



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2024 – 10:54 am GMT

PDB ID : 9HG1
Title : Crystal structure of M. smegmatis GMP reductase in complex with GMP and ATP.
Deposited on : 2024-11-18
Resolution : 2.30 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

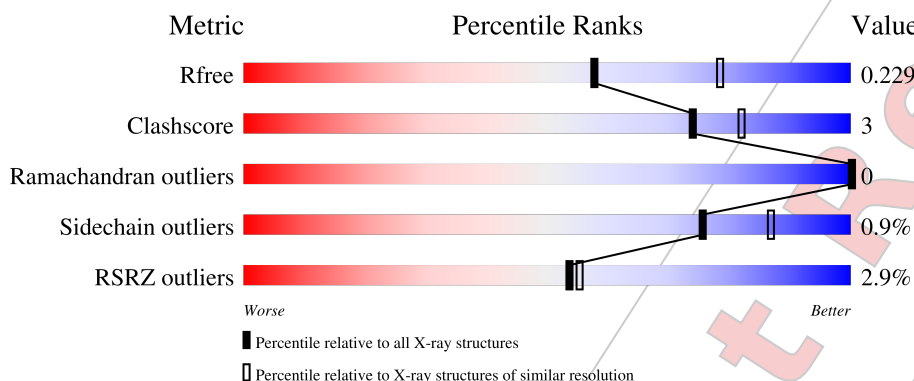
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)



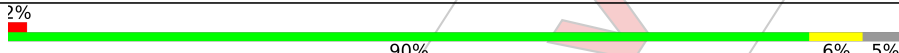



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	B	496	<div> <div>2%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	C	496	<div> <div>3%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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Mol	Chain	Length	Quality of chain
1	D	496	
1	E	496	
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 [i](#)

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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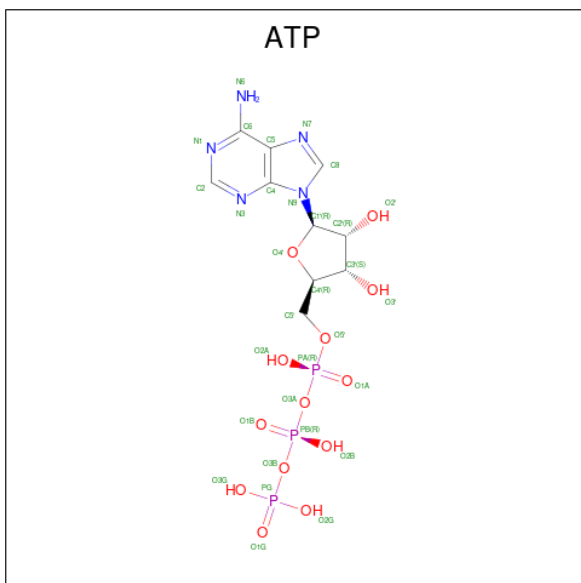
Chain	Residue	Modelled	Actual	Comment	Reference
L	491	HIS	-	expression tag	UNP A0QYE8
L	492	HIS	-	expression tag	UNP A0QYE8
L	493	HIS	-	expression tag	UNP A0QYE8
L	494	HIS	-	expression tag	UNP A0QYE8
L	495	HIS	-	expression tag	UNP A0QYE8
L	496	HIS	-	expression tag	UNP A0QYE8
M	2	VAL	-	insertion	UNP A0QYE8
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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



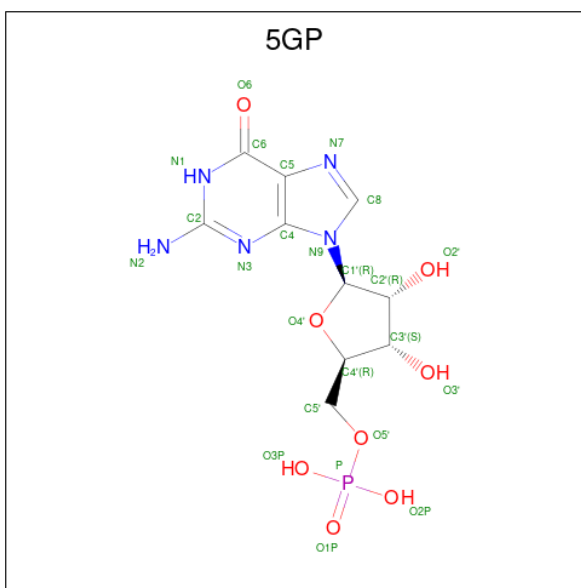
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	B	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	C	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	D	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	E	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	F	1	Total 62	C 20	N 10	O 26	P 6	0	1
2	G	1	Total 62	C 20	N 10	O 26	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 (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$) (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	
			24	10	5	8	1	
3	K	1	Total	C	N	O	P	
			24	10	5	8	1	
3	L	1	Total	C	N	O	P	
			24	10	5	8	1	
3	M	1	Total	C	N	O	P	
			24	10	5	8	1	
3	N	1	Total	C	N	O	P	
			24	10	5	8	1	
3	O	1	Total	C	N	O	P	
			24	10	5	8	1	
3	P	1	Total	C	N	O	P	
			24	10	5	8	1	

- Molecule 4 is water.

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

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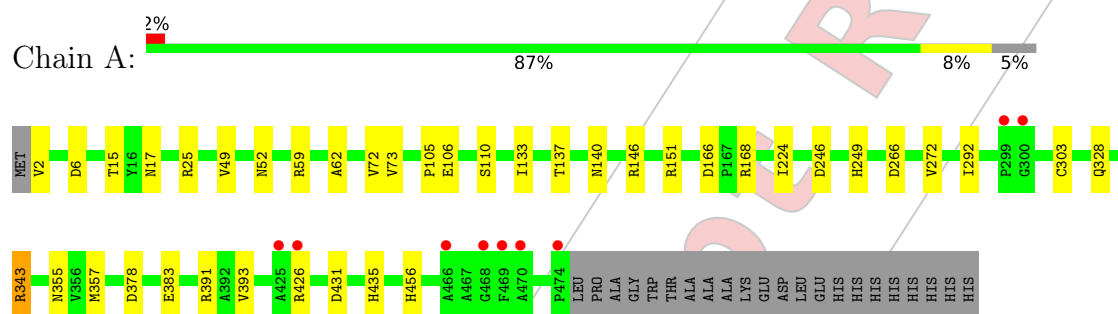
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	39	Total	O	0	0
			39	39		
4	N	30	Total	O	0	0
			30	30		
4	O	34	Total	O	0	0
			34	34		
4	P	34	Total	O	0	0
			34	34		

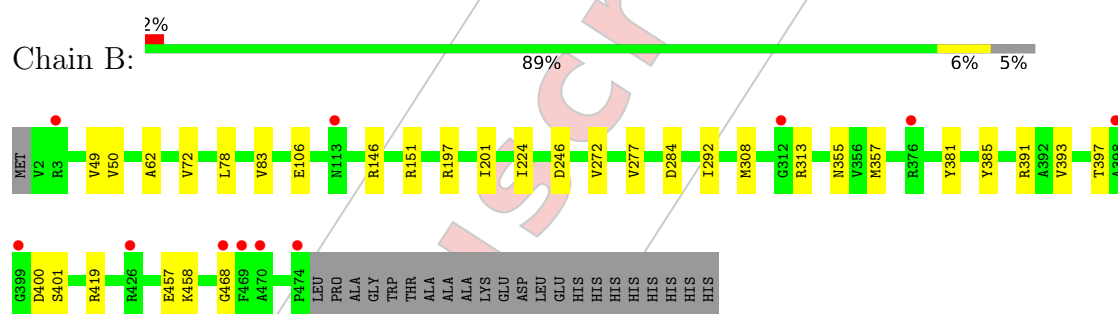
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

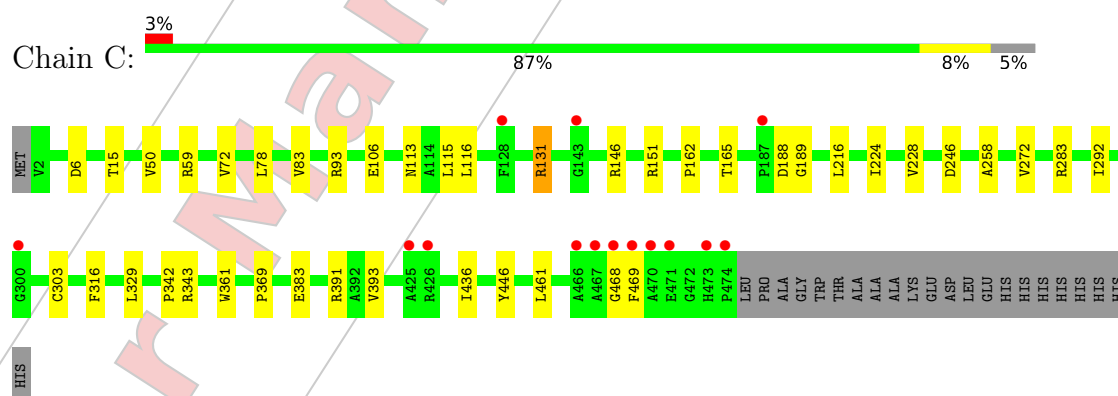
• Molecule 1: GMP reductase



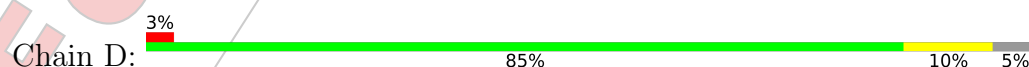
• Molecule 1: GMP reductase

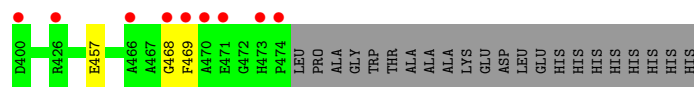


• Molecule 1: GMP reductase

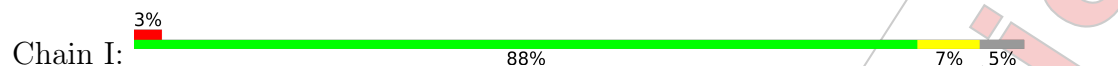


• Molecule 1: GMP reductase

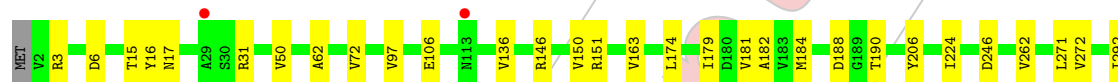
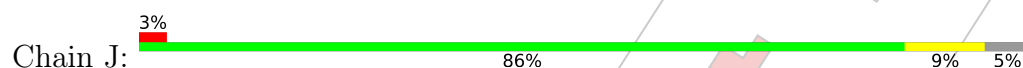




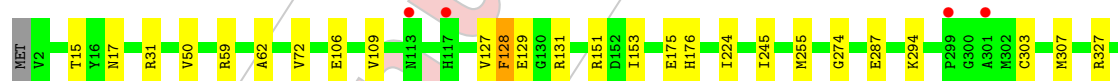
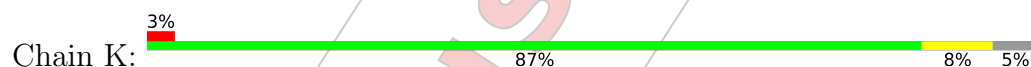
- Molecule 1: GMP reductase



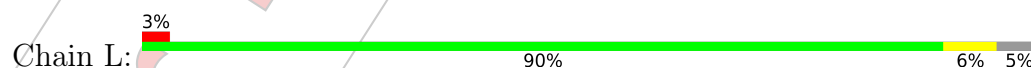
- Molecule 1: GMP reductase

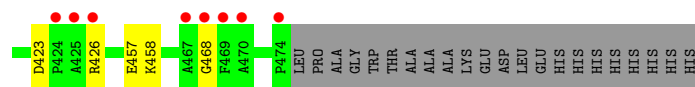


- Molecule 1: GMP reductase

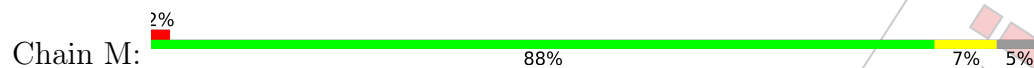


- Molecule 1: GMP reductase

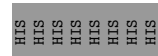
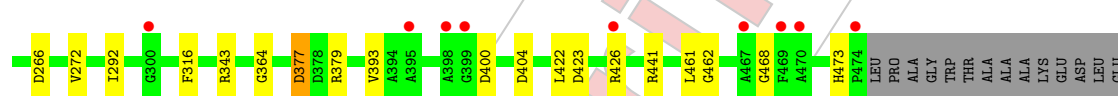
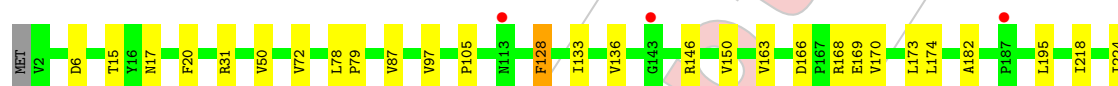
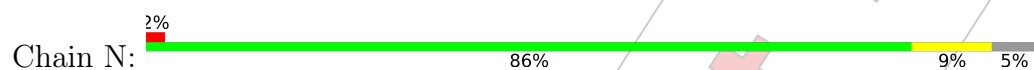




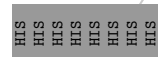
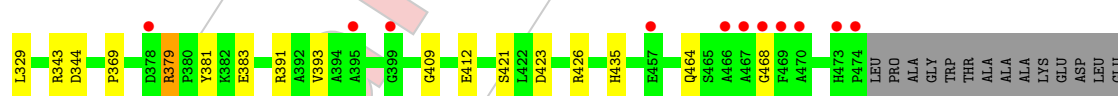
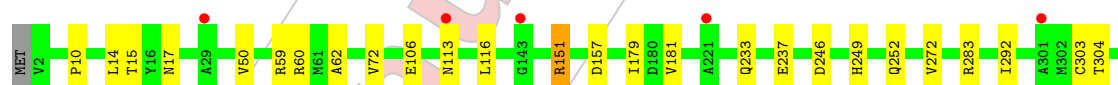
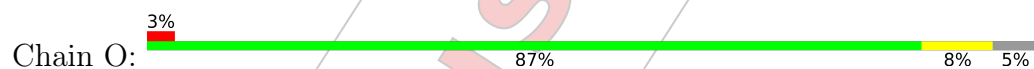
● Molecule 1: GMP reductase



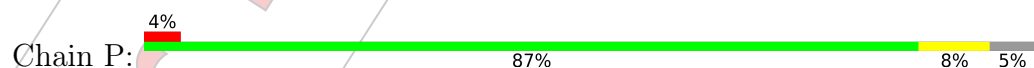
● Molecule 1: GMP reductase

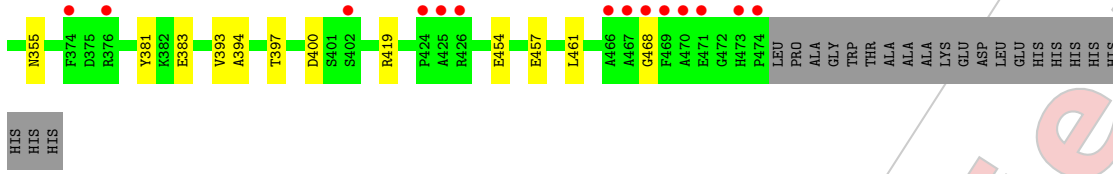


● Molecule 1: GMP reductase



● 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)	Xtrriage
Refinement program	PHENIX 1.21_5204	Depositor
R, R_{free}	0.200 , 0.230 0.199 , 0.229	Depositor DCC
R_{free} test set	16967 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/3489	0.53	0/4753
1	B	0.27	0/3483	0.52	0/4746
1	C	0.28	0/3483	0.52	0/4746
1	D	0.28	0/3489	0.52	0/4753
1	E	0.28	0/3489	0.53	0/4753
1	F	0.29	0/3484	0.53	0/4747
1	G	0.28	0/3489	0.53	0/4753
1	H	0.28	0/3483	0.52	0/4746
1	I	0.27	0/3489	0.53	0/4753
1	J	0.27	0/3484	0.52	0/4747
1	K	0.28	0/3489	0.53	0/4753
1	L	0.28	0/3485	0.53	0/4748
1	M	0.28	0/3483	0.51	0/4746
1	N	0.27	0/3489	0.52	0/4753
1	O	0.27	0/3483	0.52	0/4746
1	P	0.27	0/3489	0.53	0/4753
All	All	0.28	0/55780	0.52	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3429	0	3407	23	0
1	B	3423	0	3396	18	0
1	C	3423	0	3396	28	0
1	D	3429	0	3407	27	0
1	E	3429	0	3407	19	0
1	F	3424	0	3398	21	0
1	G	3429	0	3407	17	0
1	H	3423	0	3396	20	0
1	I	3429	0	3407	20	0
1	J	3424	0	3398	33	0
1	K	3429	0	3407	26	0
1	L	3425	0	3400	21	0
1	M	3423	0	3396	23	0
1	N	3429	0	3407	26	0
1	O	3423	0	3396	28	0
1	P	3429	0	3407	27	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	336	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 (336) 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: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:O:113:ASN:HA	1:O:116:LEU:HD12	1.75	0.66
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: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:B:146:ARG:HH12	1:G:383:GLU:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:J:146:ARG:HH12	1:O:383:GLU:HB2	1.74	0.52
1:I:302:MET:HE3	1:I:418:SER:HB2	1.91	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
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: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: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:H:369:PRO:HB3	2:H:501[A]:ATP:H5'2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:369:PRO:HB3	2:L:502[B]:ATP:H5'2	1.92	0.51
1:H:360:SER:OG	3:H:502:5GP:O3P	2.25	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:328:GLN:CD	1:J:3:ARG:HD3	2.37	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:M:262:VAL:HG11	1:M:271:LEU:HD21	1.99	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
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:K:245:ILE:HG22	1:K:255:MET:HE1	1.99	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:P:16:TYR:C	1:P:343:ARG:HH21	2.23	0.42
1:A:106:GLU:CD	1:A:151:ARG:HH22	2.17	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:J:343:ARG:HE	1:K:307:MET:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:426:ARG:HB3	1:A:431:ASP:CG	2.40	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:ARG:HH12	1:P:383:GLU:HB2	1.86	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: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
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:J:206:TYR:OH	1:J:434:ASP:OD1	2.33	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: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: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:F:426:ARG:HB3	1:F:431:ASP:CG	2.42	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:P:225:ASN:CG	1:P:394:ALA:H	2.22	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%)	345 (98%)	6 (2%)	56	72
1	B	350/372 (94%)	347 (99%)	3 (1%)	75	87
1	C	350/372 (94%)	347 (99%)	3 (1%)	75	87
1	D	351/372 (94%)	347 (99%)	4 (1%)	70	83
1	E	351/372 (94%)	348 (99%)	3 (1%)	75	87
1	F	350/372 (94%)	345 (99%)	5 (1%)	62	77
1	G	351/372 (94%)	348 (99%)	3 (1%)	75	87
1	H	350/372 (94%)	345 (99%)	5 (1%)	62	77
1	I	351/372 (94%)	347 (99%)	4 (1%)	70	83
1	J	350/372 (94%)	345 (99%)	5 (1%)	62	77
1	K	351/372 (94%)	348 (99%)	3 (1%)	75	87
1	L	350/372 (94%)	349 (100%)	1 (0%)	91	96
1	M	350/372 (94%)	348 (99%)	2 (1%)	84	92
1	N	351/372 (94%)	347 (99%)	4 (1%)	70	83
1	O	350/372 (94%)	347 (99%)	3 (1%)	75	87
1	P	351/372 (94%)	351 (100%)	0	100	100
All	All	5608/5952 (94%)	5554 (99%)	54 (1%)	75	85

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	266	ASP
1	A	328	GLN
1	A	343	ARG
1	A	355	ASN
1	A	378	ASP
1	B	355	ASN
1	B	397	THR
1	B	400	ASP
1	C	6	ASP
1	C	115	LEU
1	C	131	ARG
1	D	59	ARG
1	D	138	GLU
1	D	343	ARG
1	D	400	ASP

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Mol	Chain	Res	Type
1	E	151	ARG
1	E	389	SER
1	E	417	THR
1	F	31	ARG
1	F	328	GLN
1	F	355	ASN
1	F	377	ASP
1	F	379	ARG
1	G	6	ASP
1	G	378	ASP
1	G	417	THR
1	H	128	PHE
1	H	355	ASN
1	H	360	SER
1	H	457[A]	GLU
1	H	457[B]	GLU
1	I	6	ASP
1	I	168	ARG
1	I	379	ARG
1	I	426	ARG
1	J	6	ASP
1	J	328	GLN
1	J	355	ASN
1	J	379	ARG
1	J	426	ARG
1	K	128	PHE
1	K	287	GLU
1	K	401	SER
1	L	404	ASP
1	M	27	ASP
1	M	355	ASN
1	N	6	ASP
1	N	128	PHE
1	N	266	ASP
1	N	377	ASP
1	O	151	ARG
1	O	157	ASP
1	O	379	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	233	GLN
1	C	328	GLN
1	D	252	GLN
1	D	435	HIS
1	I	117	HIS
1	J	117	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	C	501[A]	-	26,33,33	0.73	0	31,52,52	0.65	0
3	5GP	B	502	-	22,26,26	0.56	0	26,40,40	0.79	0
2	ATP	C	501[B]	-	26,33,33	0.74	0	31,52,52	0.61	0
2	ATP	A	501[B]	-	26,33,33	0.73	0	31,52,52	0.64	0
2	ATP	F	501[A]	-	26,33,33	0.74	0	31,52,52	0.64	0
3	5GP	O	501	-	22,26,26	0.54	0	26,40,40	0.74	0
3	5GP	I	502	-	22,26,26	0.51	0	26,40,40	0.74	0
3	5GP	N	501	-	22,26,26	0.57	0	26,40,40	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	F	501[B]	-	26,33,33	0.73	0	31,52,52	0.65	0
2	ATP	J	501[A]	-	26,33,33	0.73	0	31,52,52	0.65	0
2	ATP	K	501[A]	-	26,33,33	0.74	0	31,52,52	0.65	0
2	ATP	B	501[A]	-	26,33,33	0.73	0	31,52,52	0.62	0
2	ATP	E	501[A]	-	26,33,33	0.73	0	31,52,52	0.63	0
3	5GP	A	502	-	22,26,26	0.55	0	26,40,40	0.77	0
3	5GP	D	502	-	22,26,26	0.55	0	26,40,40	0.76	0
2	ATP	J	501[B]	-	26,33,33	0.73	0	31,52,52	0.63	0
2	ATP	K	501[B]	-	26,33,33	0.74	0	31,52,52	0.63	0
2	ATP	B	501[B]	-	26,33,33	0.74	0	31,52,52	0.61	0
2	ATP	E	501[B]	-	26,33,33	0.74	0	31,52,52	0.62	0
2	ATP	M	502[A]	-	26,33,33	0.74	0	31,52,52	0.64	0
3	5GP	F	502	-	22,26,26	0.59	0	26,40,40	0.80	0
3	5GP	P	501	-	22,26,26	0.52	0	26,40,40	0.76	0
3	5GP	C	502	-	22,26,26	0.54	0	26,40,40	0.74	0
2	ATP	M	502[B]	-	26,33,33	0.74	0	31,52,52	0.63	0
3	5GP	G	502	-	22,26,26	0.47	0	26,40,40	0.79	0
2	ATP	P	502[A]	-	26,33,33	0.74	0	31,52,52	0.66	0
3	5GP	H	502	-	22,26,26	0.51	0	26,40,40	0.82	0
3	5GP	M	501	-	22,26,26	0.60	0	26,40,40	0.77	0
3	5GP	K	502	-	22,26,26	0.53	0	26,40,40	0.73	0
2	ATP	P	502[B]	-	26,33,33	0.73	0	31,52,52	0.61	0
2	ATP	O	502[A]	-	26,33,33	0.73	0	31,52,52	0.66	0
2	ATP	O	502[B]	-	26,33,33	0.73	0	31,52,52	0.62	0
2	ATP	I	501[A]	-	26,33,33	0.73	0	31,52,52	0.66	0
2	ATP	I	501[B]	-	26,33,33	0.74	0	31,52,52	0.61	0
2	ATP	H	501[A]	-	26,33,33	0.73	0	31,52,52	0.75	0
2	ATP	L	502[A]	-	26,33,33	0.73	0	31,52,52	0.65	0
2	ATP	N	502[A]	-	26,33,33	0.73	0	31,52,52	0.64	0
2	ATP	G	501[A]	-	26,33,33	0.73	0	31,52,52	0.66	0
3	5GP	L	501	-	22,26,26	0.56	0	26,40,40	0.76	0
2	ATP	D	501[A]	-	26,33,33	0.73	0	31,52,52	0.65	0
2	ATP	H	501[B]	-	26,33,33	0.74	0	31,52,52	0.66	0
2	ATP	L	502[B]	-	26,33,33	0.73	0	31,52,52	0.63	0
2	ATP	N	502[B]	-	26,33,33	0.74	0	31,52,52	0.62	0
3	5GP	E	502	-	22,26,26	0.56	0	26,40,40	0.74	0
2	ATP	G	501[B]	-	26,33,33	0.74	0	31,52,52	0.66	0
2	ATP	D	501[B]	-	26,33,33	0.74	0	31,52,52	0.64	0
2	ATP	A	501[A]	-	26,33,33	0.74	0	31,52,52	0.64	0
3	5GP	J	502	-	22,26,26	0.54	0	26,40,40	0.80	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	C	501[A]	-	-	1/18/38/38	0/3/3/3
3	5GP	B	502	-	-	0/6/26/26	0/3/3/3
2	ATP	C	501[B]	-	-	7/18/38/38	0/3/3/3
2	ATP	A	501[B]	-	-	4/18/38/38	0/3/3/3
2	ATP	F	501[A]	-	-	0/18/38/38	0/3/3/3
3	5GP	O	501	-	-	0/6/26/26	0/3/3/3
3	5GP	I	502	-	-	0/6/26/26	0/3/3/3
3	5GP	N	501	-	-	0/6/26/26	0/3/3/3
2	ATP	F	501[B]	-	-	2/18/38/38	0/3/3/3
2	ATP	J	501[A]	-	-	2/18/38/38	0/3/3/3
2	ATP	K	501[A]	-	-	2/18/38/38	0/3/3/3
2	ATP	B	501[A]	-	-	1/18/38/38	0/3/3/3
2	ATP	E	501[A]	-	-	6/18/38/38	0/3/3/3
3	5GP	A	502	-	-	0/6/26/26	0/3/3/3
3	5GP	D	502	-	-	0/6/26/26	0/3/3/3
2	ATP	J	501[B]	-	-	2/18/38/38	0/3/3/3
2	ATP	K	501[B]	-	-	9/18/38/38	0/3/3/3
2	ATP	B	501[B]	-	-	5/18/38/38	0/3/3/3
2	ATP	E	501[B]	-	-	3/18/38/38	0/3/3/3
2	ATP	M	502[A]	-	-	5/18/38/38	0/3/3/3
3	5GP	F	502	-	-	0/6/26/26	0/3/3/3
3	5GP	P	501	-	-	0/6/26/26	0/3/3/3
3	5GP	C	502	-	-	0/6/26/26	0/3/3/3
2	ATP	M	502[B]	-	-	7/18/38/38	0/3/3/3
3	5GP	G	502	-	-	0/6/26/26	0/3/3/3
2	ATP	P	502[A]	-	-	2/18/38/38	0/3/3/3
3	5GP	H	502	-	-	0/6/26/26	0/3/3/3
3	5GP	M	501	-	-	0/6/26/26	0/3/3/3
3	5GP	K	502	-	-	0/6/26/26	0/3/3/3
2	ATP	P	502[B]	-	-	6/18/38/38	0/3/3/3
2	ATP	O	502[A]	-	-	1/18/38/38	0/3/3/3
2	ATP	O	502[B]	-	-	3/18/38/38	0/3/3/3
2	ATP	I	501[A]	-	-	2/18/38/38	0/3/3/3
2	ATP	I	501[B]	-	-	9/18/38/38	0/3/3/3
2	ATP	H	501[A]	-	-	0/18/38/38	0/3/3/3
2	ATP	L	502[A]	-	-	1/18/38/38	0/3/3/3
2	ATP	N	502[A]	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	G	501[A]	-	-	0/18/38/38	0/3/3/3
3	5GP	L	501	-	-	0/6/26/26	0/3/3/3
2	ATP	D	501[A]	-	-	5/18/38/38	0/3/3/3
2	ATP	H	501[B]	-	-	2/18/38/38	0/3/3/3
2	ATP	L	502[B]	-	-	6/18/38/38	0/3/3/3
2	ATP	N	502[B]	-	-	8/18/38/38	0/3/3/3
3	5GP	E	502	-	-	0/6/26/26	0/3/3/3
2	ATP	G	501[B]	-	-	2/18/38/38	0/3/3/3
2	ATP	D	501[B]	-	-	3/18/38/38	0/3/3/3
2	ATP	A	501[A]	-	-	1/18/38/38	0/3/3/3
3	5GP	J	502	-	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (111) 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-O3A
2	E	501[A]	ATP	C5'-O5'-PA-O1A
2	I	501[B]	ATP	C5'-O5'-PA-O2A
2	K	501[B]	ATP	C5'-O5'-PA-O2A
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[B]	ATP	C5'-O5'-PA-O2A
2	N	502[B]	ATP	C5'-O5'-PA-O2A
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	P	502[B]	ATP	O4'-C4'-C5'-O5'
2	M	502[B]	ATP	C3'-C4'-C5'-O5'

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

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Mol	Chain	Res	Type	Atoms
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
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	L	502[B]	ATP	O4'-C4'-C5'-O5'
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	I	501[A]	ATP	C5'-O5'-PA-O3A
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

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Mol	Chain	Res	Type	Atoms
2	O	502[B]	ATP	PB-O3A-PA-O2A
2	P	502[A]	ATP	PA-O3A-PB-O1B
2	C	501[B]	ATP	C5'-O5'-PA-O1A
2	I	501[A]	ATP	C5'-O5'-PA-O1A
2	L	502[B]	ATP	C5'-O5'-PA-O1A
2	P	502[B]	ATP	C5'-O5'-PA-O1A

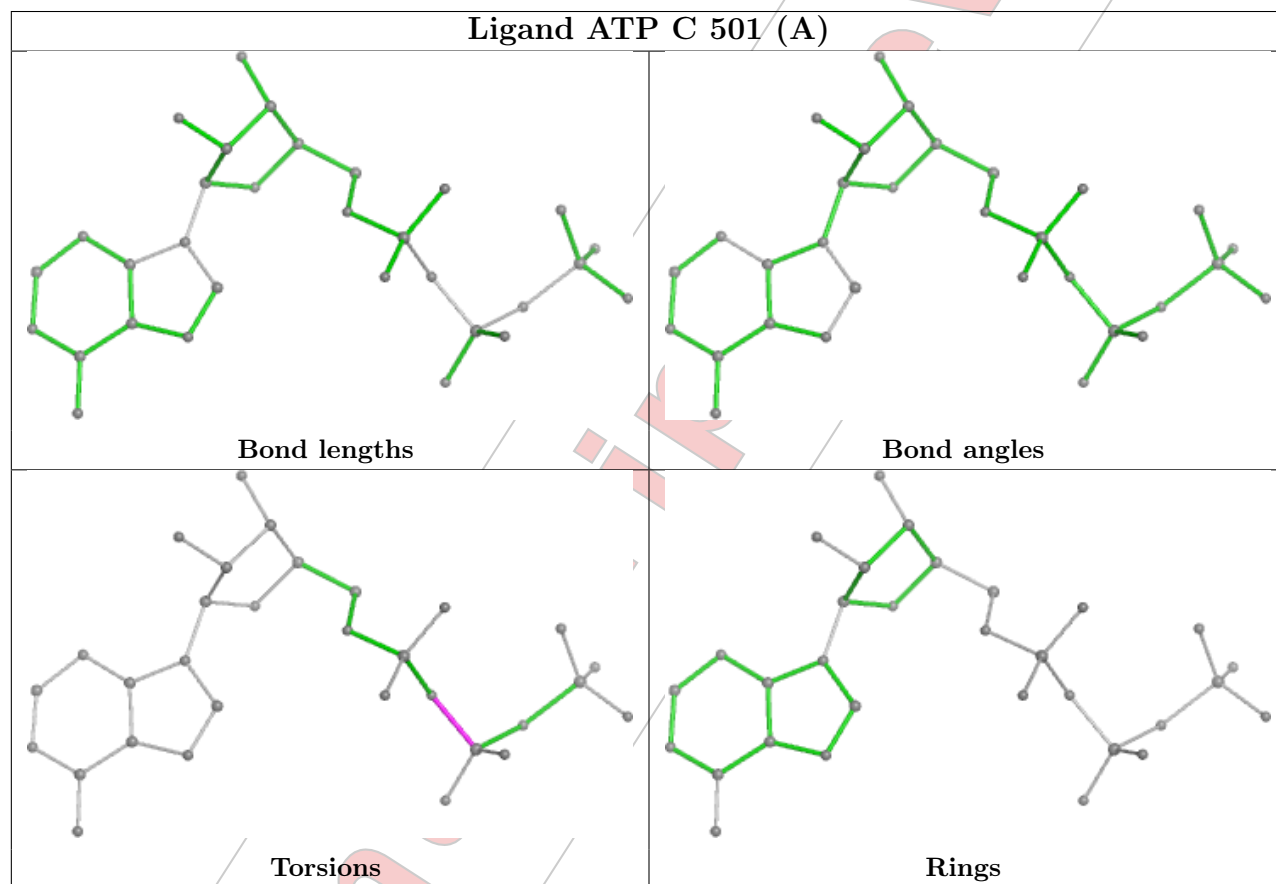
There are no ring outliers.

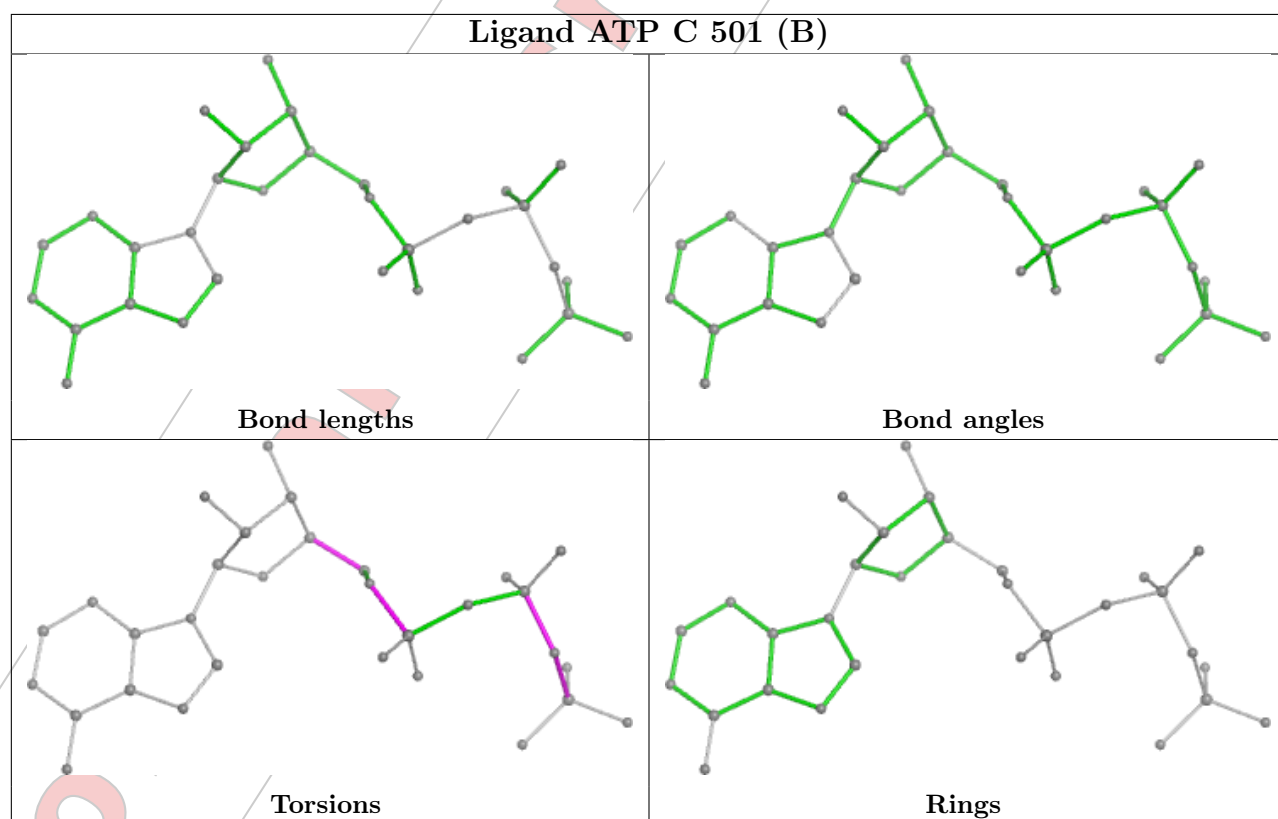
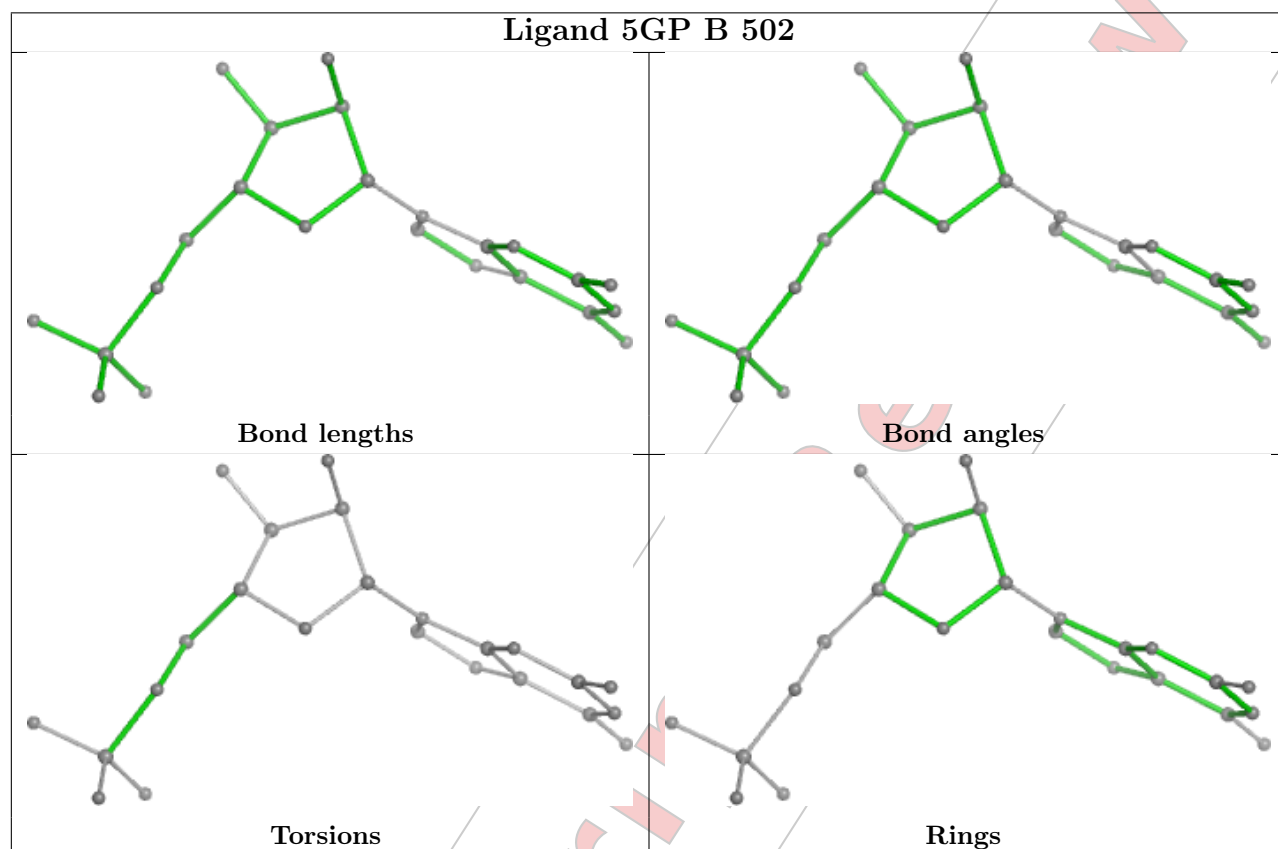
26 monomers are involved in 35 short contacts:

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

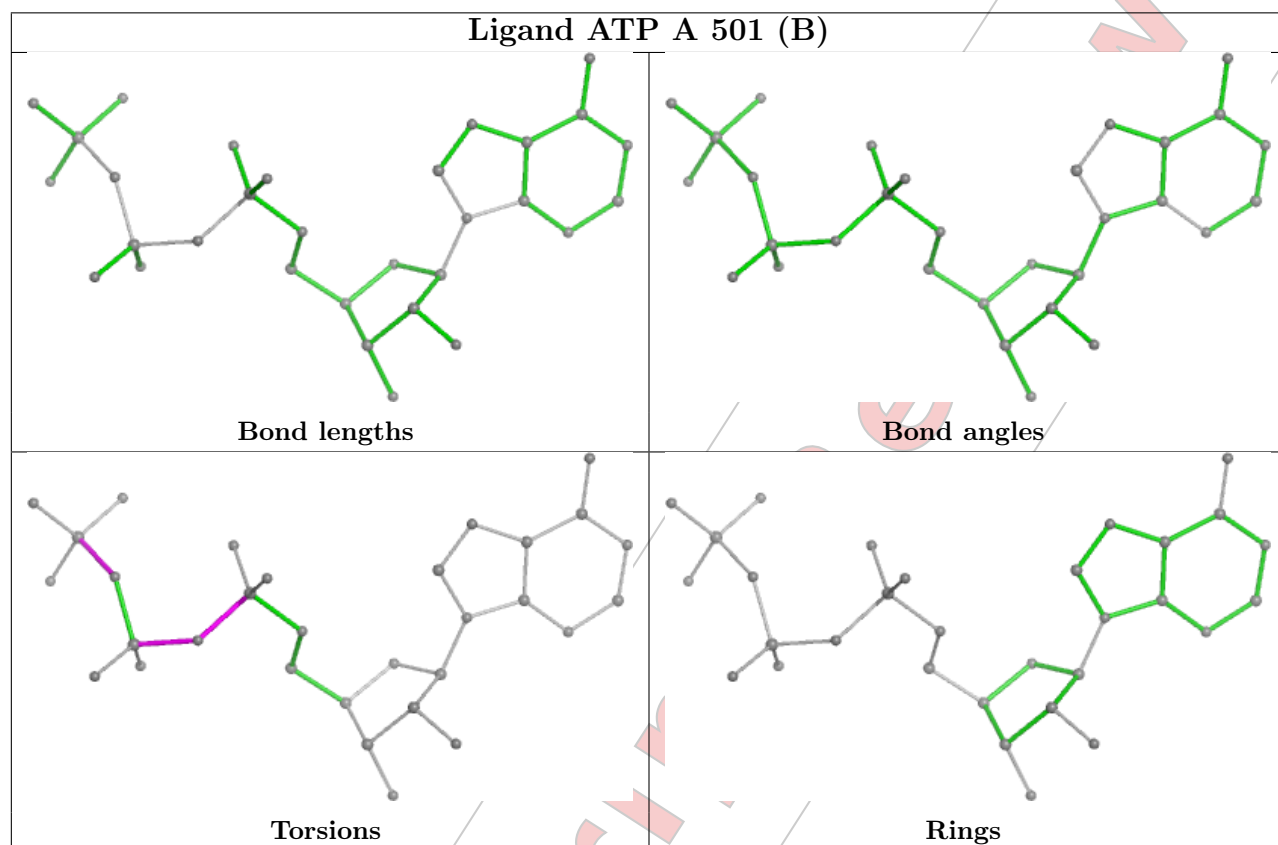
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

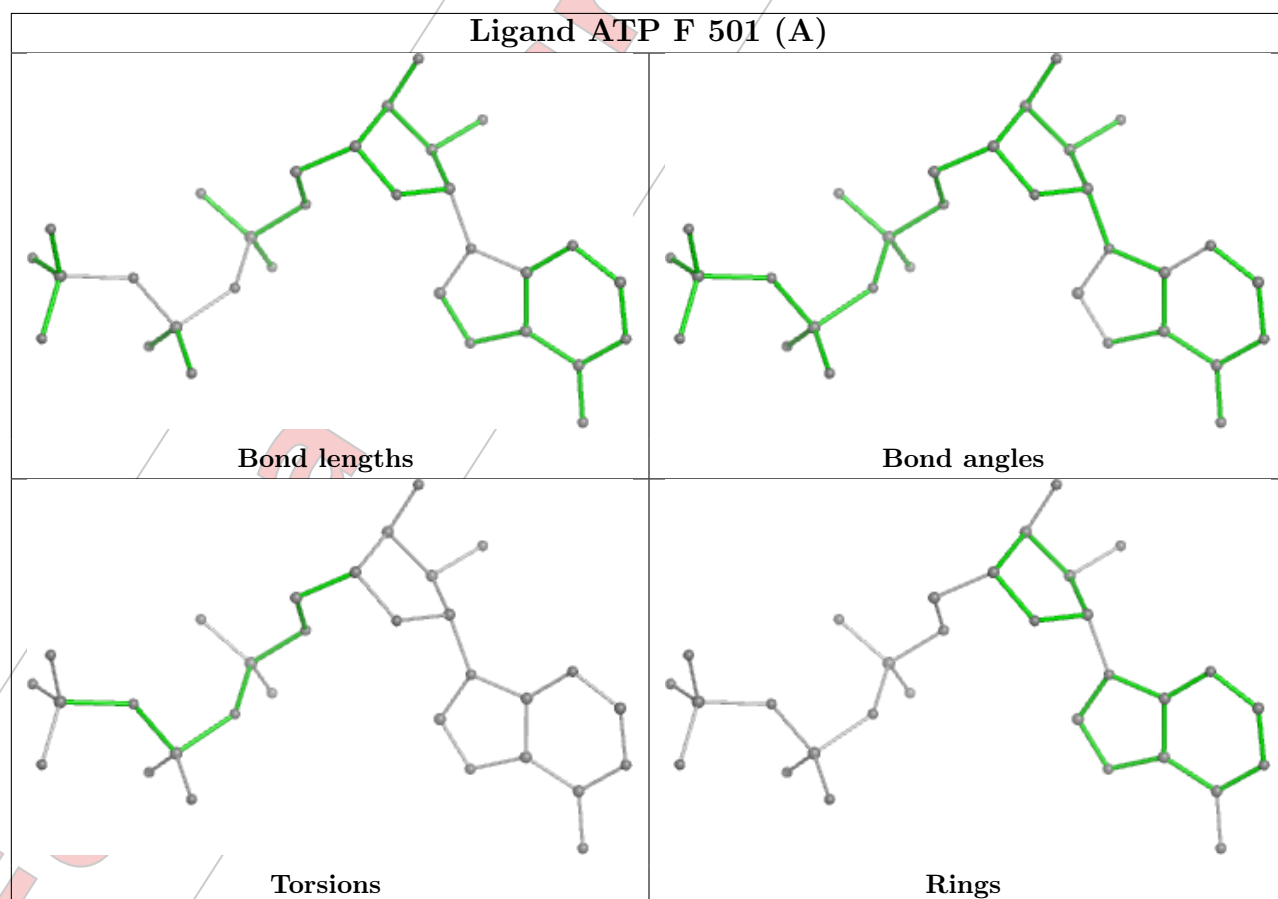




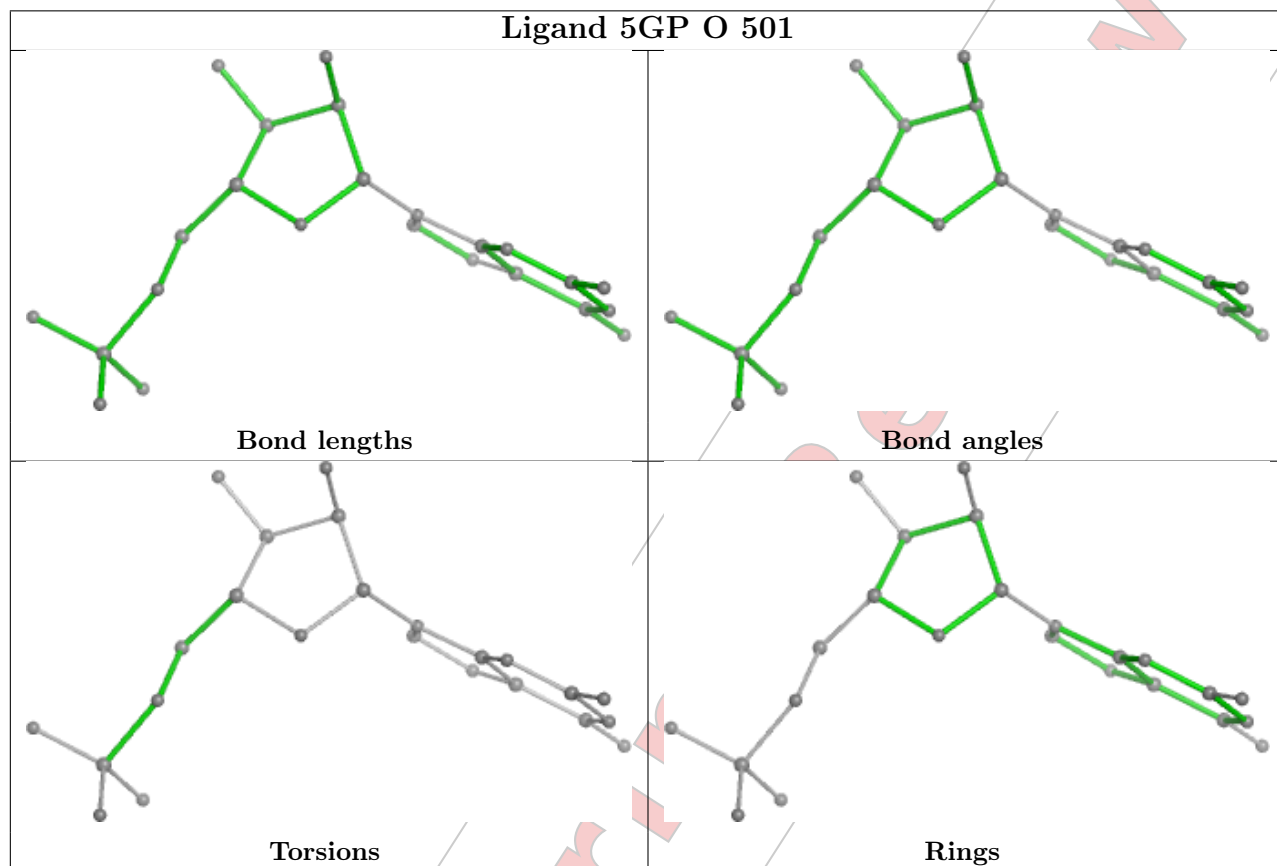
Ligand ATP A 501 (B)



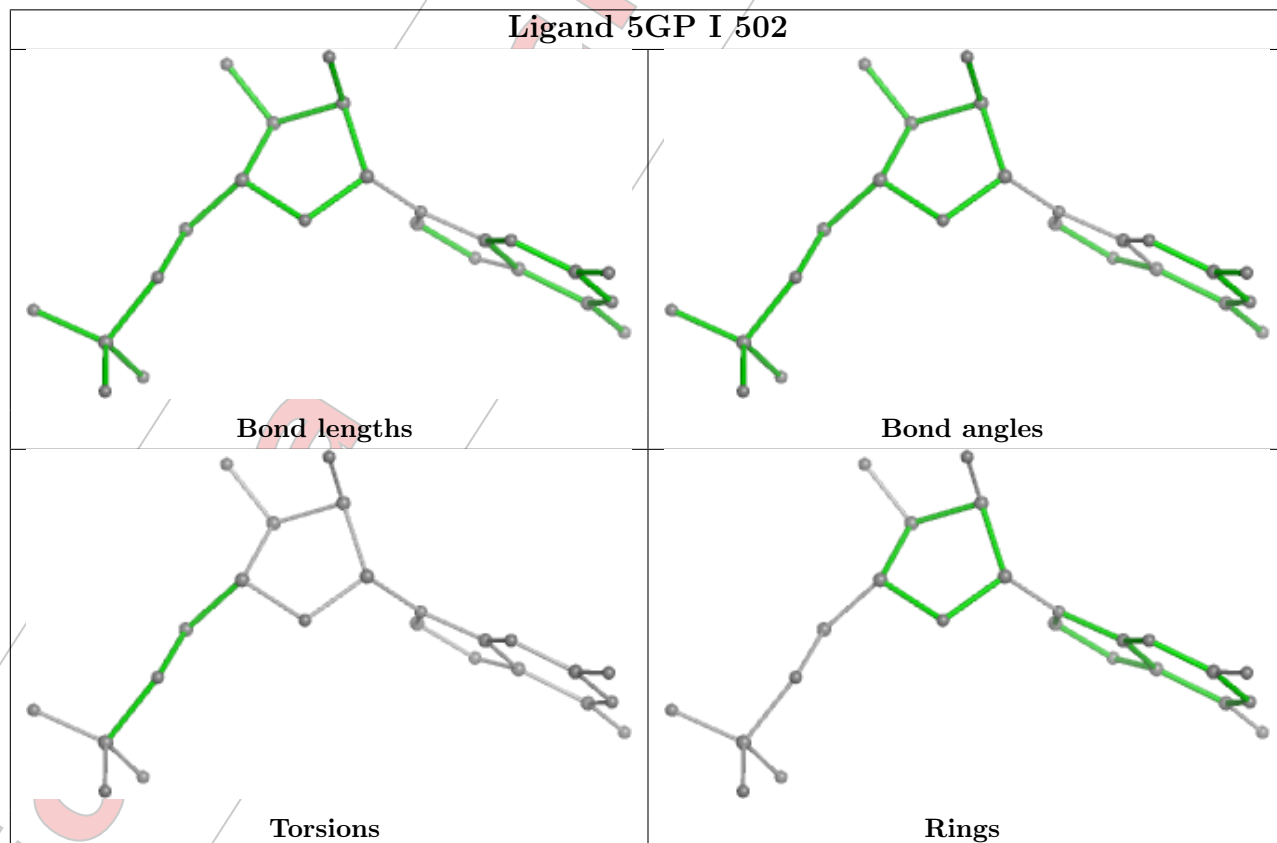
Ligand ATP F 501 (A)

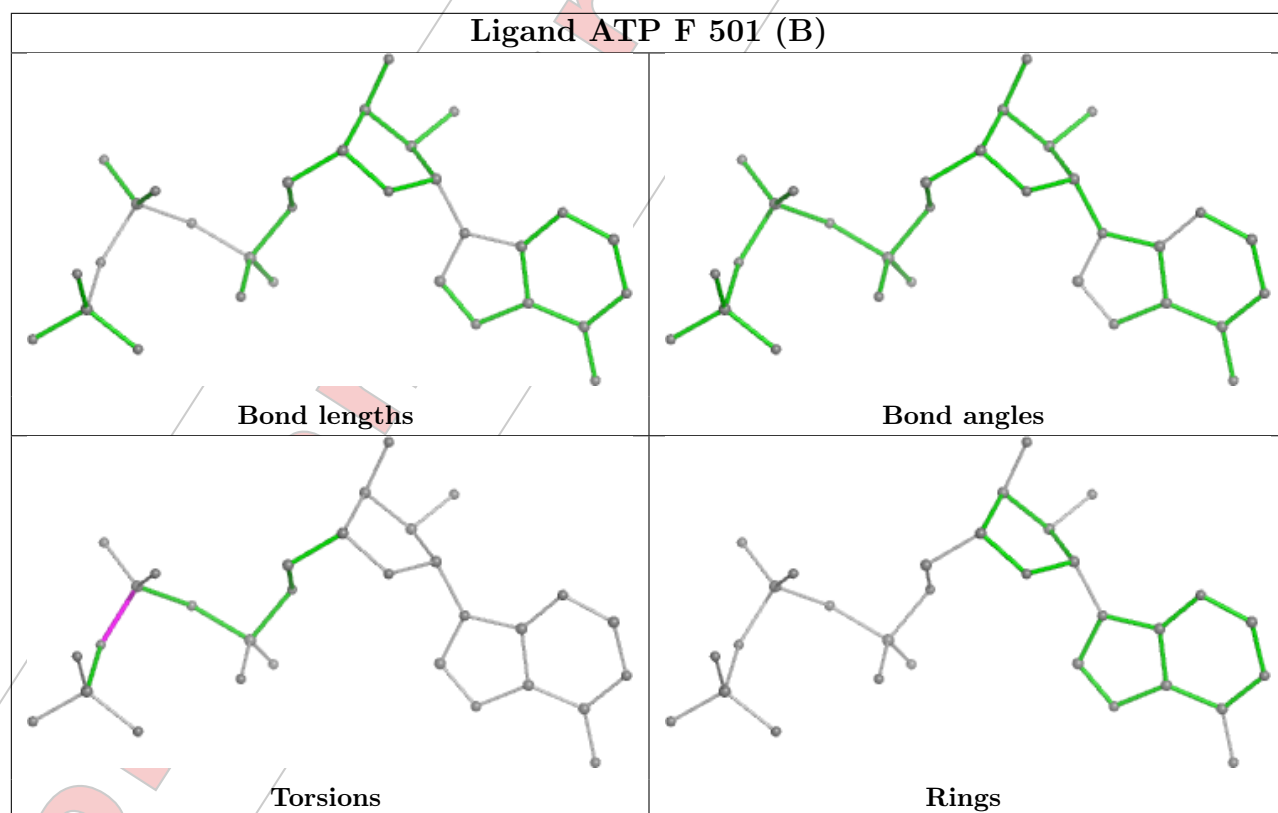
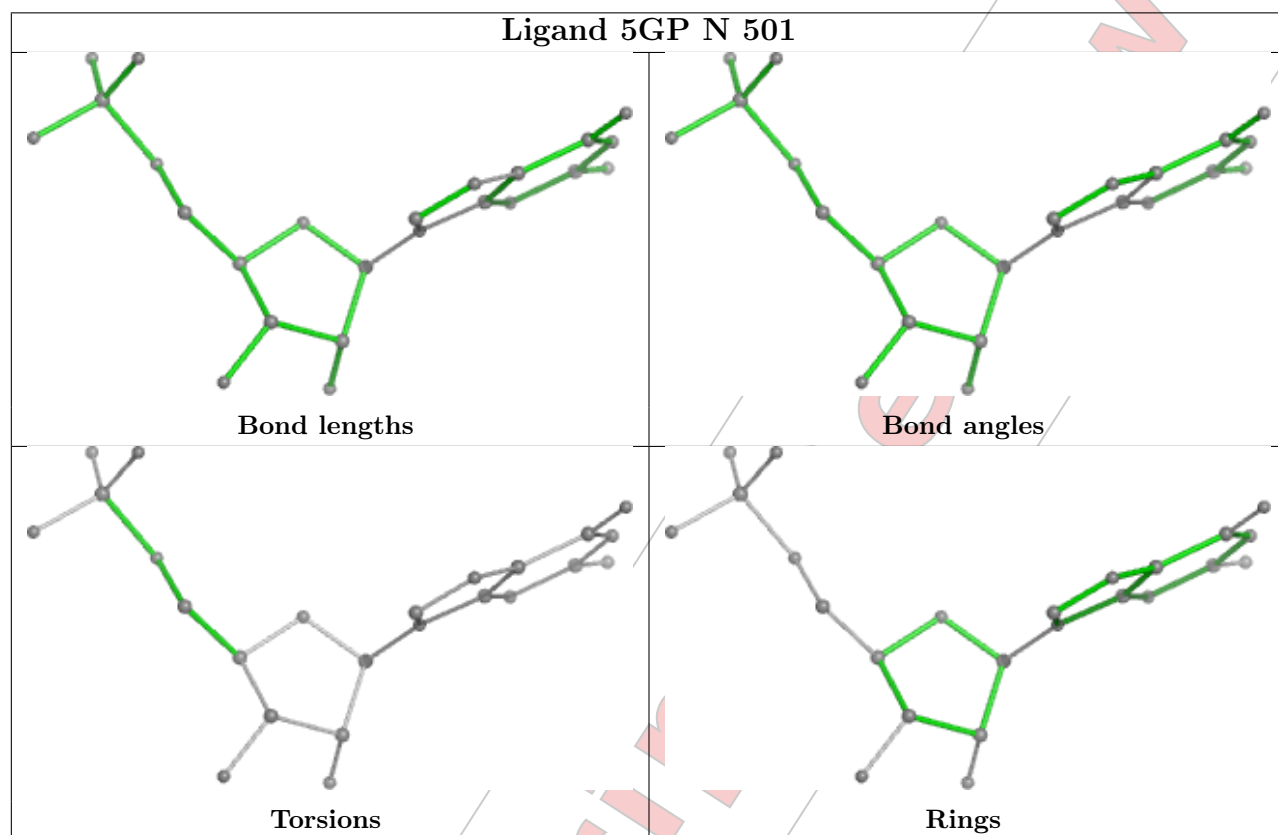


Ligand 5GP O 501

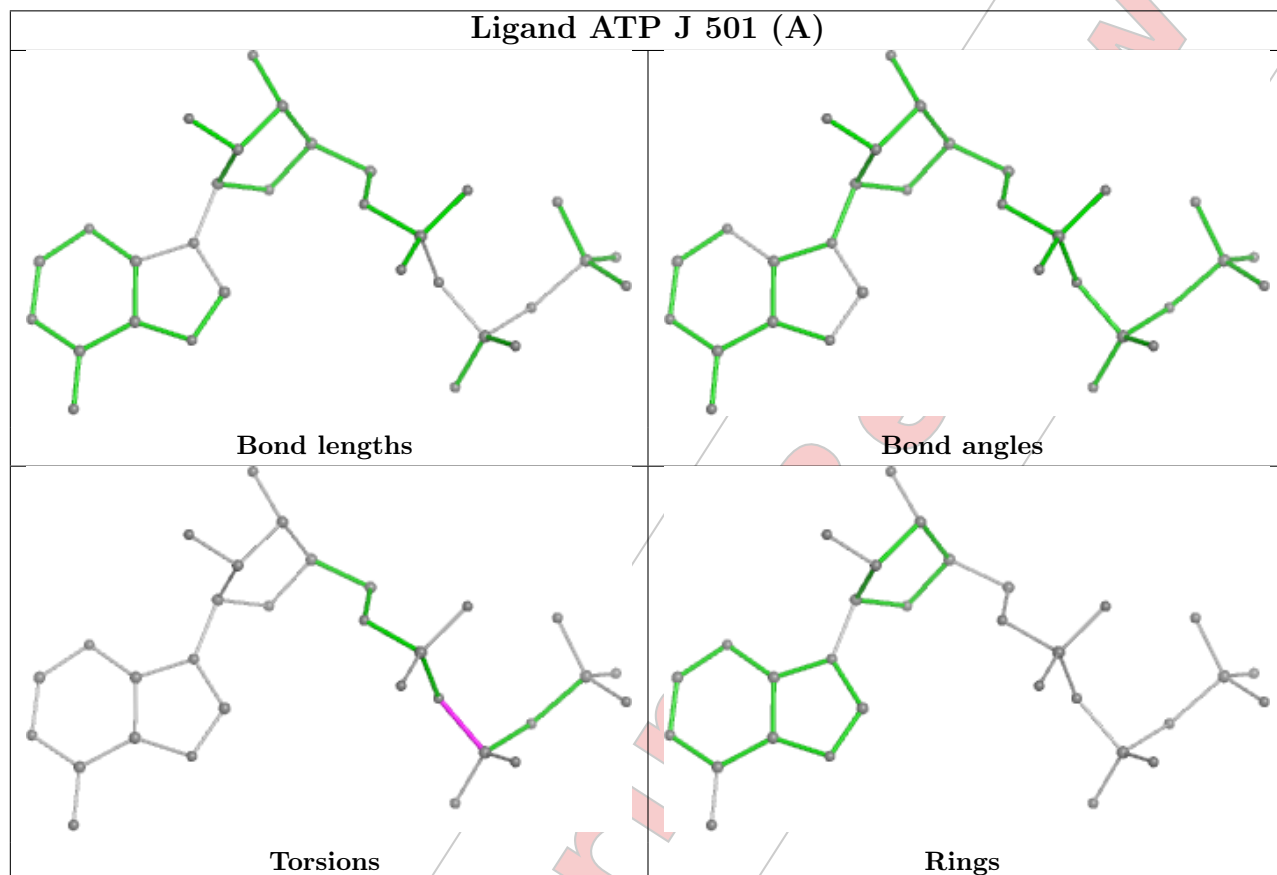


Ligand 5GP I 502

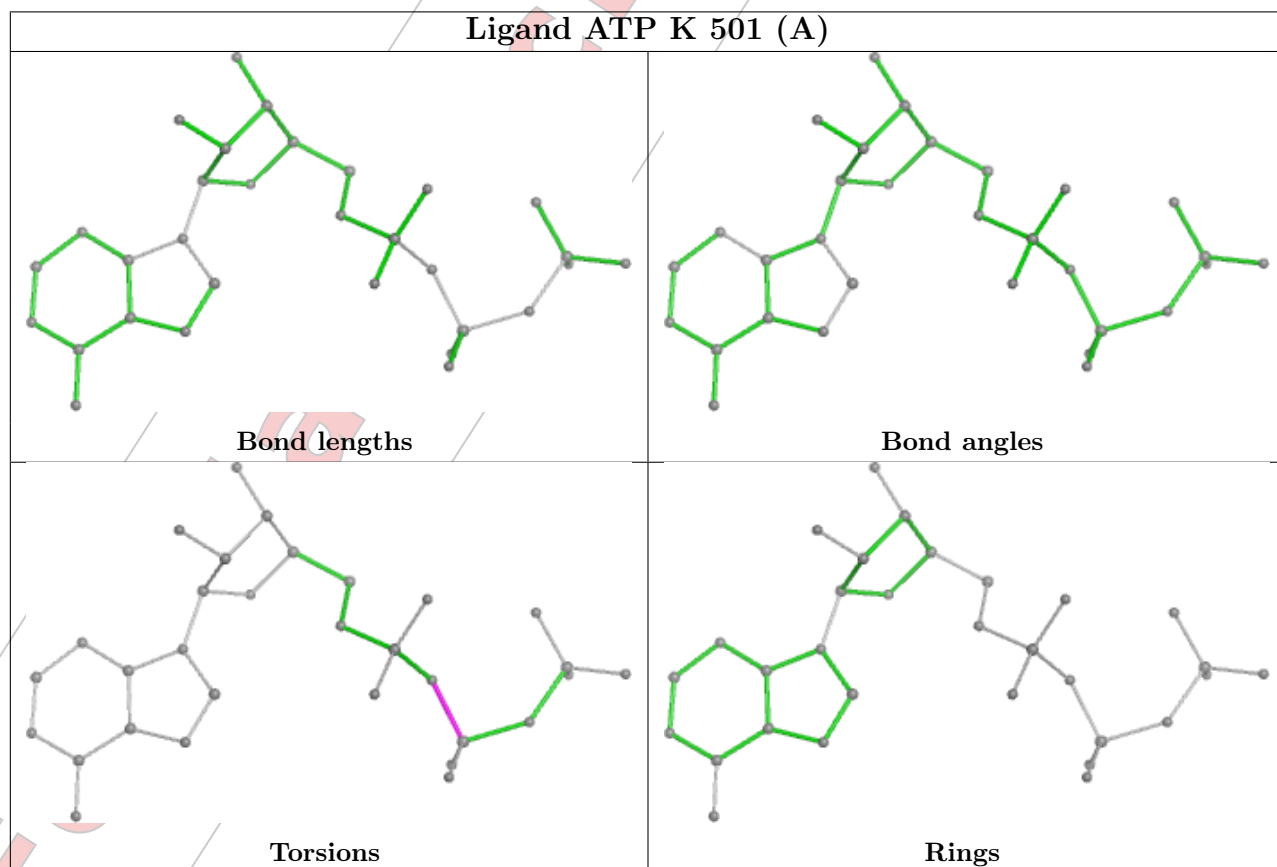


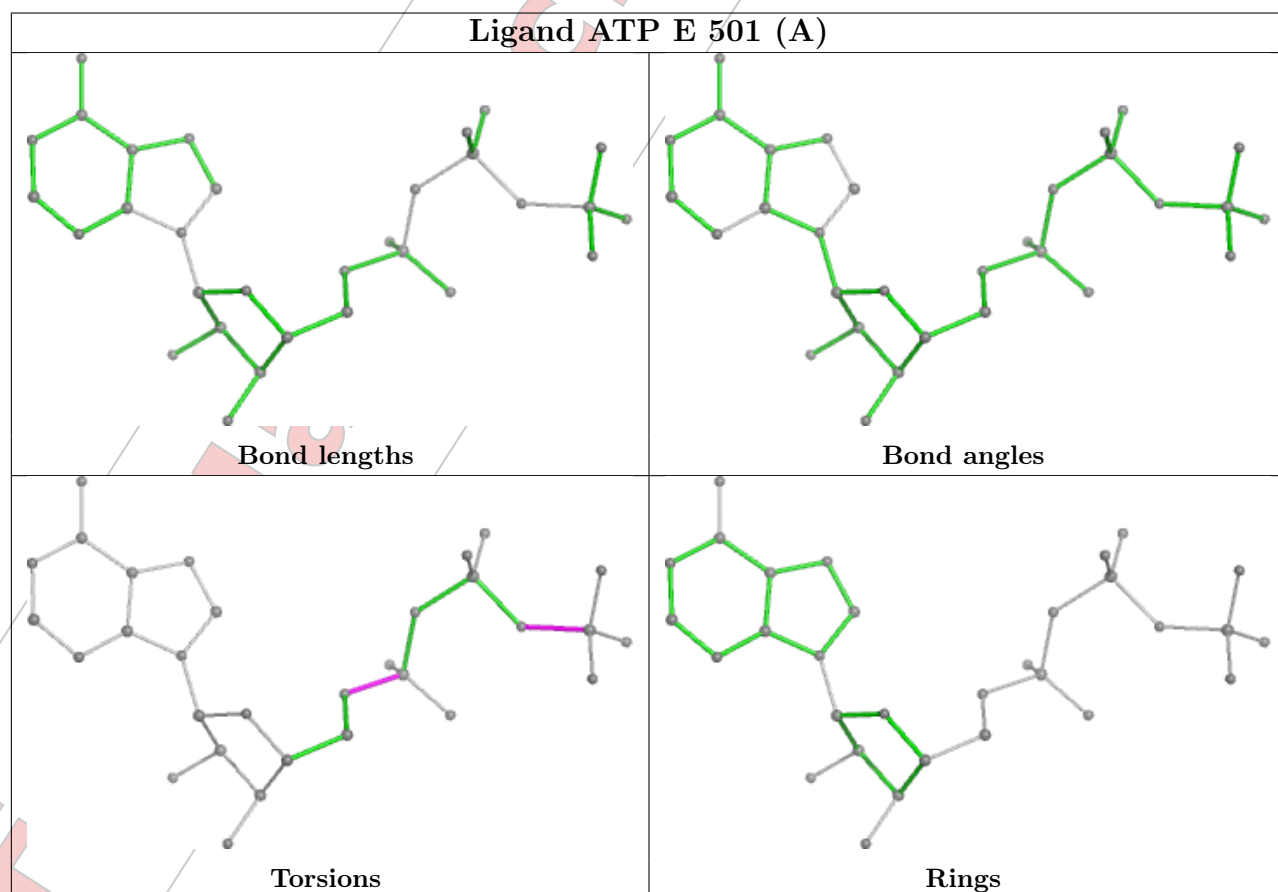
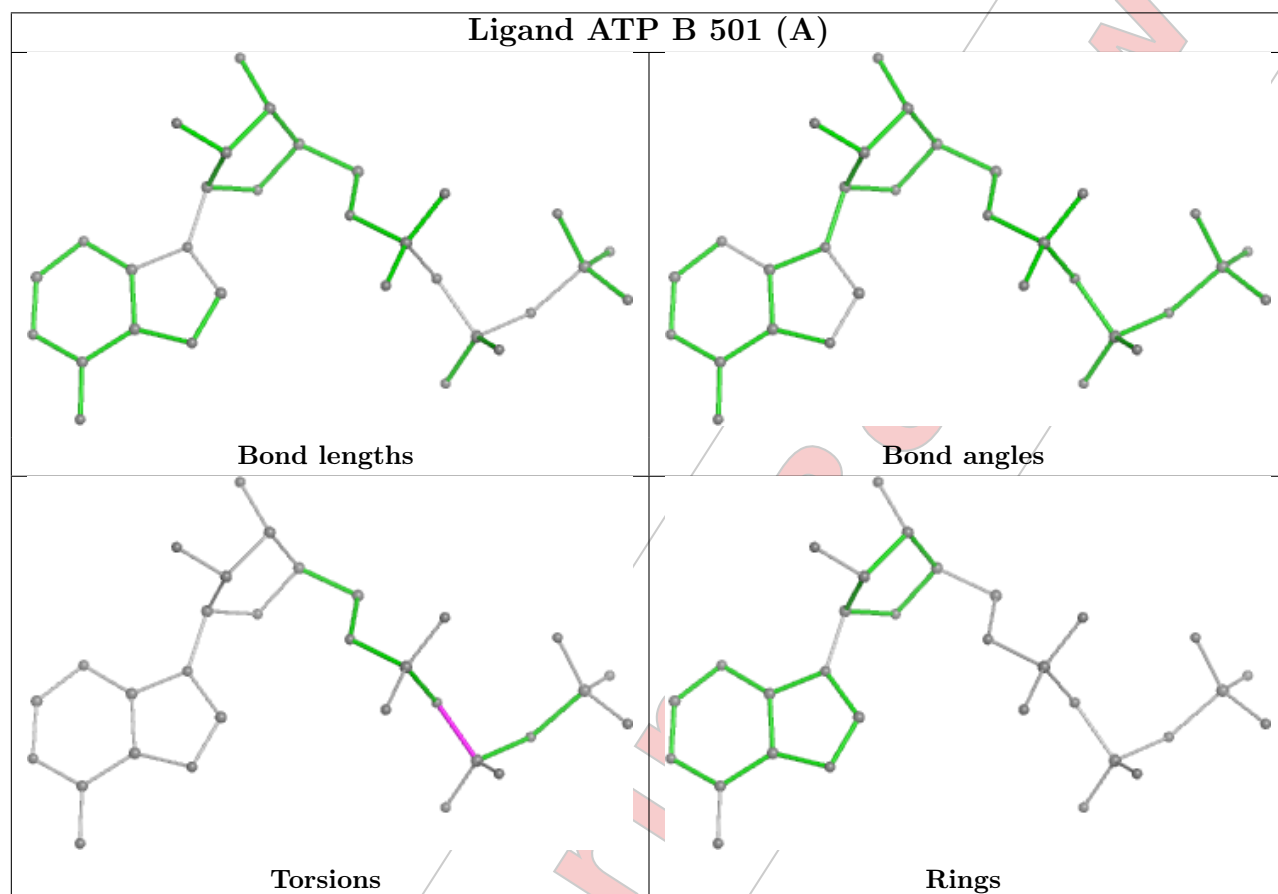


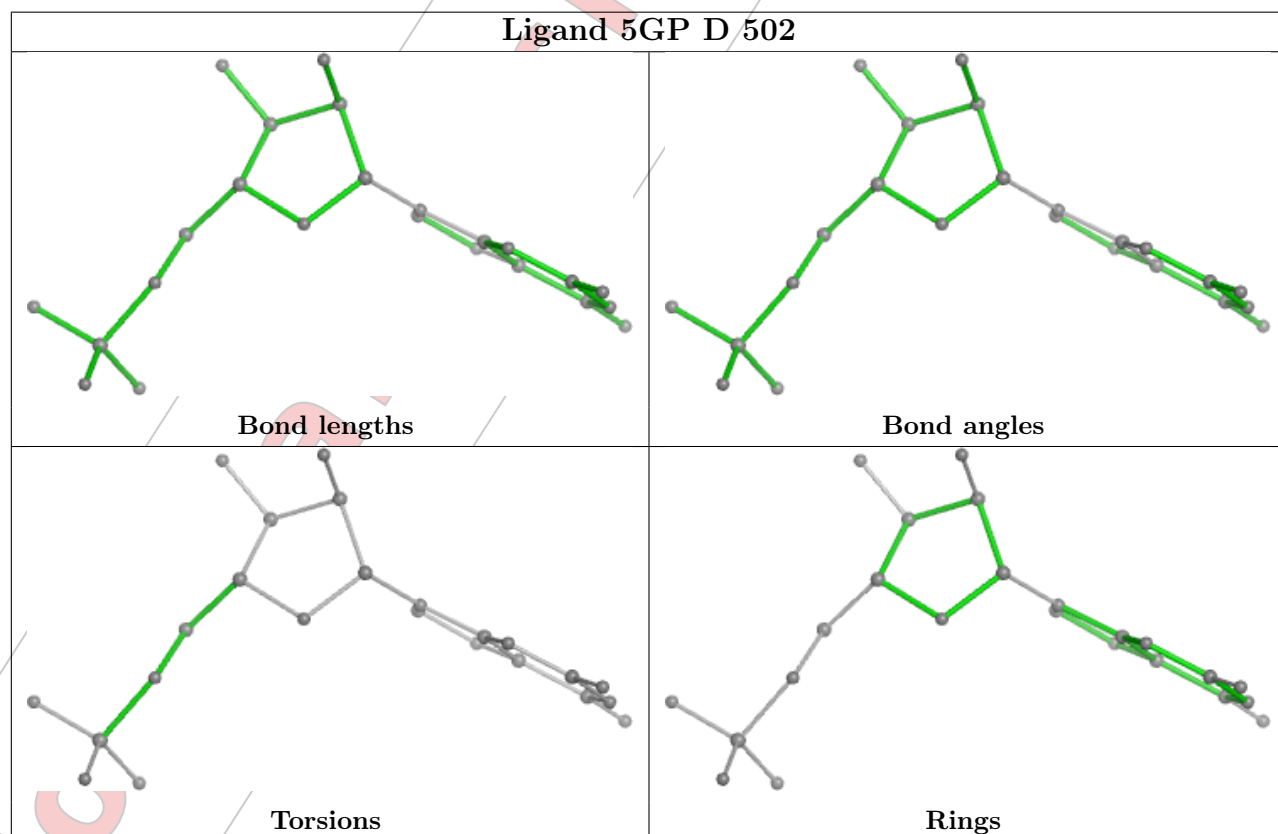
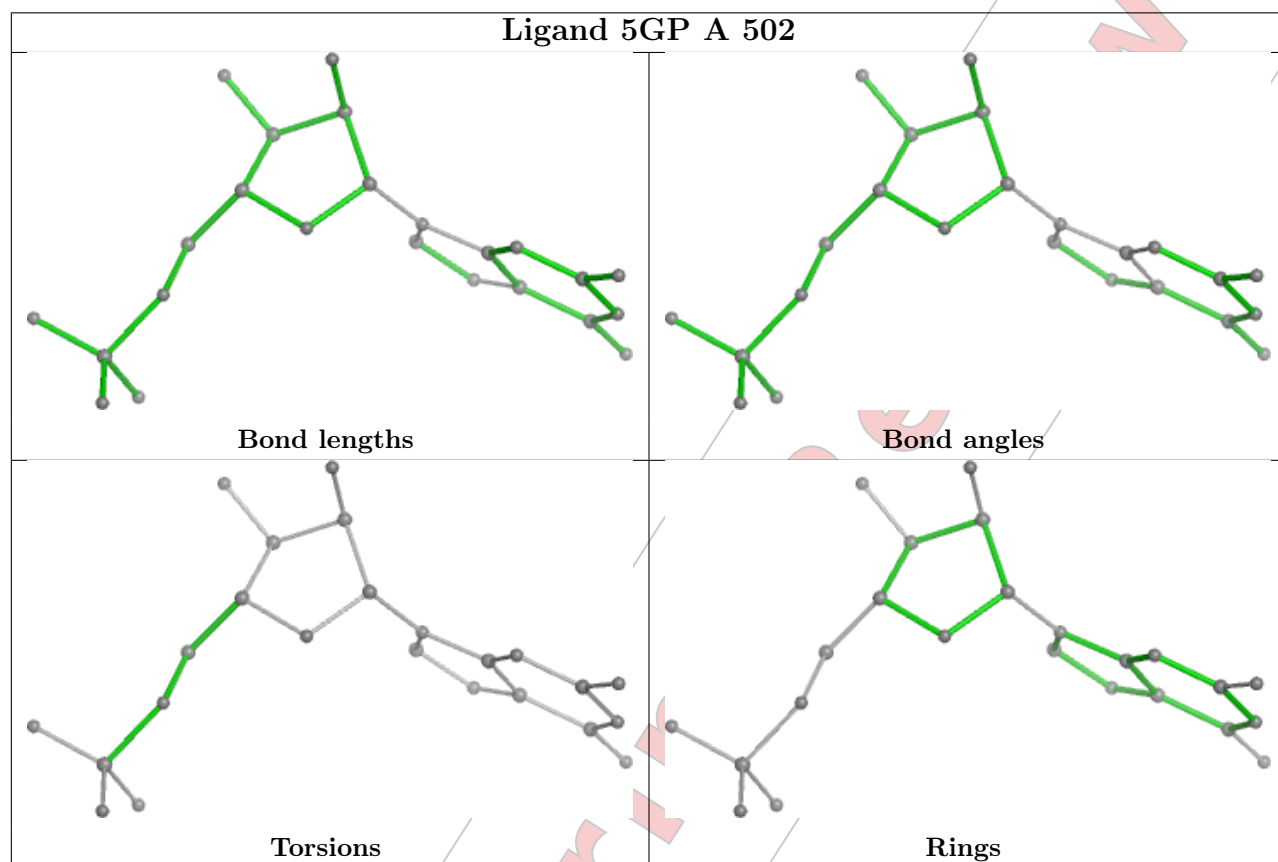
Ligand ATP J 501 (A)



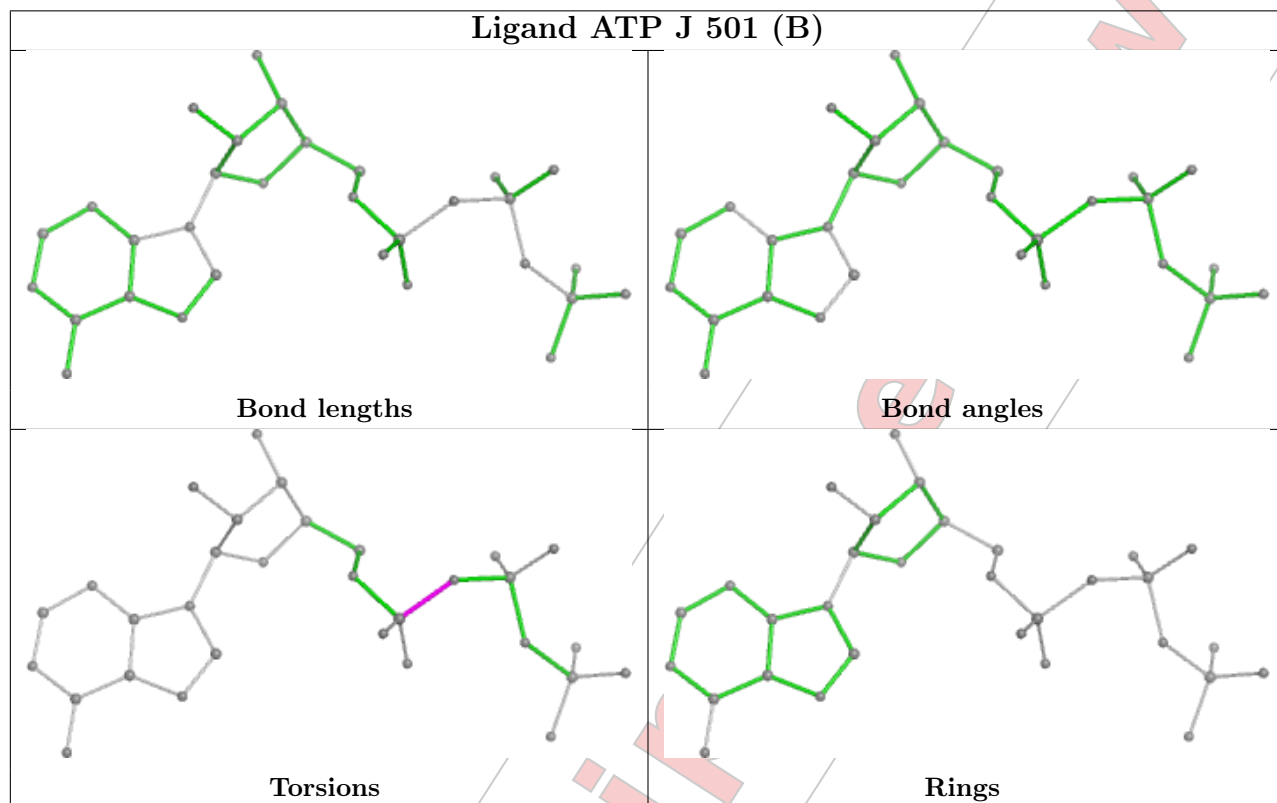
Ligand ATP K 501 (A)



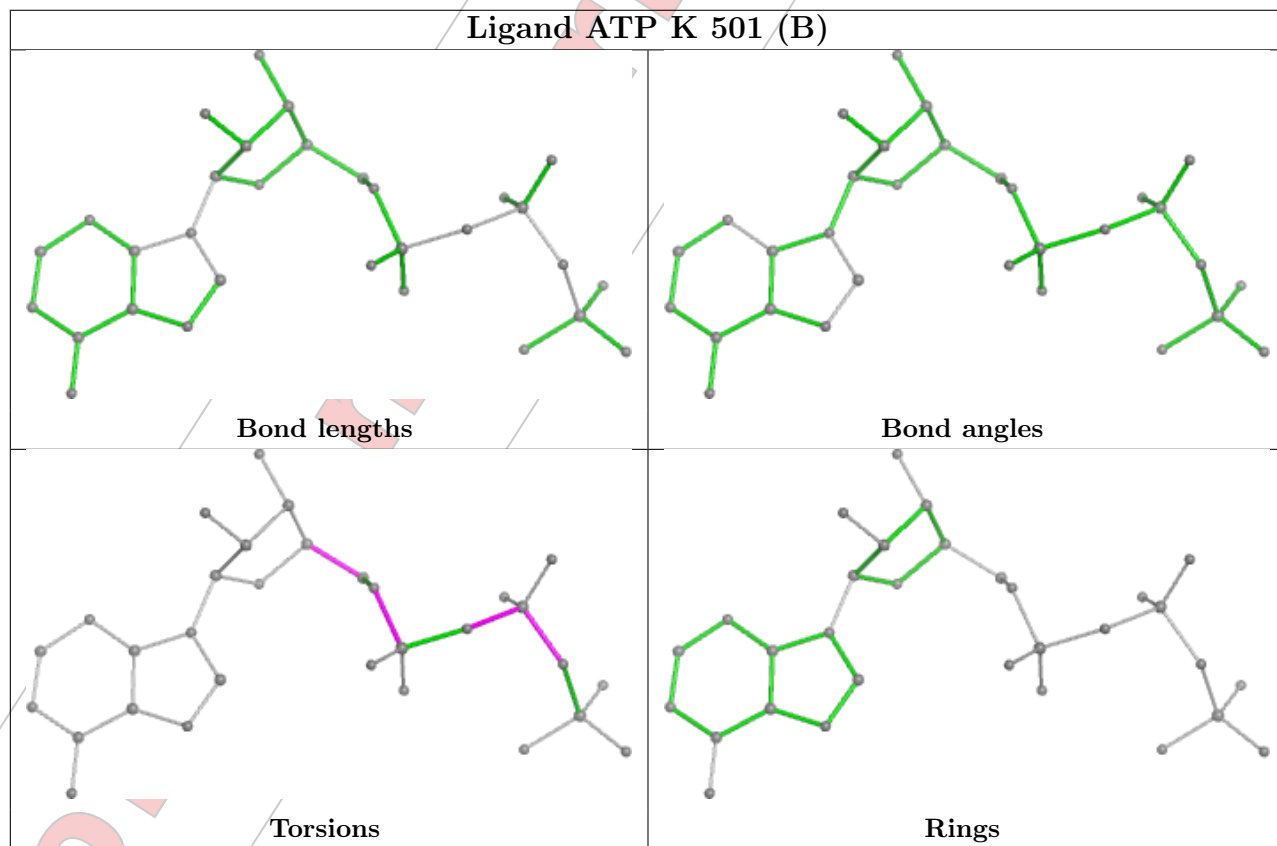




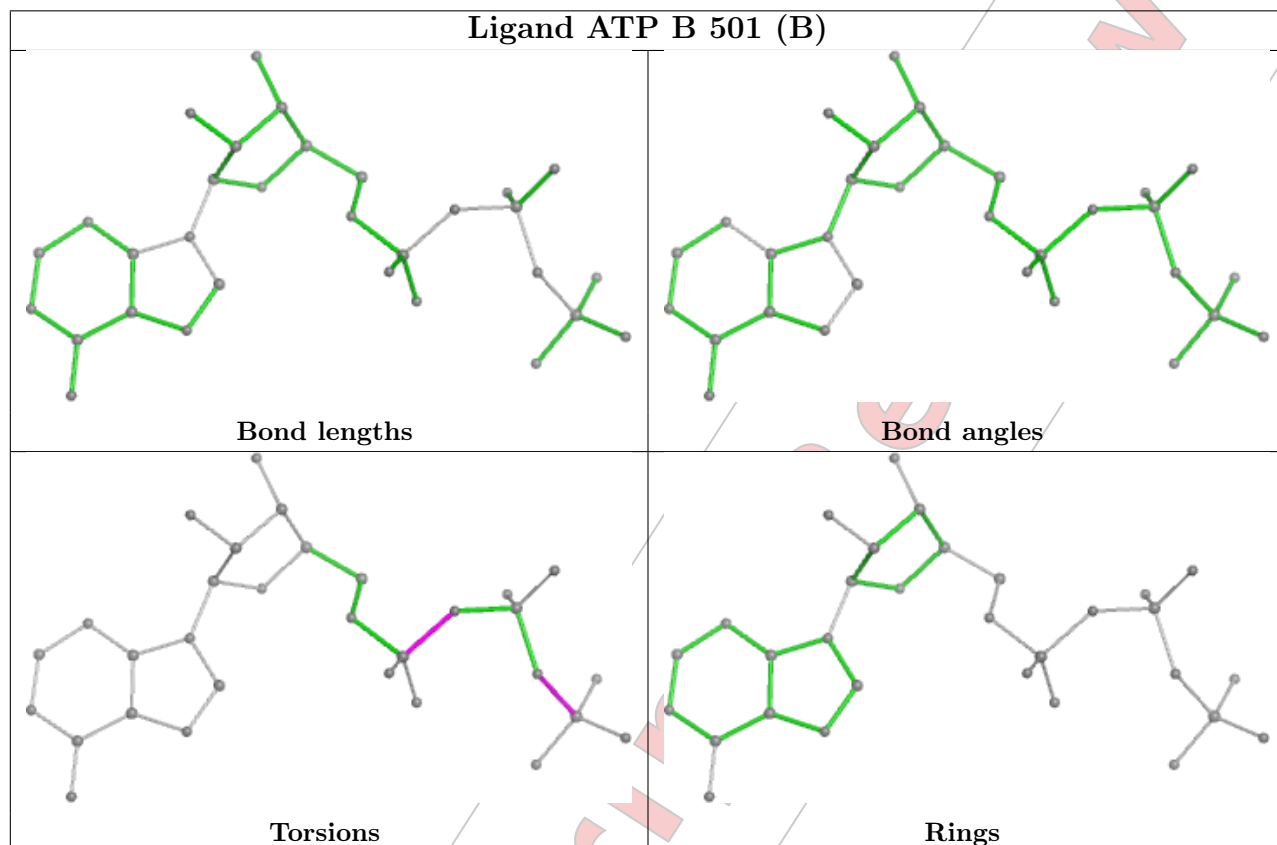
Ligand ATP J 501 (B)



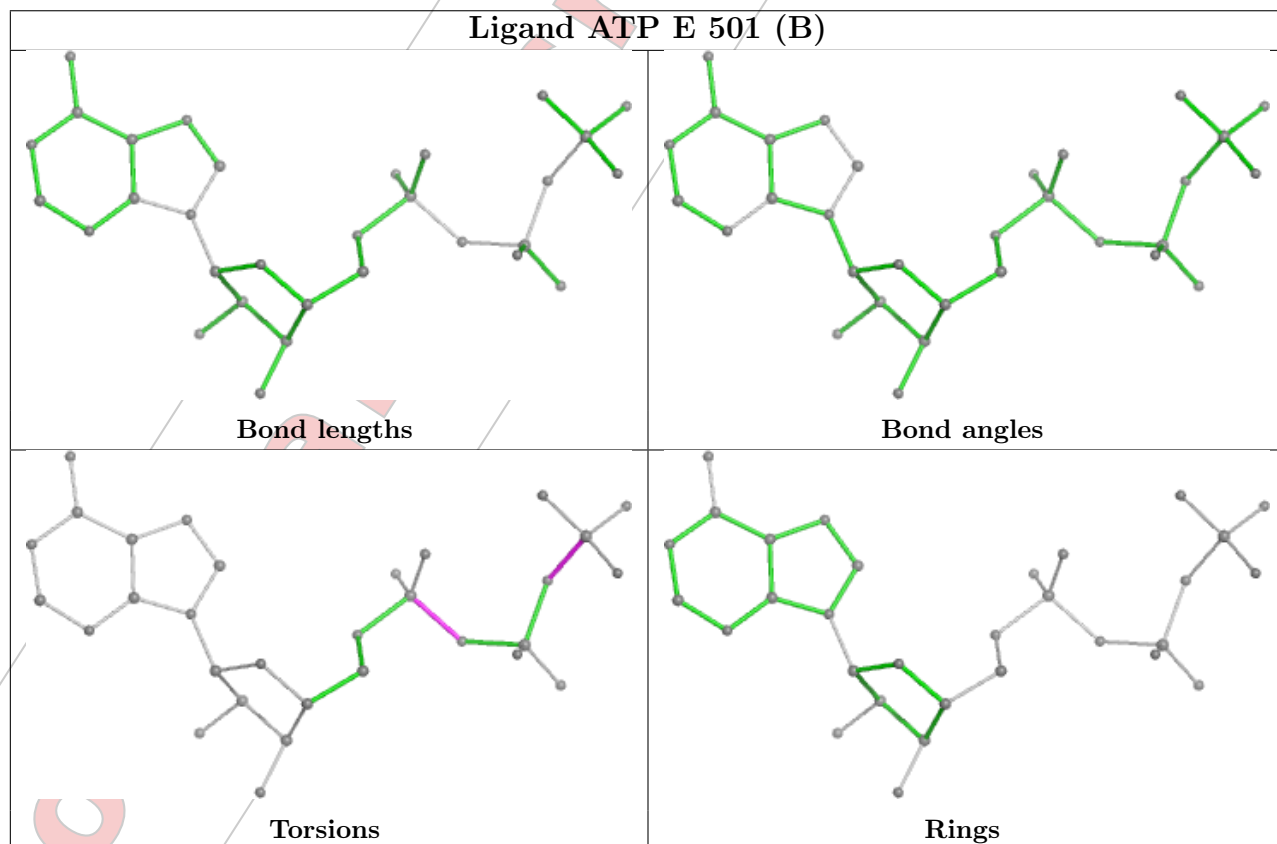
Ligand ATP K 501 (B)

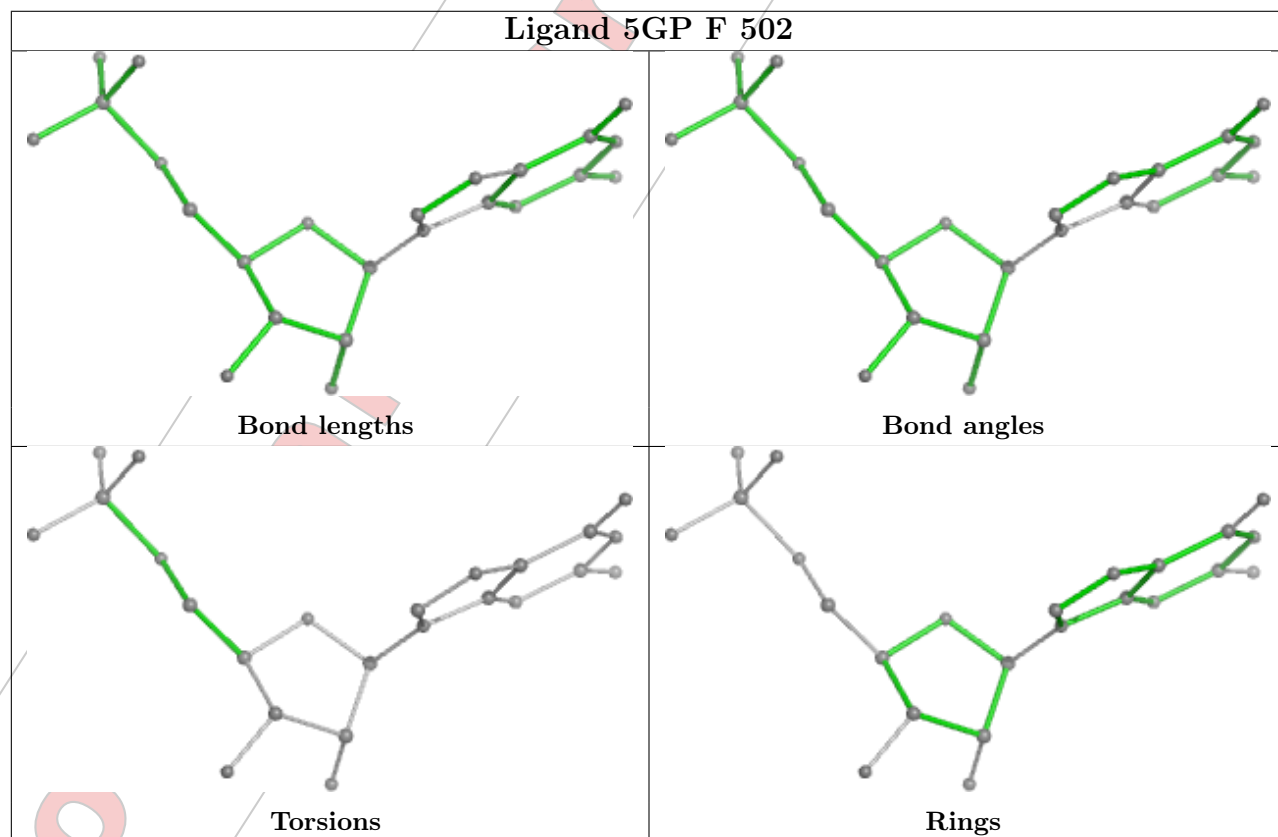
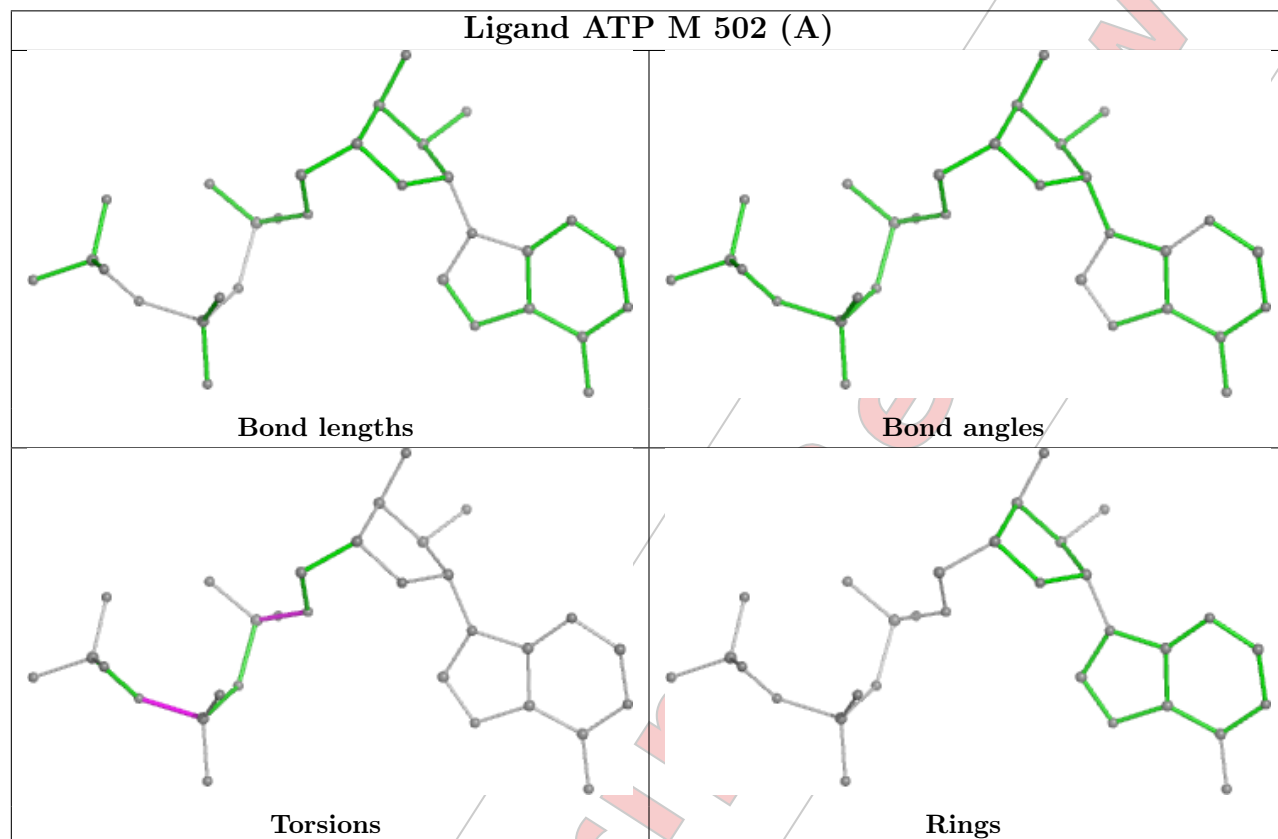


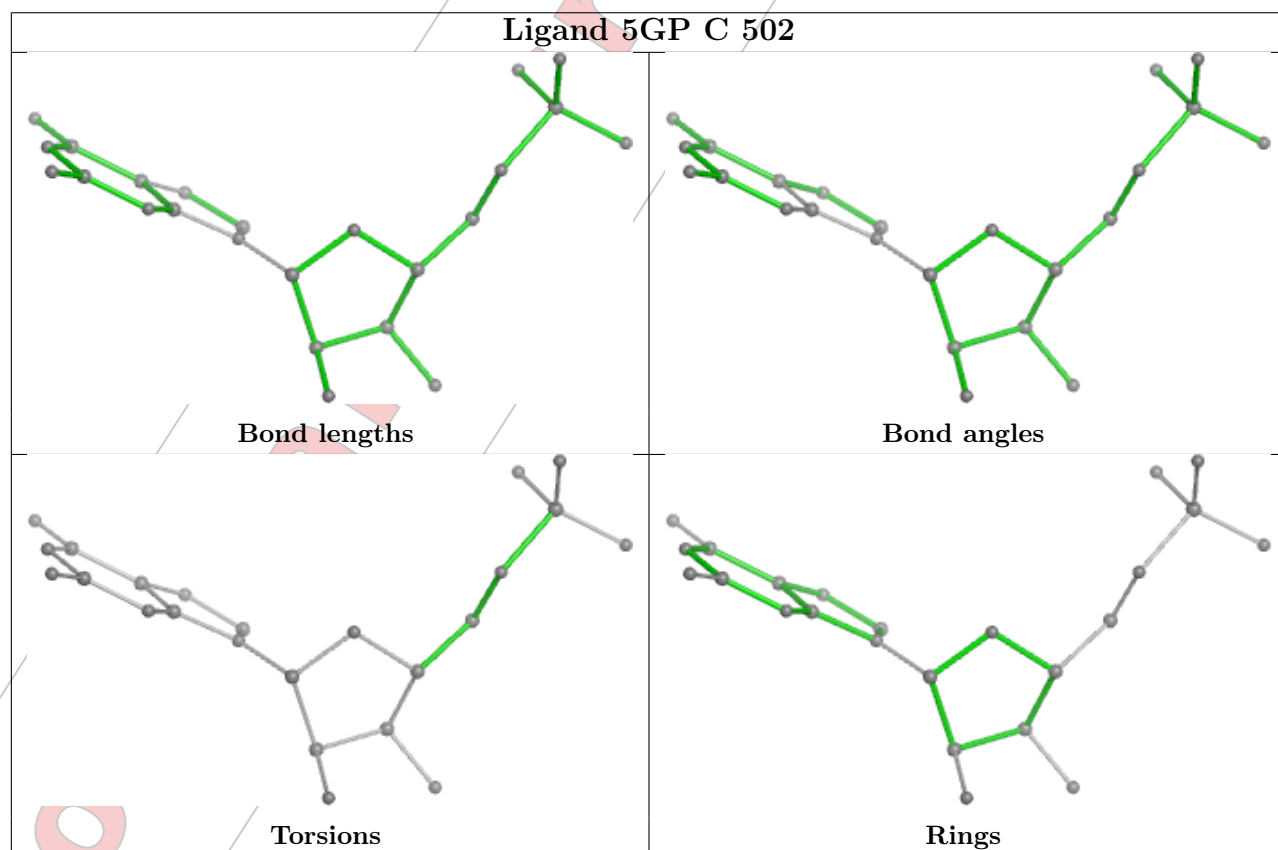
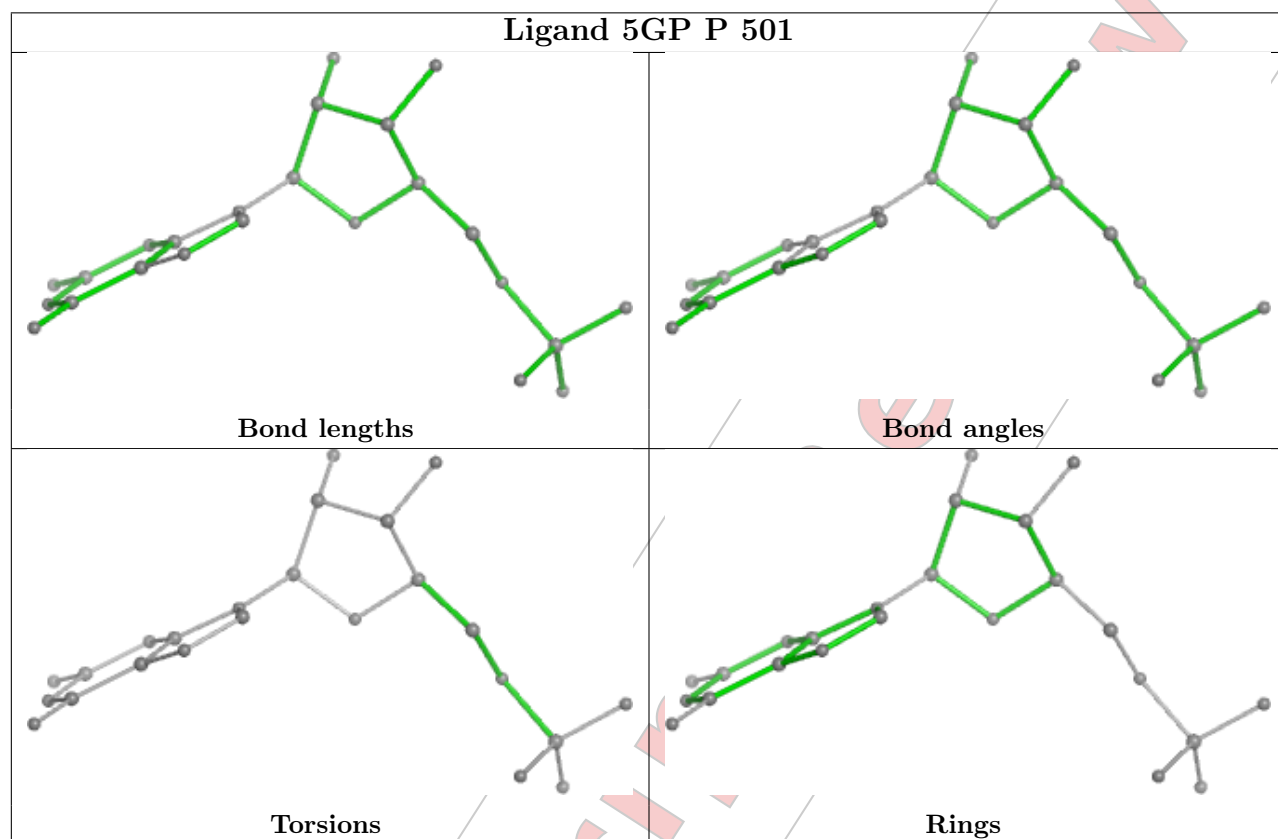
Ligand ATP B 501 (B)



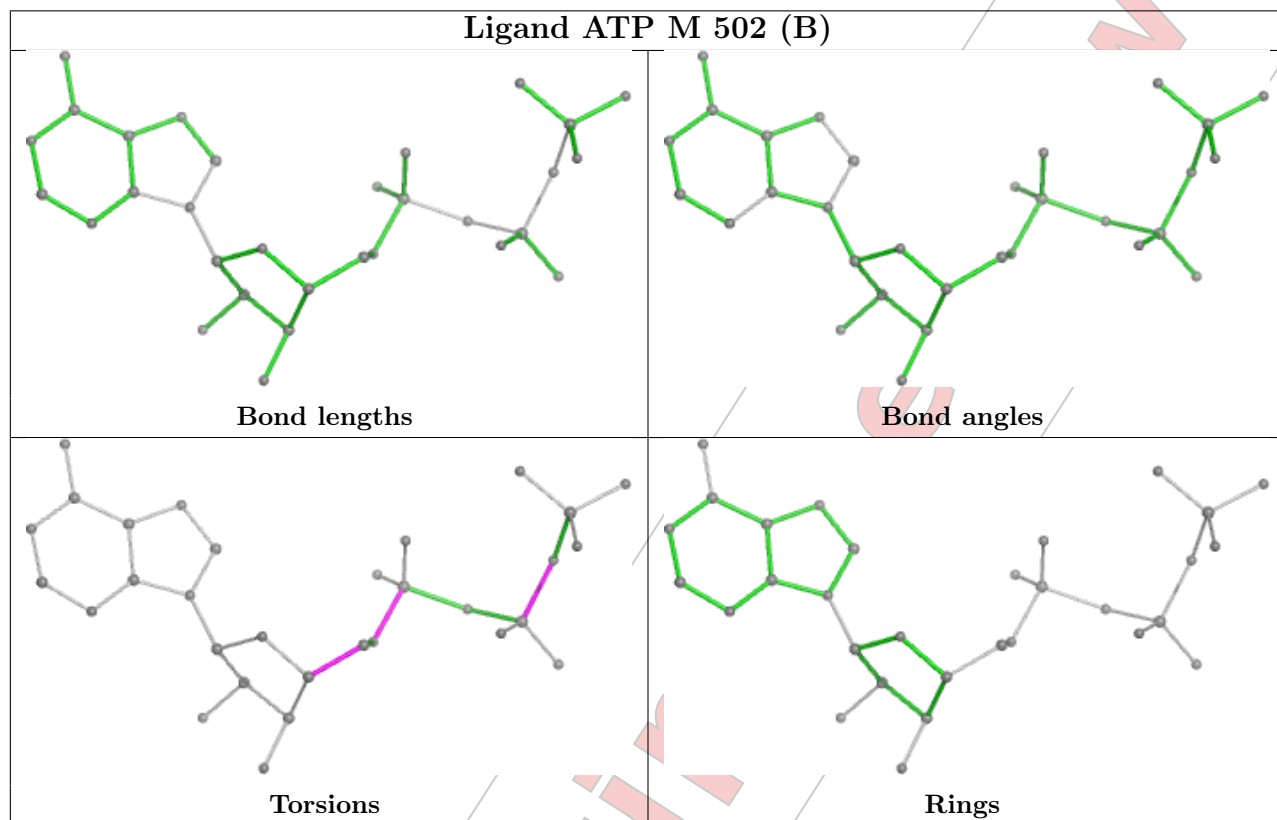
Ligand ATP E 501 (B)



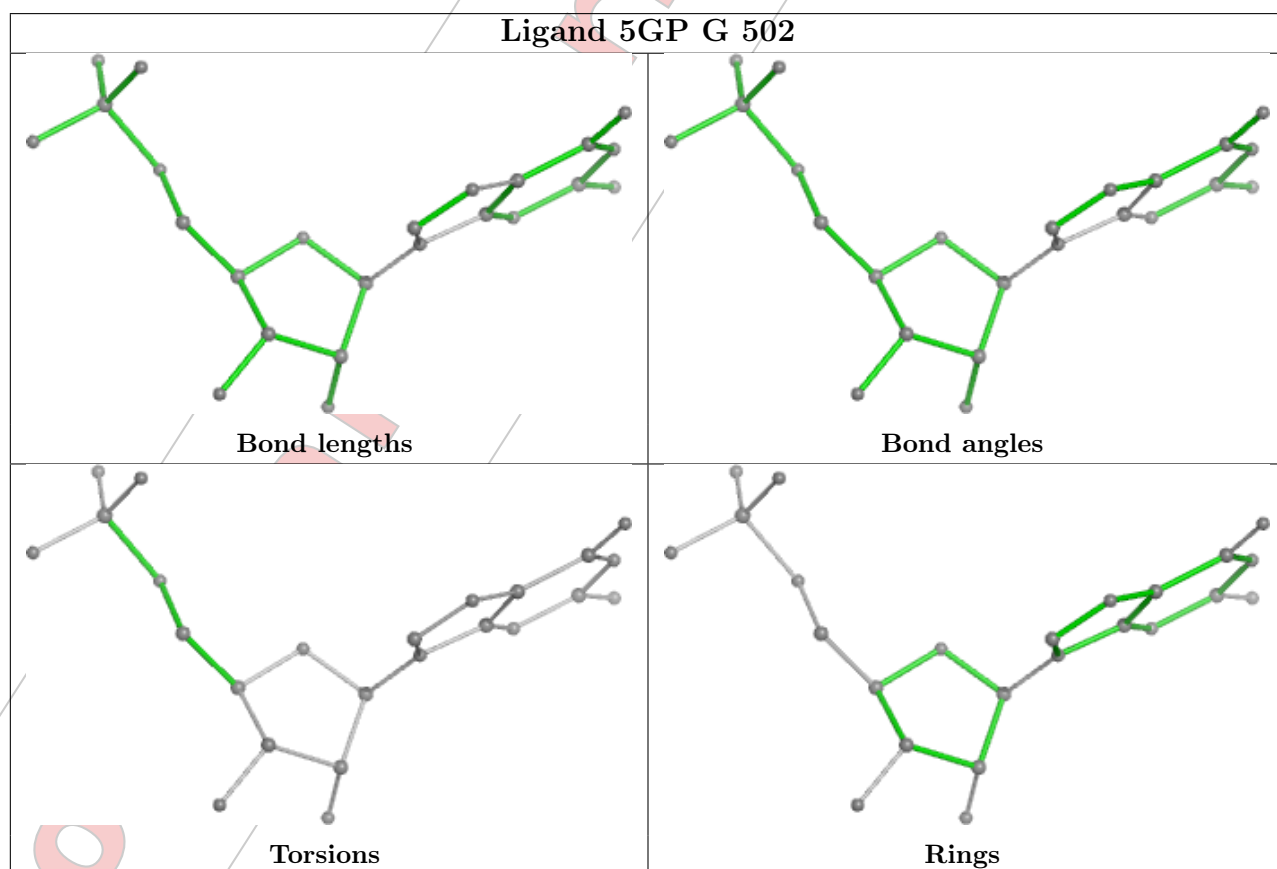


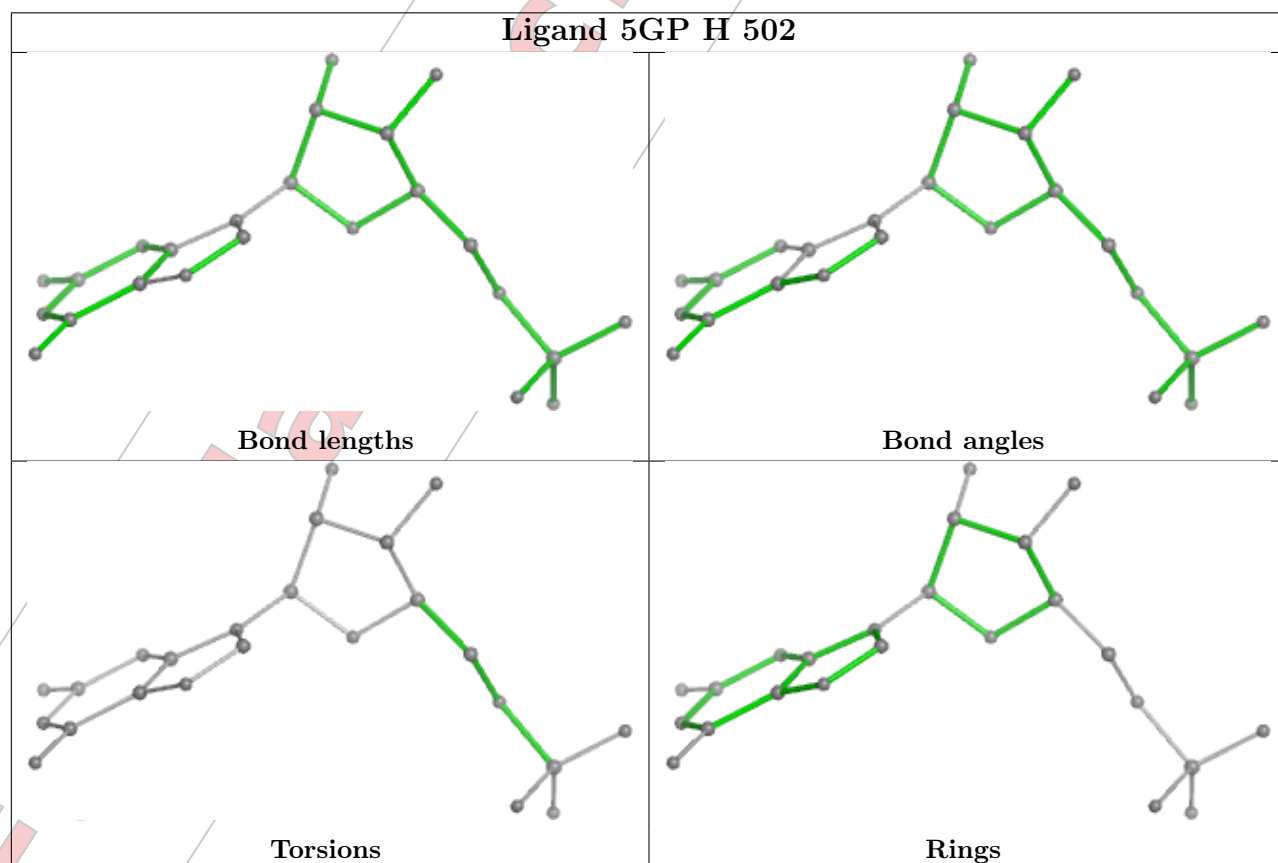
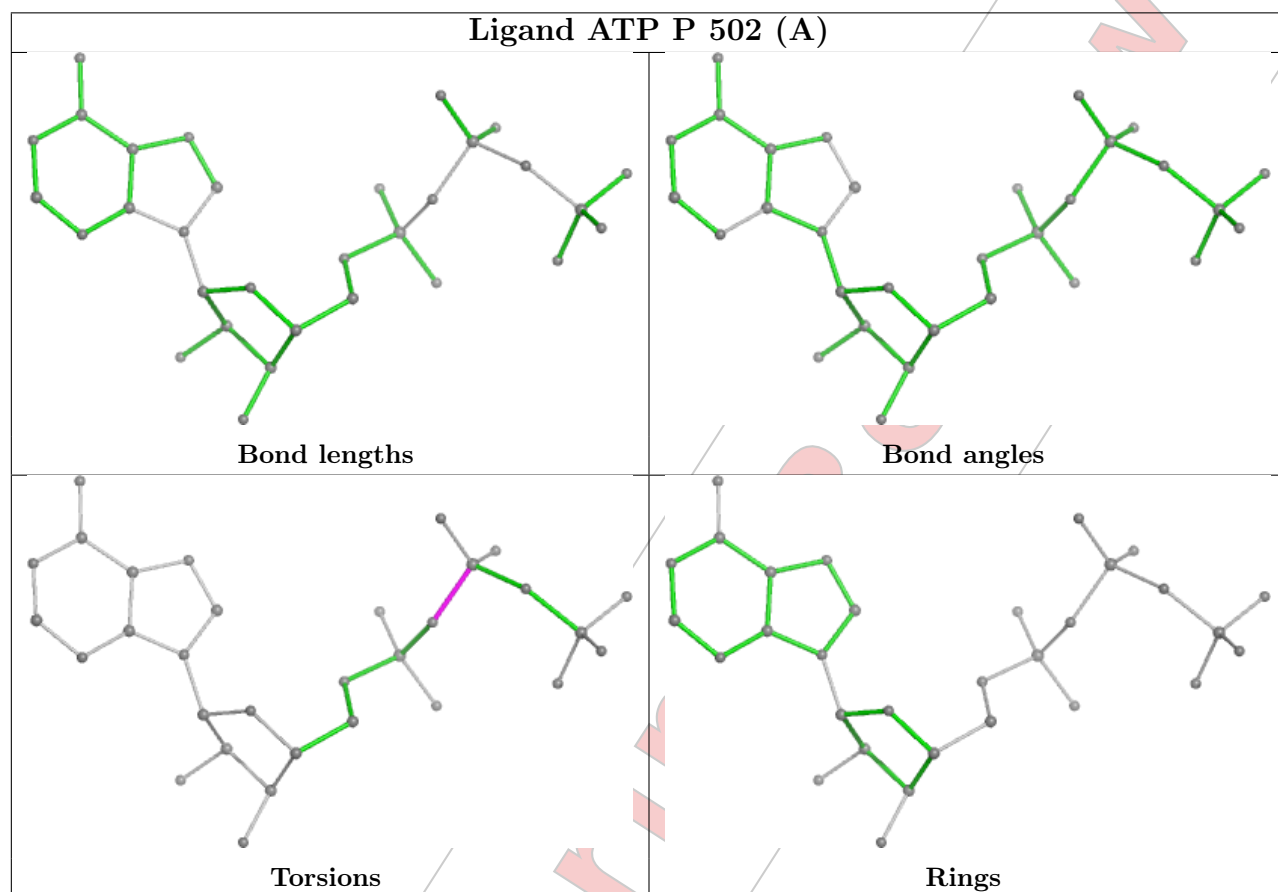


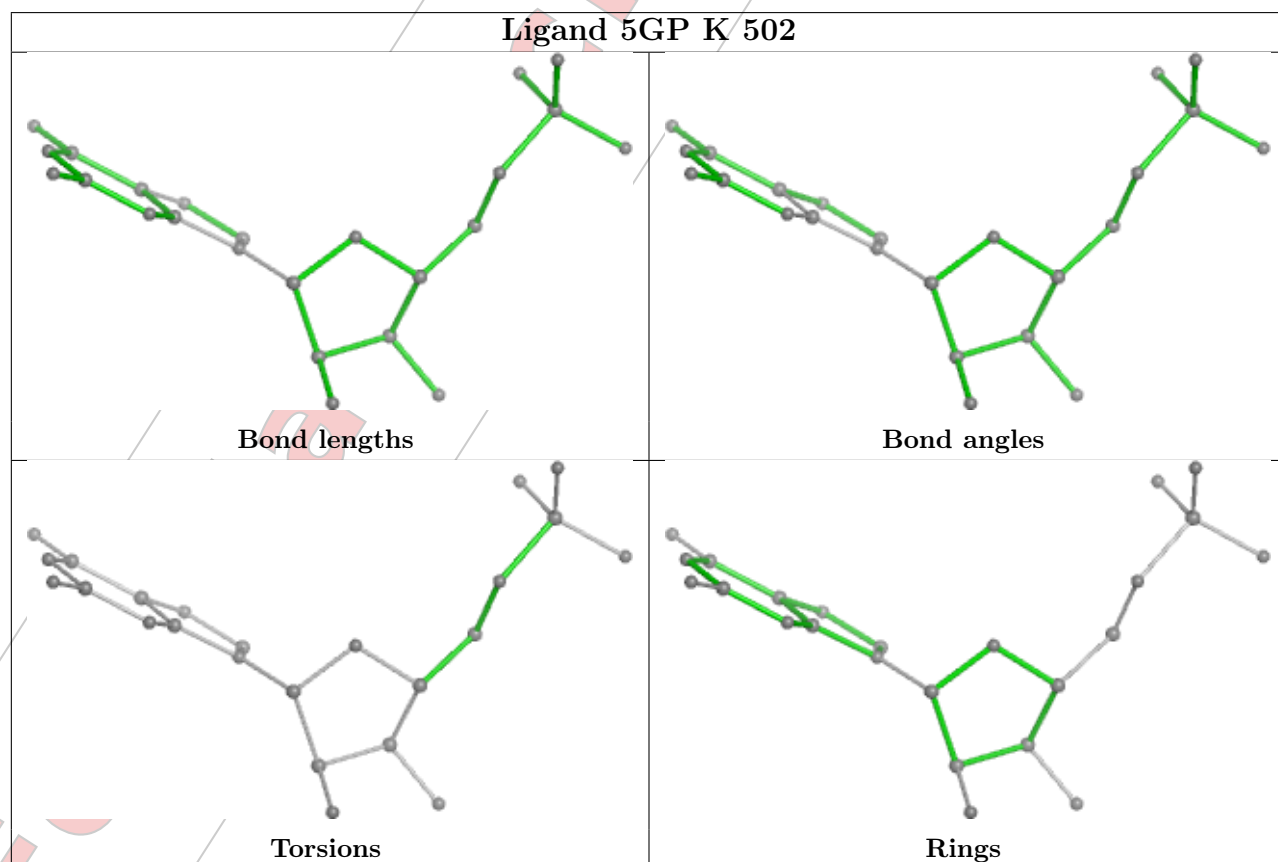
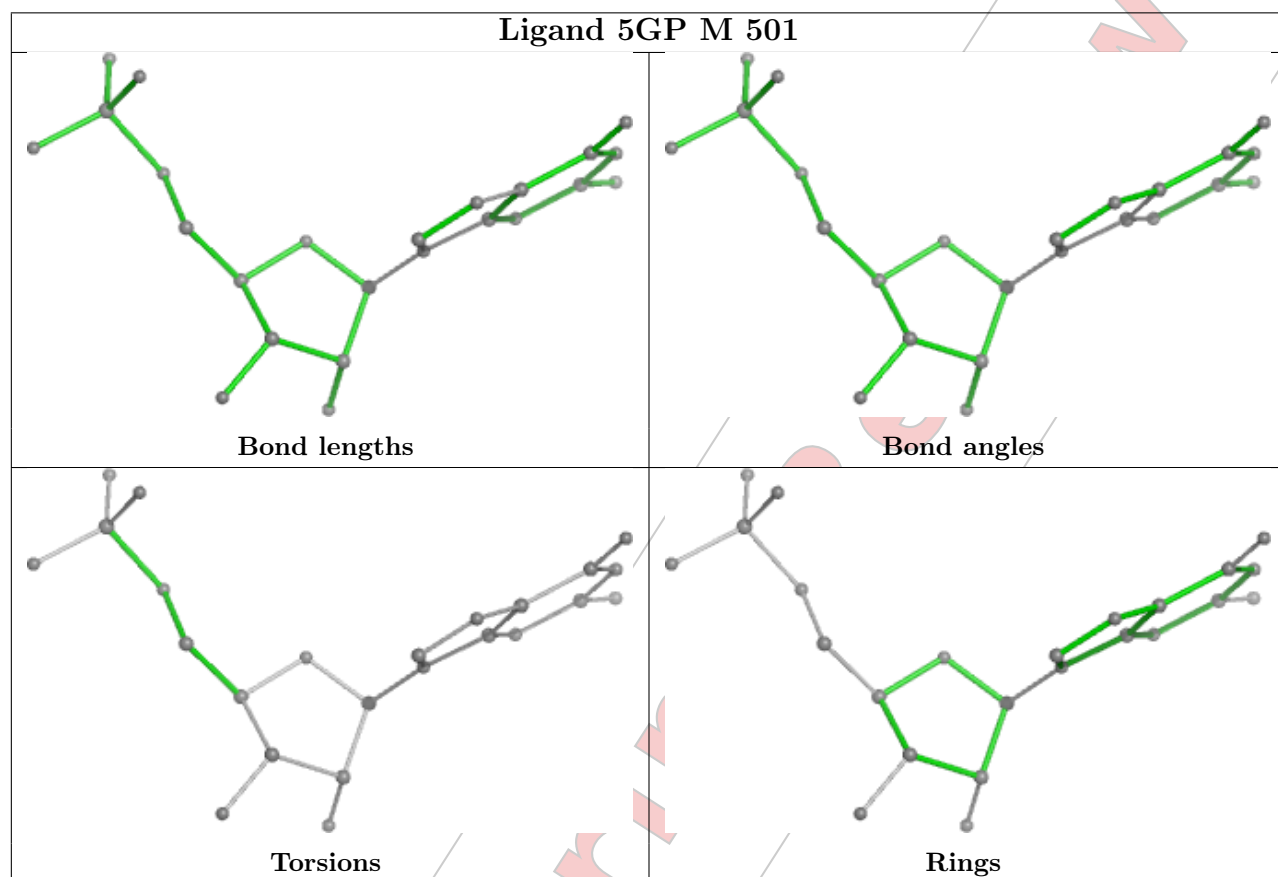
Ligand ATP M 502 (B)

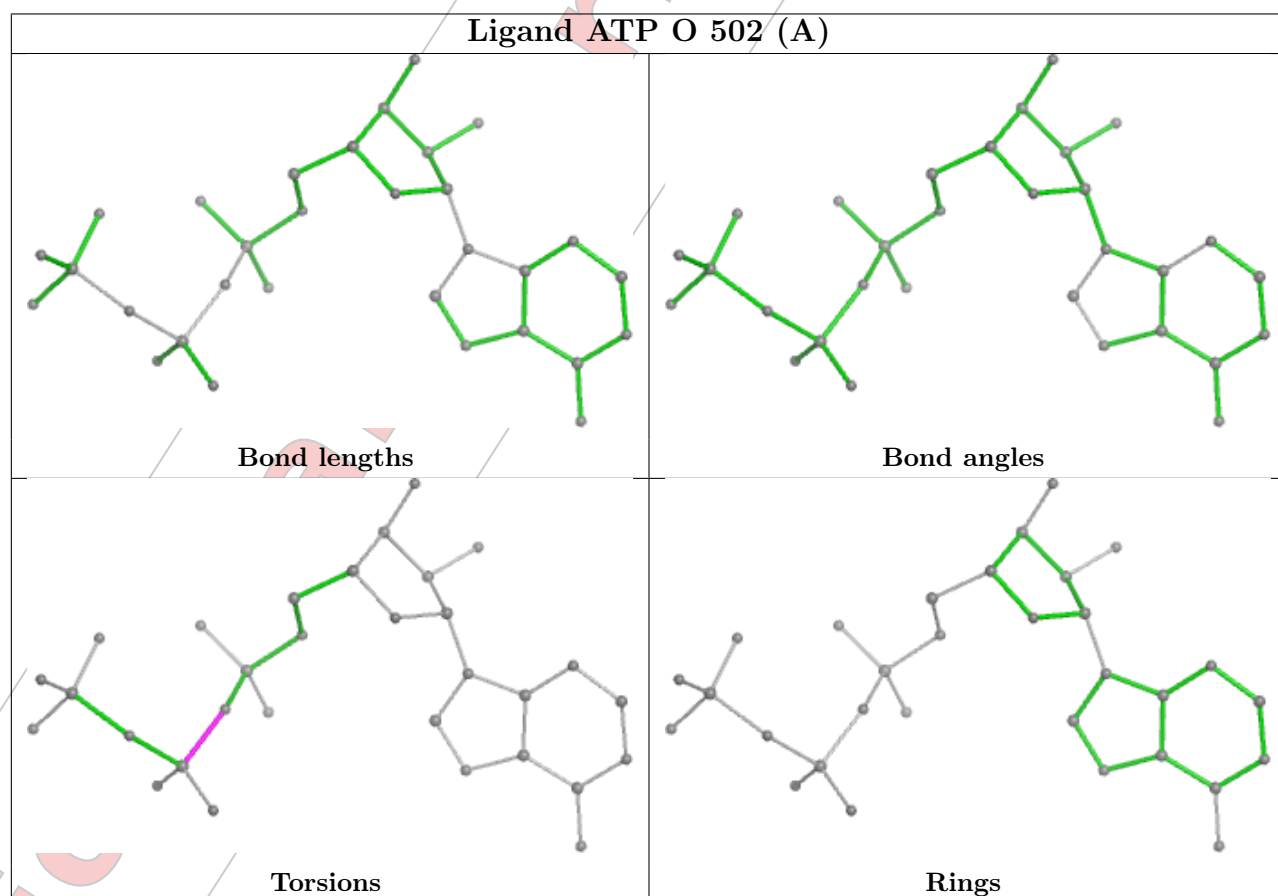
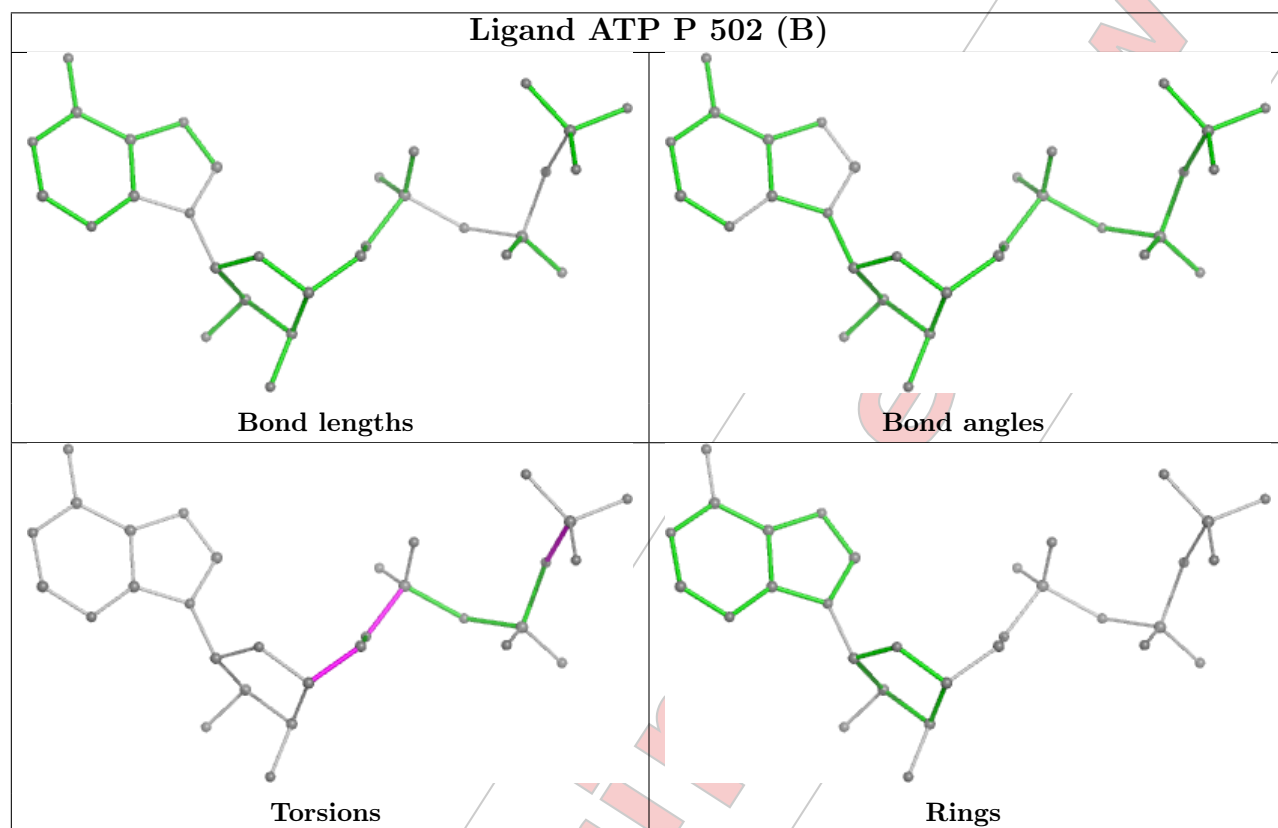


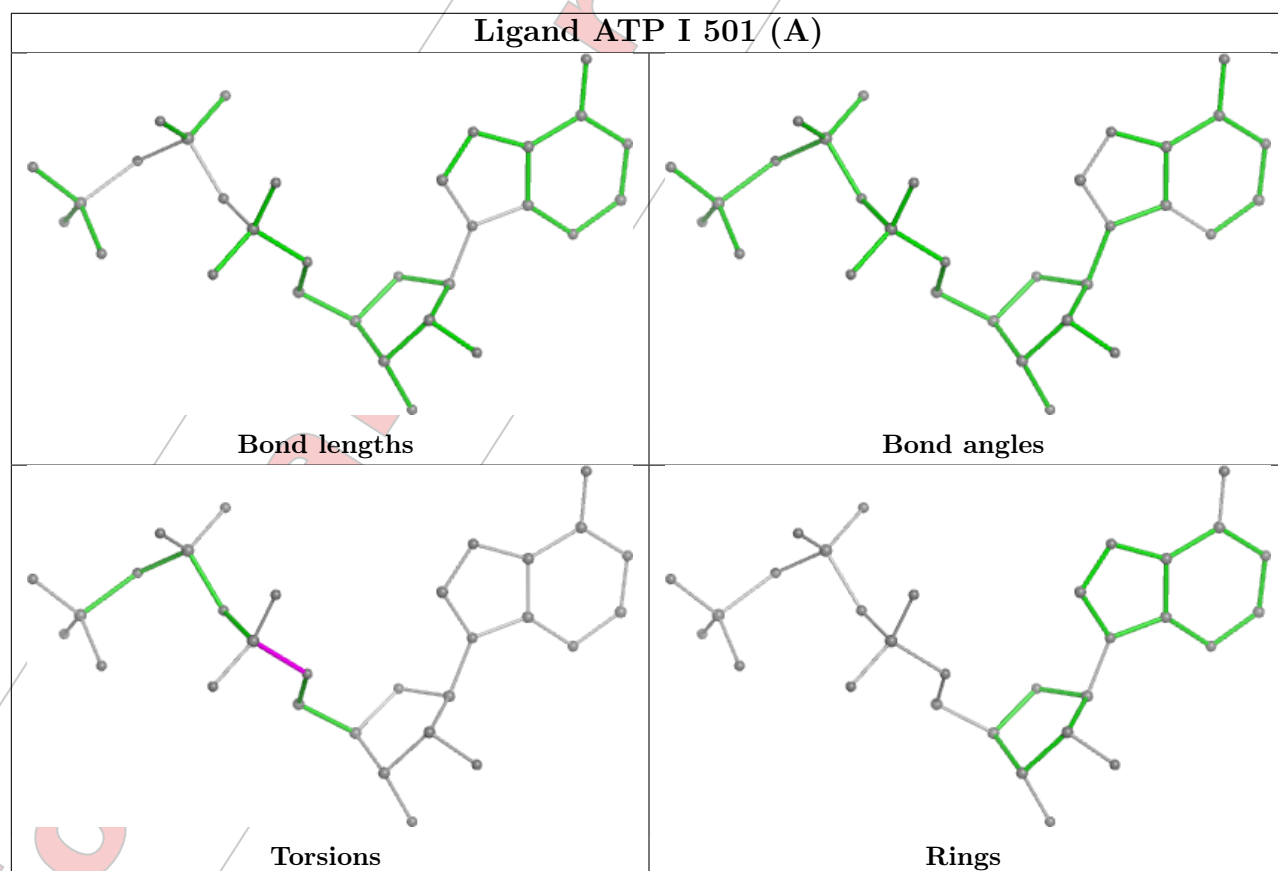
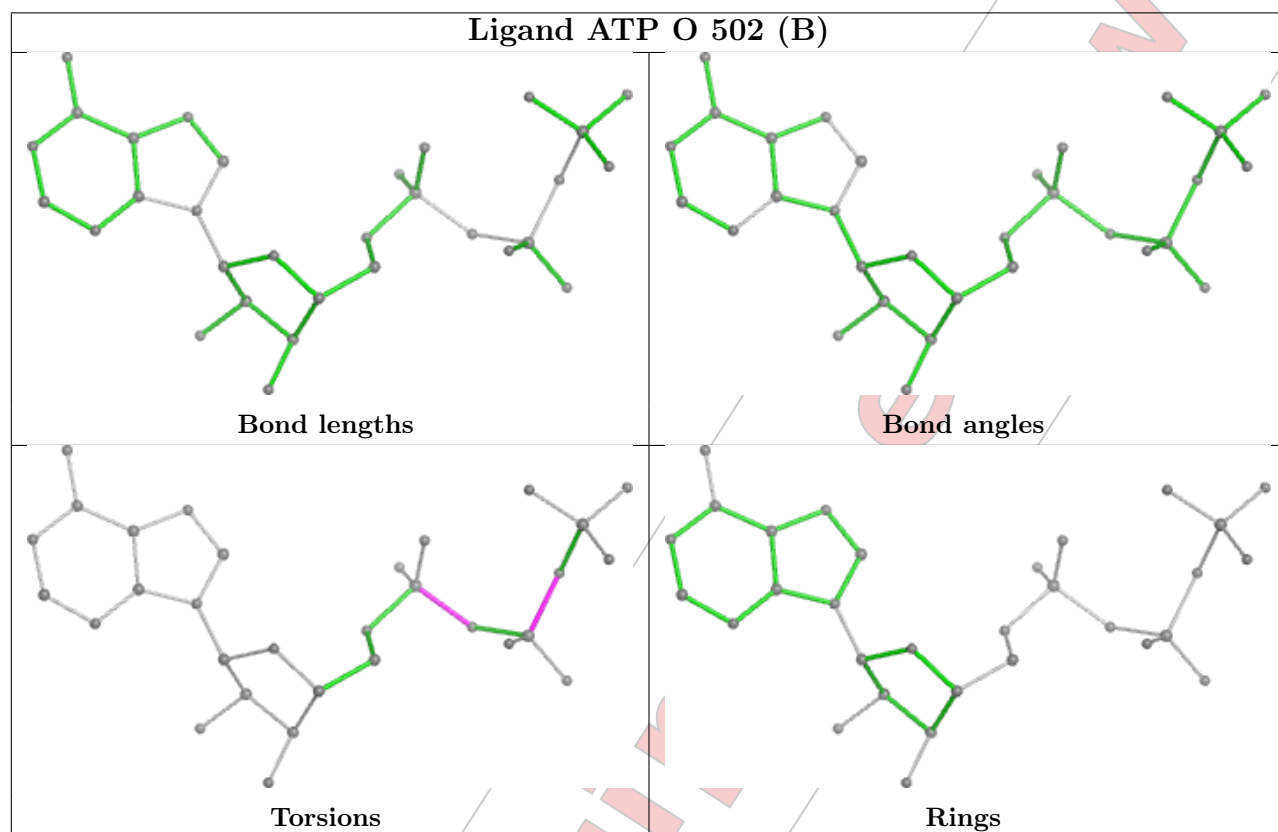
Ligand 5GP G 502



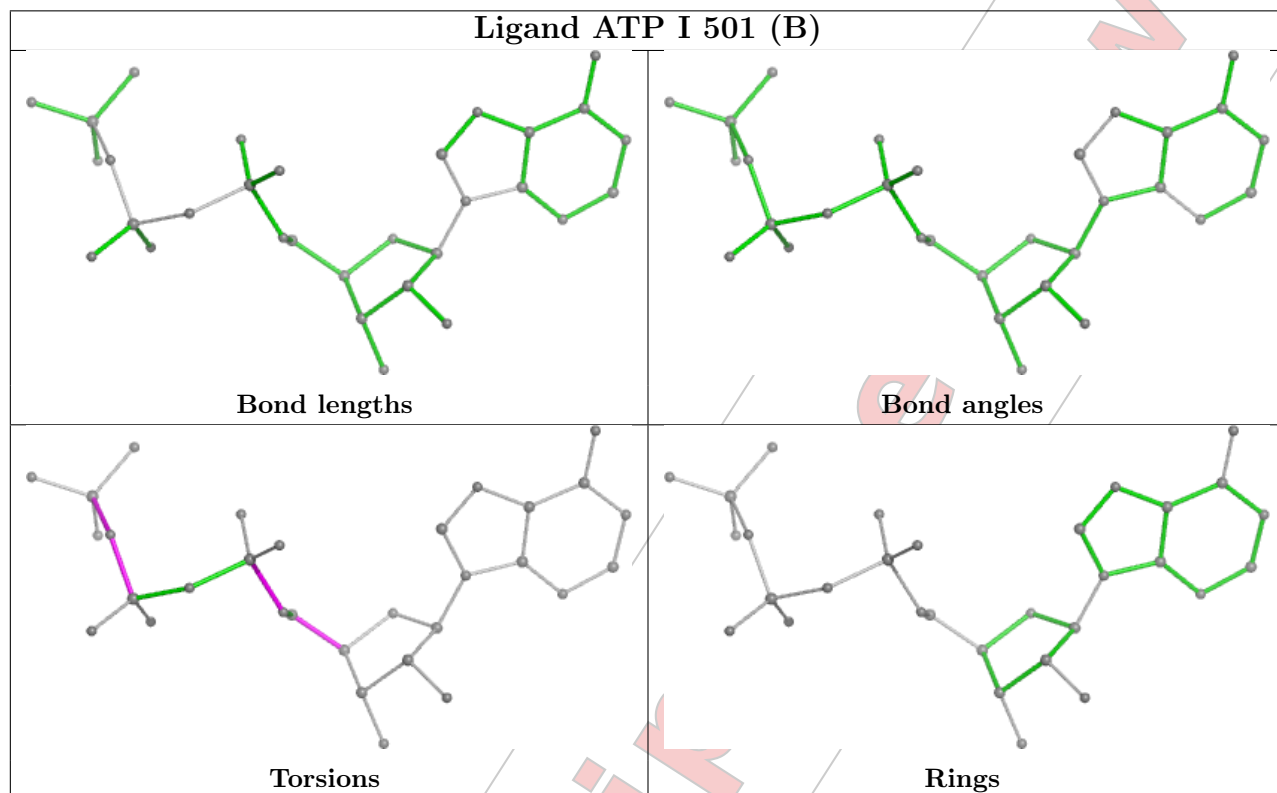




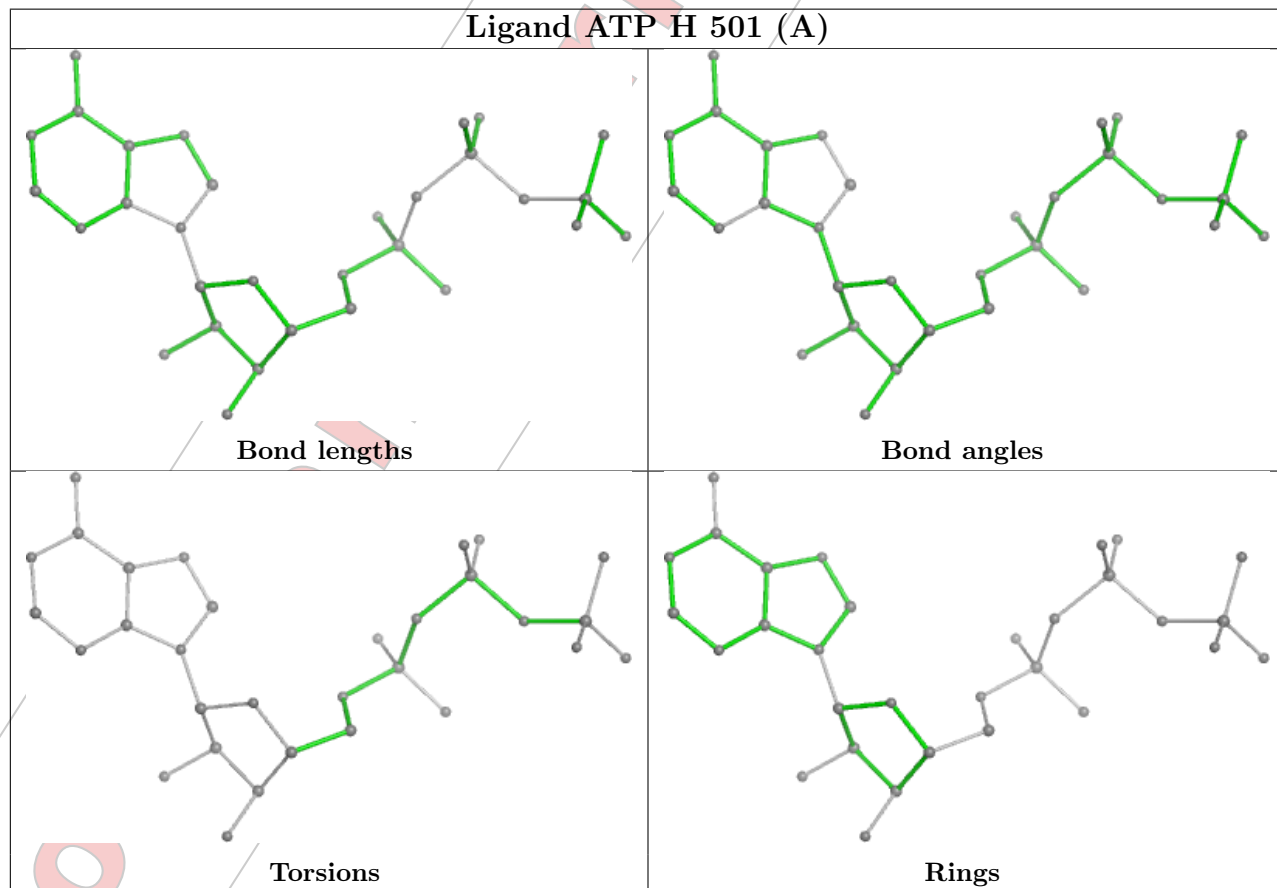




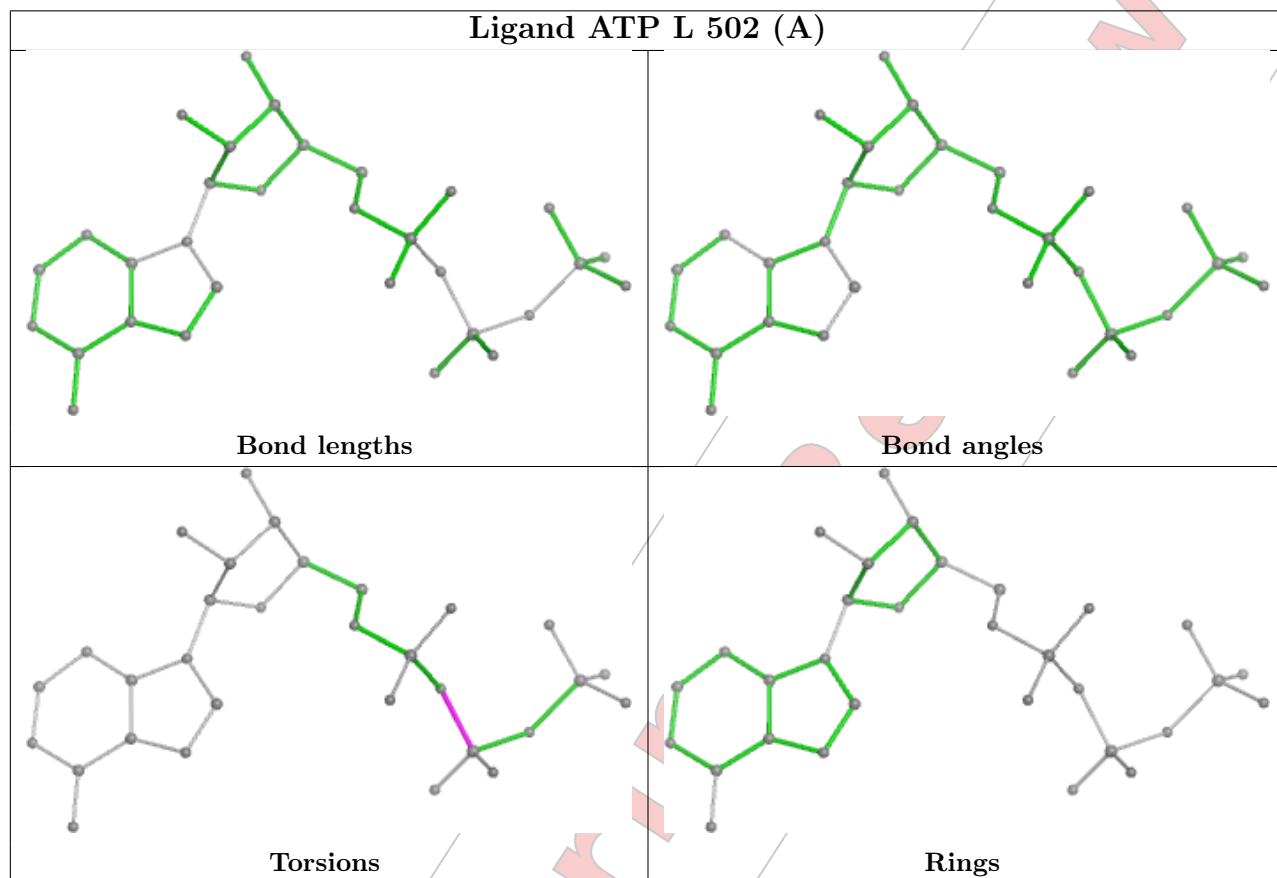
Ligand ATP I 501 (B)



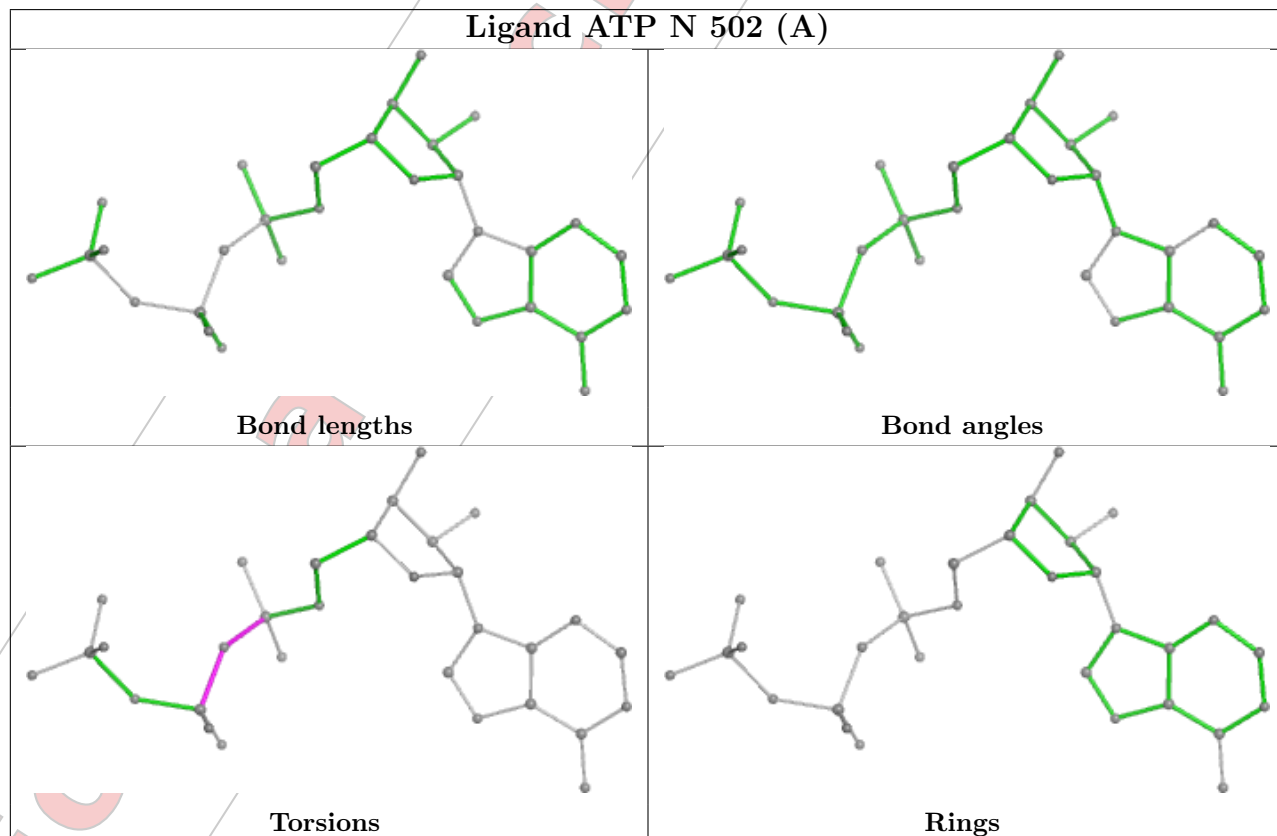
Ligand ATP H 501 (A)

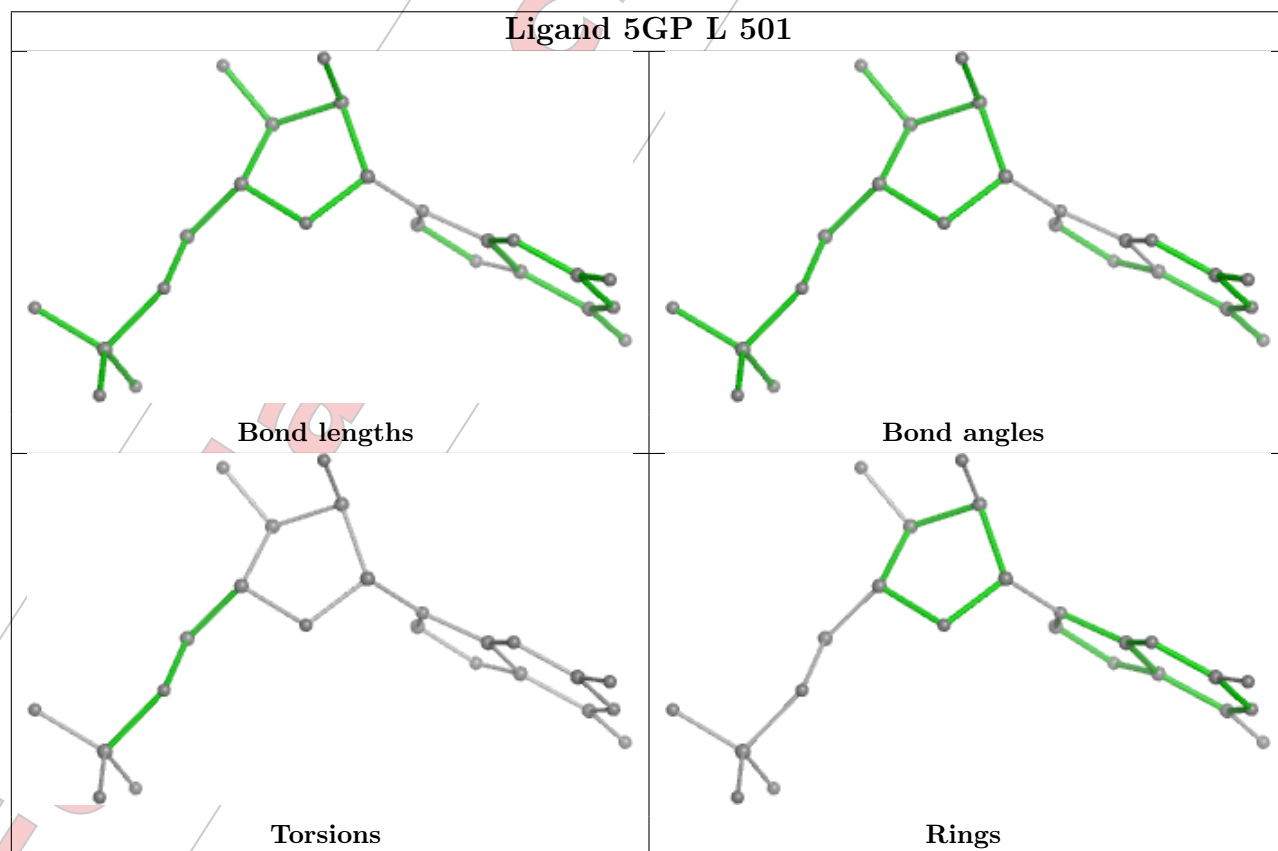
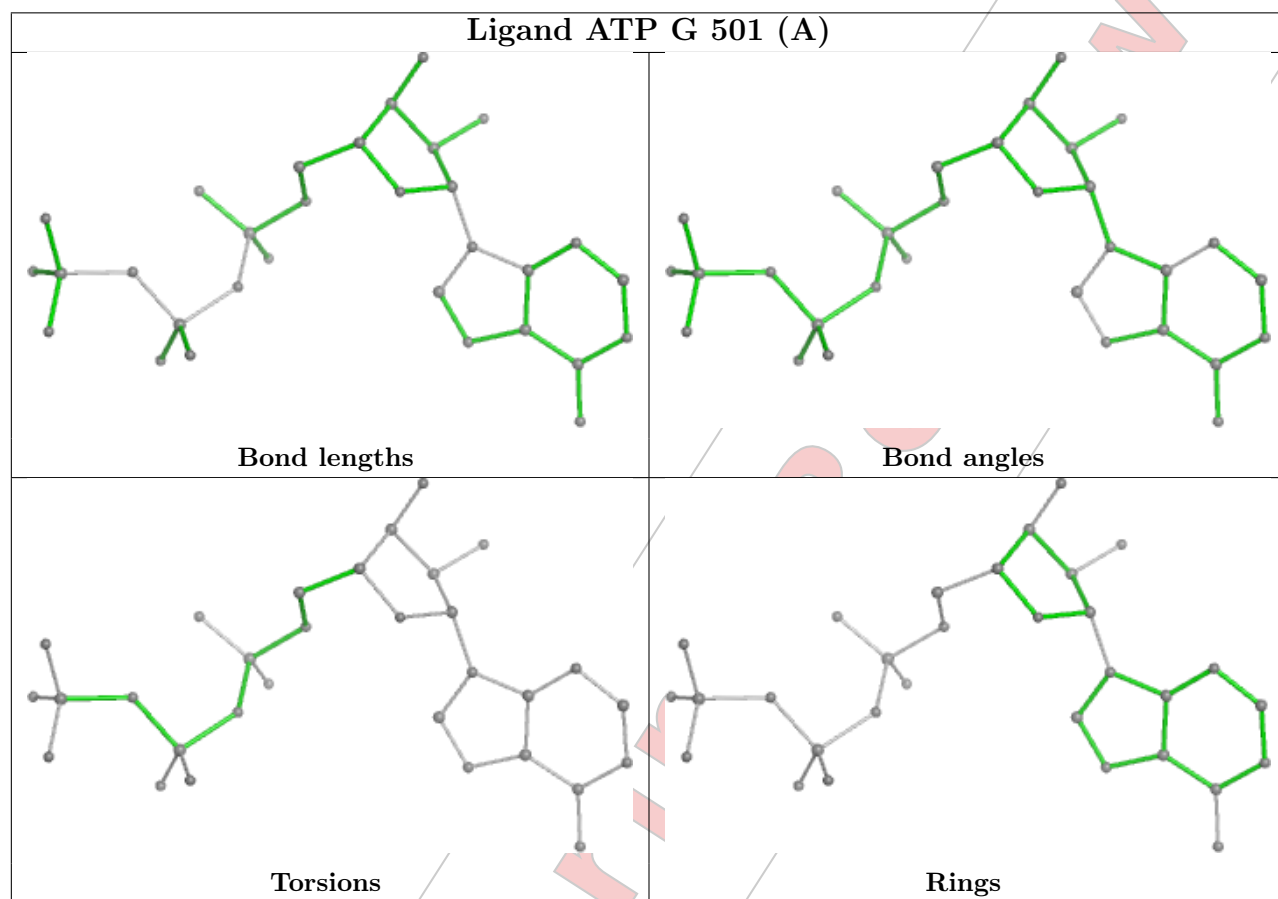


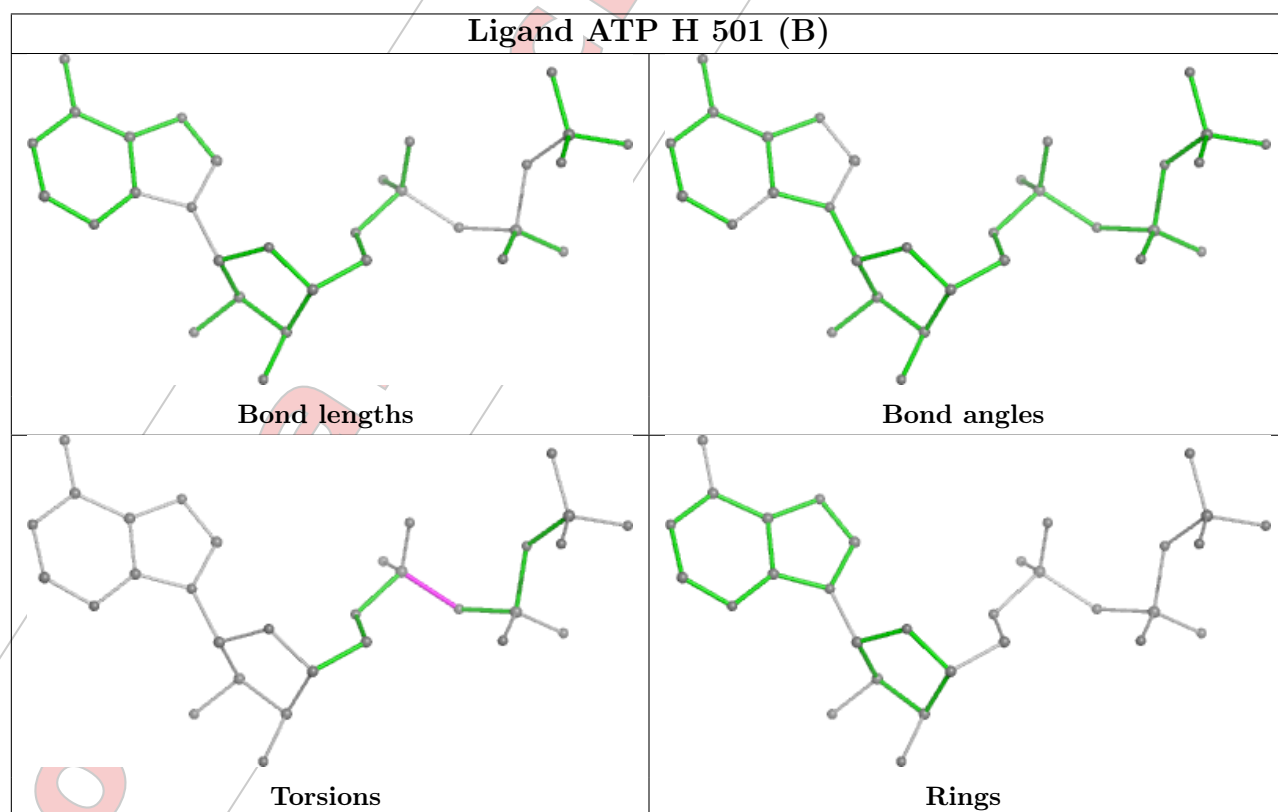
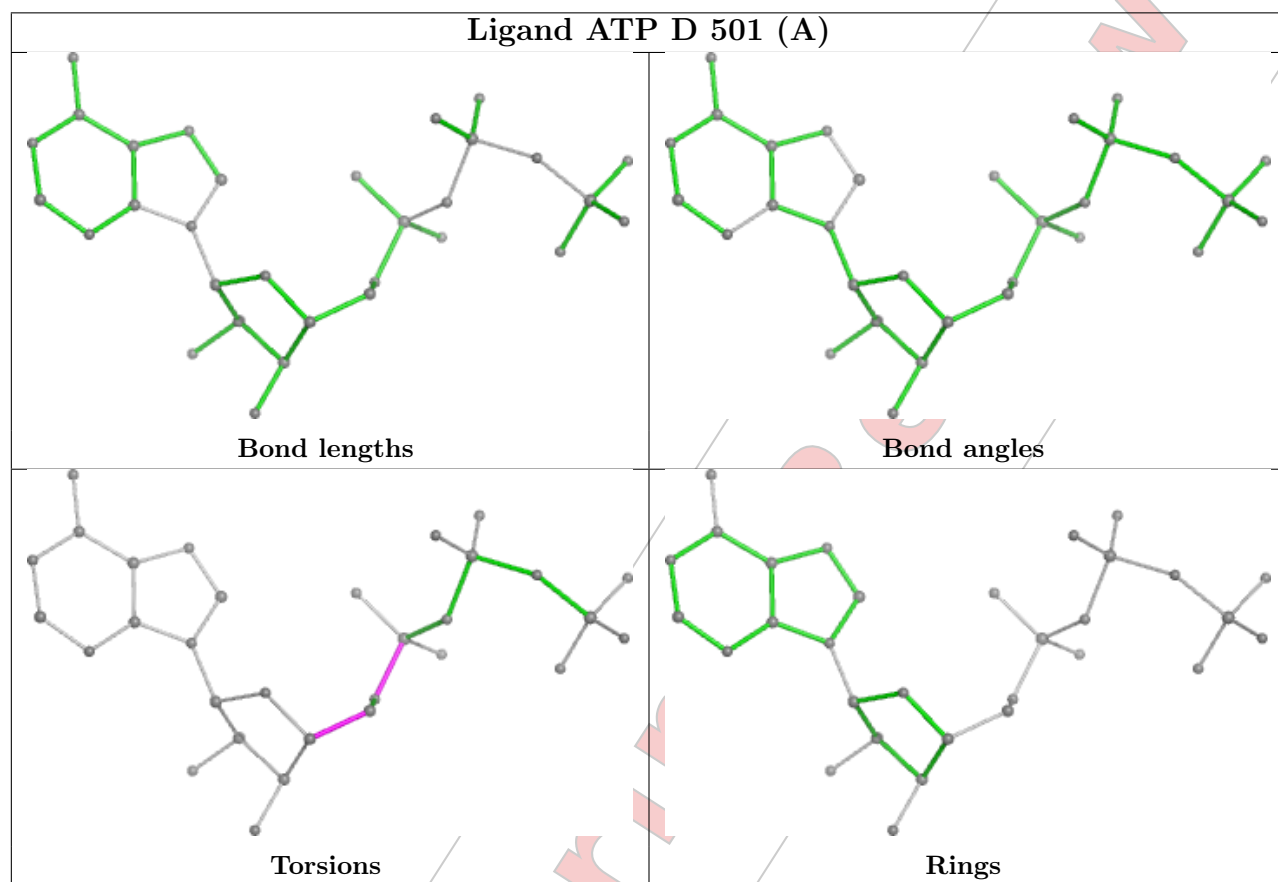
Ligand ATP L 502 (A)



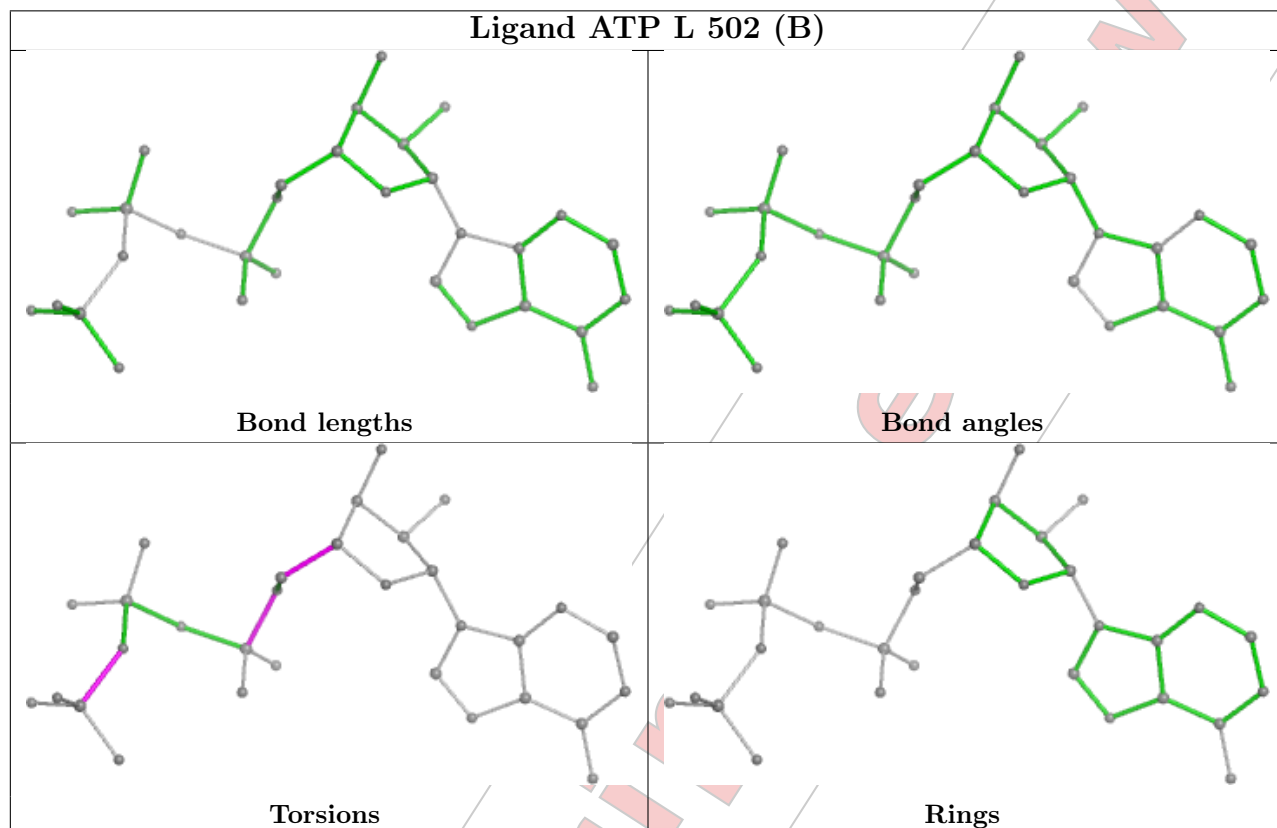
Ligand ATP N 502 (A)



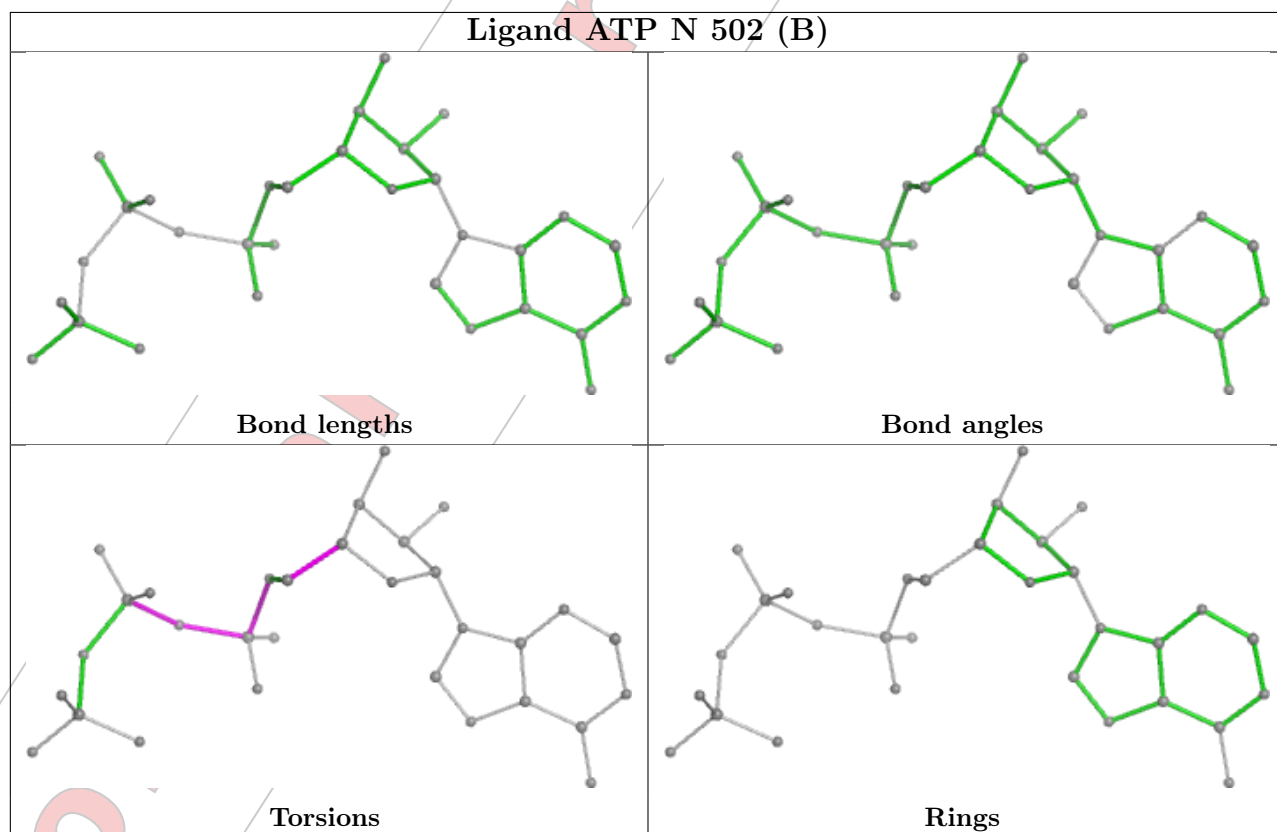


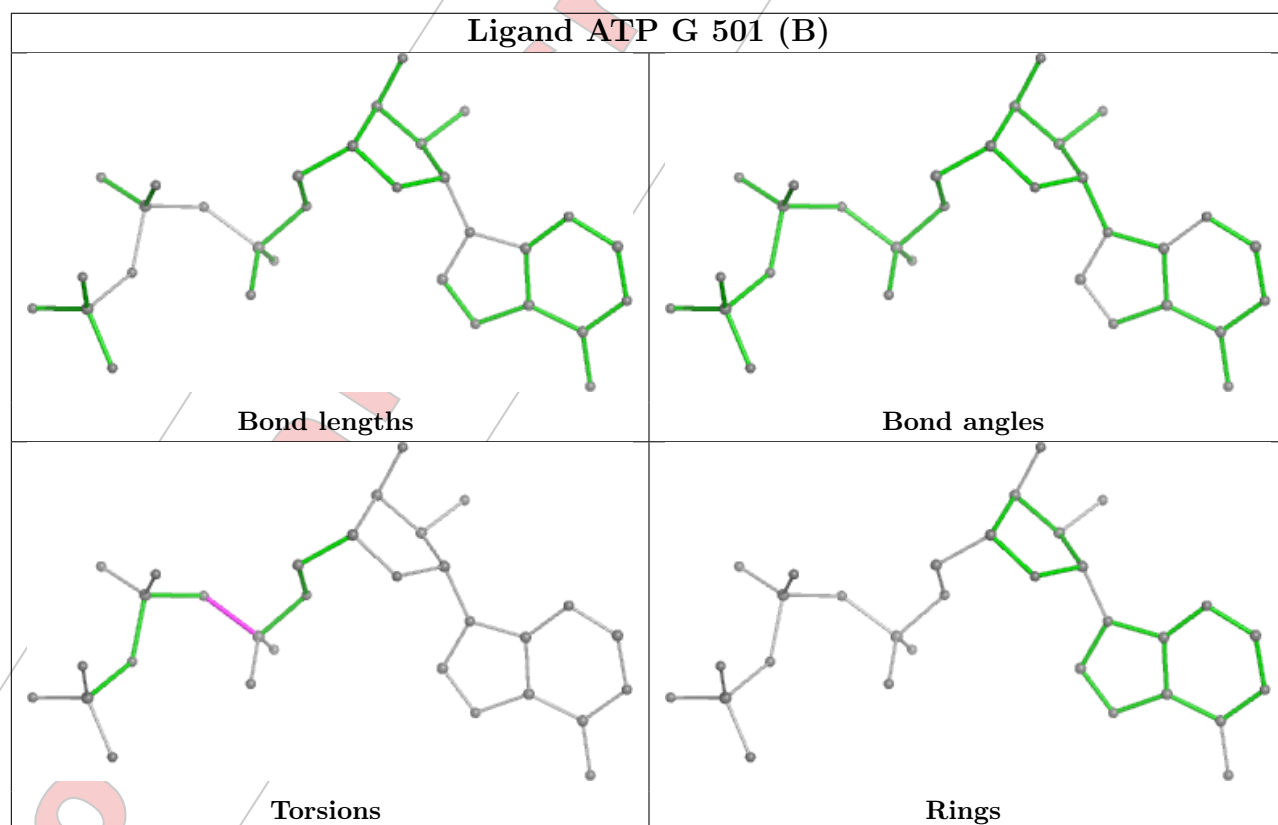
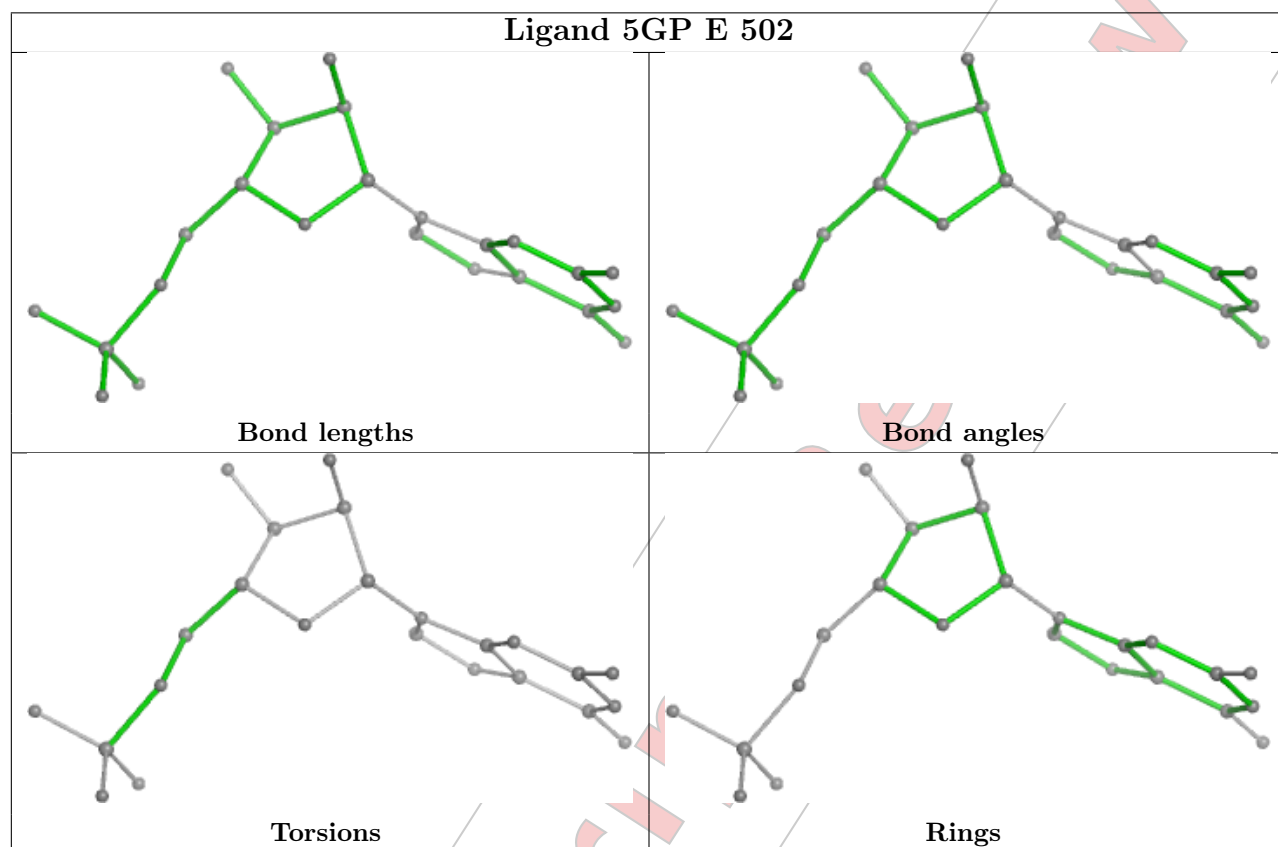


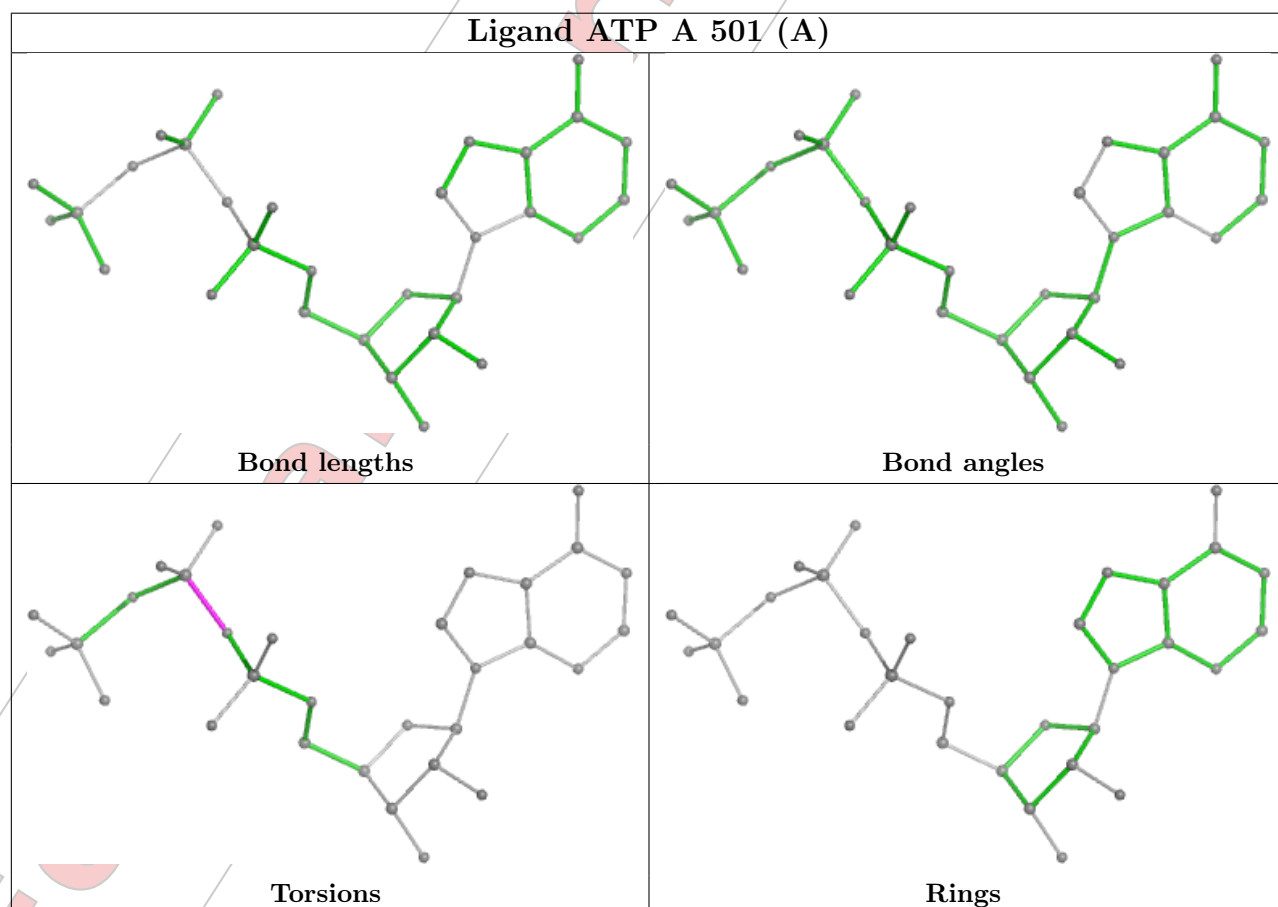
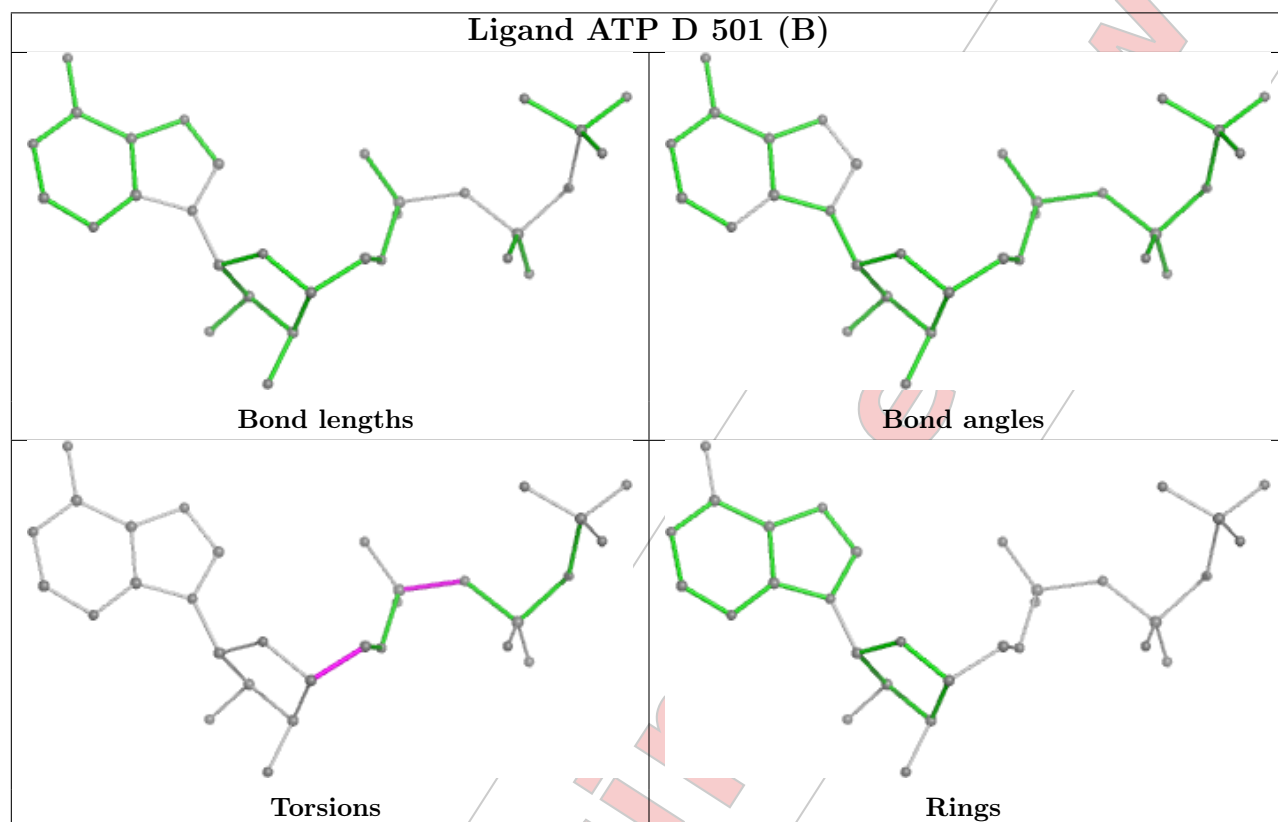
Ligand ATP L 502 (B)

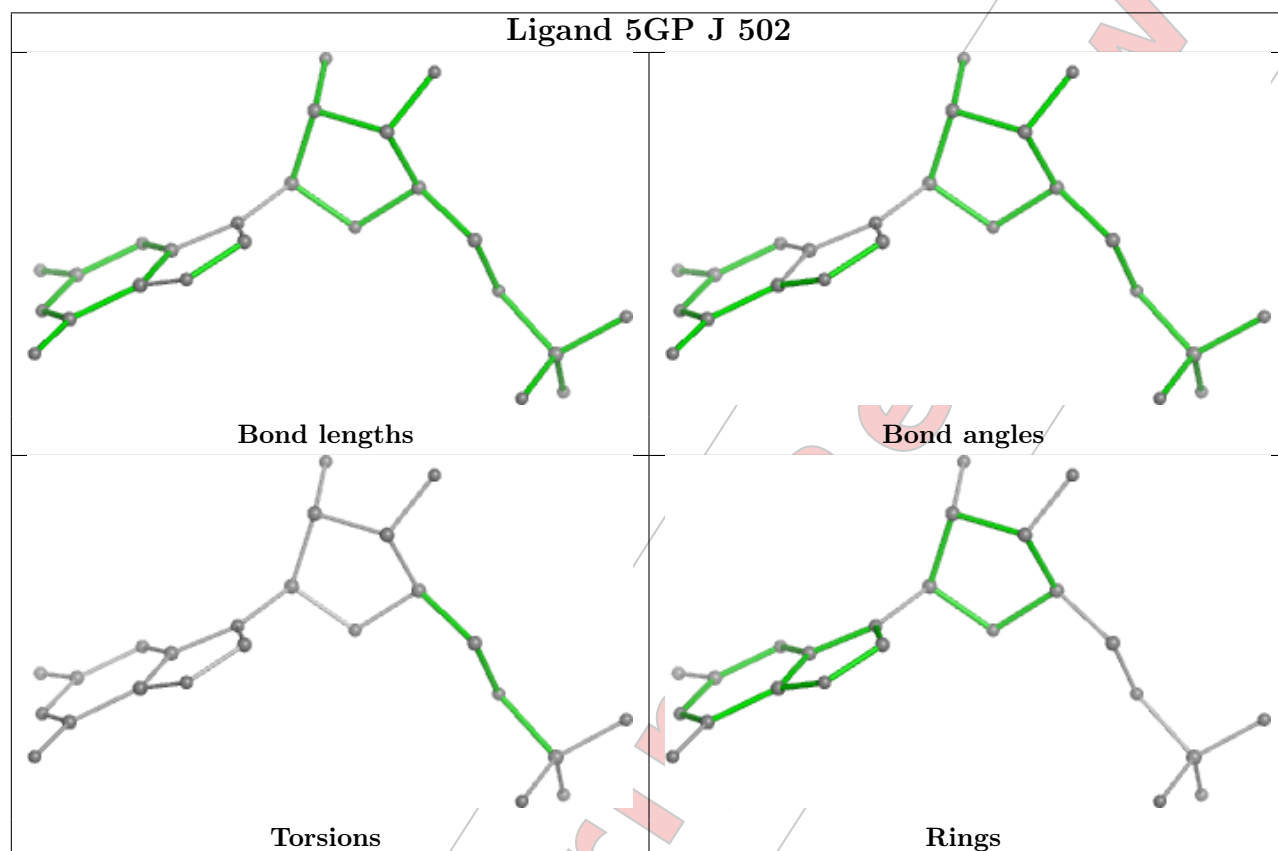


Ligand ATP N 502 (B)









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.01	9 (1%) 66 67	28, 43, 62, 82	1 (0%)
1	B	473/496 (95%)	0.08	11 (2%) 61 62	28, 46, 65, 94	1 (0%)
1	C	473/496 (95%)	0.21	14 (2%) 52 54	30, 49, 73, 95	1 (0%)
1	D	473/496 (95%)	0.30	17 (3%) 46 48	27, 51, 72, 105	1 (0%)
1	E	473/496 (95%)	0.02	17 (3%) 46 48	25, 43, 68, 100	1 (0%)
1	F	473/496 (95%)	-0.04	12 (2%) 58 59	25, 42, 64, 104	1 (0%)
1	G	473/496 (95%)	-0.00	9 (1%) 66 67	26, 41, 66, 91	1 (0%)
1	H	473/496 (95%)	-0.00	12 (2%) 58 59	25, 41, 65, 96	1 (0%)
1	I	473/496 (95%)	0.09	17 (3%) 46 48	27, 45, 67, 96	1 (0%)
1	J	473/496 (95%)	0.18	16 (3%) 48 50	28, 48, 71, 103	1 (0%)
1	K	473/496 (95%)	0.04	14 (2%) 52 54	25, 43, 69, 106	1 (0%)
1	L	473/496 (95%)	0.00	15 (3%) 50 52	27, 41, 65, 101	1 (0%)
1	M	473/496 (95%)	0.24	11 (2%) 61 62	32, 50, 70, 107	1 (0%)
1	N	473/496 (95%)	0.23	12 (2%) 58 59	30, 51, 72, 101	1 (0%)
1	O	473/496 (95%)	0.31	16 (3%) 48 50	31, 52, 75, 106	1 (0%)
1	P	473/496 (95%)	0.33	19 (4%) 43 44	30, 52, 73, 99	1 (0%)
All	All	7568/7936 (95%)	0.13	221 (2%) 54 55	25, 47, 70, 107	16 (0%)

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	468	GLY	5.8
1	K	469	PHE	5.7
1	C	469	PHE	5.6
1	D	469	PHE	5.3
1	J	469	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	N	469	PHE	5.0
1	B	469	PHE	4.8
1	H	469	PHE	4.7
1	P	469	PHE	4.7
1	L	474	PRO	4.4
1	E	398	ALA	4.2
1	B	399	GLY	4.2
1	O	469	PHE	4.1
1	N	470	ALA	4.1
1	L	299	PRO	4.1
1	L	469	PHE	4.0
1	O	468	GLY	4.0
1	H	470	ALA	4.0
1	O	470	ALA	4.0
1	H	426	ARG	3.9
1	M	469	PHE	3.9
1	F	398	ALA	3.9
1	K	398	ALA	3.9
1	J	470	ALA	3.8
1	A	469	PHE	3.8
1	O	474	PRO	3.8
1	D	468	GLY	3.8
1	J	113	ASN	3.7
1	D	426	ARG	3.7
1	I	398	ALA	3.7
1	K	474	PRO	3.7
1	P	474	PRO	3.7
1	P	468	GLY	3.7
1	E	395	ALA	3.7
1	L	468	GLY	3.6
1	D	398	ALA	3.6
1	K	470	ALA	3.6
1	M	299	PRO	3.6
1	E	469	PHE	3.5
1	D	187	PRO	3.5
1	J	474	PRO	3.5
1	K	299	PRO	3.5
1	D	470	ALA	3.4
1	P	2	VAL	3.4
1	N	474	PRO	3.4
1	J	468	GLY	3.4
1	M	474	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	426	ARG	3.3
1	D	299	PRO	3.3
1	F	470	ALA	3.3
1	C	474	PRO	3.3
1	F	469	PHE	3.3
1	I	469	PHE	3.3
1	A	468	GLY	3.3
1	M	398	ALA	3.3
1	P	299	PRO	3.3
1	F	468	GLY	3.3
1	A	300	GLY	3.2
1	M	300	GLY	3.2
1	M	113	ASN	3.2
1	P	376	ARG	3.2
1	D	300	GLY	3.2
1	E	399	GLY	3.2
1	G	128	PHE	3.2
1	I	468	GLY	3.2
1	M	468	GLY	3.2
1	B	113	ASN	3.1
1	P	470	ALA	3.1
1	I	300	GLY	3.1
1	H	473	HIS	3.1
1	C	470	ALA	3.1
1	N	399	GLY	3.0
1	B	398	ALA	3.0
1	G	468	GLY	3.0
1	K	395	ALA	3.0
1	N	398	ALA	3.0
1	B	474	PRO	3.0
1	F	113	ASN	3.0
1	B	470	ALA	3.0
1	G	395	ALA	3.0
1	O	301	ALA	3.0
1	B	468	GLY	2.9
1	E	303	CYS	2.9
1	I	474	PRO	2.9
1	L	470	ALA	2.9
1	N	395	ALA	2.9
1	P	426	ARG	2.8
1	E	468	GLY	2.8
1	J	398	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	395	ALA	2.8
1	A	474	PRO	2.8
1	G	129	GLU	2.8
1	O	395	ALA	2.8
1	C	468	GLY	2.8
1	I	113	ASN	2.8
1	G	469	PHE	2.7
1	M	470	ALA	2.7
1	J	471	GLU	2.7
1	H	474	PRO	2.7
1	I	303	CYS	2.7
1	O	113	ASN	2.6
1	A	470	ALA	2.6
1	O	399	GLY	2.6
1	D	474	PRO	2.6
1	F	299	PRO	2.6
1	O	466	ALA	2.6
1	P	466	ALA	2.6
1	C	467	ALA	2.6
1	D	303	CYS	2.6
1	E	426	ARG	2.6
1	J	426	ARG	2.6
1	H	128	PHE	2.5
1	D	405	ARG	2.5
1	J	303	CYS	2.5
1	D	467	ALA	2.5
1	E	301	ALA	2.5
1	A	426	ARG	2.5
1	J	401	SER	2.5
1	C	471	GLU	2.5
1	N	300	GLY	2.5
1	P	29	ALA	2.5
1	K	426	ARG	2.5
1	D	402	SER	2.5
1	C	466	ALA	2.5
1	I	470	ALA	2.5
1	J	473	HIS	2.5
1	A	425	ALA	2.4
1	P	473	HIS	2.4
1	F	376	ARG	2.4
1	G	396	ARG	2.4
1	A	299	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	471	GLU	2.4
1	L	404	ASP	2.4
1	N	143	GLY	2.4
1	K	301	ALA	2.4
1	C	187	PRO	2.4
1	I	299	PRO	2.4
1	J	376	ARG	2.4
1	L	426	ARG	2.4
1	C	425	ALA	2.4
1	L	425	ALA	2.4
1	E	474	PRO	2.4
1	G	474	PRO	2.4
1	O	473	HIS	2.4
1	A	466	ALA	2.4
1	D	425	ALA	2.4
1	J	29	ALA	2.4
1	L	467	ALA	2.4
1	P	425	ALA	2.4
1	I	397	THR	2.3
1	J	299	PRO	2.3
1	H	400	ASP	2.3
1	B	376	ARG	2.3
1	E	470	ALA	2.3
1	O	221	ALA	2.3
1	F	303	CYS	2.3
1	I	396	ARG	2.3
1	I	395	ALA	2.3
1	D	2	VAL	2.3
1	C	128	PHE	2.3
1	N	187	PRO	2.3
1	E	473	HIS	2.3
1	P	300	GLY	2.3
1	K	113	ASN	2.3
1	O	467	ALA	2.3
1	I	426	ARG	2.3
1	K	473	HIS	2.3
1	E	299	PRO	2.2
1	N	426	ARG	2.2
1	L	374	PHE	2.2
1	H	29	ALA	2.2
1	H	466	ALA	2.2
1	M	426	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	402	SER	2.2
1	H	468	GLY	2.2
1	E	379	ARG	2.2
1	E	425	ALA	2.2
1	L	424	PRO	2.2
1	O	29	ALA	2.2
1	M	303	CYS	2.2
1	I	399	GLY	2.2
1	G	426	ARG	2.2
1	F	474	PRO	2.2
1	H	398	ALA	2.2
1	P	128	PHE	2.2
1	F	426	ARG	2.1
1	N	467	ALA	2.1
1	C	143	GLY	2.1
1	L	303	CYS	2.1
1	J	467	ALA	2.1
1	K	467	ALA	2.1
1	L	395	ALA	2.1
1	D	471	GLU	2.1
1	B	3	ARG	2.1
1	C	300	GLY	2.1
1	F	401	SER	2.1
1	K	117	HIS	2.1
1	E	113	ASN	2.1
1	F	397	THR	2.1
1	I	466	ALA	2.1
1	O	457[A]	GLU	2.1
1	C	426	ARG	2.1
1	E	378	ASP	2.1
1	L	378	ASP	2.1
1	B	312	GLY	2.1
1	J	472	GLY	2.1
1	N	113	ASN	2.1
1	P	424	PRO	2.1
1	G	152	ASP	2.0
1	I	298	GLY	2.0
1	O	143	GLY	2.0
1	C	473	HIS	2.0
1	E	376	ARG	2.0
1	I	405	ARG	2.0
1	P	467	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	471	GLU	2.0
1	M	385	TYR	2.0
1	K	399	GLY	2.0
1	O	378	ASP	2.0
1	P	374	PHE	2.0
1	L	418	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^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

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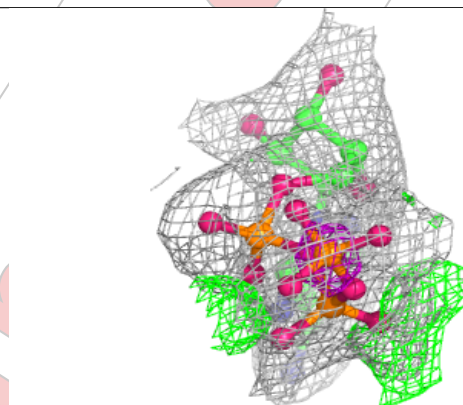
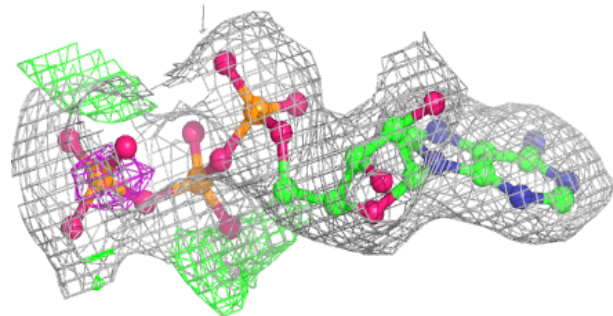
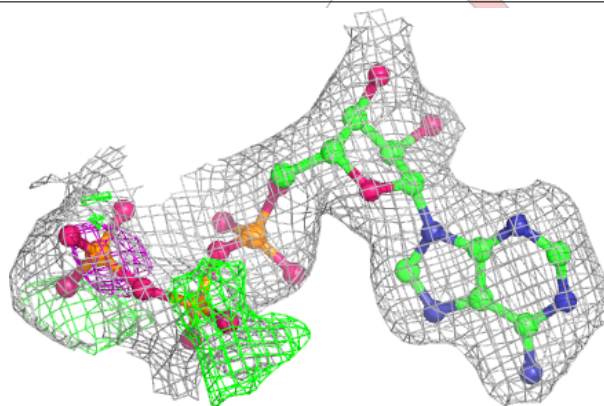
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	M	502[B]	31/31	0.90	0.09	43,45,54,55	31
2	ATP	J	501[A]	31/31	0.91	0.09	46,49,55,59	31
2	ATP	J	501[B]	31/31	0.91	0.09	46,49,56,57	31
2	ATP	N	502[A]	31/31	0.91	0.09	44,45,54,54	31
2	ATP	N	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.

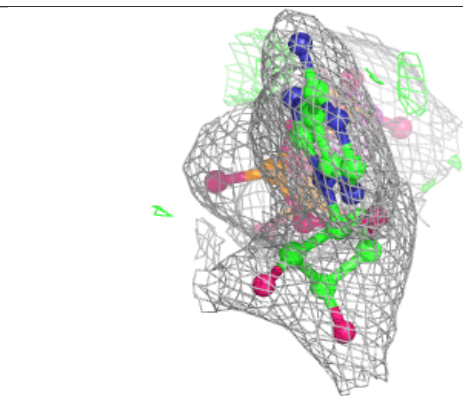
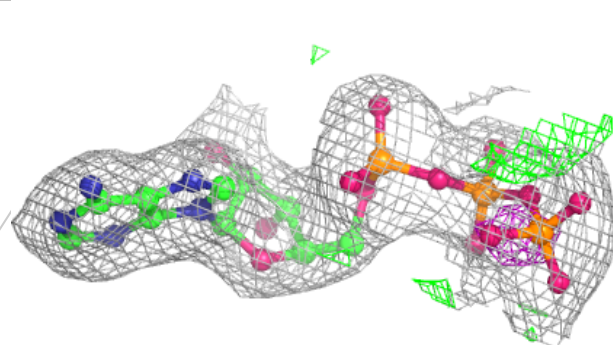
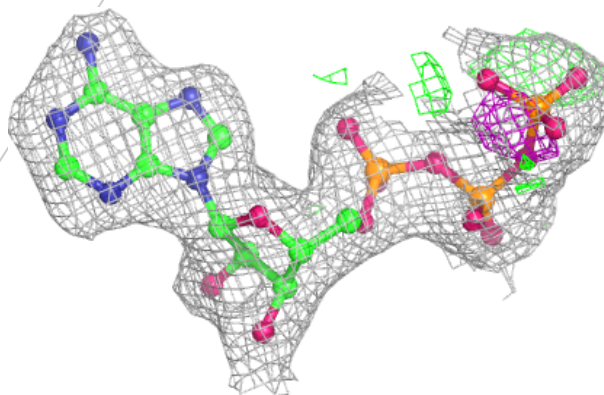
Electron density around ATP D 501 (A):

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



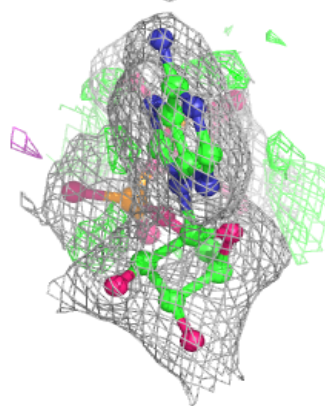
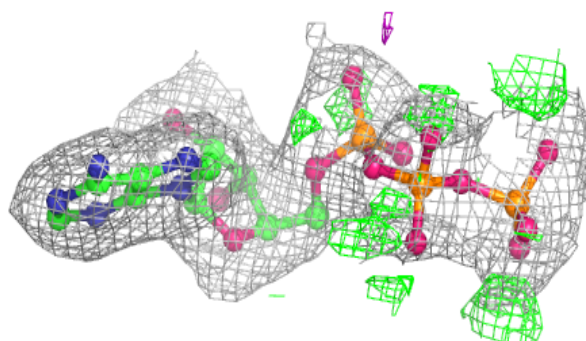
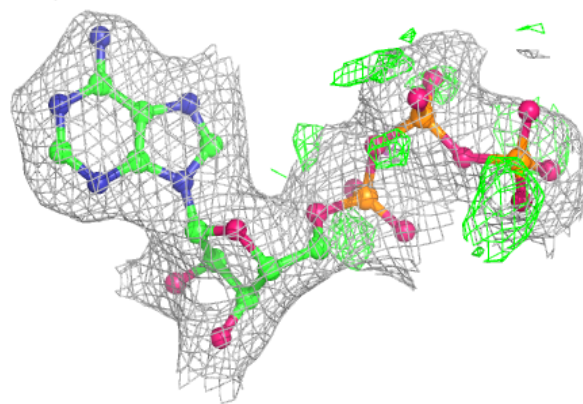
Electron density around ATP D 501 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



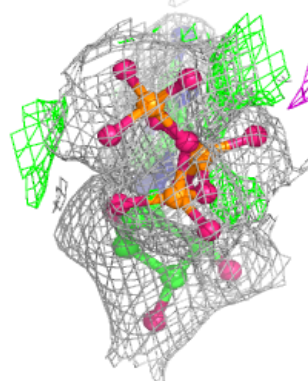
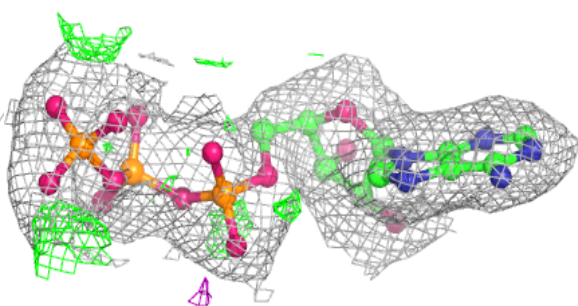
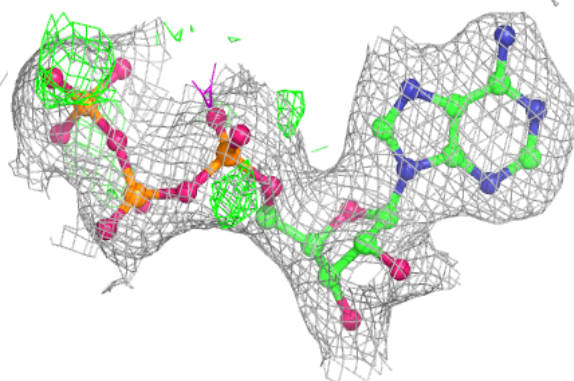
Electron density around ATP E 501 (A):

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



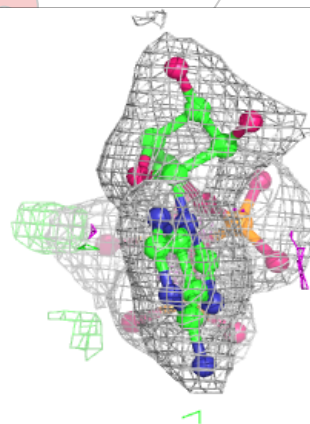
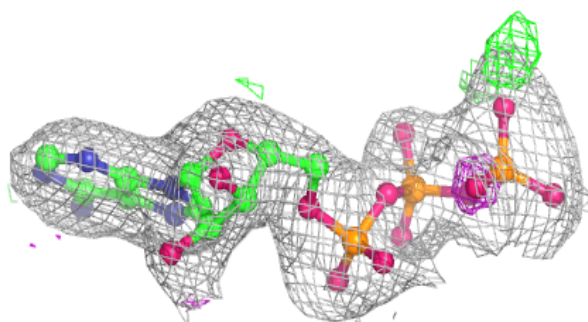
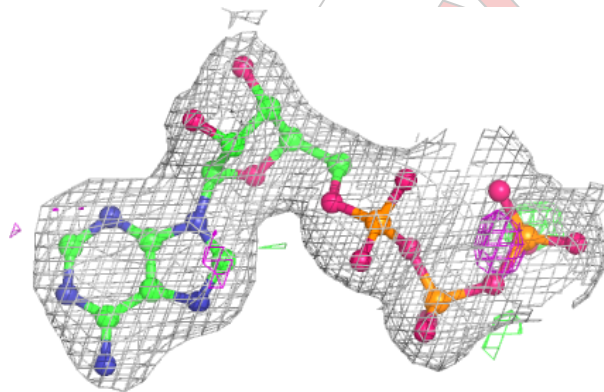
Electron density around ATP E 501 (B):

$2mF_o-DF_c$ (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):

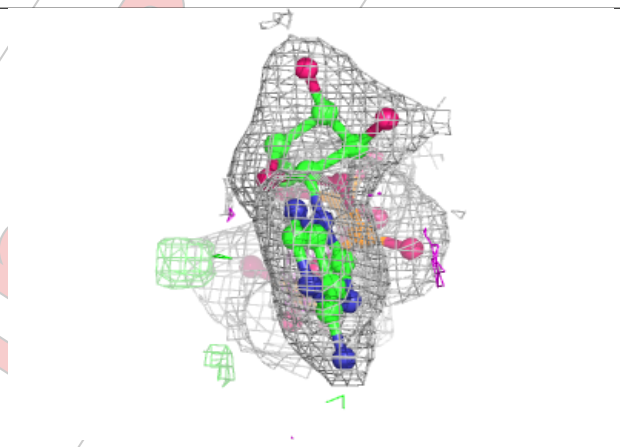
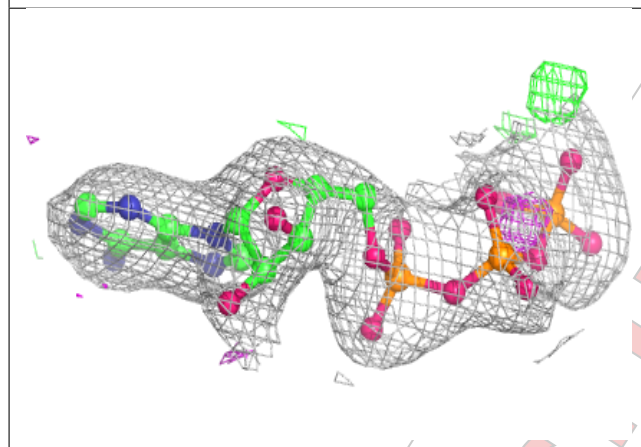
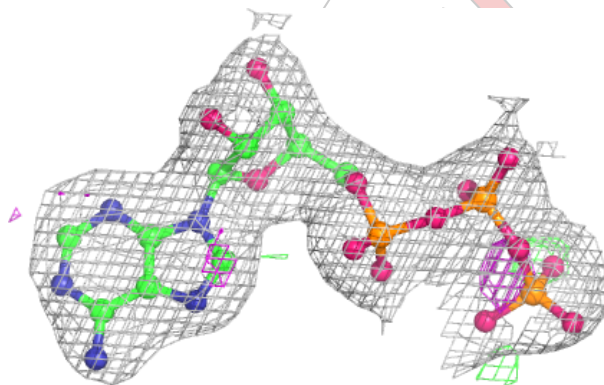
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



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Electron density around ATP K 501 (B):

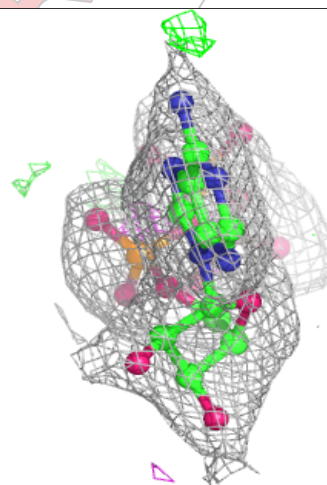
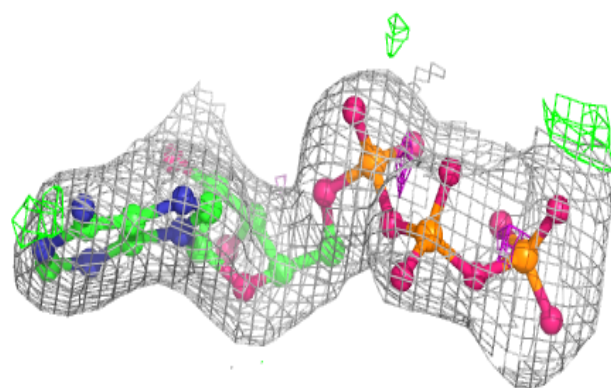
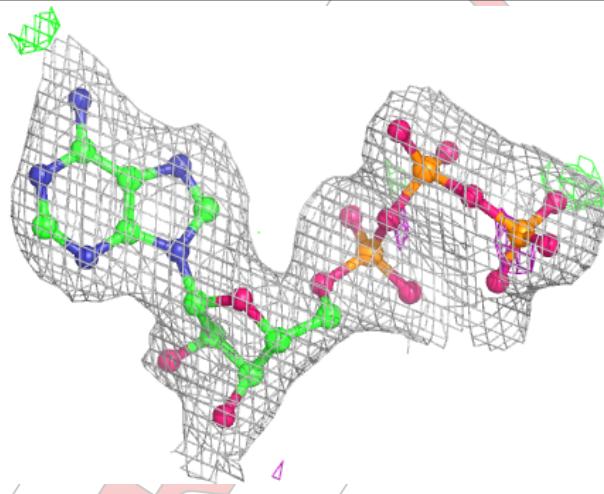
2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



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Electron density around ATP O 502 (A):

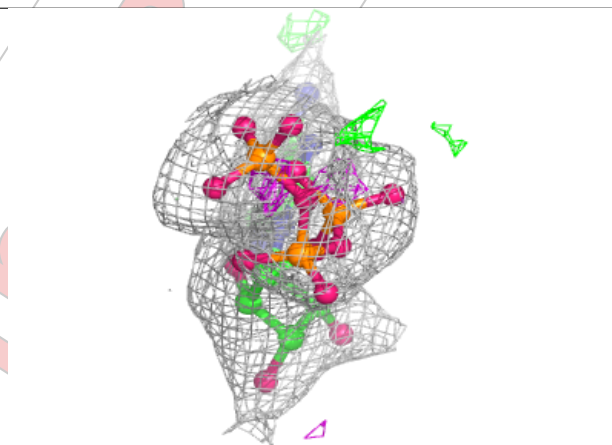
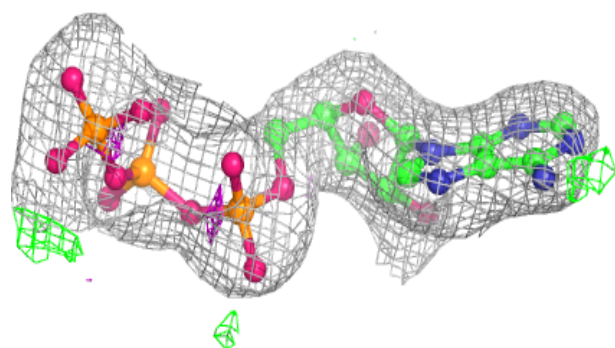
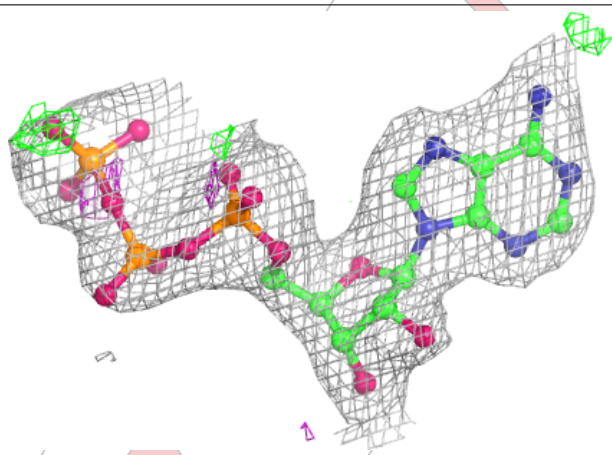
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
 and green (positive)



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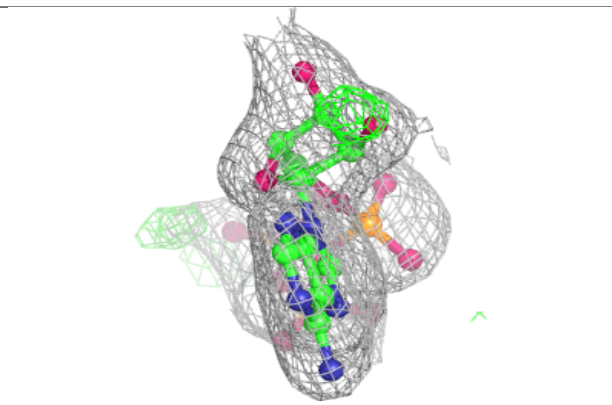
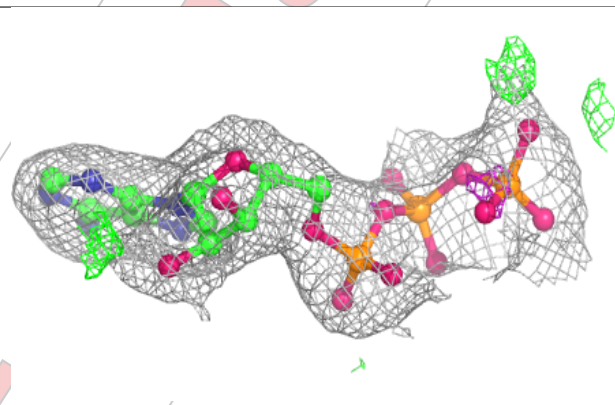
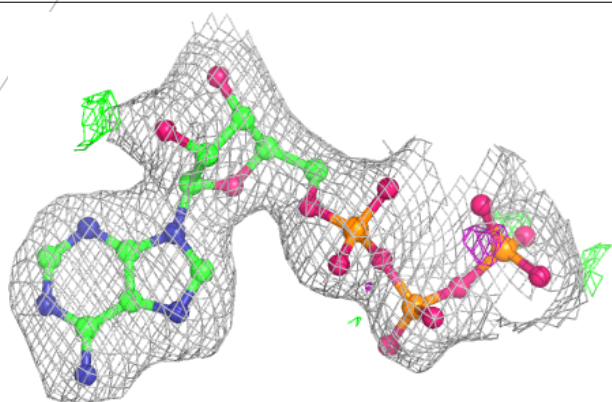
Electron density around ATP O 502 (B):

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



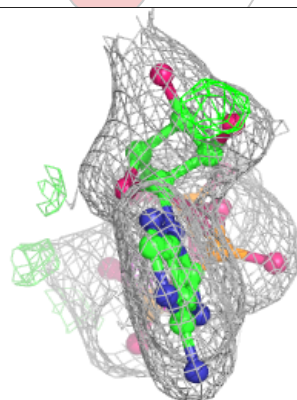
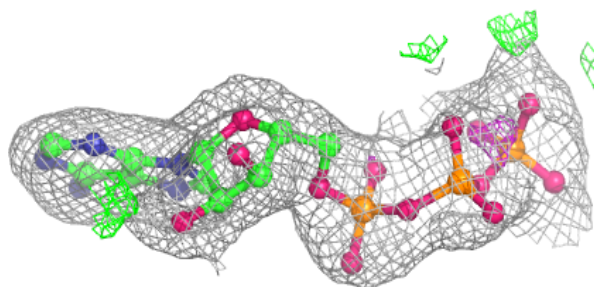
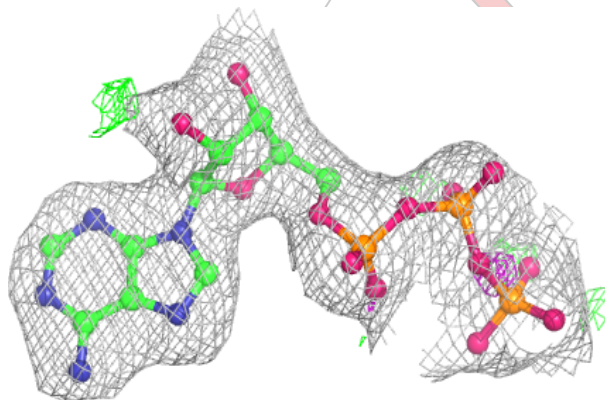
Electron density around ATP B 501 (A):

$2mF_o-DF_c$ (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):

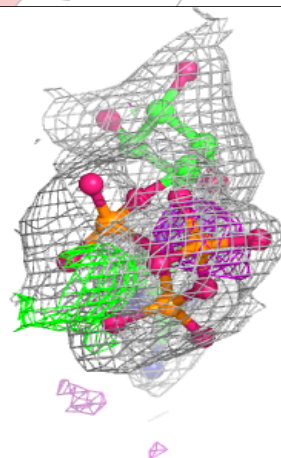
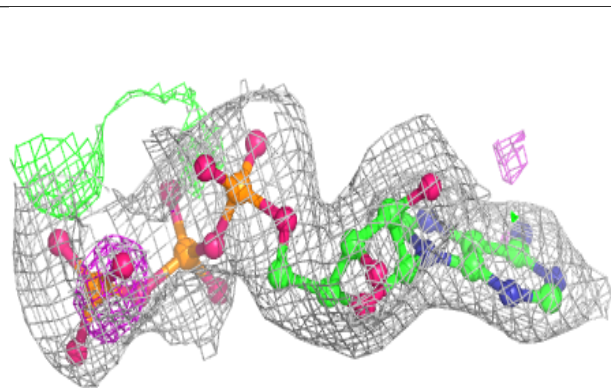
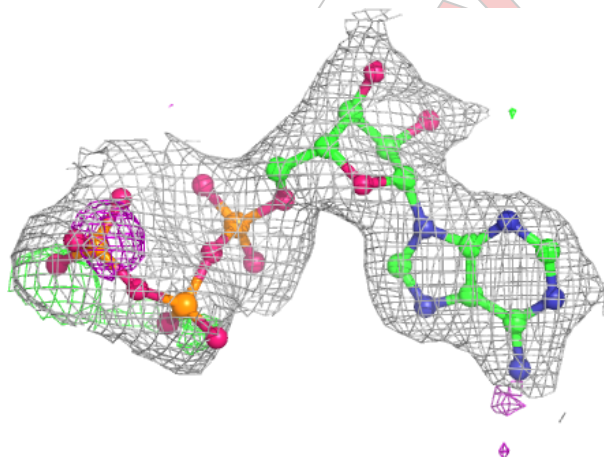
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



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Electron density around ATP L 502 (A):

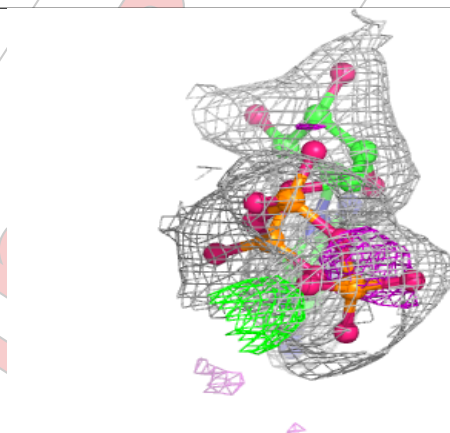
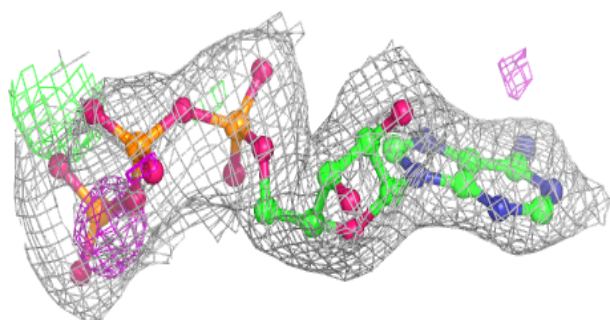
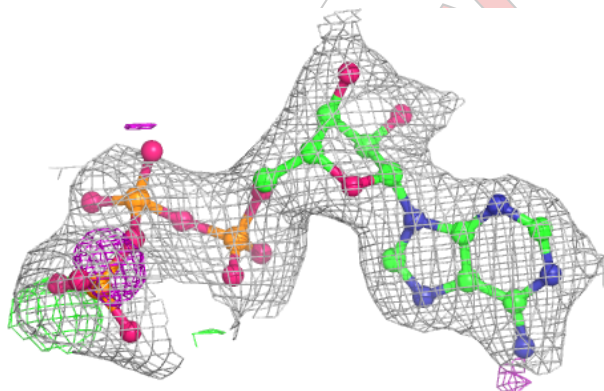
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
 and green (positive)



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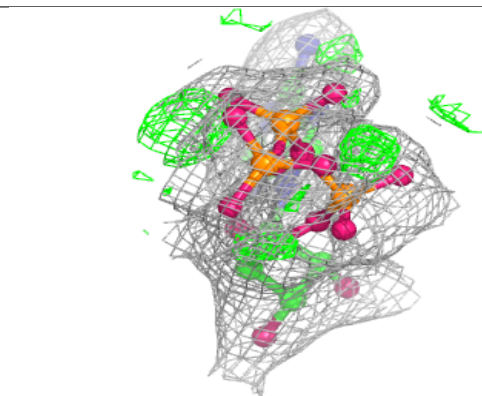
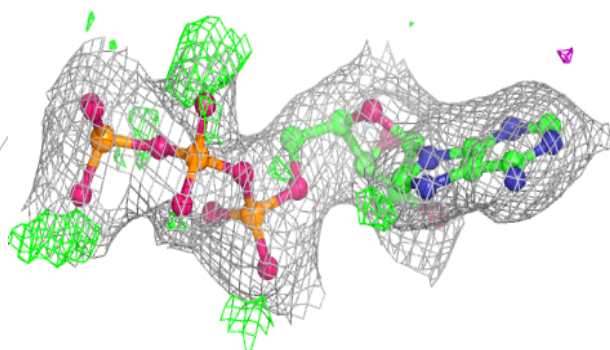
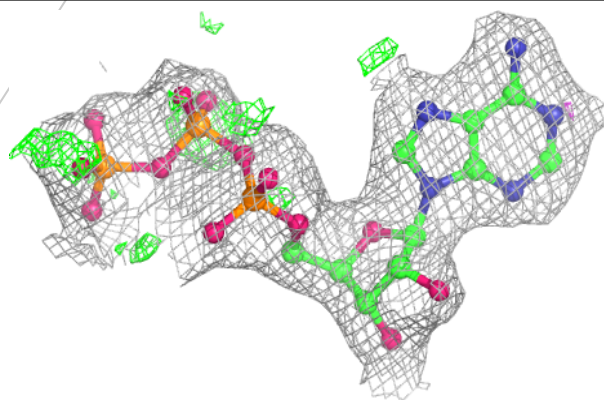
Electron density around ATP L 502 (B):

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 and green (positive)



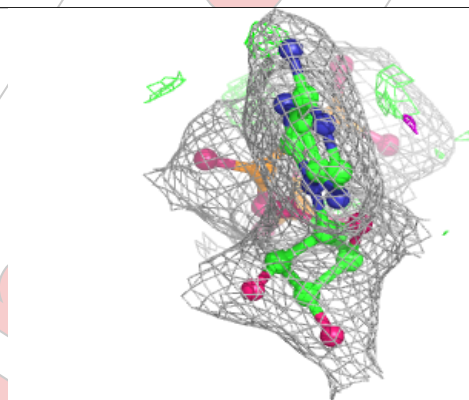
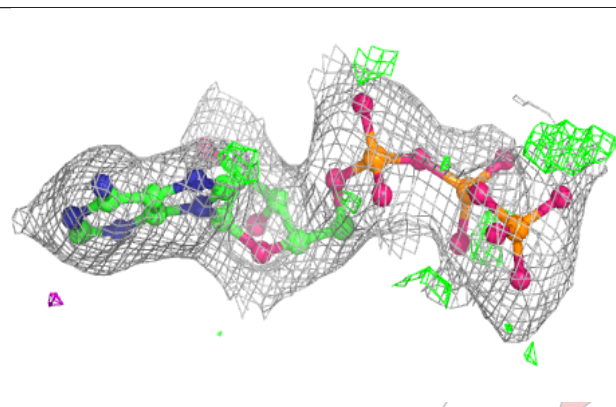
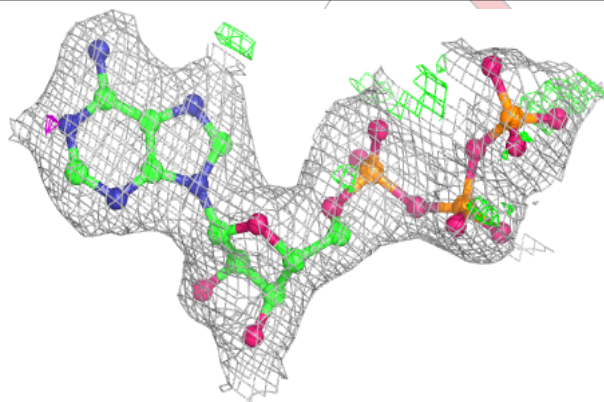
Electron density around ATP G 501 (A):

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



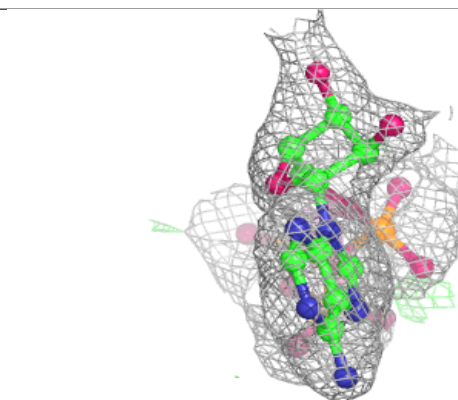
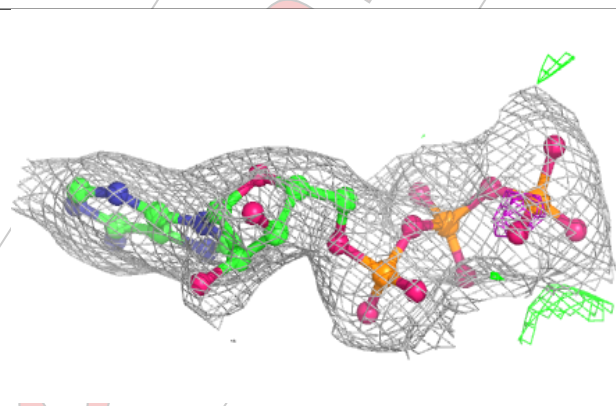
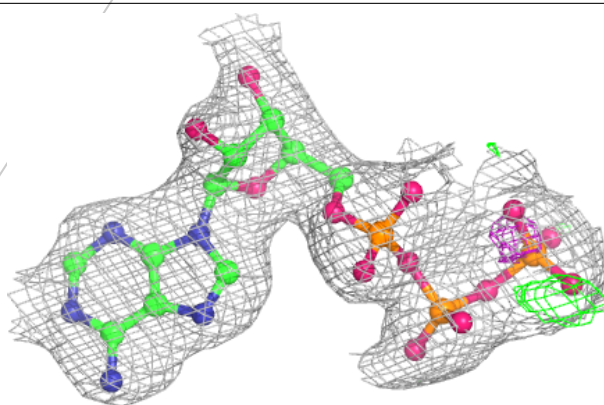
Electron density around ATP G 501 (B):

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



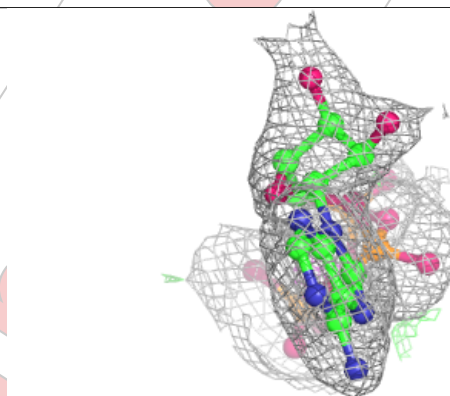
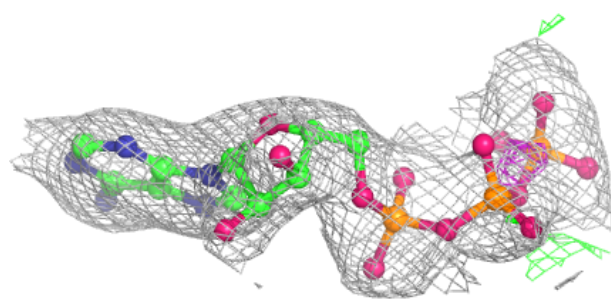
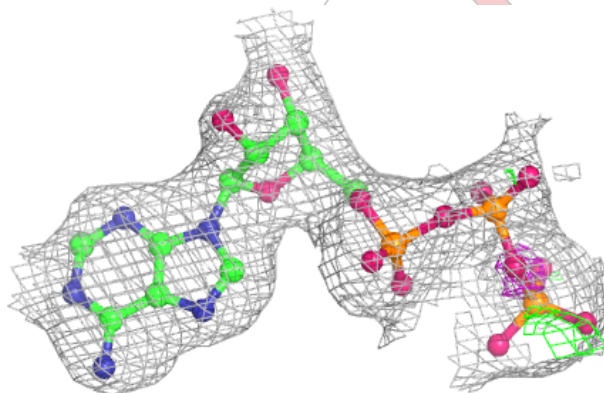
Electron density around ATP P 502 (A):

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



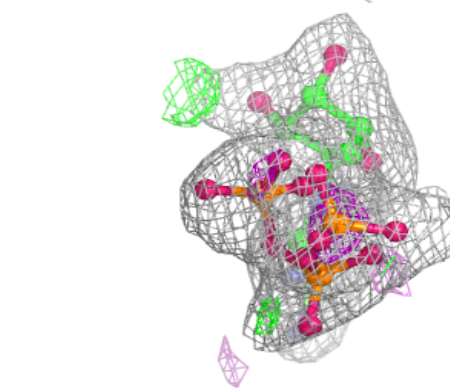
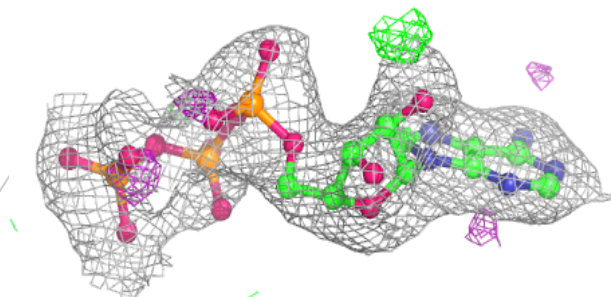
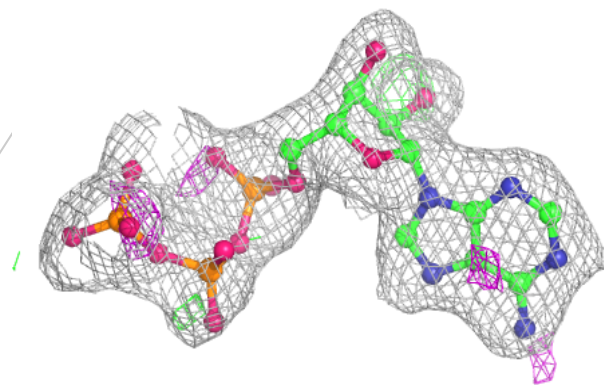
Electron density around ATP P 502 (B):

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



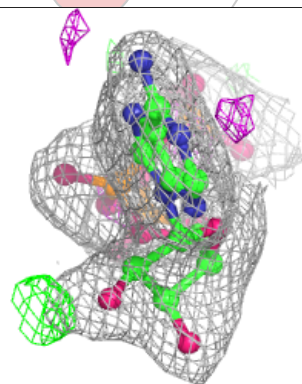
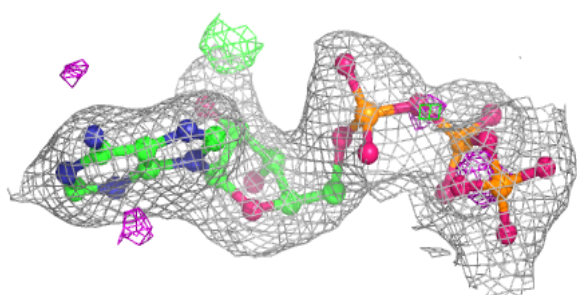
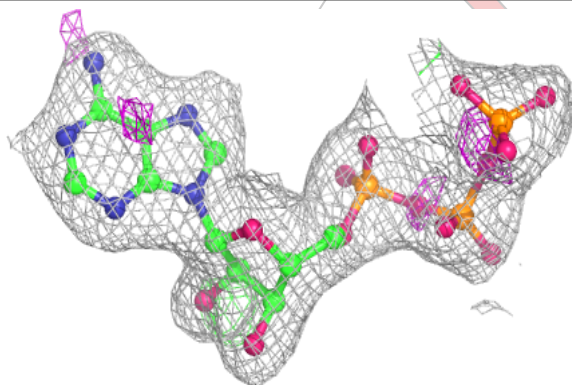
Electron density around ATP M 502 (A):

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



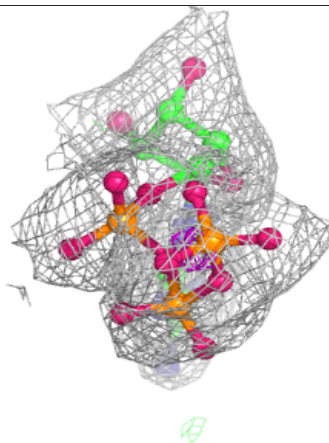
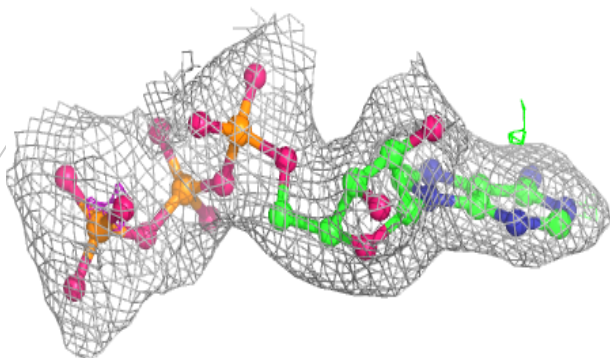
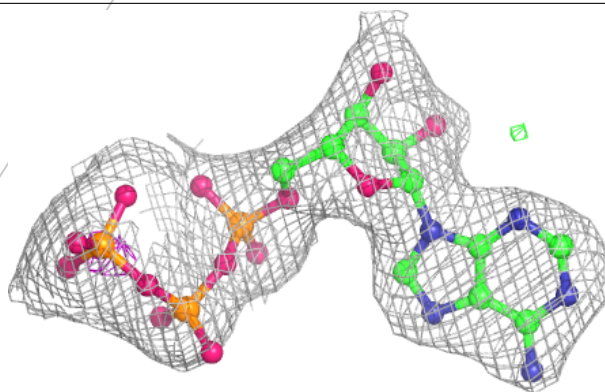
Electron density around ATP M 502 (B):

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



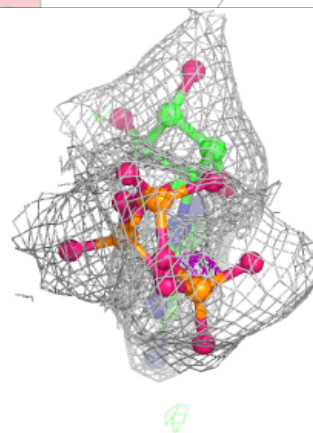
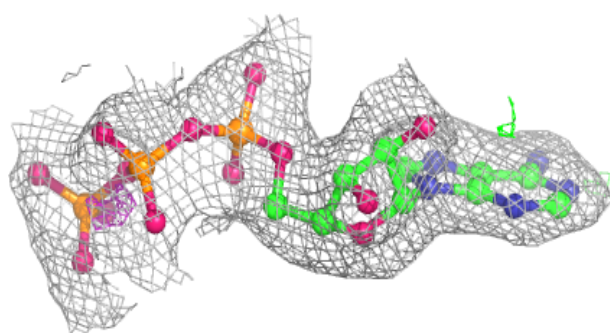
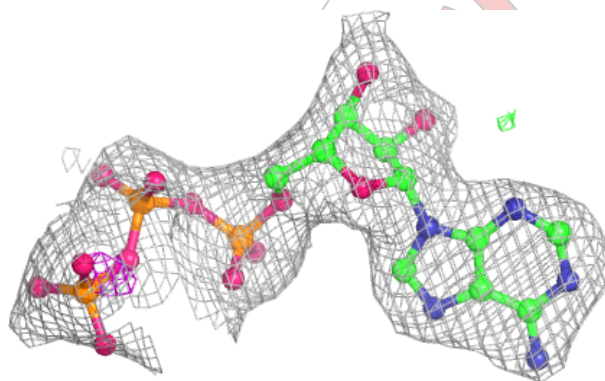
Electron density around ATP J 501 (A):

$2mF_o-DF_c$ (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):

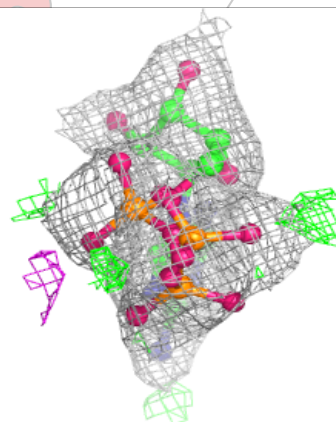
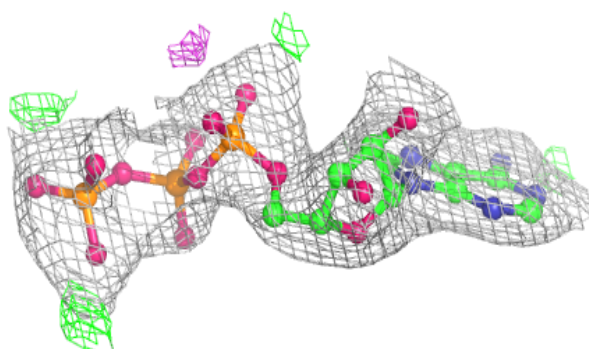
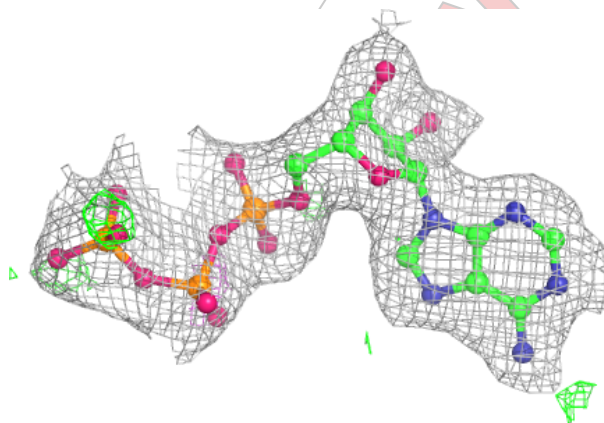
2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



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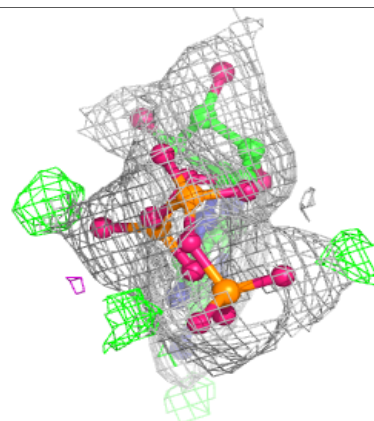
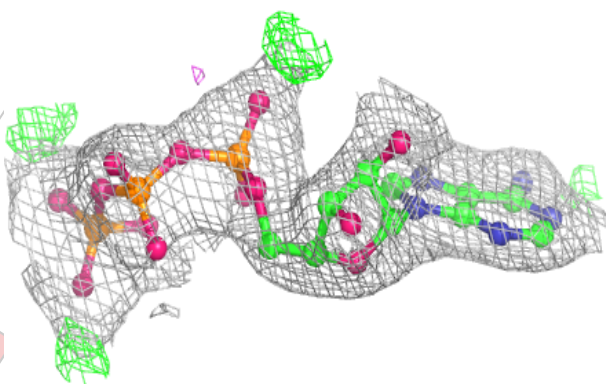
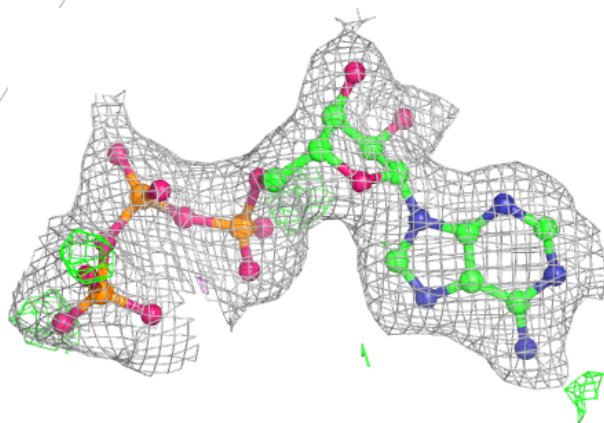
Electron density around ATP N 502 (A):

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



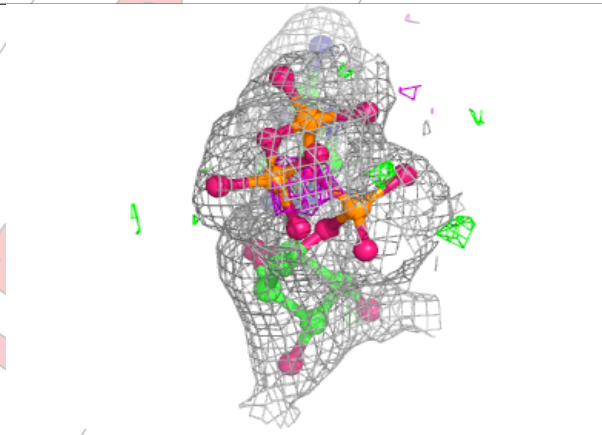
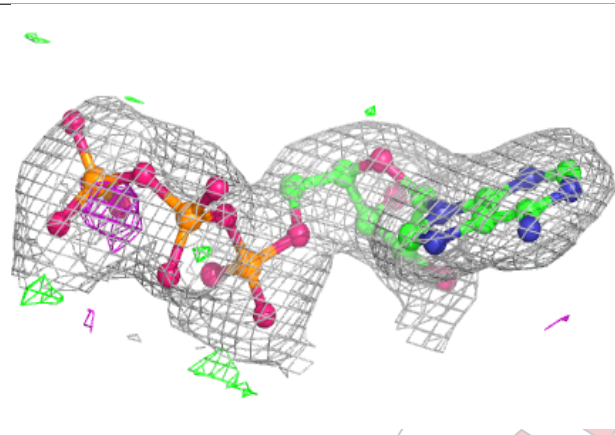
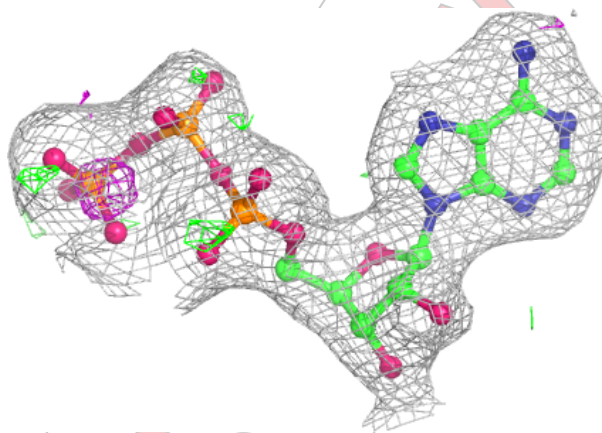
Electron density around ATP N 502 (B):

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



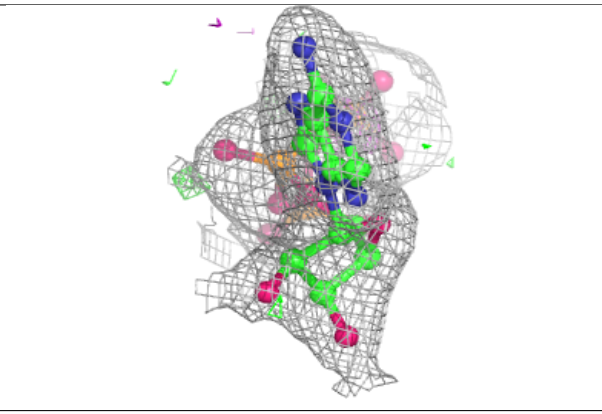
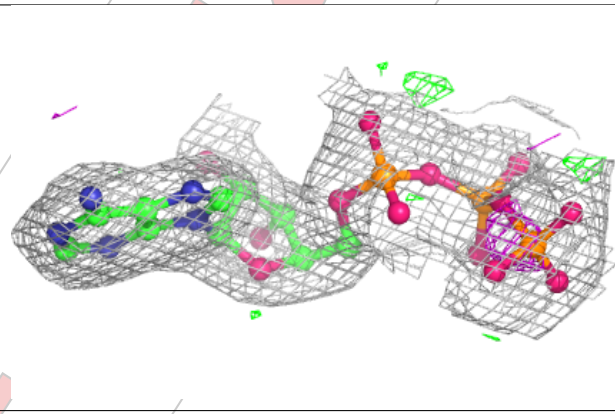
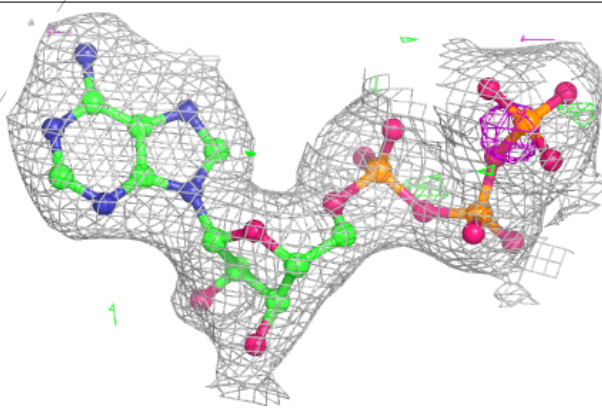
Electron density around ATP A 501 (A):

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



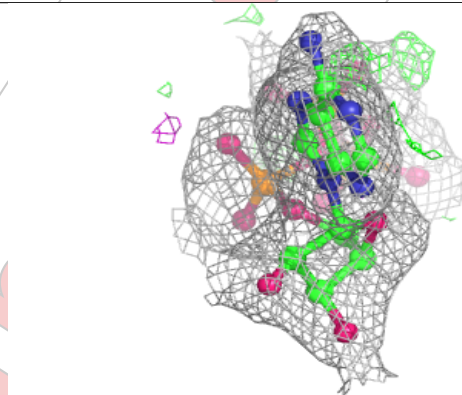
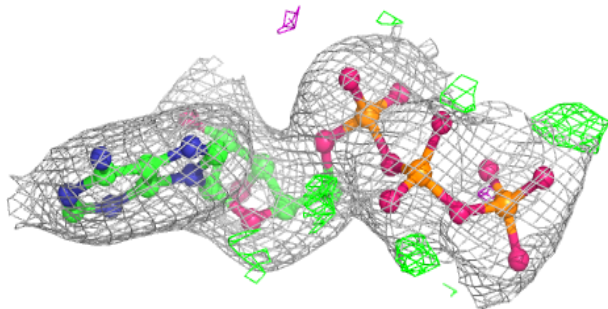
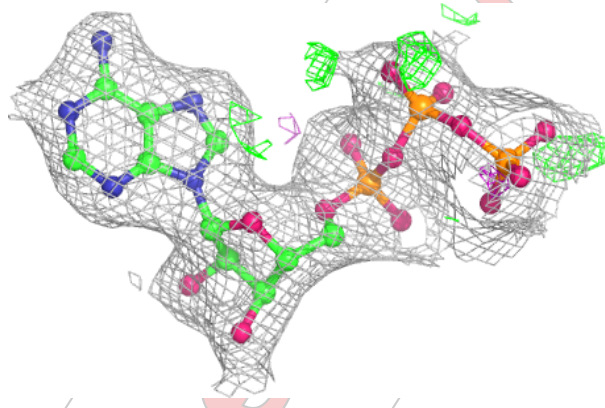
Electron density around ATP A 501 (B):

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



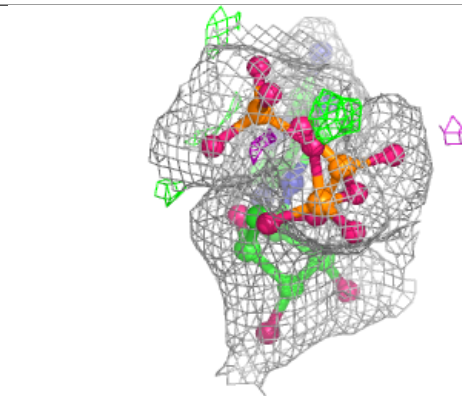
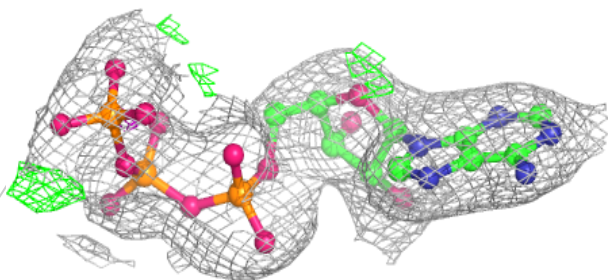
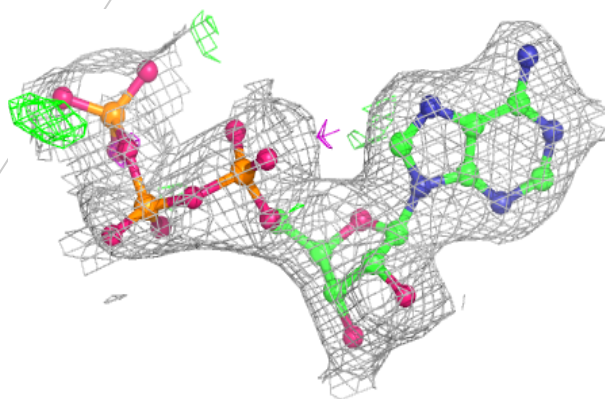
Electron density around ATP I 501 (A):

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



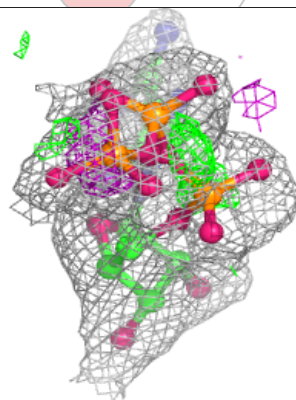
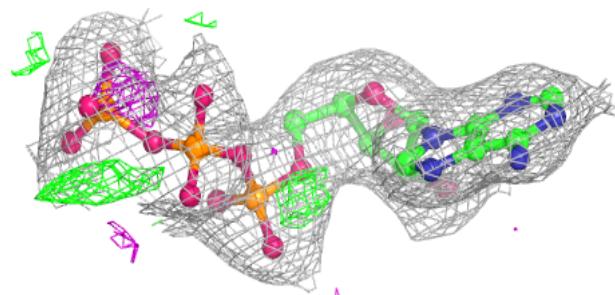
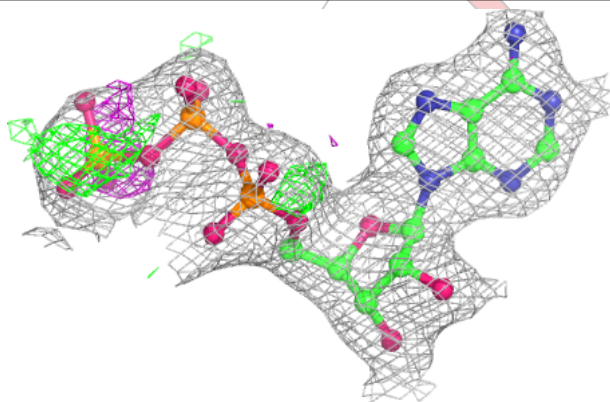
Electron density around ATP I 501 (B):

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



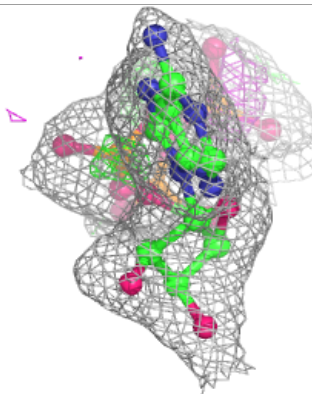
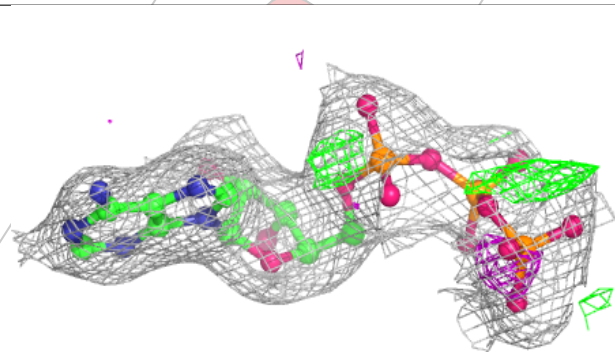
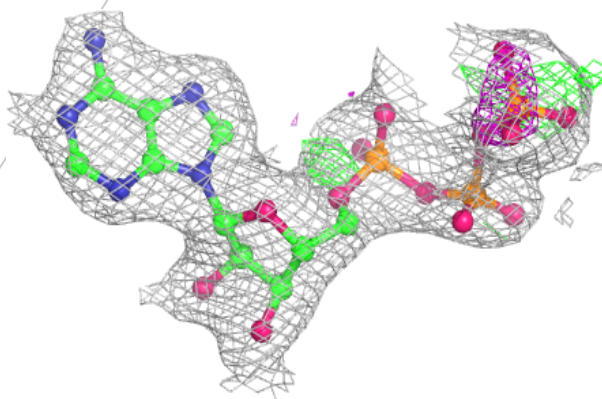
Electron density around ATP H 501 (A):

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



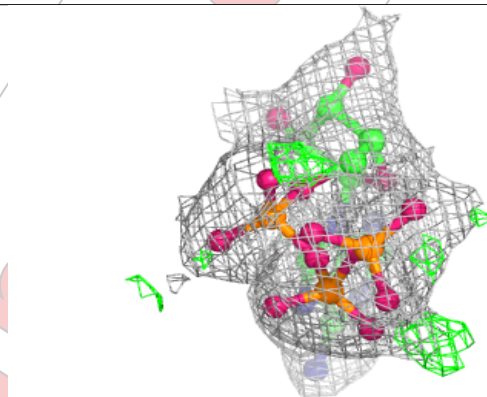
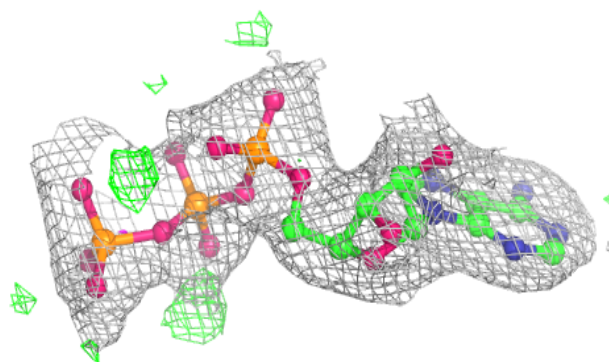
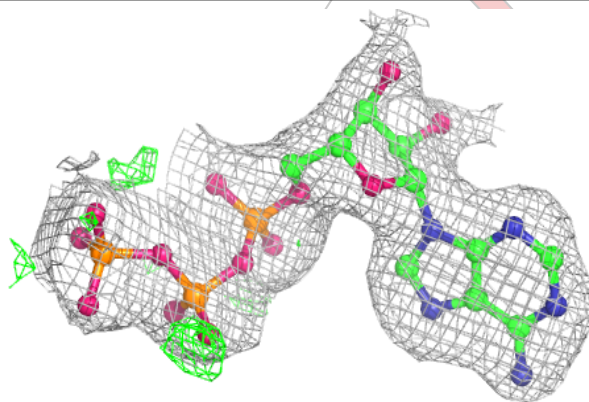
Electron density around ATP H 501 (B):

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



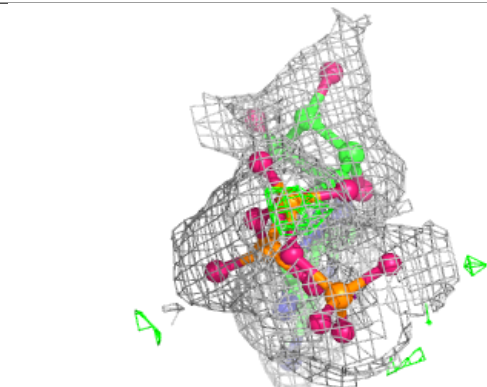
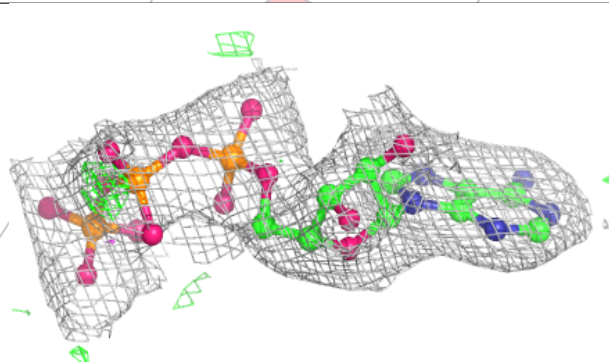
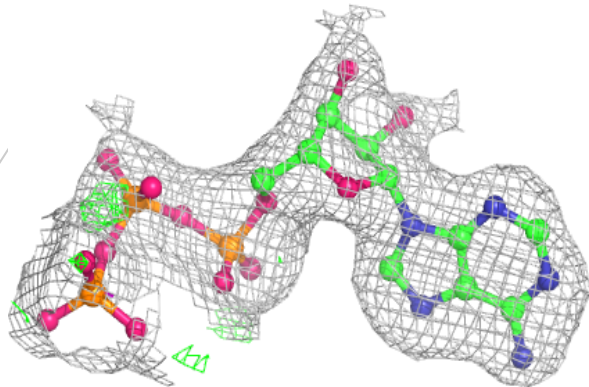
Electron density around ATP F 501 (A):

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



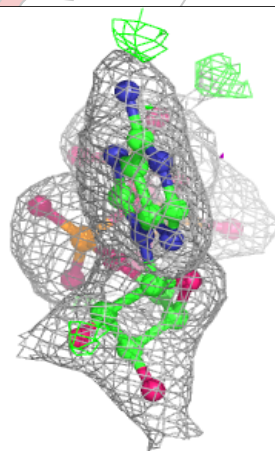
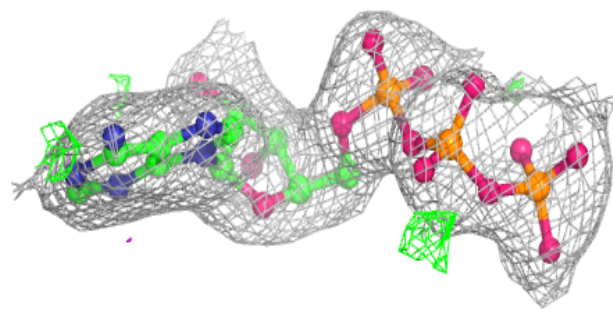
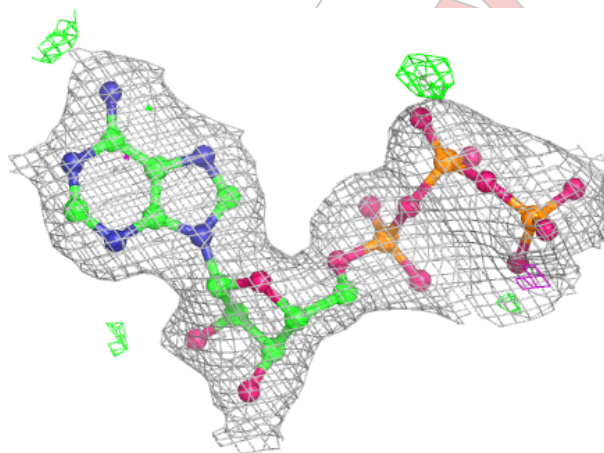
Electron density around ATP F 501 (B):

$2mF_o - DF_c$ (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):

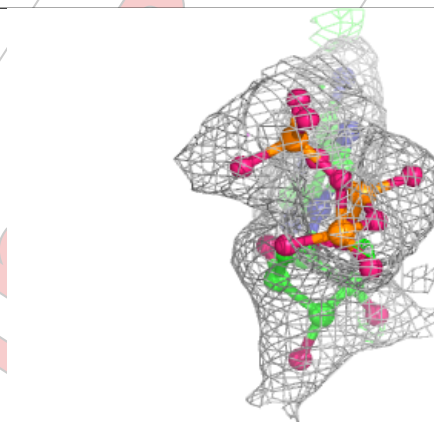
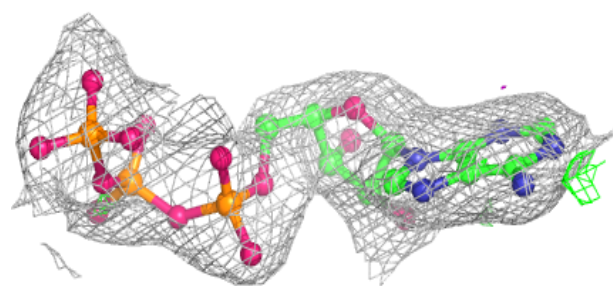
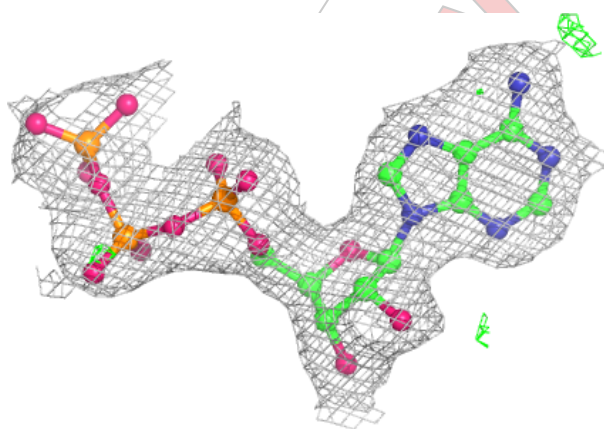
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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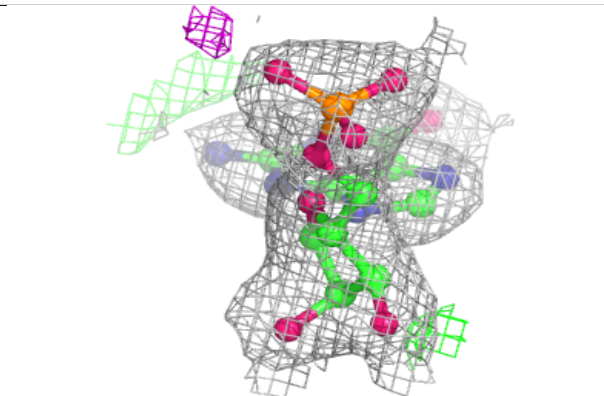
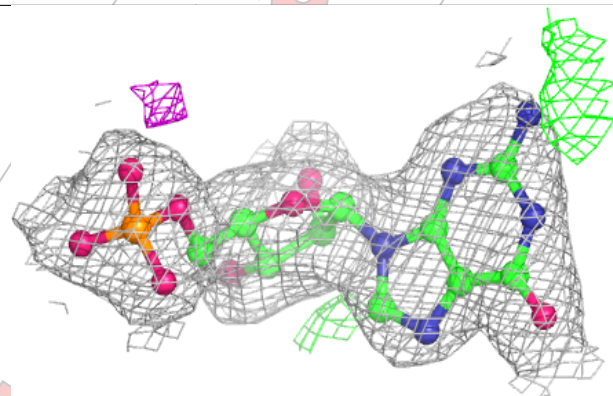
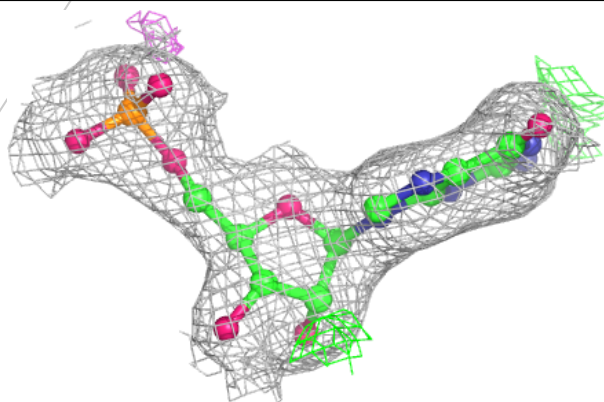
Electron density around ATP C 501 (B):

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



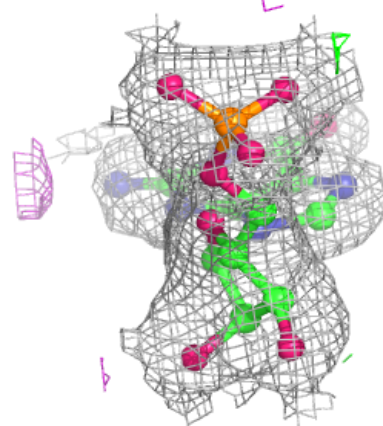
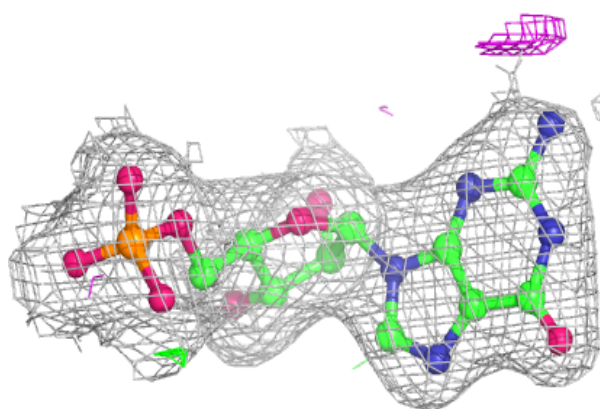
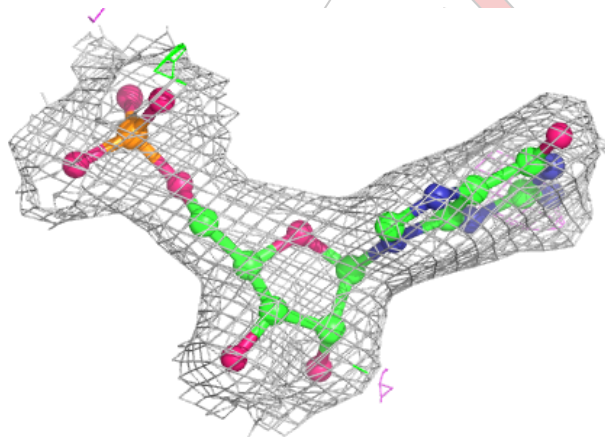
Electron density around 5GP P 501:

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



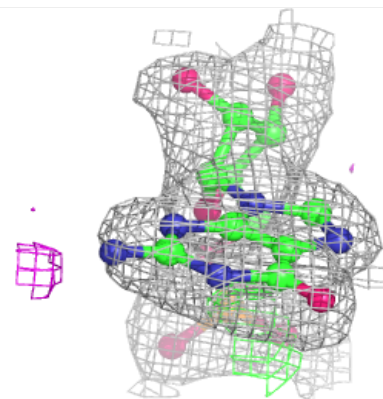
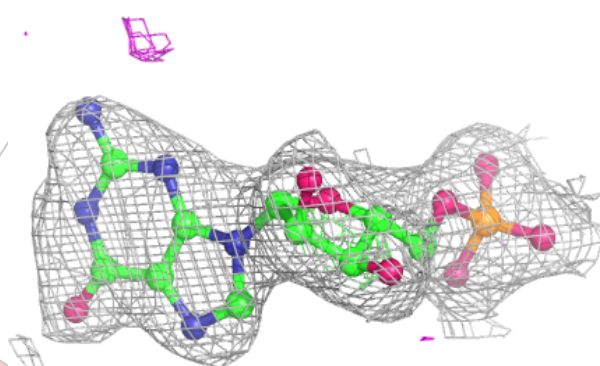
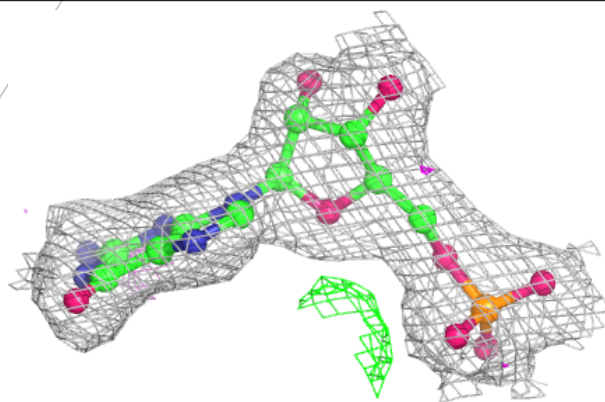
Electron density around 5GP F 502:

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



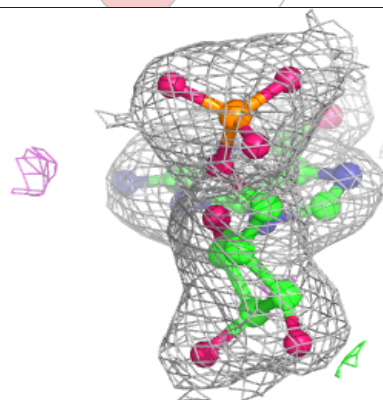
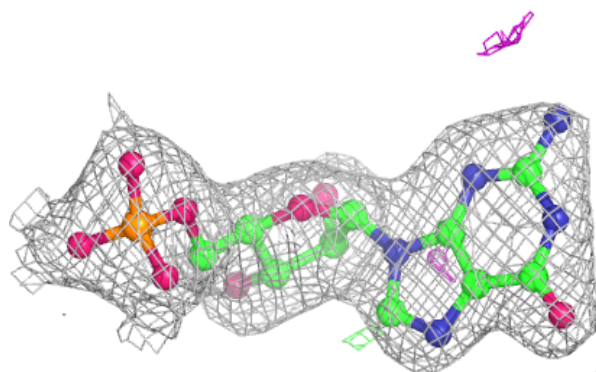
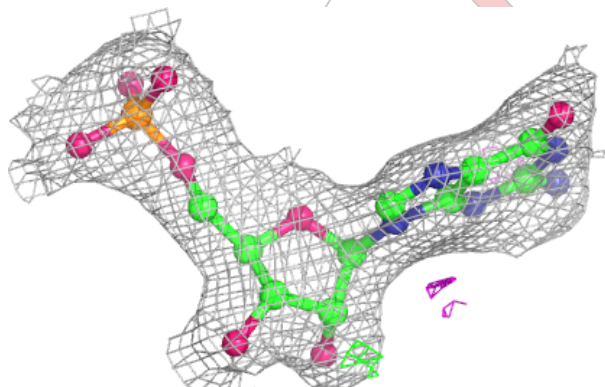
Electron density around 5GP I 502:

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



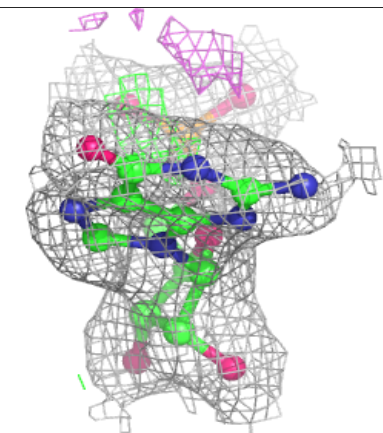
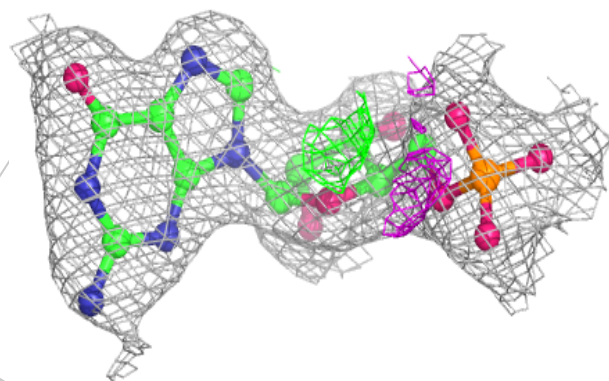
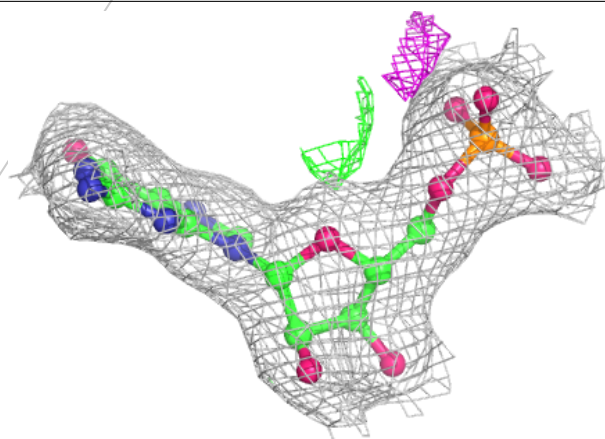
Electron density around 5GP J 502:

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



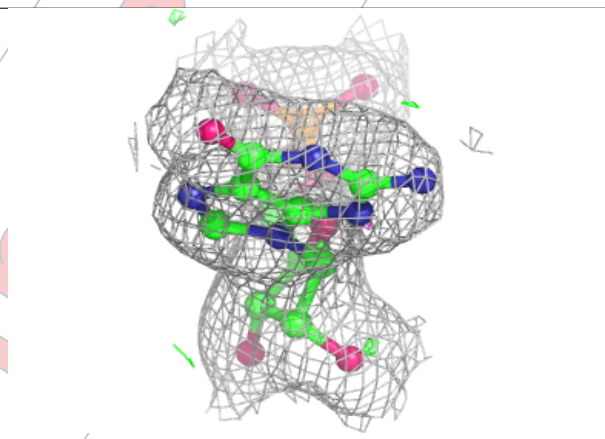
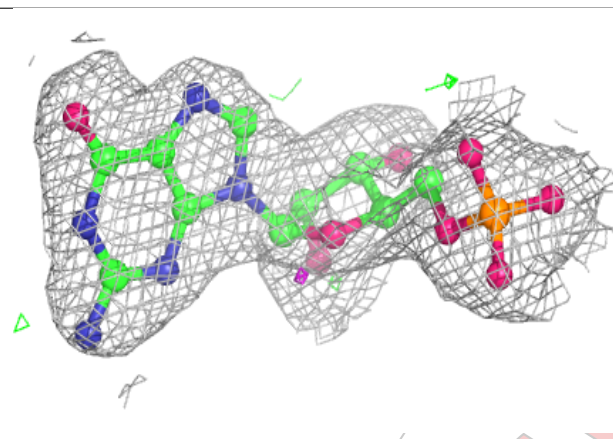
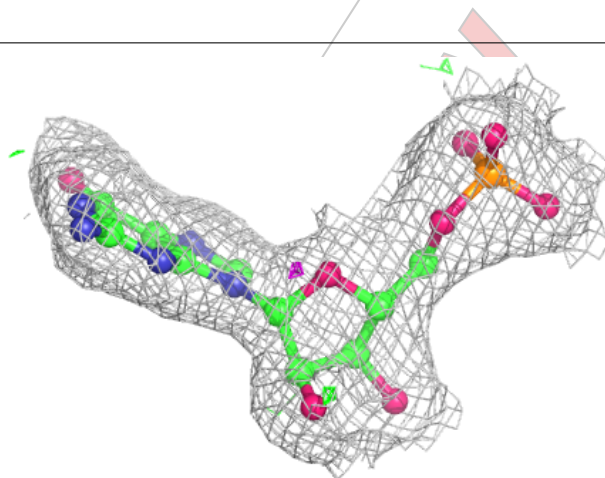
Electron density around 5GP K 502:

$2mF_o-DF_c$ (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:

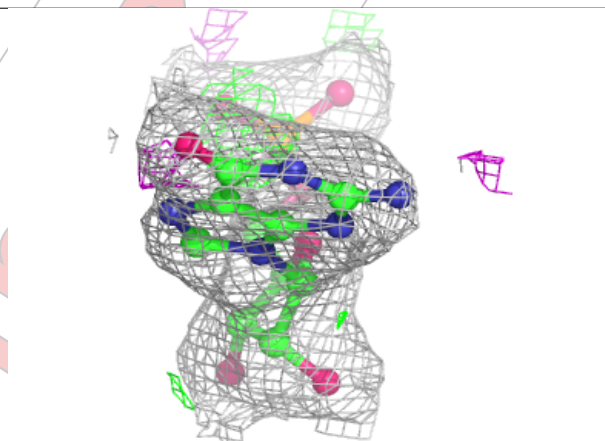
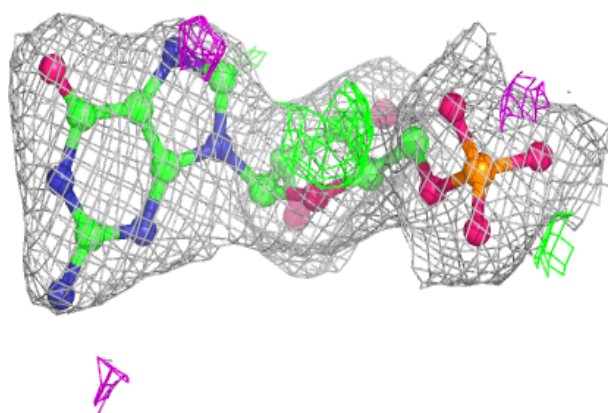
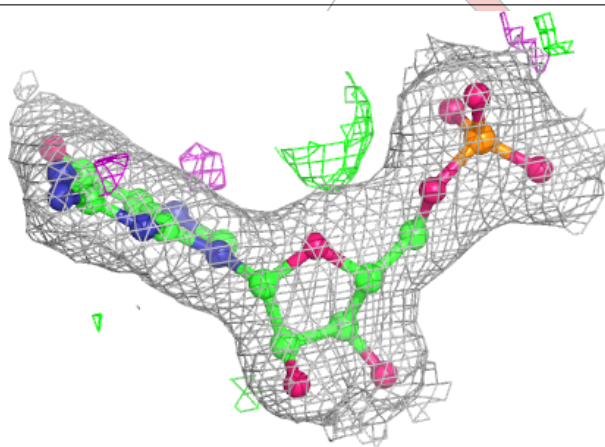
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



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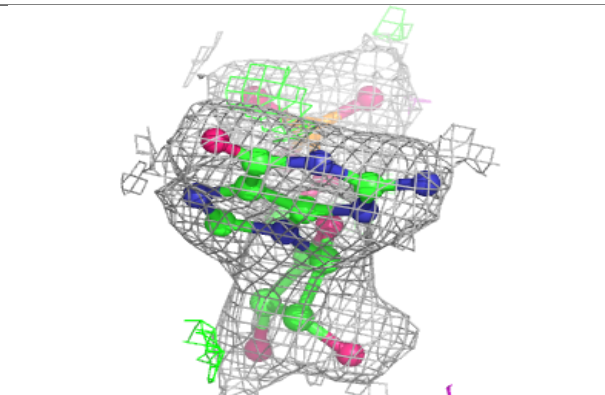
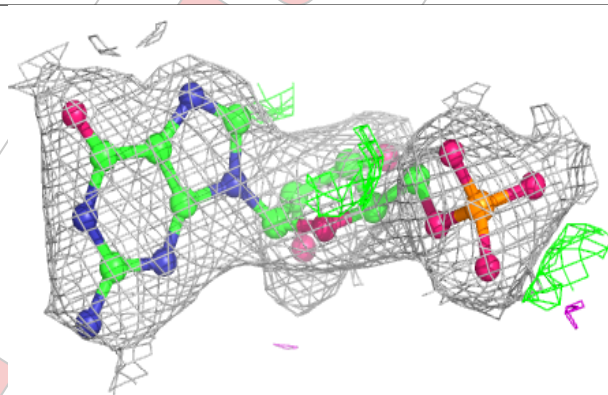
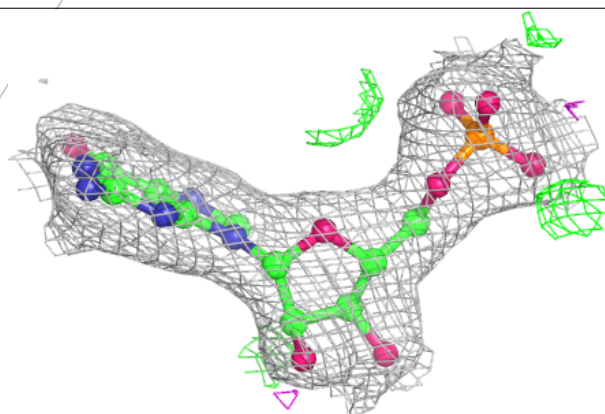
Electron density around 5GP M 501:

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



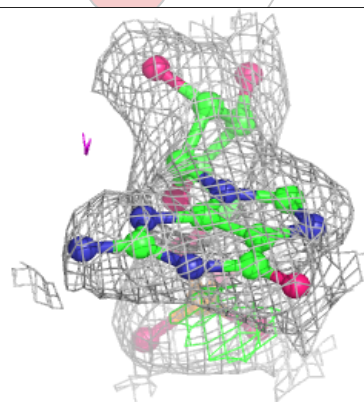
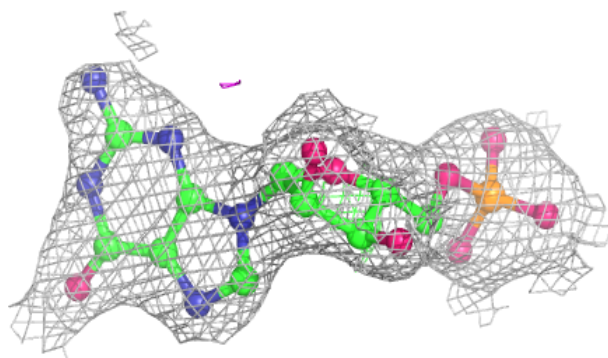
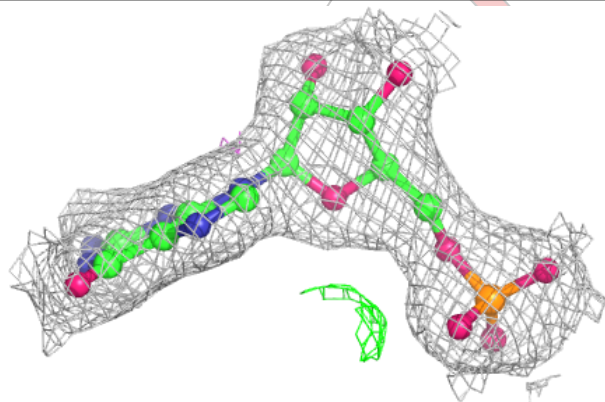
Electron density around 5GP N 501:

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



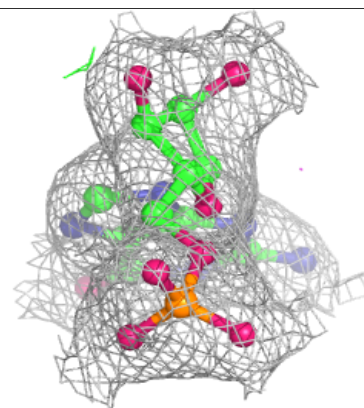
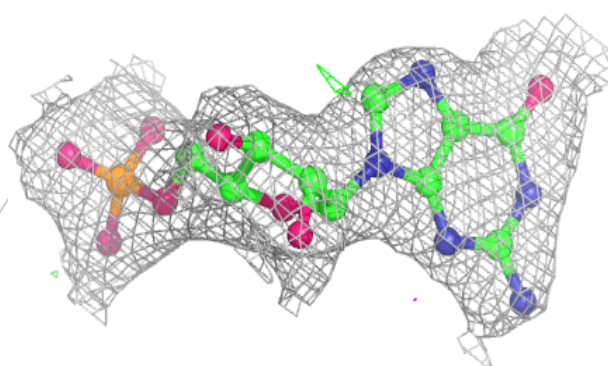
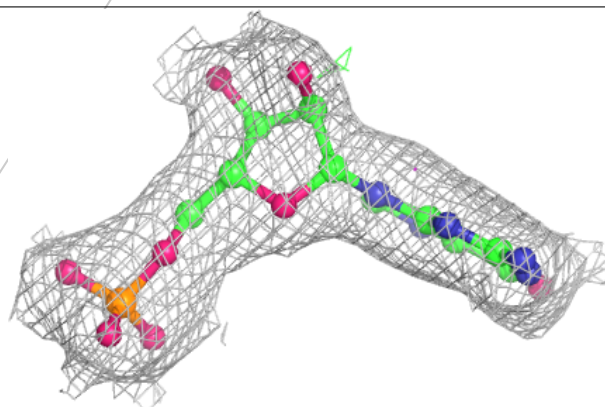
Electron density around 5GP O 501:

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



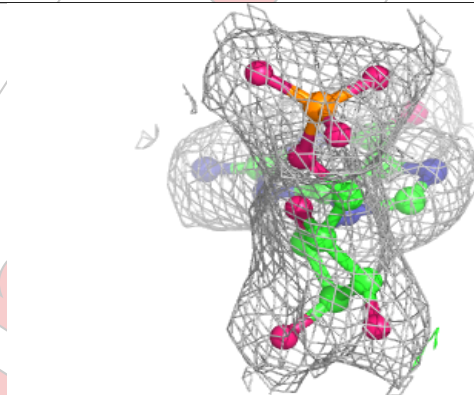
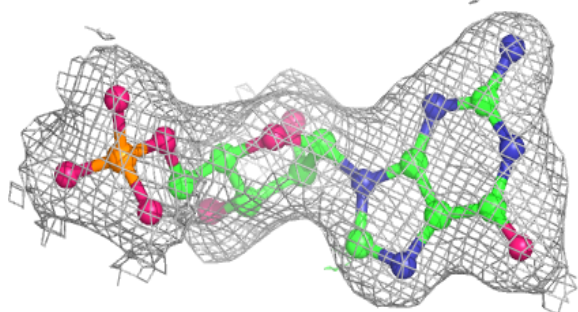
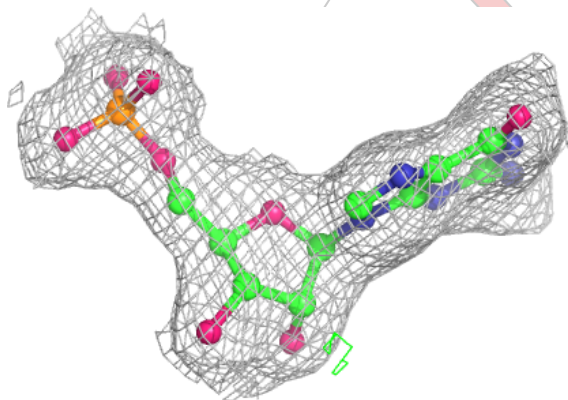
Electron density around 5GP D 502:

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



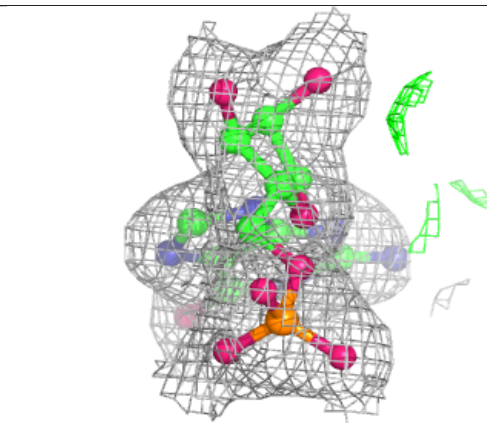
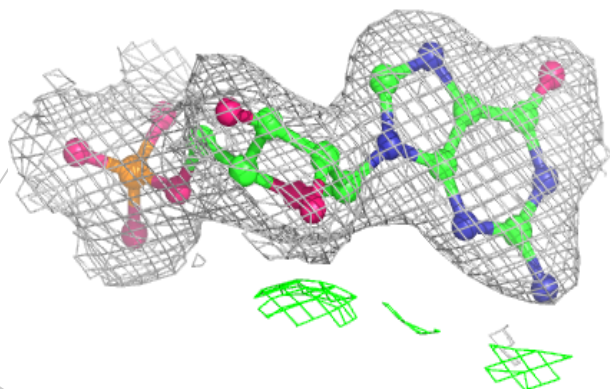
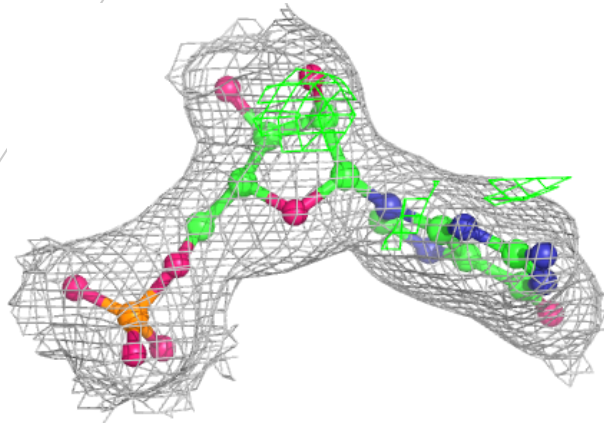
Electron density around 5GP G 502:

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



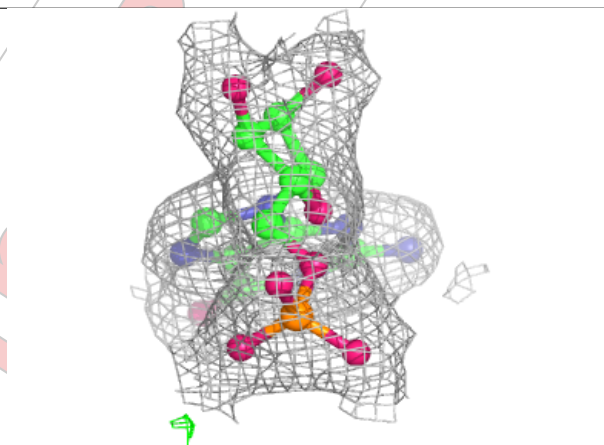
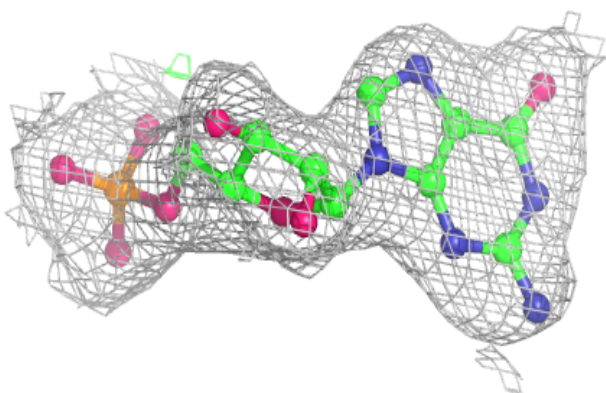
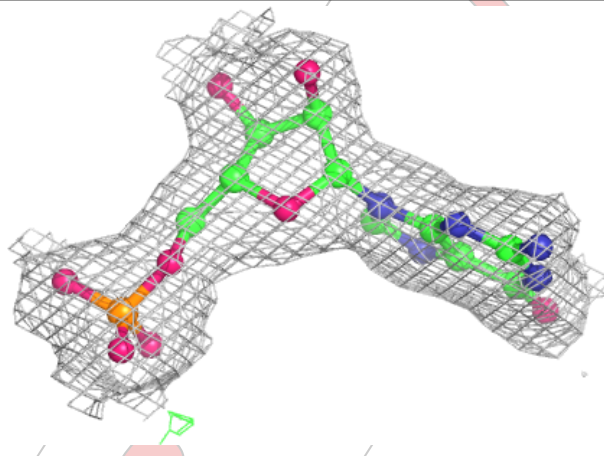
Electron density around 5GP H 502:

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



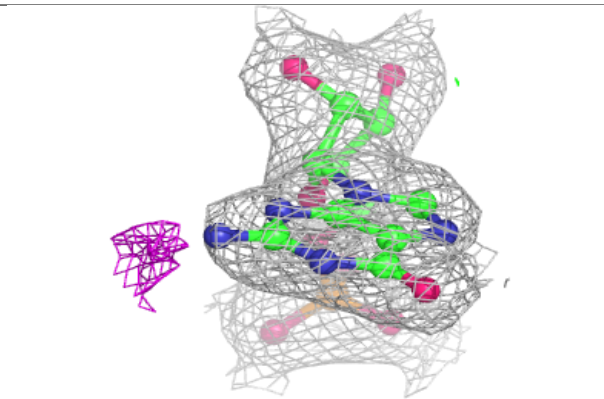
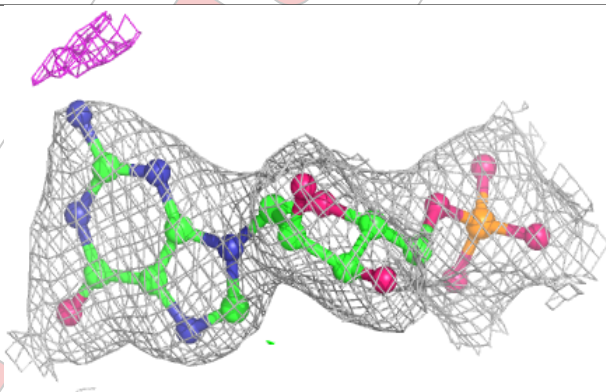
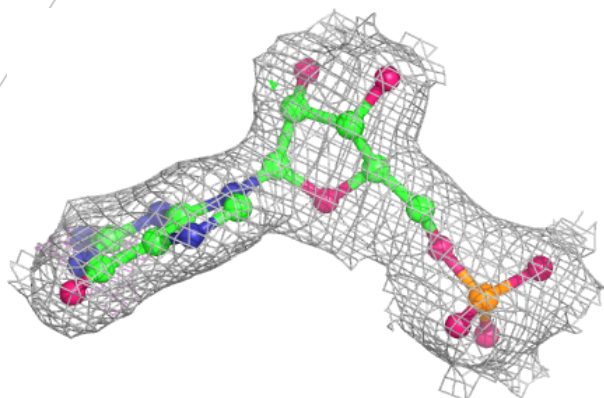
Electron density around 5GP A 502:

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



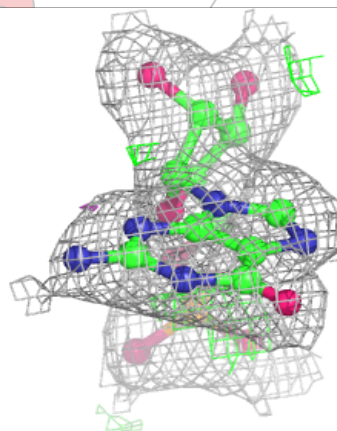
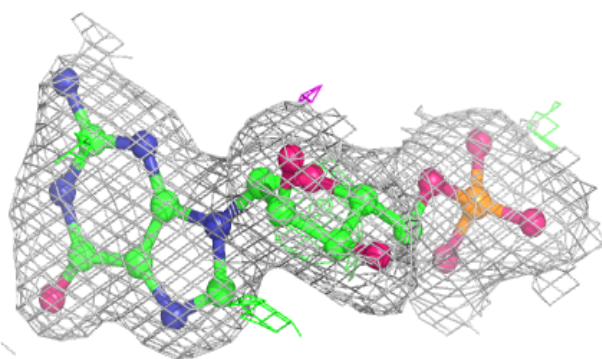
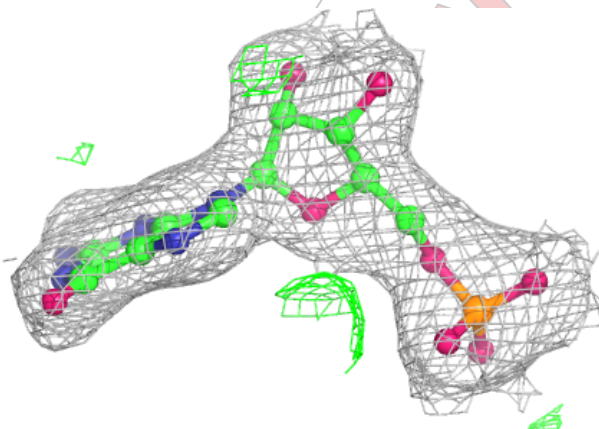
Electron density around 5GP E 502:

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

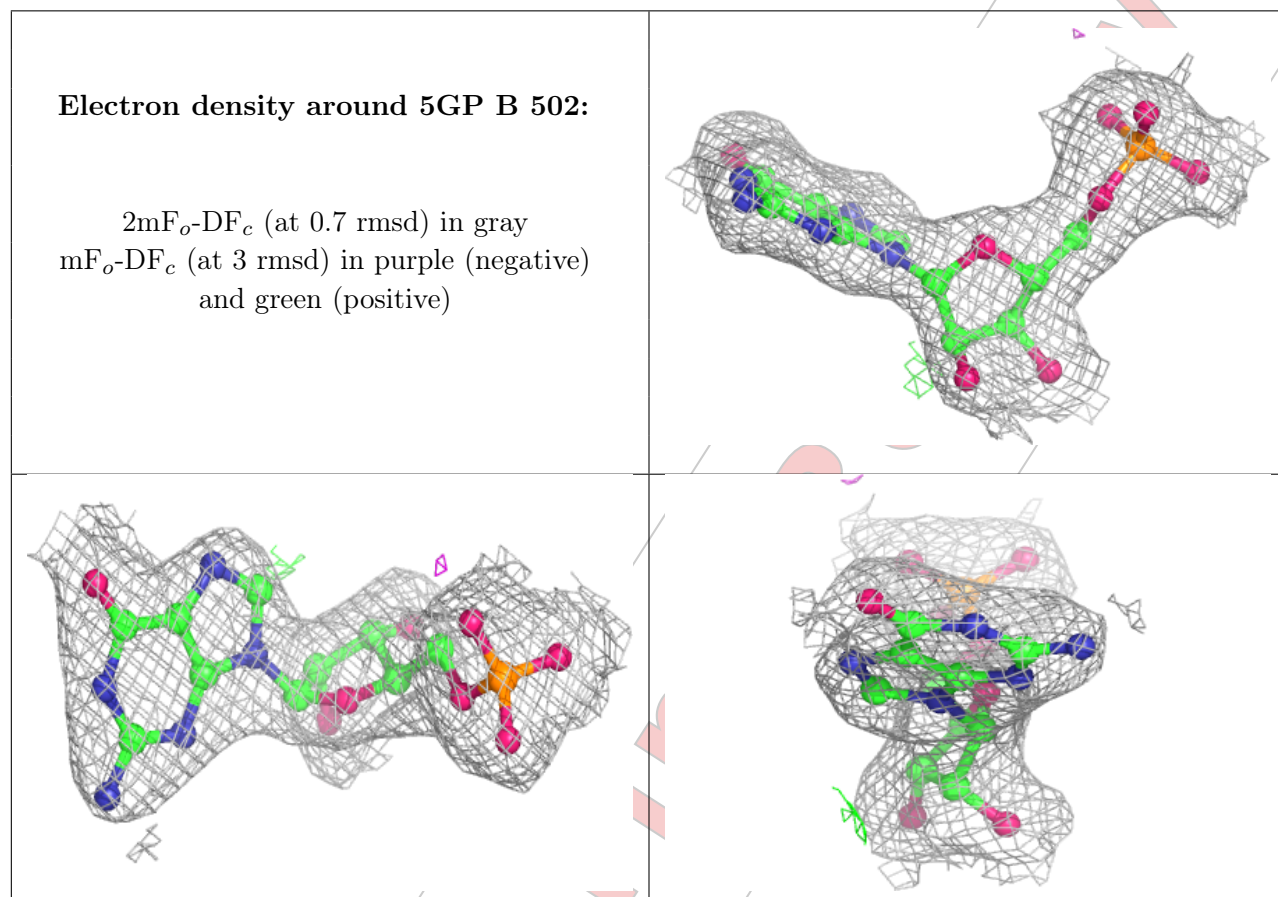


Electron density around 5GP C 502:

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



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6.5 Other polymers ⓘ

There are no such residues in this entry.