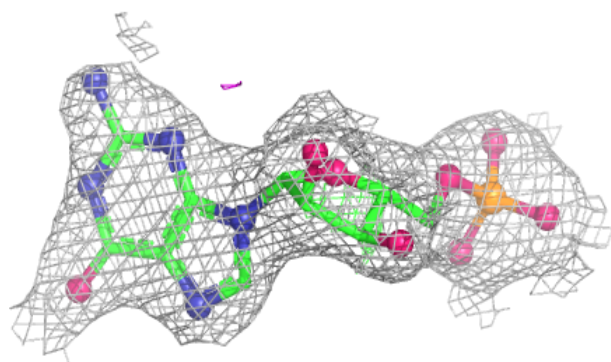
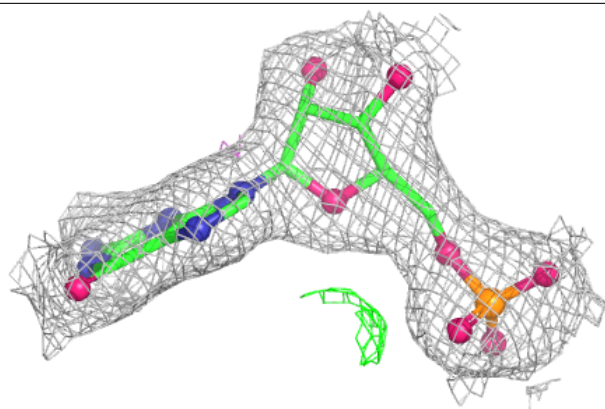
**Electron density around 5GP N 501:**

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

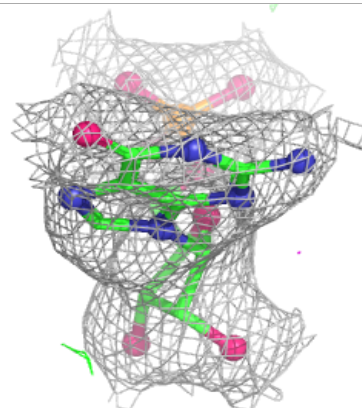
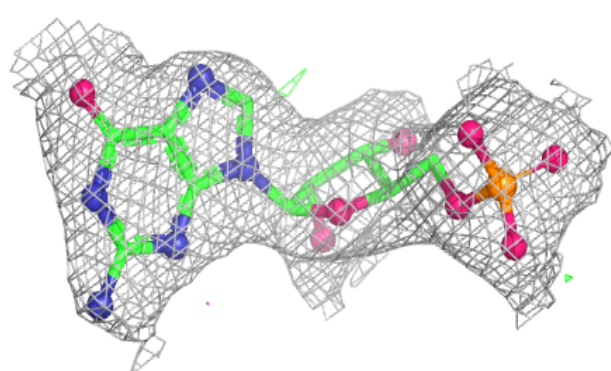
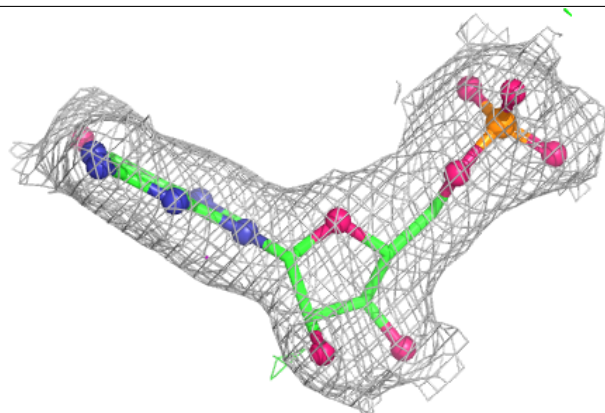


Electron density around 5GP O 501:

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

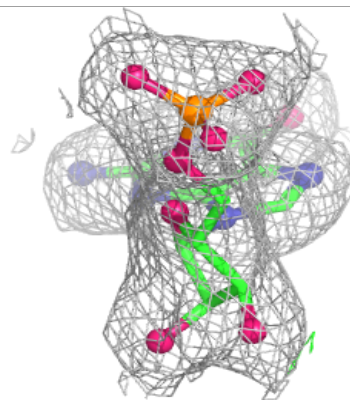
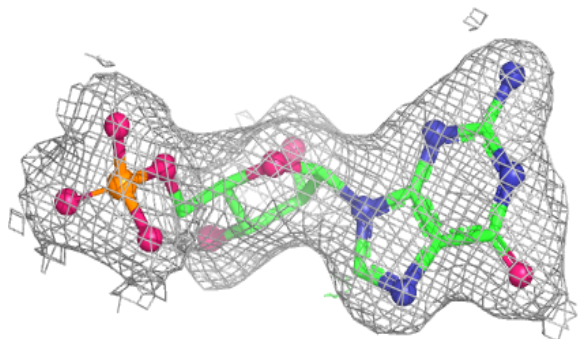
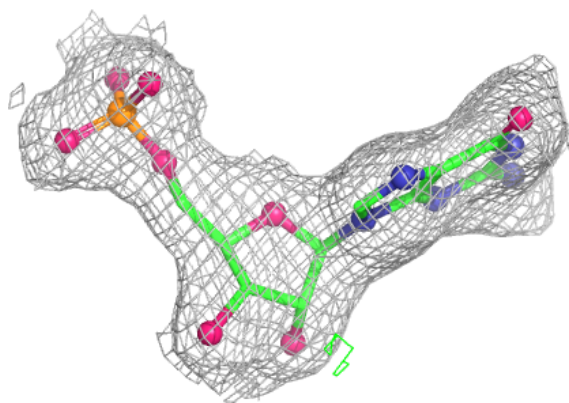
**Electron density around 5GP D 502:**

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

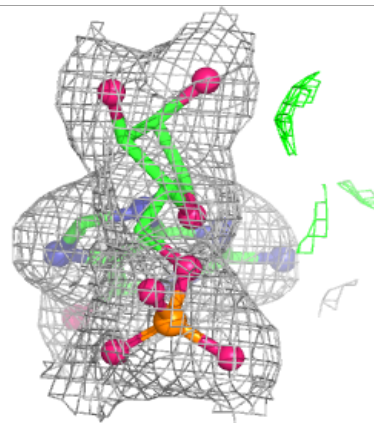
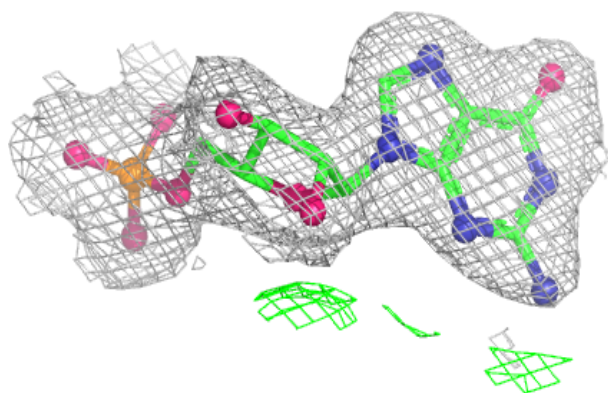
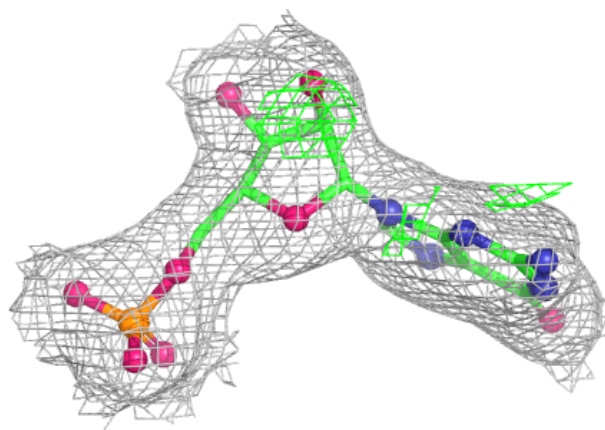


Electron density around 5GP G 502:

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

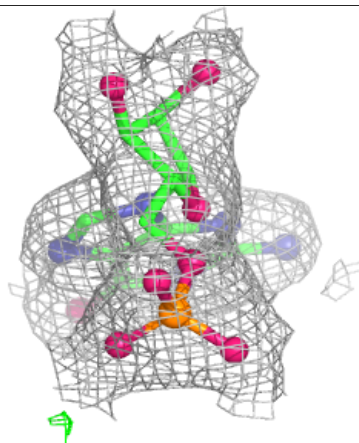
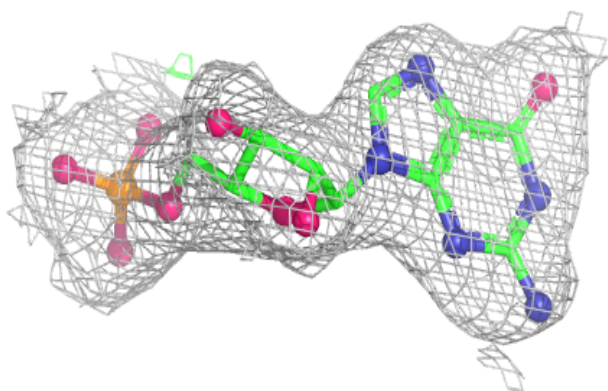
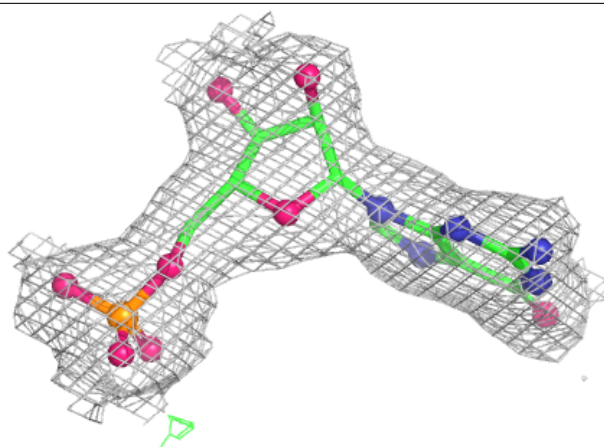
**Electron density around 5GP H 502:**

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

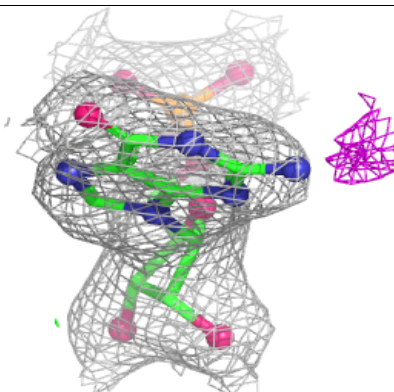
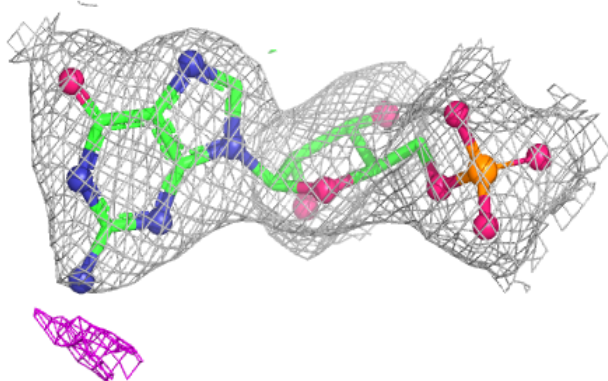
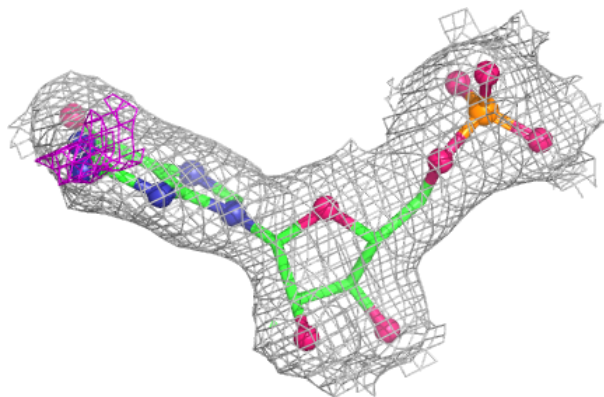


Electron density around 5GP A 502:

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

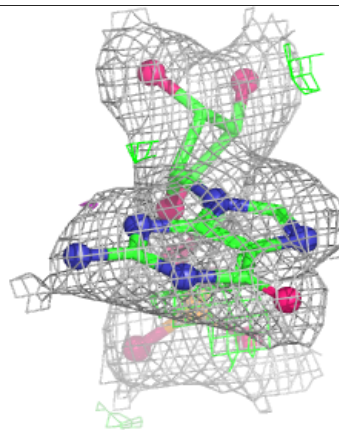
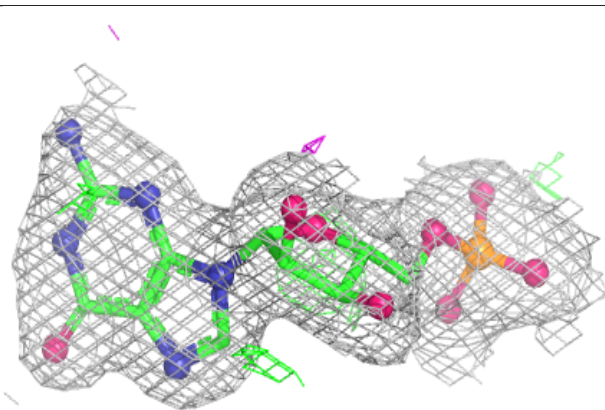
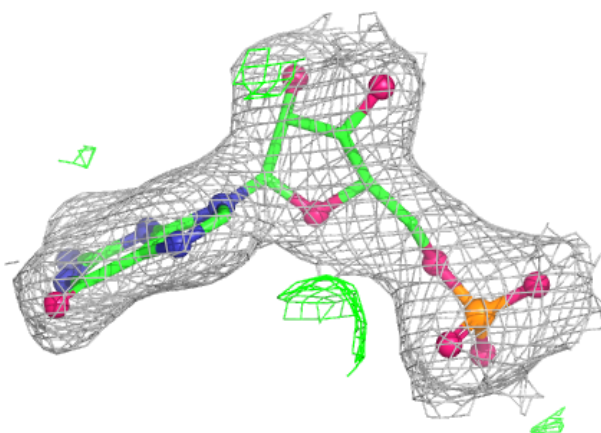
**Electron density around 5GP E 502:**

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



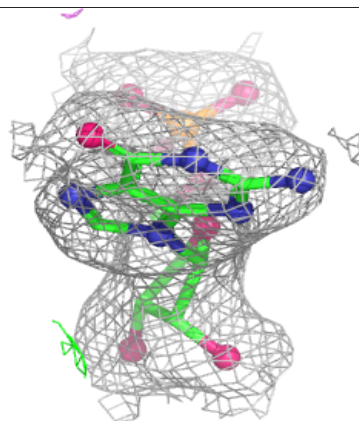
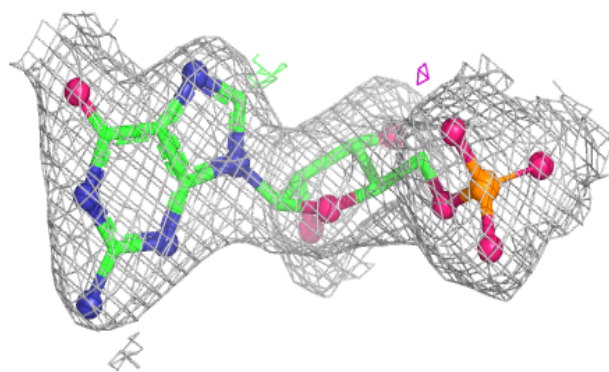
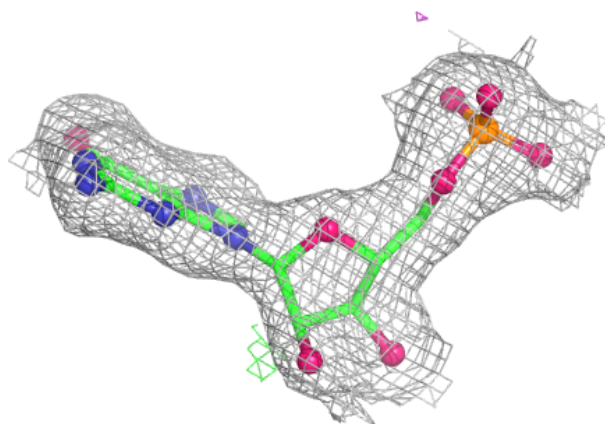
Electron density around 5GP C 502:

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



Electron density around 5GP B 502:

$2mF_o-DF_c$ (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.