



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2024 – 11:11 am GMT

PDB ID : 9HG2  
Title : Crystal structure of M. smegmatis GMP reductase in complex with IMP and ATP.  
Deposited on : 2024-11-18  
Resolution : 1.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, 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)

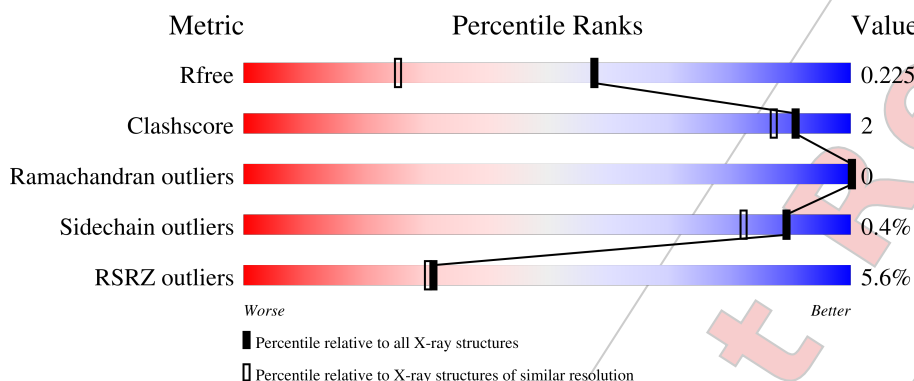
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	<div> <div>4%</div> <div>89%</div> <div>7%</div> </div>
1	B	496	<div> <div>4%</div> <div>90%</div> <div>7%</div> </div>
1	C	496	<div> <div>5%</div> <div>89%</div> <div>7%</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	 4% 89% 7%
1	E	496	 4% 90% 7%
1	F	496	 4% 90% 7%
1	G	496	 4% 91% 7%
1	H	496	 3% 90% 7%
1	I	496	 9% 90% 7%
1	J	496	 6% 89% 7%
1	K	496	 5% 89% 7%
1	L	496	 7% 89% 7%
1	M	496	 6% 89% 7%
1	N	496	 5% 88% 7%
1	O	496	 6% 89% 7%
1	P	496	 7% 89% 7%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 57872 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	461	Total	C	N	O	S	0	4	0
			3359	2096	602	646	15			
1	B	460	Total	C	N	O	S	0	3	0
			3339	2083	596	646	14			
1	C	461	Total	C	N	O	S	0	4	0
			3360	2095	598	652	15			
1	D	460	Total	C	N	O	S	0	3	0
			3348	2087	597	650	14			
1	E	460	Total	C	N	O	S	0	4	0
			3352	2090	601	647	14			
1	F	461	Total	C	N	O	S	0	3	0
			3356	2092	598	651	15			
1	G	461	Total	C	N	O	S	0	3	0
			3341	2085	594	647	15			
1	H	461	Total	C	N	O	S	0	3	0
			3348	2089	597	647	15			
1	I	461	Total	C	N	O	S	0	3	0
			3345	2086	597	647	15			
1	J	461	Total	C	N	O	S	0	3	0
			3348	2090	598	645	15			
1	K	460	Total	C	N	O	S	0	3	0
			3342	2086	596	646	14			
1	L	461	Total	C	N	O	S	0	3	0
			3341	2085	594	647	15			
1	M	461	Total	C	N	O	S	0	3	0
			3339	2084	594	646	15			
1	N	460	Total	C	N	O	S	0	3	0
			3336	2082	596	644	14			
1	O	461	Total	C	N	O	S	0	3	0
			3351	2090	597	649	15			
1	P	460	Total	C	N	O	S	0	3	0
			3334	2080	594	646	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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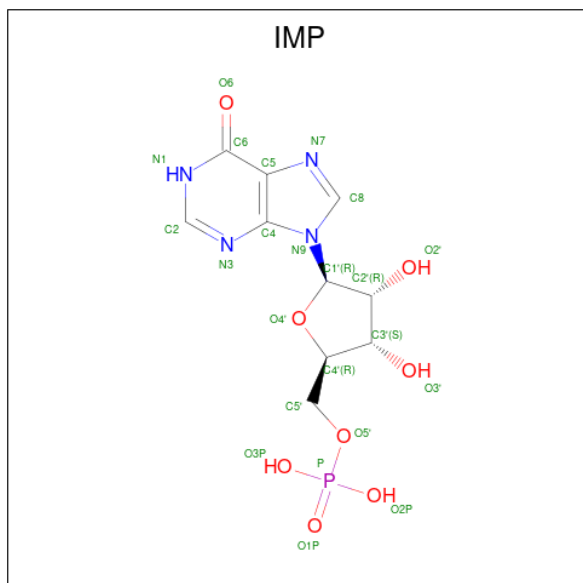
Chain	Residue	Modelled	Actual	Comment	Reference
L	491	HIS	-	expression tag	UNP A0QYE8
L	492	HIS	-	expression tag	UNP A0QYE8
L	493	HIS	-	expression tag	UNP A0QYE8
L	494	HIS	-	expression tag	UNP A0QYE8
L	495	HIS	-	expression tag	UNP A0QYE8
L	496	HIS	-	expression tag	UNP A0QYE8
M	2	VAL	-	insertion	UNP A0QYE8
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 INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



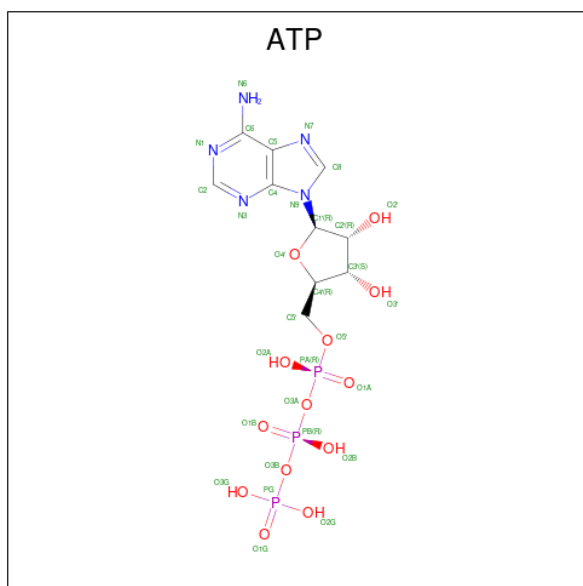
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	I	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	J	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	K	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	L	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	M	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	N	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	P	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	B	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	C	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	D	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	E	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	F	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	G	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	H	1	Total	C	N	O	P	0	1
			62	20	10	26	6		
3	I	1	Total	C	N	O	P	0	1
			62	20	10	26	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	N	O	P	
			62	20	10	26	6	
3	K	1	Total	C	N	O	P	
			62	20	10	26	6	
3	L	1	Total	C	N	O	P	
			62	20	10	26	6	
3	M	1	Total	C	N	O	P	
			62	20	10	26	6	
3	N	1	Total	C	N	O	P	
			62	20	10	26	6	
3	O	1	Total	C	N	O	P	
			62	20	10	26	6	
3	P	1	Total	C	N	O	P	
			62	20	10	26	6	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O		
			213	213	0	0
4	B	189	Total	O		
			189	189	0	0
4	C	211	Total	O		
			211	211	0	0
4	D	251	Total	O		
			251	251	0	0
4	E	241	Total	O		
			241	241	0	0
4	F	235	Total	O		
			235	235	0	0
4	G	236	Total	O		
			236	236	0	0
4	H	244	Total	O		
			244	244	0	0
4	I	116	Total	O		
			116	116	0	0
4	J	212	Total	O		
			212	212	0	0
4	K	200	Total	O		
			200	200	0	0
4	L	134	Total	O		
			134	134	0	0

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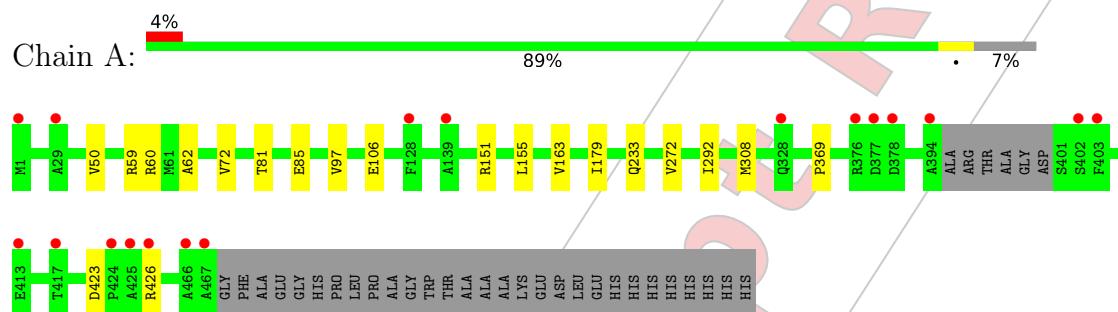
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	119	Total 119	O 119	0	0
4	N	149	Total 149	O 149	0	0
4	O	120	Total 120	O 120	0	0
4	P	103	Total 103	O 103	0	0

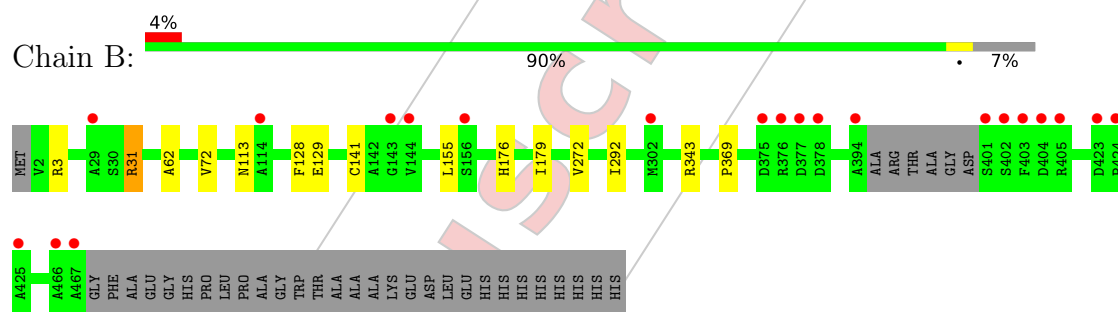
### 3 Residue-property plots

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.

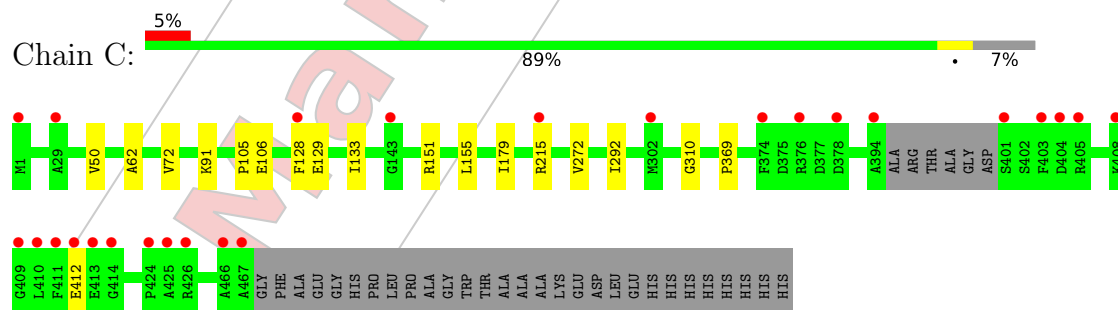
#### • Molecule 1: GMP reductase



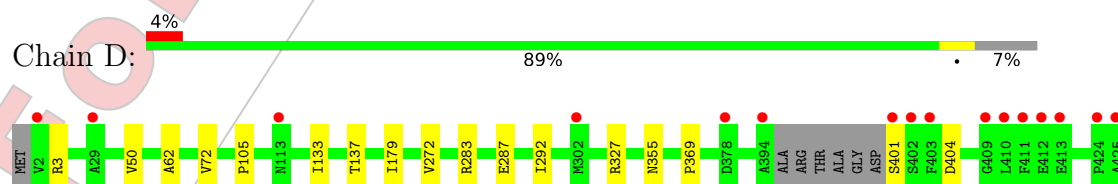
#### • Molecule 1: GMP reductase

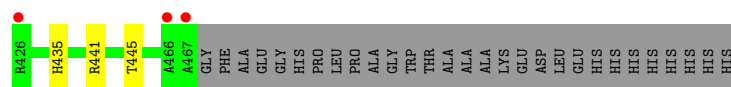


#### • Molecule 1: GMP reductase

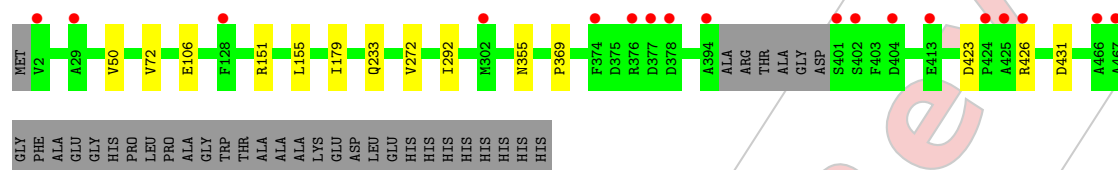
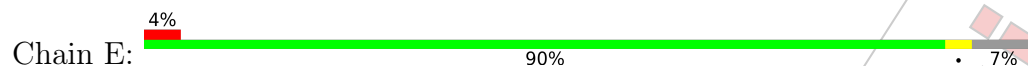


#### • Molecule 1: GMP reductase

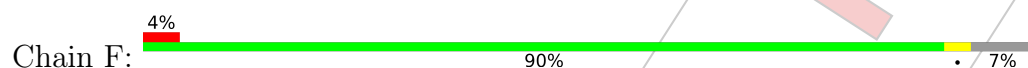




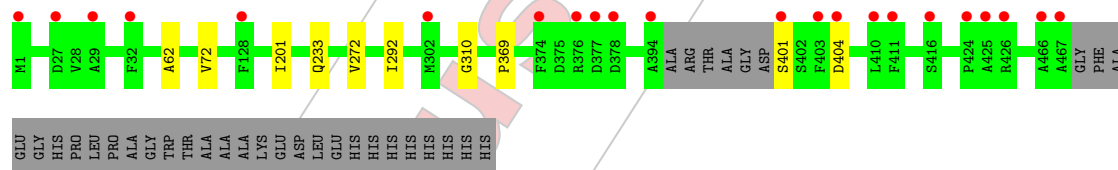
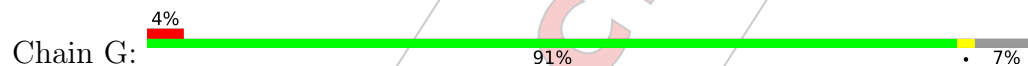
- Molecule 1: GMP reductase



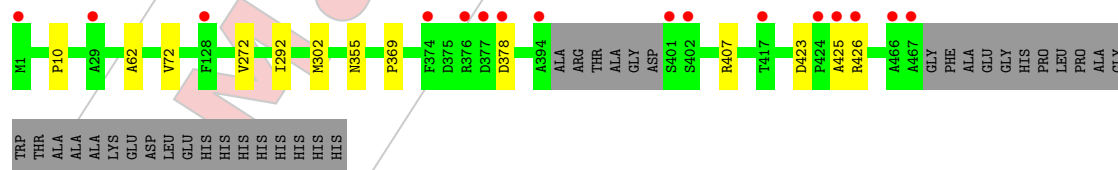
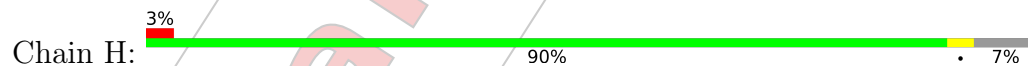
- Molecule 1: GMP reductase



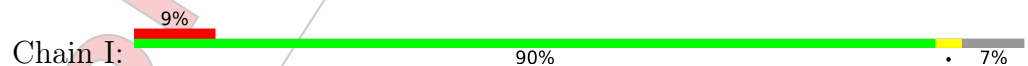
- Molecule 1: GMP reductase

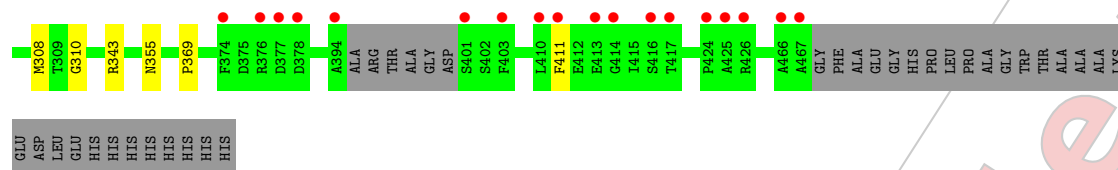


- Molecule 1: GMP reductase

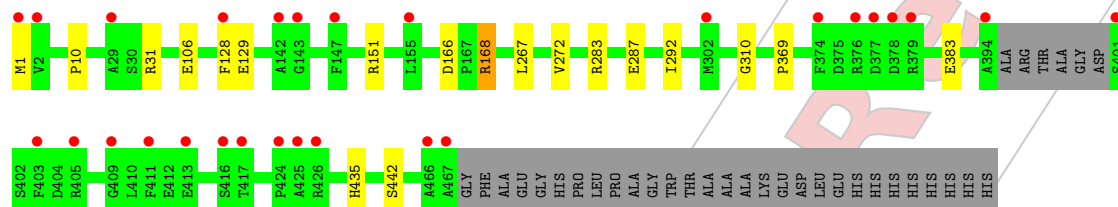
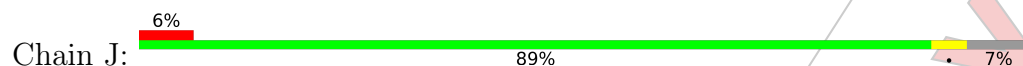


- Molecule 1: GMP reductase

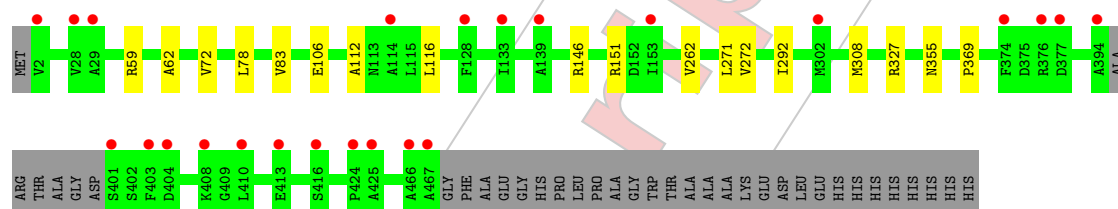
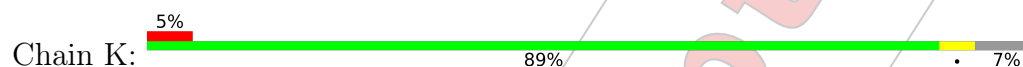




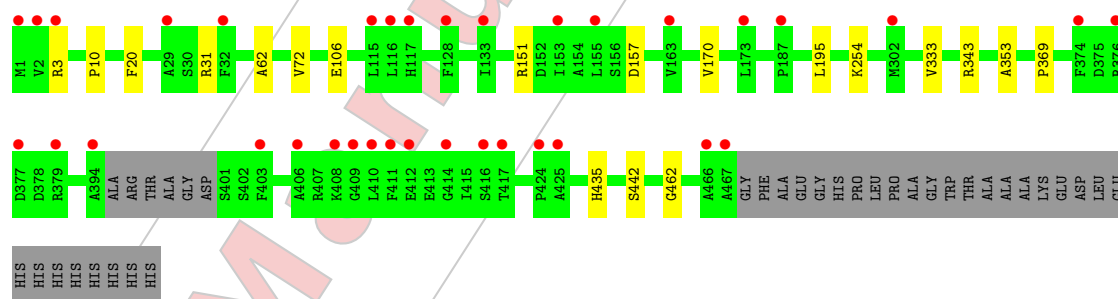
• Molecule 1: GMP reductase



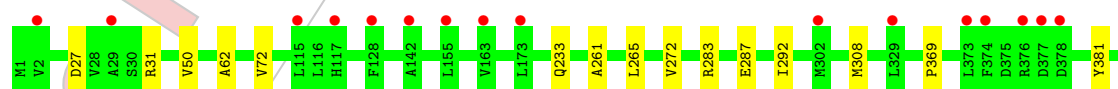
• Molecule 1: GMP reductase

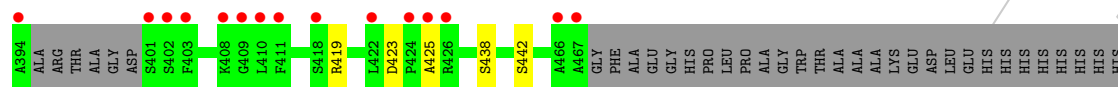


• Molecule 1: GMP reductase

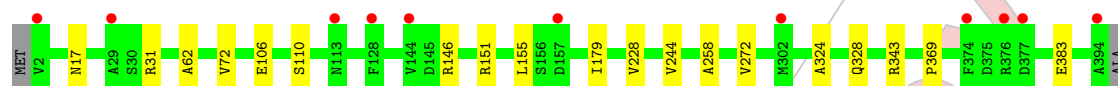
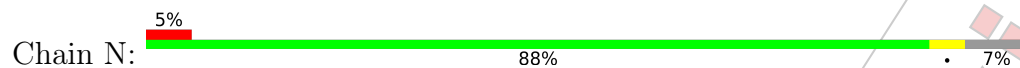


• Molecule 1: GMP reductase

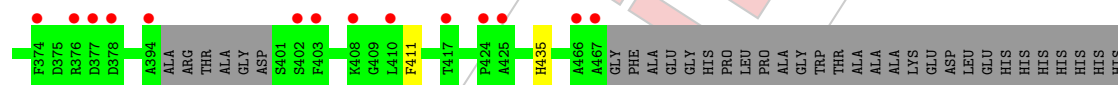
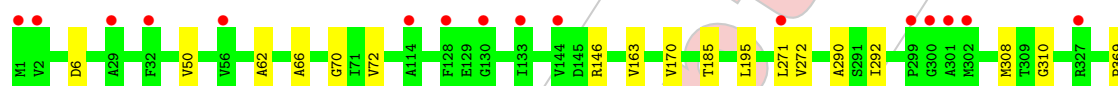
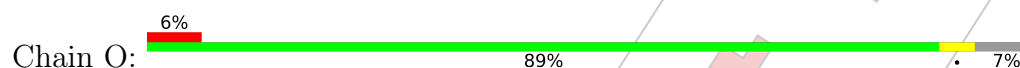




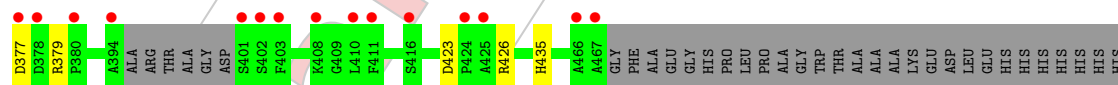
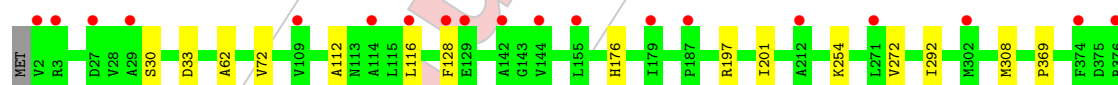
- Molecule 1: GMP reductase



- 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, $\alpha$ , $\beta$ , $\gamma$	113.94Å 115.74Å 178.92Å 77.75° 83.32° 65.60°	Depositor
Resolution (Å)	45.50 – 1.60 45.50 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.50-1.60) 99.1 (45.50-1.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.21_5204	Depositor
R, $R_{free}$	0.202 , 0.225 0.203 , 0.225	Depositor DCC
$R_{free}$ test set	53151 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	57872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.29	0/3420	0.56	0/4655
1	B	0.29	0/3398	0.55	0/4629
1	C	0.30	0/3421	0.56	0/4658
1	D	0.30	0/3407	0.56	0/4640
1	E	0.30	0/3413	0.56	0/4647
1	F	0.31	0/3415	0.57	0/4650
1	G	0.31	0/3400	0.56	0/4632
1	H	0.31	0/3407	0.56	0/4640
1	I	0.27	0/3404	0.53	0/4637
1	J	0.30	0/3407	0.55	0/4639
1	K	0.29	0/3401	0.55	0/4632
1	L	0.28	0/3400	0.54	0/4632
1	M	0.27	0/3398	0.53	0/4630
1	N	0.27	0/3395	0.54	0/4625
1	O	0.27	0/3410	0.53	0/4644
1	P	0.27	0/3393	0.53	0/4623
All	All	0.29	0/54489	0.55	0/74213

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	3359	0	3369	13	0
1	B	3339	0	3330	10	0
1	C	3360	0	3357	12	0
1	D	3348	0	3343	13	0
1	E	3352	0	3355	9	0
1	F	3356	0	3355	10	0
1	G	3341	0	3331	7	0
1	H	3348	0	3344	7	0
1	I	3345	0	3338	12	0
1	J	3348	0	3351	14	0
1	K	3342	0	3336	13	0
1	L	3341	0	3331	15	0
1	M	3339	0	3326	12	0
1	N	3336	0	3328	17	0
1	O	3351	0	3346	13	0
1	P	3334	0	3321	12	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	0	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
2	I	23	0	11	0	0
2	J	23	0	11	0	0
2	K	23	0	11	0	0
2	L	23	0	11	0	0
2	M	23	0	11	0	0
2	N	23	0	11	0	0
2	O	23	0	11	0	0
2	P	23	0	11	0	0
3	A	62	0	24	2	0
3	B	62	0	24	2	0
3	C	62	0	24	2	0
3	D	62	0	24	2	0
3	E	62	0	24	2	0
3	F	62	0	24	2	0
3	G	62	0	24	2	0
3	H	62	0	24	1	0
3	I	62	0	24	2	0
3	J	62	0	24	2	0
3	K	62	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	62	0	24	2	0
3	M	62	0	24	2	0
3	N	62	0	24	1	0
3	O	62	0	24	1	0
3	P	62	0	24	1	0
4	A	213	0	0	0	0
4	B	189	0	0	0	0
4	C	211	0	0	0	0
4	D	251	0	0	2	0
4	E	241	0	0	0	0
4	F	235	0	0	1	0
4	G	236	0	0	0	0
4	H	244	0	0	1	0
4	I	116	0	0	2	0
4	J	212	0	0	2	0
4	K	200	0	0	1	0
4	L	134	0	0	0	0
4	M	119	0	0	0	0
4	N	149	0	0	0	0
4	O	120	0	0	0	0
4	P	103	0	0	0	0
All	All	57872	0	54021	169	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 2.

All (169) 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:N:31:ARG:NH2	1:O:411:PHE:O	2.29	0.65
1:C:369:PRO:HB3	3:C:502[B]:ATP:H5'2	1.81	0.62
1:M:272:VAL:HG22	1:M:292:ILE:HB	1.83	0.61
1:A:369:PRO:HB3	3:A:502[B]:ATP:H5'2	1.84	0.59
1:B:369:PRO:HB3	3:B:502[B]:ATP:H5'2	1.84	0.59
1:E:369:PRO:HB3	3:E:502[A]:ATP:H5'2	1.85	0.58
1:F:369:PRO:HB3	3:F:502[A]:ATP:H5'2	1.85	0.57
1:C:155:LEU:HD12	1:C:179:ILE:HD11	1.87	0.57
1:J:369:PRO:HB3	3:J:502[A]:ATP:H5'2	1.87	0.57
1:M:423:ASP:OD2	1:M:425:ALA:N	2.29	0.57
1:C:272:VAL:HG22	1:C:292:ILE:HB	1.86	0.57
1:E:423:ASP:CG	1:E:426:ARG:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:SER:HB3	1:D:404:ASP:OD2	2.06	0.56
1:G:369:PRO:HB3	3:G:502[A]:ATP:H5'2	1.87	0.56
1:K:59:ARG:NH1	3:K:502[B]:ATP:O2A	2.38	0.56
1:L:157:ASP:OD2	1:P:176:HIS:NE2	2.34	0.56
1:P:377:ASP:HB2	1:P:379:ARG:HD3	1.88	0.55
1:I:272:VAL:HG22	1:I:292:ILE:HB	1.89	0.55
1:G:401:SER:HB3	1:G:404:ASP:OD2	2.08	0.54
1:N:62:ALA:HA	1:N:72:VAL:HG21	1.90	0.54
1:E:155:LEU:HD12	1:E:179:ILE:HD11	1.90	0.54
1:J:369:PRO:HB3	3:J:502[B]:ATP:H5'2	1.89	0.53
1:C:128:PHE:O	1:C:129:GLU:HG2	2.09	0.53
1:K:369:PRO:HB3	3:K:502[A]:ATP:H5'2	1.91	0.53
1:L:106:GLU:OE2	1:L:151:ARG:NH1	2.39	0.53
1:H:369:PRO:HB3	3:H:502[A]:ATP:H5'2	1.91	0.52
1:A:106:GLU:OE2	1:A:151:ARG:NH2	2.42	0.52
1:D:369:PRO:HB3	3:D:502[A]:ATP:H5'2	1.91	0.52
1:F:369:PRO:HB3	3:F:502[B]:ATP:H5'2	1.90	0.52
1:J:272:VAL:HG22	1:J:292:ILE:HB	1.90	0.52
1:L:369:PRO:HB3	3:L:502[B]:ATP:H5'2	1.91	0.52
1:N:369:PRO:HB3	3:N:502[B]:ATP:H5'2	1.91	0.52
1:P:369:PRO:HB3	3:P:502[A]:ATP:H5'2	1.92	0.52
1:J:106:GLU:OE2	1:J:151:ARG:NH2	2.40	0.51
1:D:105:PRO:HG3	1:D:133:ILE:HD11	1.92	0.51
1:L:369:PRO:HB3	3:L:502[A]:ATP:H5'2	1.91	0.51
1:K:59:ARG:NH1	3:K:502[A]:ATP:O1A	2.44	0.51
1:M:31:ARG:HD3	1:M:442[A]:SER:OG	2.11	0.51
1:D:272:VAL:HG22	1:D:292:ILE:HB	1.93	0.51
1:E:423:ASP:OD2	1:E:426:ARG:HB2	2.12	0.51
1:K:106:GLU:OE2	1:K:151:ARG:NH2	2.38	0.51
1:L:31:ARG:HD3	1:L:442[A]:SER:OG	2.11	0.50
1:J:383:GLU:OE1	1:O:146:ARG:NH2	2.40	0.50
1:N:106:GLU:OE2	1:N:151:ARG:NH2	2.41	0.50
1:F:155:LEU:HD12	1:F:179:ILE:HD11	1.94	0.49
1:L:62:ALA:HA	1:L:72:VAL:HG21	1.95	0.49
1:B:272:VAL:HG22	1:B:292:ILE:HB	1.93	0.49
1:P:112:ALA:O	1:P:116:LEU:HD13	2.12	0.49
1:A:272:VAL:HG22	1:A:292:ILE:HB	1.94	0.49
1:I:62:ALA:HA	1:I:72:VAL:HG21	1.93	0.49
1:I:369:PRO:HB3	3:I:502[B]:ATP:H5'2	1.94	0.49
1:B:31:ARG:HH22	1:C:412:GLU:HA	1.77	0.49
1:P:197:ARG:O	1:P:201:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:GLU:OE2	1:F:151:ARG:NH2	2.30	0.48
1:H:423:ASP:OD1	1:H:425:ALA:N	2.36	0.48
1:M:369:PRO:HB3	3:M:502[B]:ATP:H5'2	1.94	0.48
1:G:62:ALA:HA	1:G:72:VAL:HG21	1.96	0.48
1:O:435:HIS:NE2	1:P:308:MET:SD	2.87	0.48
1:N:110:SER:HB2	1:N:146:ARG:HG2	1.96	0.48
1:C:91:LYS:HB3	1:C:215:ARG:HE	1.79	0.48
1:C:369:PRO:HB3	3:C:502[A]:ATP:H5'2	1.96	0.48
1:E:272:VAL:HG22	1:E:292:ILE:HB	1.96	0.48
1:K:62:ALA:HA	1:K:72:VAL:HG21	1.96	0.48
1:D:62:ALA:HA	1:D:72:VAL:HG21	1.96	0.47
1:F:131:ARG:NH1	1:F:188:ASP:O	2.47	0.47
1:O:369:PRO:HB3	3:O:502[A]:ATP:H5'2	1.95	0.47
1:A:308:MET:SD	1:D:435:HIS:NE2	2.88	0.47
1:H:62:ALA:HA	1:H:72:VAL:HG21	1.97	0.47
1:G:201:ILE:HG23	1:H:407:ARG:HA	1.96	0.46
1:N:324:ALA:O	1:N:328:GLN:HG3	2.15	0.46
1:H:10:PRO:HB3	4:H:686:HOH:O	2.14	0.46
1:N:31:ARG:HD3	1:N:442[A]:SER:OG	2.15	0.46
1:O:163:VAL:HG12	1:O:185:THR:O	2.16	0.46
1:I:369:PRO:HB3	3:I:502[A]:ATP:H5'2	1.98	0.46
1:A:155:LEU:HD12	1:A:179:ILE:HD11	1.97	0.46
1:D:369:PRO:HB3	3:D:502[B]:ATP:H5'2	1.97	0.46
1:I:308:MET:SD	1:L:435:HIS:NE2	2.89	0.46
1:N:228:VAL:HG11	1:N:258:ALA:HB1	1.98	0.46
1:G:272:VAL:HG22	1:G:292:ILE:HB	1.97	0.46
1:E:426:ARG:HG2	1:E:431:ASP:HB3	1.97	0.45
1:M:261:ALA:O	1:M:265:LEU:HD13	2.15	0.45
1:I:310:GLY:HA2	1:L:343:ARG:HG3	1.98	0.45
1:G:369:PRO:HB3	3:G:502[B]:ATP:H5'2	1.99	0.45
1:M:50:VAL:HB	1:M:72:VAL:HG22	1.99	0.45
1:M:62:ALA:HA	1:M:72:VAL:HG21	1.99	0.45
1:C:62:ALA:HA	1:C:72:VAL:HG21	1.97	0.45
1:H:272:VAL:HG22	1:H:292:ILE:HB	1.99	0.45
4:I:656:HOH:O	1:L:10:PRO:HB3	2.16	0.45
1:K:146:ARG:NH2	1:N:383:GLU:OE1	2.38	0.45
1:I:59:ARG:HG3	1:I:60:ARG:N	2.32	0.45
1:P:30:SER:HB3	1:P:33:ASP:OD2	2.17	0.45
1:E:369:PRO:HB3	3:E:502[B]:ATP:H5'2	1.98	0.45
1:M:283:ARG:HD3	1:M:287:GLU:OE2	2.17	0.45
1:N:106:GLU:OE2	1:N:151:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:267:LEU:HB2	4:J:780:HOH:O	2.17	0.44
1:O:50:VAL:HB	1:O:72:VAL:HG22	1.99	0.44
1:N:17:ASN:OD1	1:N:343:ARG:NH2	2.49	0.44
1:B:62:ALA:HA	1:B:72:VAL:HG21	1.99	0.44
1:B:176:HIS:NE2	1:F:157:ASP:OD2	2.48	0.44
1:A:81:THR:O	1:A:85:GLU:HG3	2.18	0.44
1:I:343:ARG:HG3	1:J:310:GLY:HA2	1.99	0.44
1:N:343:ARG:HG3	1:O:310:GLY:HA2	2.00	0.44
1:P:254:LYS:HE2	1:P:254:LYS:HB3	1.84	0.44
1:A:97:VAL:HG21	1:A:163:VAL:HG23	2.00	0.43
1:D:283:ARG:HD3	4:D:740:HOH:O	2.18	0.43
1:I:411:PHE:O	1:L:31:ARG:NH2	2.51	0.43
1:A:50:VAL:HB	1:A:72:VAL:HG22	2.00	0.43
1:I:201:ILE:HD13	1:I:201:ILE:HA	1.91	0.43
1:L:170:VAL:HG11	1:L:195:LEU:HD23	2.01	0.43
1:O:272:VAL:HG22	1:O:292:ILE:HB	2.01	0.43
1:A:369:PRO:HB3	3:A:502[A]:ATP:H5'2	2.00	0.43
1:D:137:THR:HG21	1:D:179:ILE:HD12	2.00	0.43
1:M:369:PRO:HB3	3:M:502[A]:ATP:H5'2	2.01	0.43
1:K:262:VAL:HG11	1:K:271:LEU:HD21	2.00	0.43
1:L:333:VAL:HG23	1:L:353:ALA:HA	1.99	0.43
1:B:155:LEU:HD12	1:B:179:ILE:HD11	2.01	0.43
1:D:50:VAL:HB	1:D:72:VAL:HG22	2.00	0.43
1:D:283:ARG:O	1:D:287:GLU:HG3	2.19	0.43
1:J:31:ARG:NE	1:J:442[A]:SER:OG	2.51	0.43
1:J:168:ARG:N	1:J:168:ARG:HD3	2.34	0.43
1:C:105:PRO:HG3	1:C:133:ILE:HD11	2.01	0.43
1:F:62:ALA:HA	1:F:72:VAL:HG21	2.00	0.43
1:N:435:HIS:NE2	1:O:308:MET:SD	2.92	0.43
1:K:112:ALA:O	1:K:116:LEU:HD23	2.19	0.42
1:P:62:ALA:HA	1:P:72:VAL:HG21	2.01	0.42
1:P:272:VAL:HG22	1:P:292:ILE:HB	2.01	0.42
1:A:62:ALA:HA	1:A:72:VAL:HG21	2.00	0.42
1:C:50:VAL:HB	1:C:72:VAL:HG22	2.00	0.42
1:O:62:ALA:HA	1:O:72:VAL:HG21	2.01	0.42
1:B:128:PHE:O	1:B:129:GLU:HG2	2.19	0.42
1:K:78:LEU:HD23	1:K:83:VAL:HG22	2.01	0.42
1:A:106:GLU:OE2	1:A:151:ARG:NH1	2.49	0.42
1:M:381:TYR:CE2	1:M:419:ARG:HG2	2.55	0.42
1:N:155:LEU:HD12	1:N:179:ILE:HD11	2.02	0.42
1:N:244:VAL:HG22	1:N:272:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:ALA:HA	1:O:70:GLY:O	2.20	0.42
1:B:343:ARG:HG3	1:C:310:GLY:HA2	2.02	0.41
1:L:254:LYS:HE3	1:L:254:LYS:HB3	1.82	0.41
1:E:106:GLU:OE2	1:E:151:ARG:NH1	2.49	0.41
1:K:327:ARG:HD2	4:K:717:HOH:O	2.19	0.41
1:B:369:PRO:HB3	3:B:502[A]:ATP:H5'2	2.00	0.41
1:J:435:HIS:NE2	1:K:308:MET:SD	2.94	0.41
1:L:31:ARG:HH11	1:L:442[A]:SER:HG	1.66	0.41
1:O:170:VAL:HG11	1:O:195:LEU:HD23	2.02	0.41
1:D:327:ARG:HD2	4:D:757:HOH:O	2.20	0.41
1:J:10:PRO:HB3	4:J:727:HOH:O	2.21	0.41
1:K:272:VAL:HG22	1:K:292:ILE:HB	2.01	0.41
1:F:50:VAL:HB	1:F:72:VAL:HG22	2.02	0.41
1:F:152:ASP:OD1	4:F:601:HOH:O	2.22	0.41
1:F:343:ARG:HG3	1:G:310:GLY:HA2	2.03	0.41
1:L:20:PHE:CZ	1:L:462:GLY:HA3	2.56	0.41
1:A:59:ARG:HG3	1:A:60:ARG:N	2.36	0.41
1:D:441:ARG:O	1:D:445:THR:HG23	2.21	0.41
1:J:283:ARG:O	1:J:287:GLU:HG3	2.21	0.41
1:C:106:GLU:OE2	1:C:151:ARG:NH2	2.50	0.41
1:N:62:ALA:HA	1:N:72:VAL:CG2	2.50	0.41
1:B:113:ASN:HD22	1:B:141:CYS:CB	2.34	0.40
1:P:423:ASP:HB3	1:P:426:ARG:HB2	2.04	0.40
1:E:50:VAL:HB	1:E:72:VAL:HG22	2.04	0.40
1:J:166:ASP:OD1	1:J:168:ARG:NE	2.53	0.40
1:M:308:MET:SD	1:P:435:HIS:NE2	2.94	0.40
1:O:271:LEU:HD22	1:O:290:ALA:HA	2.02	0.40
1:A:423:ASP:HB3	1:A:426:ARG:HB2	2.03	0.40
1:I:10:PRO:HG3	1:I:14:LEU:HD21	2.03	0.40
1:K:369:PRO:HB3	3:K:502[B]:ATP:H5'2	2.03	0.40
1:H:423:ASP:HB3	1:H:426:ARG:HB2	2.03	0.40
1:I:254:LYS:HG3	4:I:659:HOH:O	2.21	0.40
1:J:128:PHE:CE1	1:J:129:GLU:HG3	2.57	0.40
1:M:438:SER:HB2	1:N:411:PHE:CD1	2.57	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	461/496 (93%)	452 (98%)	9 (2%)	0	100	100
1	B	459/496 (92%)	452 (98%)	7 (2%)	0	100	100
1	C	461/496 (93%)	452 (98%)	9 (2%)	0	100	100
1	D	459/496 (92%)	451 (98%)	8 (2%)	0	100	100
1	E	460/496 (93%)	450 (98%)	10 (2%)	0	100	100
1	F	460/496 (93%)	451 (98%)	9 (2%)	0	100	100
1	G	460/496 (93%)	451 (98%)	9 (2%)	0	100	100
1	H	460/496 (93%)	451 (98%)	9 (2%)	0	100	100
1	I	460/496 (93%)	451 (98%)	9 (2%)	0	100	100
1	J	460/496 (93%)	450 (98%)	10 (2%)	0	100	100
1	K	459/496 (92%)	450 (98%)	9 (2%)	0	100	100
1	L	460/496 (93%)	448 (97%)	12 (3%)	0	100	100
1	M	460/496 (93%)	450 (98%)	10 (2%)	0	100	100
1	N	459/496 (92%)	450 (98%)	9 (2%)	0	100	100
1	O	460/496 (93%)	450 (98%)	10 (2%)	0	100	100
1	P	459/496 (92%)	452 (98%)	7 (2%)	0	100	100
All	All	7357/7936 (93%)	7211 (98%)	146 (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	347/372 (93%)	346 (100%)	1 (0%)	91	85
1	B	344/372 (92%)	342 (99%)	2 (1%)	84	74
1	C	348/372 (94%)	348 (100%)	0	100	100
1	D	347/372 (93%)	345 (99%)	2 (1%)	84	74
1	E	347/372 (93%)	345 (99%)	2 (1%)	84	74
1	F	348/372 (94%)	348 (100%)	0	100	100
1	G	344/372 (92%)	343 (100%)	1 (0%)	91	85
1	H	345/372 (93%)	342 (99%)	3 (1%)	75	62
1	I	345/372 (93%)	344 (100%)	1 (0%)	91	85
1	J	345/372 (93%)	343 (99%)	2 (1%)	84	74
1	K	344/372 (92%)	343 (100%)	1 (0%)	91	85
1	L	344/372 (92%)	343 (100%)	1 (0%)	91	85
1	M	343/372 (92%)	341 (99%)	2 (1%)	84	74
1	N	343/372 (92%)	343 (100%)	0	100	100
1	O	346/372 (93%)	345 (100%)	1 (0%)	91	85
1	P	343/372 (92%)	342 (100%)	1 (0%)	91	85
All	All	5523/5952 (93%)	5503 (100%)	20 (0%)	89	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	B	3	ARG
1	B	31	ARG
1	D	3	ARG
1	D	355	ASN
1	E	233	GLN
1	E	355	ASN
1	G	233	GLN
1	H	302	MET
1	H	355	ASN
1	H	378	ASP
1	I	355	ASN
1	J	1	MET
1	J	168	ARG
1	K	355	ASN
1	L	3	ARG

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Mol	Chain	Res	Type
1	M	27	ASP
1	M	233	GLN
1	O	6	ASP
1	P	128	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	328	GLN
1	N	328	GLN
1	P	113	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	ATP	F	502[B]	-	26,33,33	0.74	0	31,52,52	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	IMP	G	501	-	21,25,25	0.63	0	24,38,38	0.78	0
3	ATP	K	502[B]	-	26,33,33	0.74	0	31,52,52	0.68	0
3	ATP	L	502[B]	-	26,33,33	0.73	0	31,52,52	0.69	0
3	ATP	C	502[A]	-	26,33,33	0.74	0	31,52,52	0.65	0
2	IMP	O	501	-	21,25,25	0.62	0	24,38,38	0.83	0
3	ATP	N	502[B]	-	26,33,33	0.74	0	31,52,52	0.63	0
3	ATP	I	502[B]	-	26,33,33	0.74	0	31,52,52	0.65	0
3	ATP	H	502[B]	-	26,33,33	0.74	0	31,52,52	0.67	0
2	IMP	J	501	-	21,25,25	0.65	0	24,38,38	0.80	0
2	IMP	P	501	-	21,25,25	0.62	0	24,38,38	0.75	0
2	IMP	F	501	-	21,25,25	0.61	0	24,38,38	0.84	0
3	ATP	A	502[A]	-	26,33,33	0.74	0	31,52,52	0.69	0
3	ATP	J	502[B]	-	26,33,33	0.74	0	31,52,52	0.70	0
3	ATP	C	502[B]	-	26,33,33	0.74	0	31,52,52	0.66	0
3	ATP	M	502[B]	-	26,33,33	0.73	0	31,52,52	0.64	0
2	IMP	I	501	-	21,25,25	0.57	0	24,38,38	0.77	0
3	ATP	A	502[B]	-	26,33,33	0.74	0	31,52,52	0.63	0
3	ATP	O	502[A]	-	26,33,33	0.74	0	31,52,52	0.64	0
2	IMP	K	501	-	21,25,25	0.65	0	24,38,38	0.76	0
2	IMP	C	501	-	21,25,25	0.65	0	24,38,38	0.82	0
3	ATP	O	502[B]	-	26,33,33	0.74	0	31,52,52	0.65	0
2	IMP	D	501	-	21,25,25	0.63	0	24,38,38	0.87	0
3	ATP	E	502[A]	-	26,33,33	0.74	0	31,52,52	0.68	0
2	IMP	B	501	-	21,25,25	0.64	0	24,38,38	0.74	0
2	IMP	L	501	-	21,25,25	0.61	0	24,38,38	0.80	0
3	ATP	D	502[A]	-	26,33,33	0.74	0	31,52,52	0.67	0
3	ATP	B	502[A]	-	26,33,33	0.74	0	31,52,52	0.66	0
2	IMP	N	501	-	21,25,25	0.64	0	24,38,38	0.78	0
3	ATP	E	502[B]	-	26,33,33	0.74	0	31,52,52	0.70	0
3	ATP	G	502[A]	-	26,33,33	0.74	0	31,52,52	0.70	0
3	ATP	D	502[B]	-	26,33,33	0.74	0	31,52,52	0.68	0
3	ATP	B	502[B]	-	26,33,33	0.74	0	31,52,52	0.64	0
2	IMP	M	501	-	21,25,25	0.60	0	24,38,38	0.78	0
2	IMP	E	501	-	21,25,25	0.65	0	24,38,38	0.76	0
3	ATP	M	502[A]	-	26,33,33	0.73	0	31,52,52	0.63	0
3	ATP	P	502[A]	-	26,33,33	0.74	0	31,52,52	0.63	0
3	ATP	G	502[B]	-	26,33,33	0.74	0	31,52,52	0.65	0
3	ATP	K	502[A]	-	26,33,33	0.74	0	31,52,52	0.63	0
3	ATP	F	502[A]	-	26,33,33	0.74	0	31,52,52	0.67	0
3	ATP	L	502[A]	-	26,33,33	0.74	0	31,52,52	0.66	0
3	ATP	N	502[A]	-	26,33,33	0.74	0	31,52,52	0.64	0
2	IMP	A	501	-	21,25,25	0.67	0	24,38,38	0.76	0
2	IMP	H	501	-	21,25,25	0.64	0	24,38,38	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	P	502[B]	-	26,33,33	0.74	0	31,52,52	0.64	0
3	ATP	I	502[A]	-	26,33,33	0.74	0	31,52,52	0.65	0
3	ATP	H	502[A]	-	26,33,33	0.74	0	31,52,52	0.69	0
3	ATP	J	502[A]	-	26,33,33	0.74	0	31,52,52	0.67	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
3	ATP	F	502[B]	-	-	2/18/38/38	0/3/3/3
2	IMP	G	501	-	-	0/6/26/26	0/3/3/3
3	ATP	K	502[B]	-	-	1/18/38/38	0/3/3/3
3	ATP	L	502[B]	-	-	1/18/38/38	0/3/3/3
3	ATP	C	502[A]	-	-	2/18/38/38	0/3/3/3
2	IMP	O	501	-	-	0/6/26/26	0/3/3/3
3	ATP	N	502[B]	-	-	4/18/38/38	0/3/3/3
3	ATP	I	502[B]	-	-	0/18/38/38	0/3/3/3
3	ATP	H	502[B]	-	-	0/18/38/38	0/3/3/3
2	IMP	J	501	-	-	0/6/26/26	0/3/3/3
2	IMP	P	501	-	-	0/6/26/26	0/3/3/3
2	IMP	F	501	-	-	0/6/26/26	0/3/3/3
3	ATP	A	502[A]	-	-	3/18/38/38	0/3/3/3
3	ATP	J	502[B]	-	-	2/18/38/38	0/3/3/3
3	ATP	C	502[B]	-	-	4/18/38/38	0/3/3/3
3	ATP	M	502[B]	-	-	4/18/38/38	0/3/3/3
2	IMP	I	501	-	-	0/6/26/26	0/3/3/3
3	ATP	A	502[B]	-	-	4/18/38/38	0/3/3/3
3	ATP	O	502[A]	-	-	6/18/38/38	0/3/3/3
2	IMP	K	501	-	-	0/6/26/26	0/3/3/3
2	IMP	C	501	-	-	0/6/26/26	0/3/3/3
3	ATP	O	502[B]	-	-	2/18/38/38	0/3/3/3
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
3	ATP	E	502[A]	-	-	2/18/38/38	0/3/3/3
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
2	IMP	L	501	-	-	0/6/26/26	0/3/3/3
3	ATP	D	502[A]	-	-	2/18/38/38	0/3/3/3
3	ATP	B	502[A]	-	-	3/18/38/38	0/3/3/3
2	IMP	N	501	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	502[B]	-	-	3/18/38/38	0/3/3/3
3	ATP	G	502[A]	-	-	6/18/38/38	0/3/3/3
3	ATP	D	502[B]	-	-	2/18/38/38	0/3/3/3
3	ATP	B	502[B]	-	-	3/18/38/38	0/3/3/3
2	IMP	M	501	-	-	0/6/26/26	0/3/3/3
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
3	ATP	M	502[A]	-	-	0/18/38/38	0/3/3/3
3	ATP	P	502[A]	-	-	4/18/38/38	0/3/3/3
3	ATP	G	502[B]	-	-	2/18/38/38	0/3/3/3
3	ATP	K	502[A]	-	-	2/18/38/38	0/3/3/3
3	ATP	F	502[A]	-	-	1/18/38/38	0/3/3/3
3	ATP	L	502[A]	-	-	2/18/38/38	0/3/3/3
3	ATP	N	502[A]	-	-	0/18/38/38	0/3/3/3
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
2	IMP	H	501	-	-	0/6/26/26	0/3/3/3
3	ATP	P	502[B]	-	-	2/18/38/38	0/3/3/3
3	ATP	I	502[A]	-	-	7/18/38/38	0/3/3/3
3	ATP	H	502[A]	-	-	2/18/38/38	0/3/3/3
3	ATP	J	502[A]	-	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	ATP	PB-O3B-PG-O3G
3	B	502[A]	ATP	PB-O3B-PG-O3G
3	C	502[A]	ATP	PB-O3B-PG-O3G
3	C	502[B]	ATP	PB-O3B-PG-O2G
3	D	502[B]	ATP	PB-O3B-PG-O3G
3	E	502[B]	ATP	PB-O3B-PG-O3G
3	F	502[B]	ATP	PB-O3B-PG-O3G
3	G	502[A]	ATP	PB-O3B-PG-O2G
3	I	502[A]	ATP	PB-O3B-PG-O2G
3	O	502[A]	ATP	PB-O3B-PG-O2G
3	P	502[A]	ATP	PB-O3B-PG-O2G
3	P	502[A]	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	P	502[B]	ATP	PB-O3B-PG-O3G
3	K	502[B]	ATP	PB-O3B-PG-O1G
3	N	502[B]	ATP	PB-O3B-PG-O1G
3	B	502[B]	ATP	PB-O3A-PA-O1A
3	D	502[A]	ATP	PA-O3A-PB-O1B
3	G	502[B]	ATP	PA-O3A-PB-O1B
3	J	502[B]	ATP	PA-O3A-PB-O1B
3	C	502[B]	ATP	PB-O3B-PG-O1G
3	A	502[B]	ATP	PB-O3B-PG-O2G
3	A	502[B]	ATP	PB-O3B-PG-O3G
3	M	502[B]	ATP	PB-O3B-PG-O2G
3	N	502[B]	ATP	PB-O3B-PG-O2G
3	F	502[A]	ATP	PB-O3A-PA-O2A
3	G	502[A]	ATP	PB-O3A-PA-O2A
3	J	502[A]	ATP	PG-O3B-PB-O2B
3	K	502[A]	ATP	PB-O3A-PA-O2A
3	L	502[B]	ATP	PA-O3A-PB-O1B
3	M	502[B]	ATP	PB-O3A-PA-O2A
3	O	502[A]	ATP	PB-O3A-PA-O2A
3	O	502[B]	ATP	PG-O3B-PB-O2B
3	F	502[B]	ATP	PB-O3B-PG-O1G
3	A	502[B]	ATP	PB-O3A-PA-O2A
3	B	502[B]	ATP	PB-O3A-PA-O2A
3	C	502[B]	ATP	PG-O3B-PB-O2B
3	C	502[B]	ATP	PB-O3A-PA-O2A
3	E	502[A]	ATP	PB-O3A-PA-O2A
3	H	502[A]	ATP	PA-O3A-PB-O1B
3	H	502[A]	ATP	PB-O3A-PA-O2A
3	I	502[A]	ATP	PB-O3A-PA-O2A
3	L	502[A]	ATP	PA-O3A-PB-O1B
3	M	502[B]	ATP	PB-O3A-PA-O1A
3	N	502[B]	ATP	PB-O3A-PA-O2A
3	P	502[A]	ATP	PB-O3A-PA-O1A
3	P	502[A]	ATP	PB-O3A-PA-O2A
3	B	502[A]	ATP	PB-O3B-PG-O1G
3	C	502[A]	ATP	PB-O3B-PG-O1G
3	D	502[B]	ATP	PB-O3B-PG-O1G
3	O	502[B]	ATP	PB-O3B-PG-O1G
3	A	502[B]	ATP	PA-O3A-PB-O1B
3	G	502[B]	ATP	PA-O3A-PB-O2B
3	I	502[A]	ATP	PA-O3A-PB-O1B
3	A	502[A]	ATP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	I	502[A]	ATP	PB-O3B-PG-O1G
3	P	502[B]	ATP	PB-O3B-PG-O1G
3	A	502[A]	ATP	PB-O3B-PG-O2G
3	B	502[A]	ATP	PB-O3B-PG-O2G
3	B	502[B]	ATP	PB-O3B-PG-O3G
3	E	502[A]	ATP	PB-O3B-PG-O3G
3	E	502[B]	ATP	PB-O3B-PG-O2G
3	G	502[A]	ATP	PB-O3B-PG-O3G
3	I	502[A]	ATP	PB-O3B-PG-O3G
3	M	502[B]	ATP	PB-O3B-PG-O3G
3	O	502[A]	ATP	PB-O3B-PG-O3G
3	D	502[A]	ATP	PB-O3A-PA-O1A
3	G	502[A]	ATP	PG-O3B-PB-O2B
3	G	502[A]	ATP	PB-O3A-PA-O1A
3	I	502[A]	ATP	PG-O3B-PB-O1B
3	I	502[A]	ATP	PB-O3A-PA-O1A
3	J	502[A]	ATP	PG-O3B-PB-O1B
3	J	502[B]	ATP	PB-O3A-PA-O2A
3	K	502[A]	ATP	PB-O3A-PA-O1A
3	L	502[A]	ATP	PB-O3A-PA-O2A
3	N	502[B]	ATP	PB-O3A-PA-O1A
3	O	502[A]	ATP	PG-O3B-PB-O2B
3	O	502[A]	ATP	PB-O3A-PA-O1A
3	E	502[B]	ATP	PB-O3B-PG-O1G
3	G	502[A]	ATP	PB-O3B-PG-O1G
3	O	502[A]	ATP	PB-O3B-PG-O1G

There are no ring outliers.

28 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502[B]	ATP	1	0
3	K	502[B]	ATP	2	0
3	L	502[B]	ATP	1	0
3	C	502[A]	ATP	1	0
3	N	502[B]	ATP	1	0
3	I	502[B]	ATP	1	0
3	A	502[A]	ATP	1	0
3	J	502[B]	ATP	1	0
3	C	502[B]	ATP	1	0
3	M	502[B]	ATP	1	0
3	A	502[B]	ATP	1	0

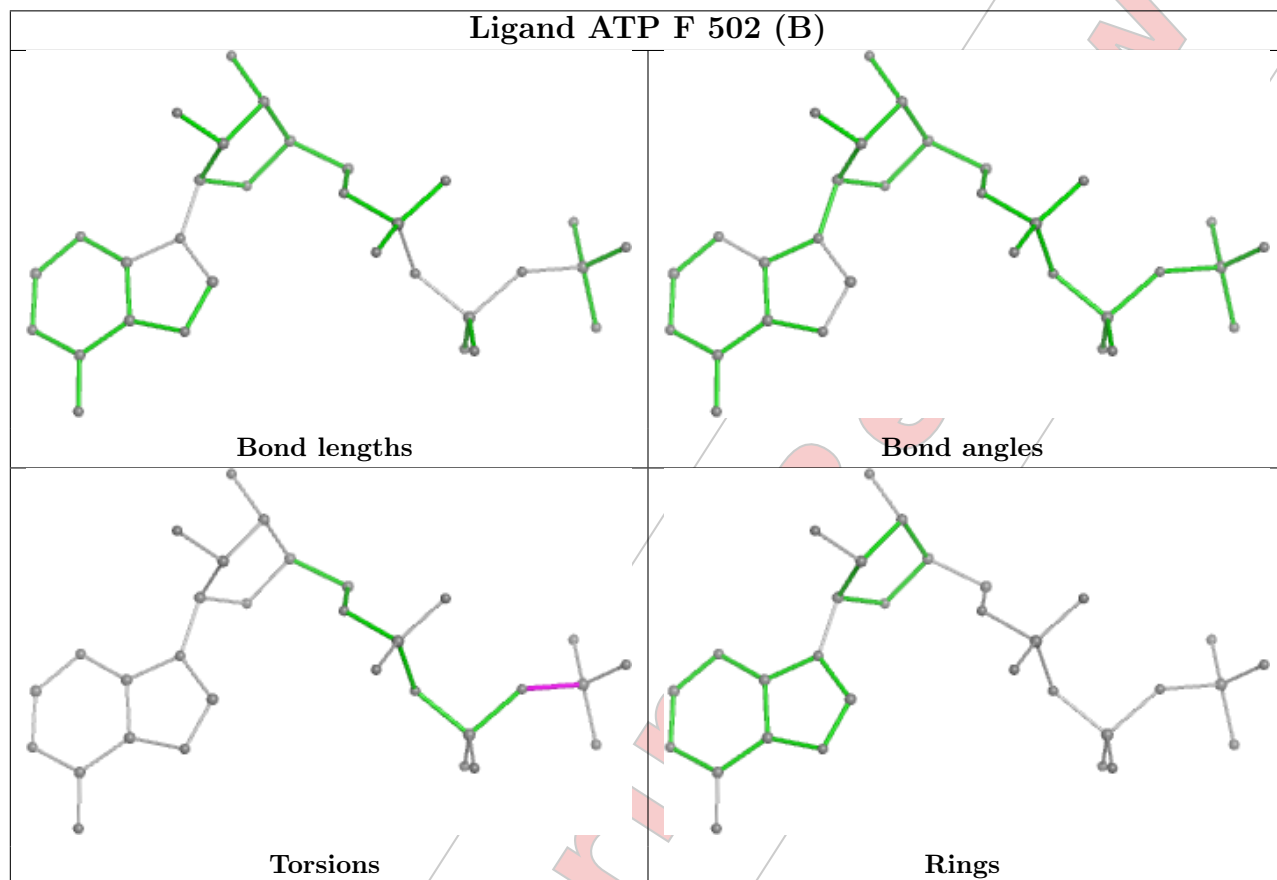
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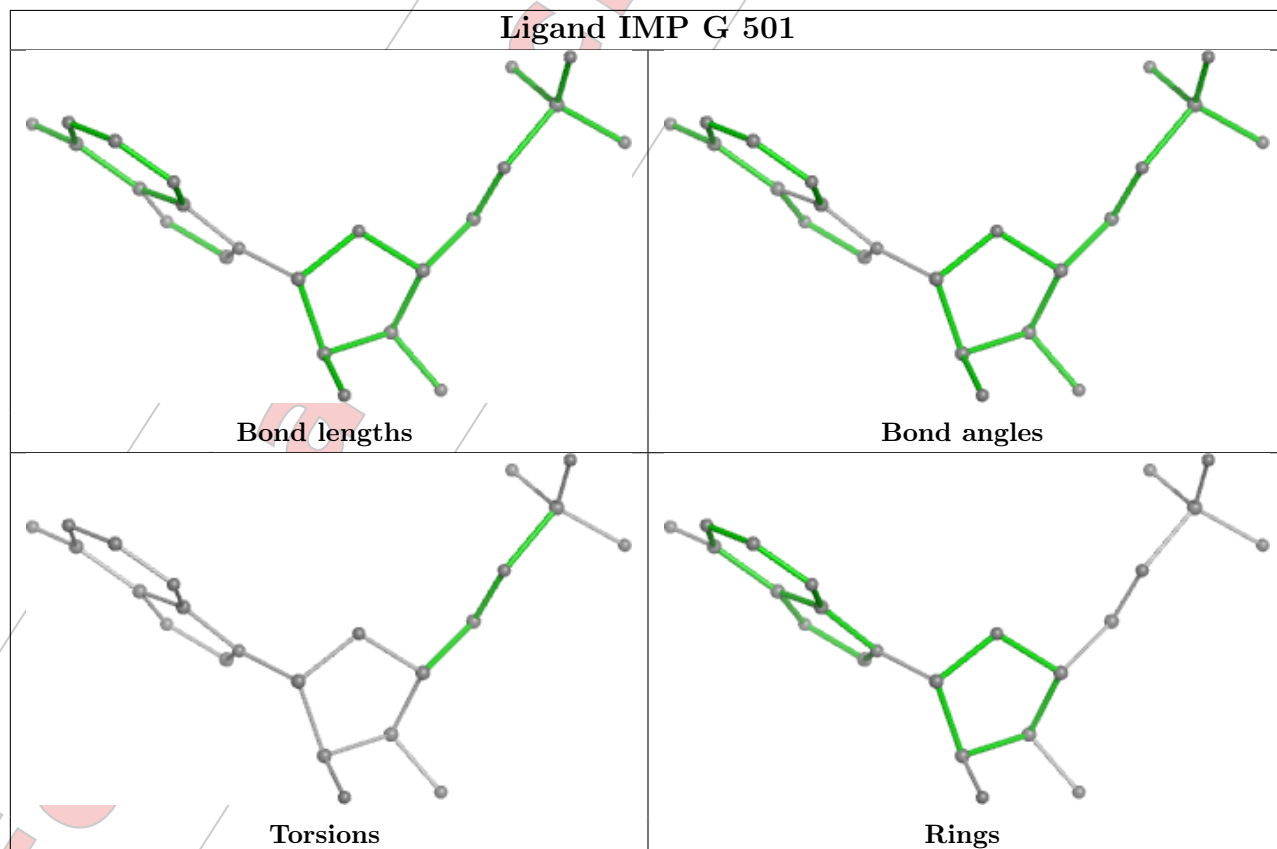
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	502[A]	ATP	1	0
3	E	502[A]	ATP	1	0
3	D	502[A]	ATP	1	0
3	B	502[A]	ATP	1	0
3	E	502[B]	ATP	1	0
3	G	502[A]	ATP	1	0
3	D	502[B]	ATP	1	0
3	B	502[B]	ATP	1	0
3	M	502[A]	ATP	1	0
3	P	502[A]	ATP	1	0
3	G	502[B]	ATP	1	0
3	K	502[A]	ATP	2	0
3	F	502[A]	ATP	1	0
3	L	502[A]	ATP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

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

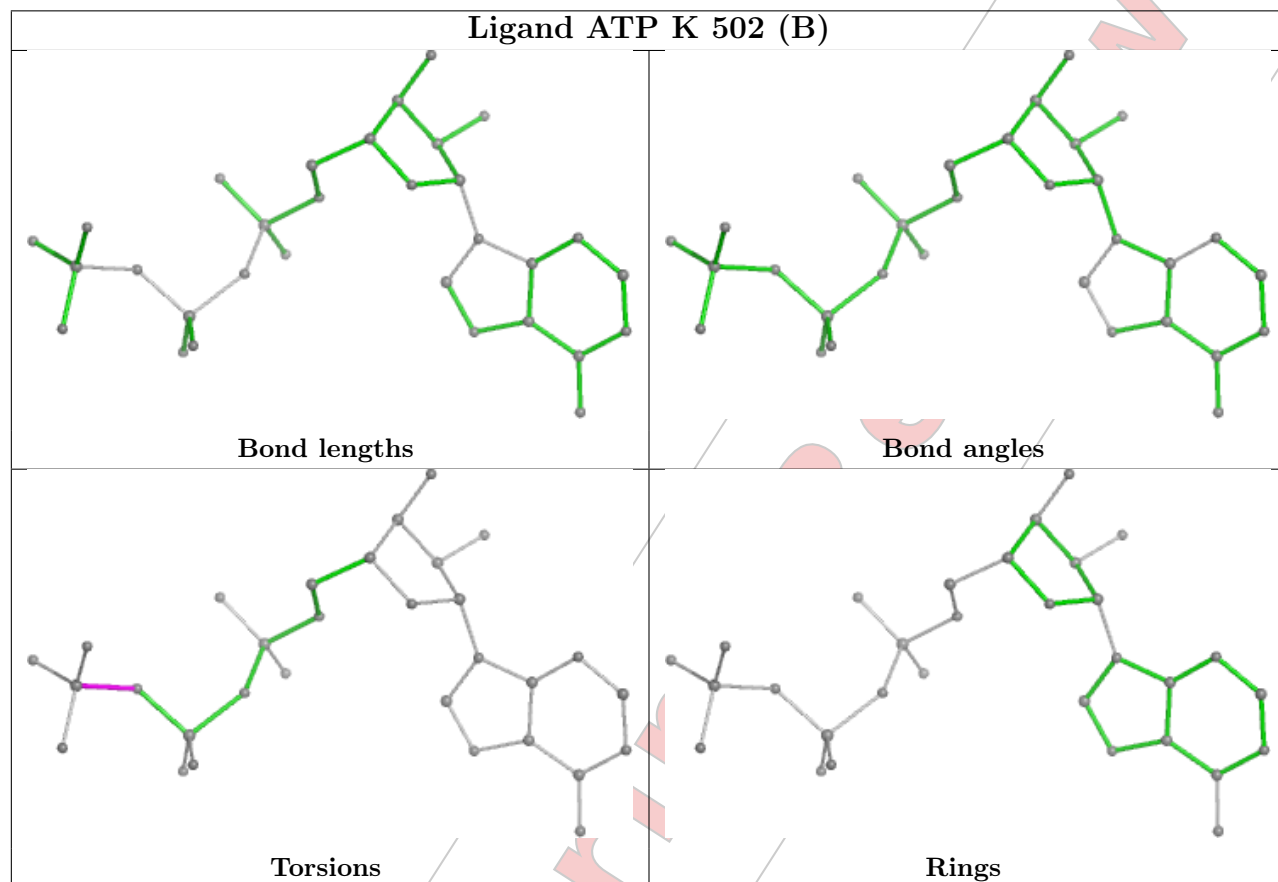
Ligand ATP F 502 (B)



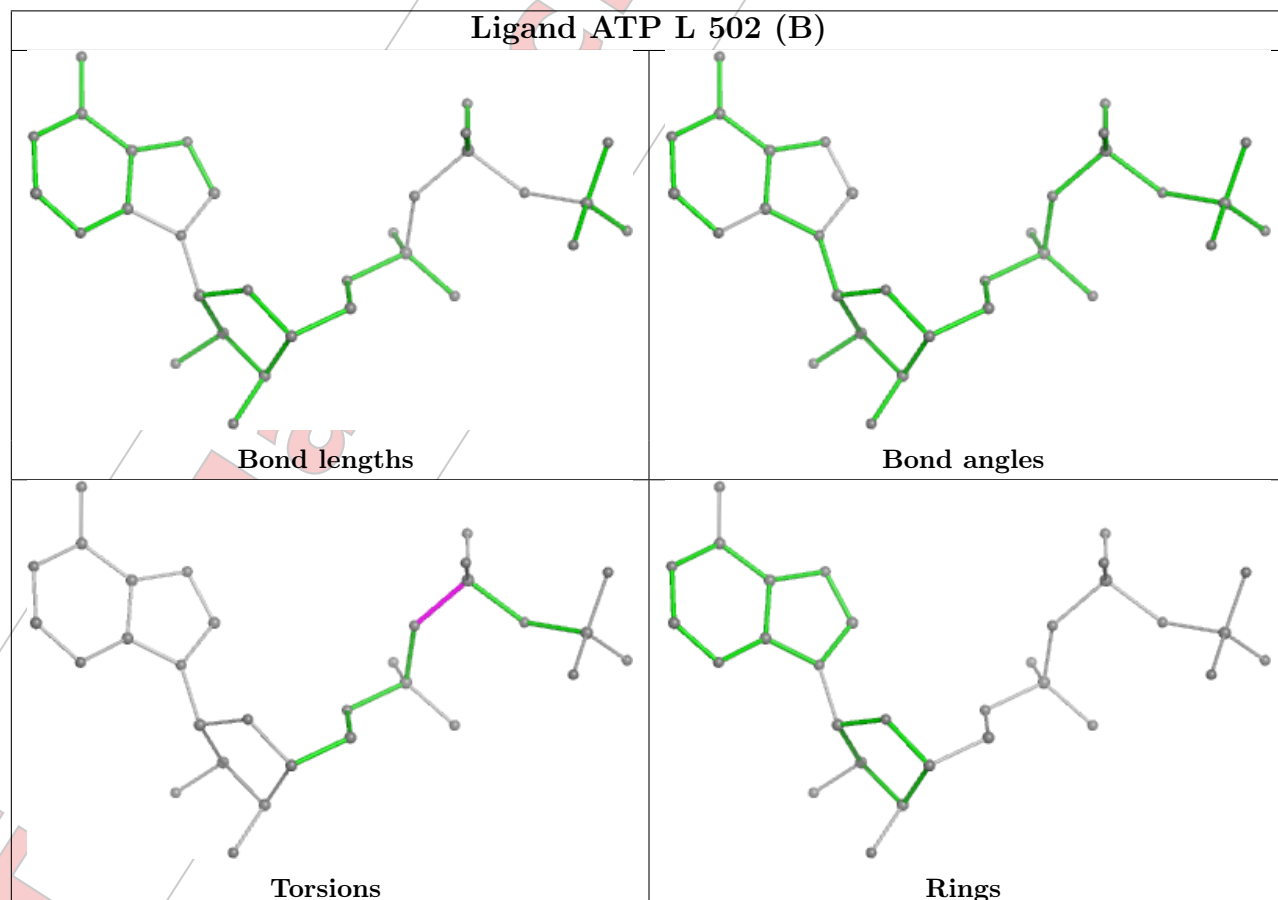
Ligand IMP G 501

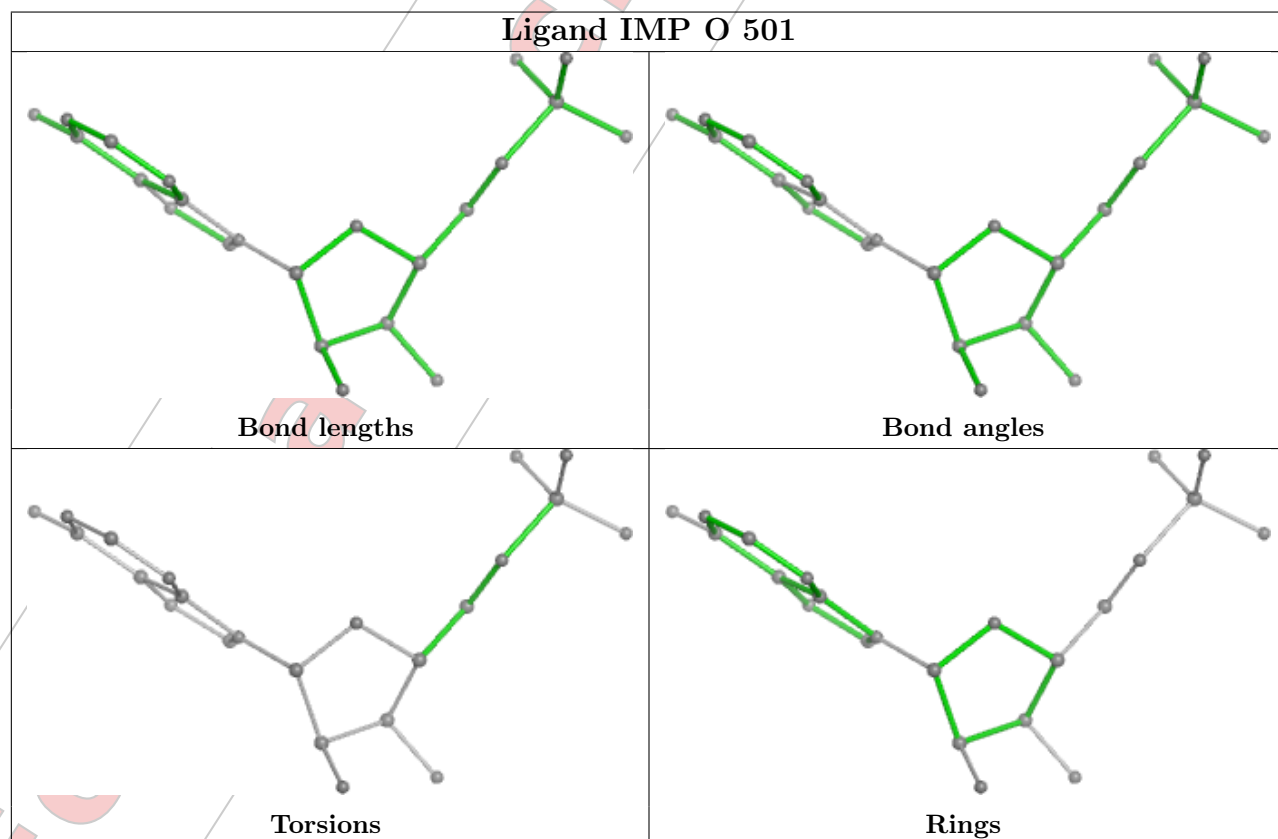
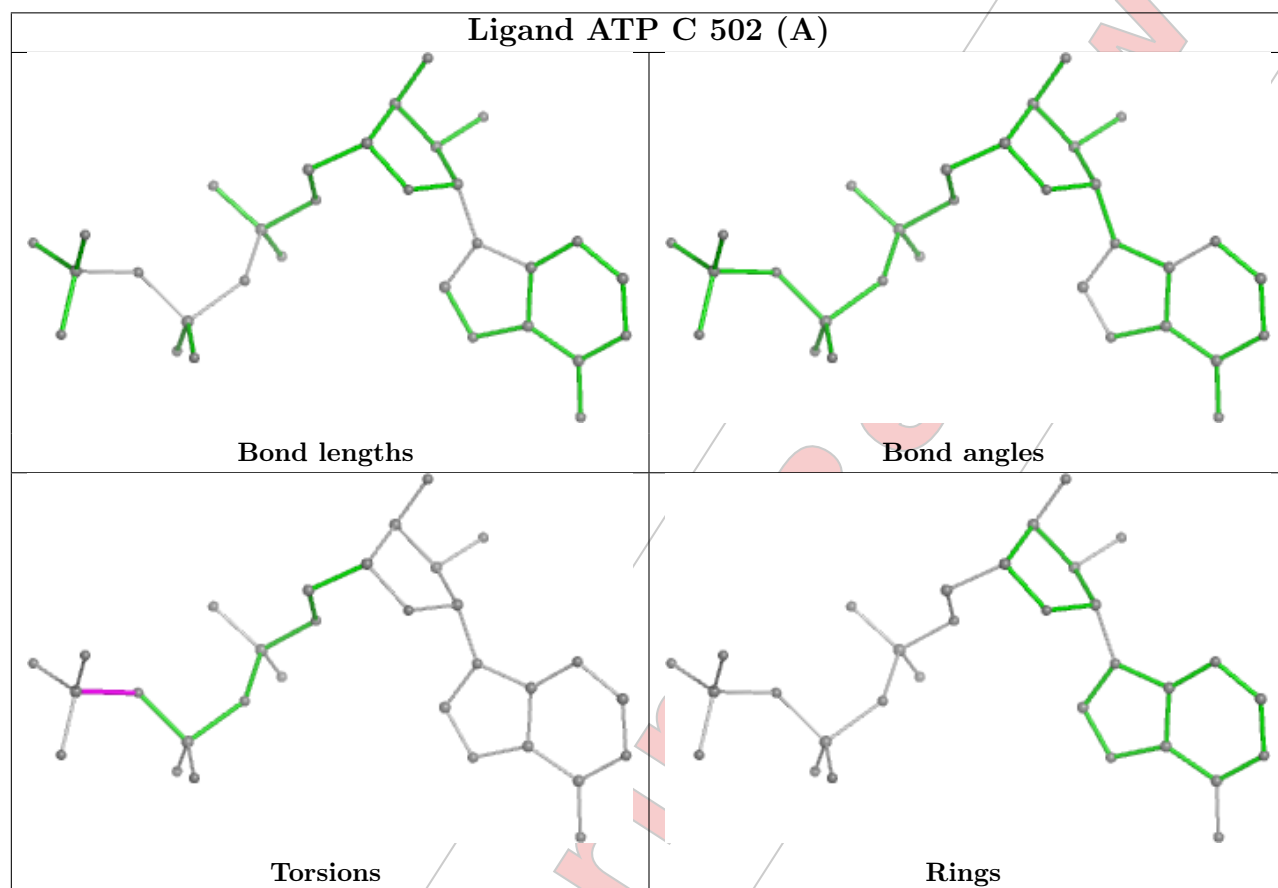


Ligand ATP K 502 (B)

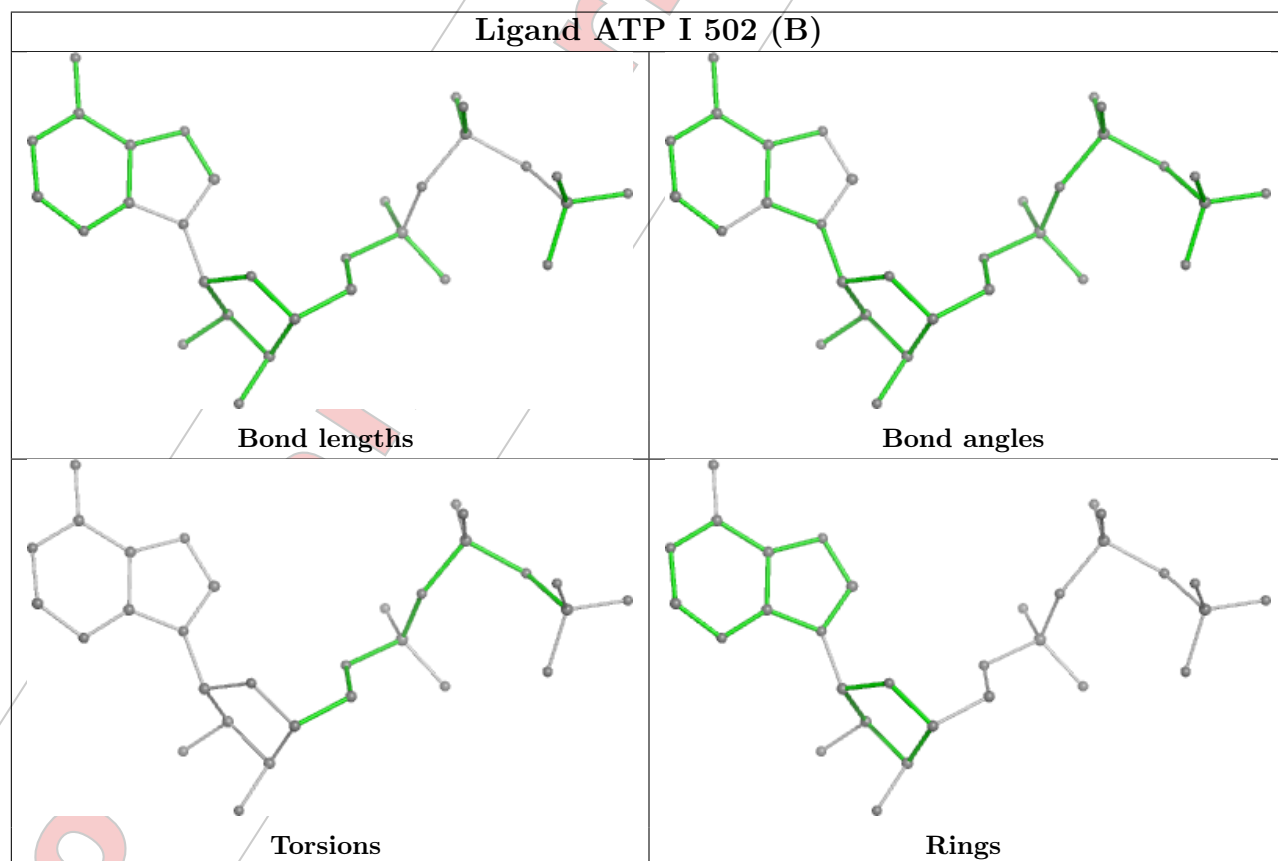
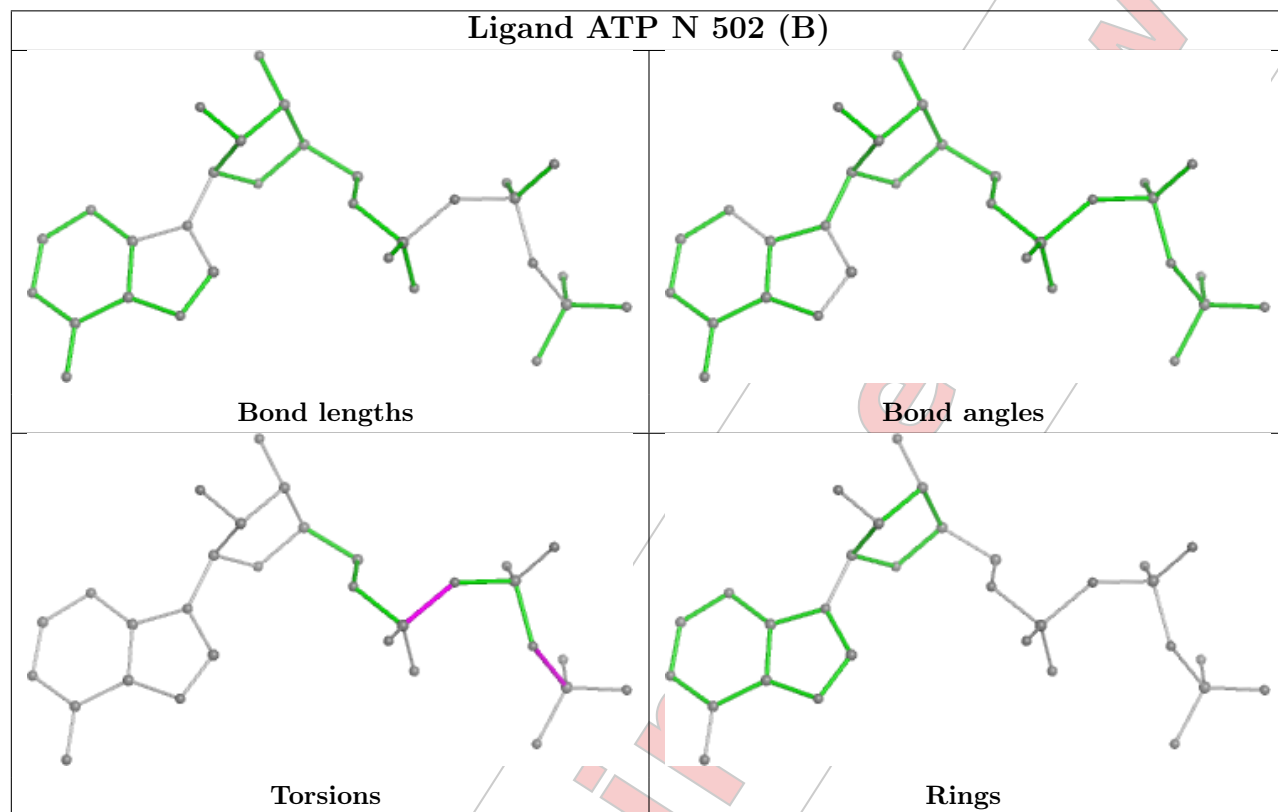


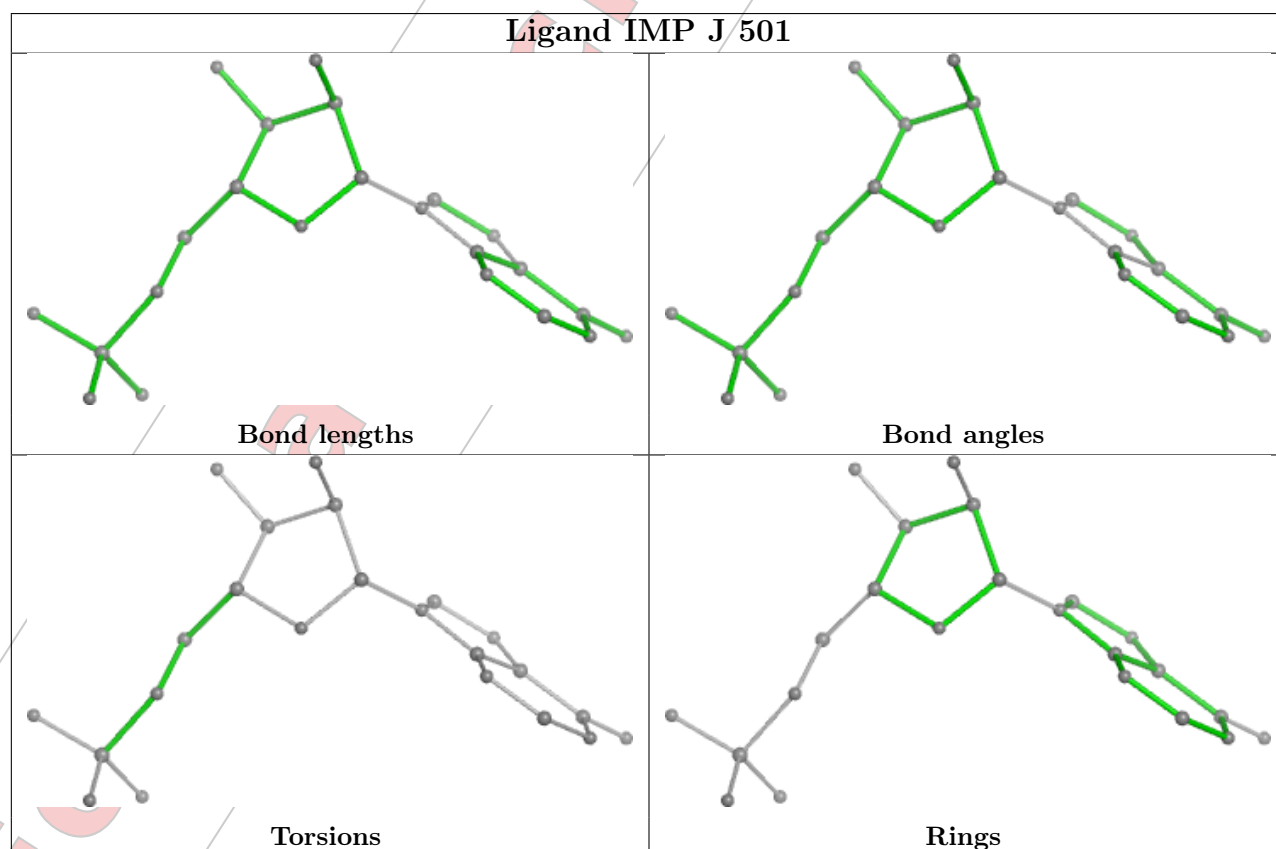
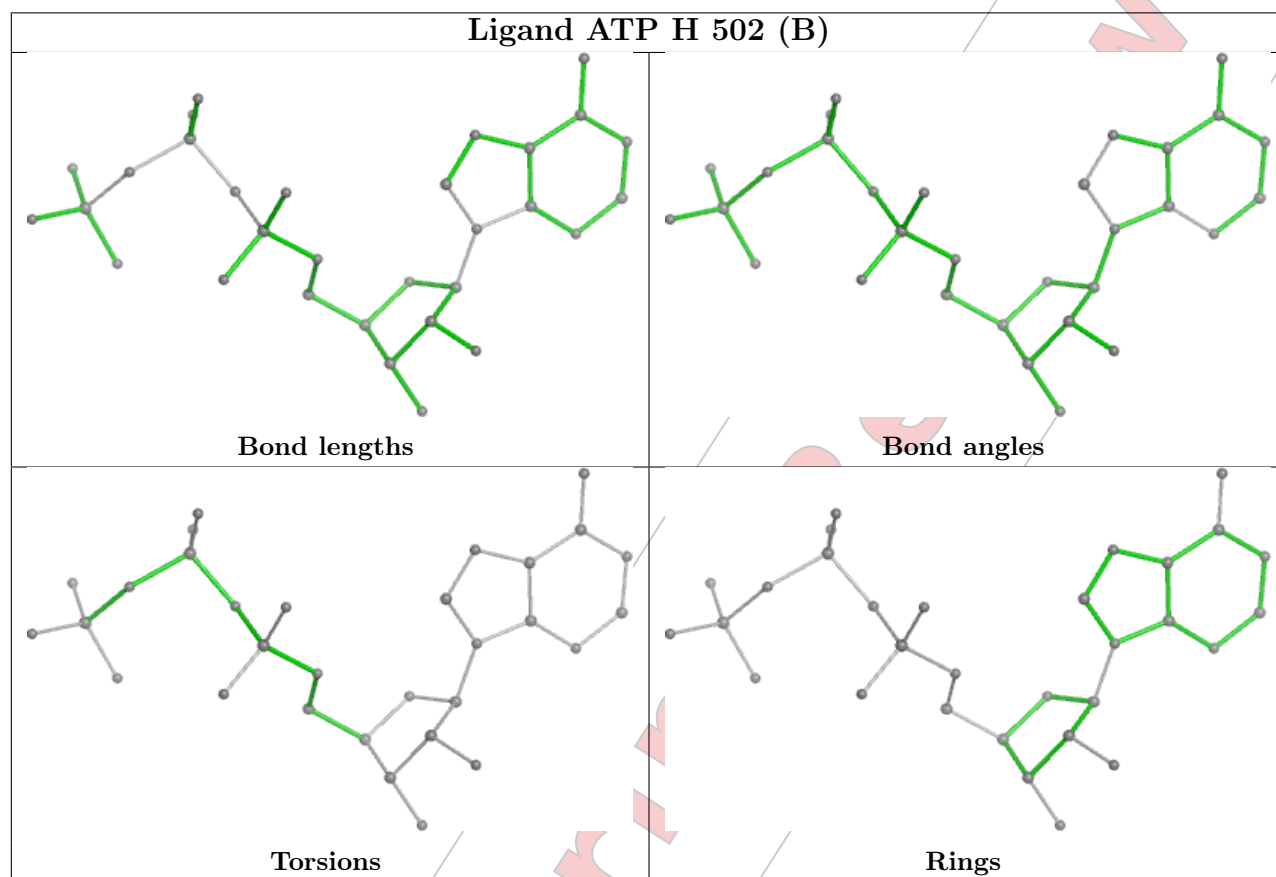
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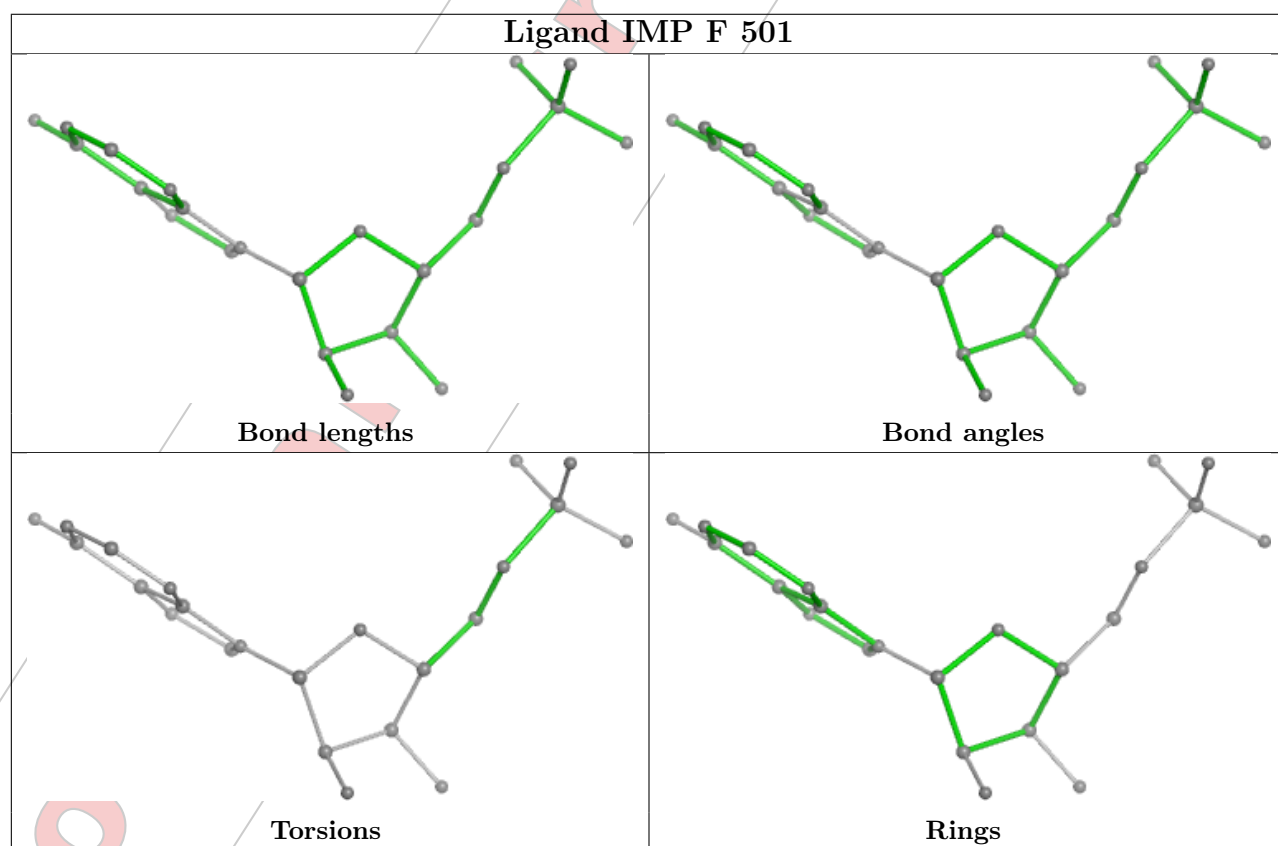
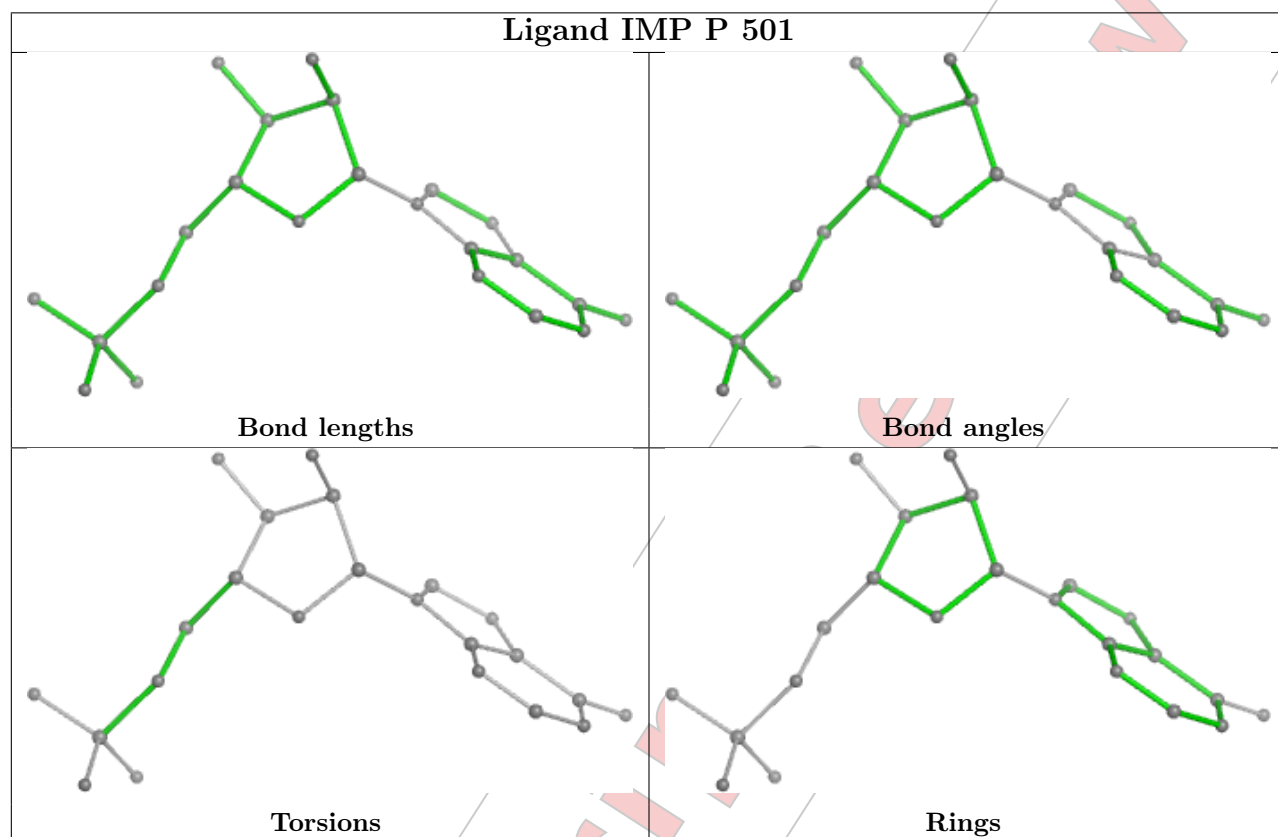




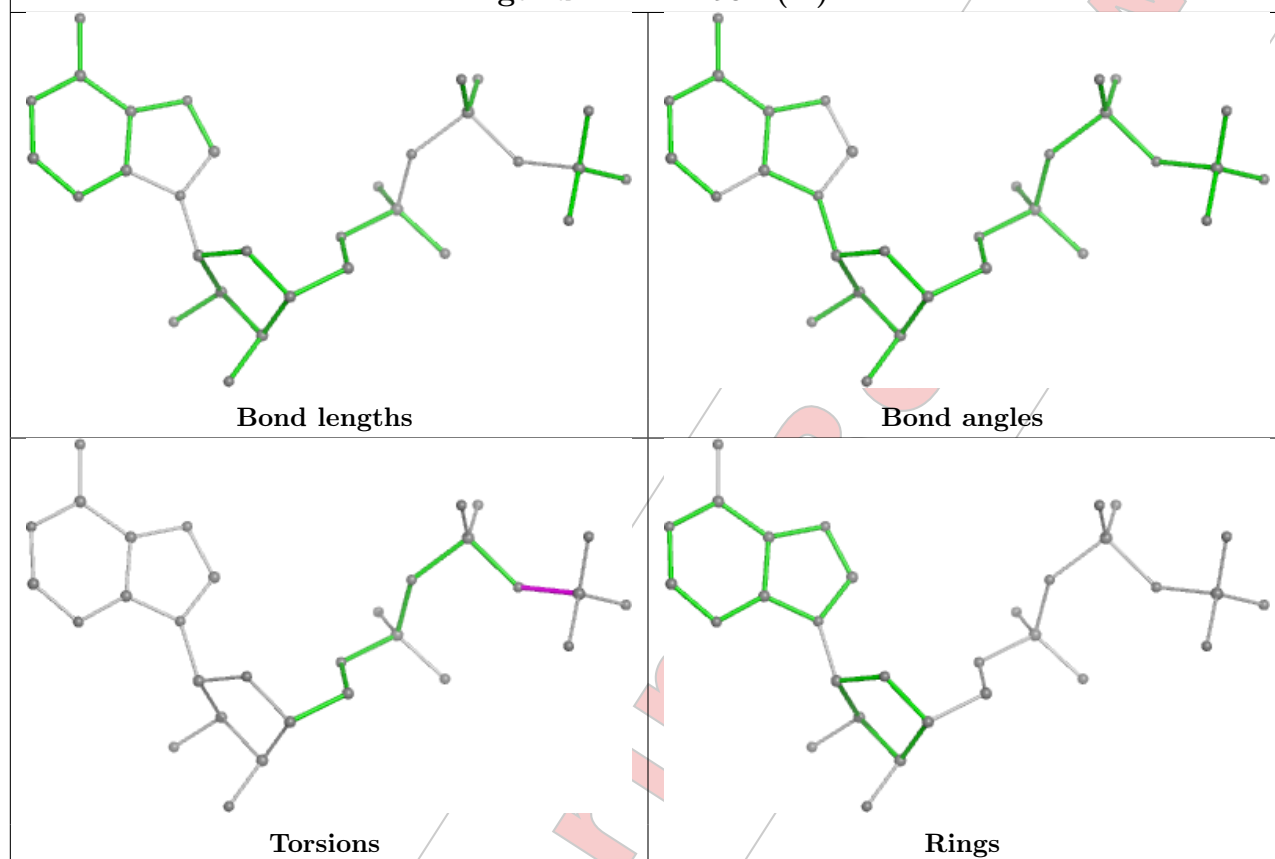




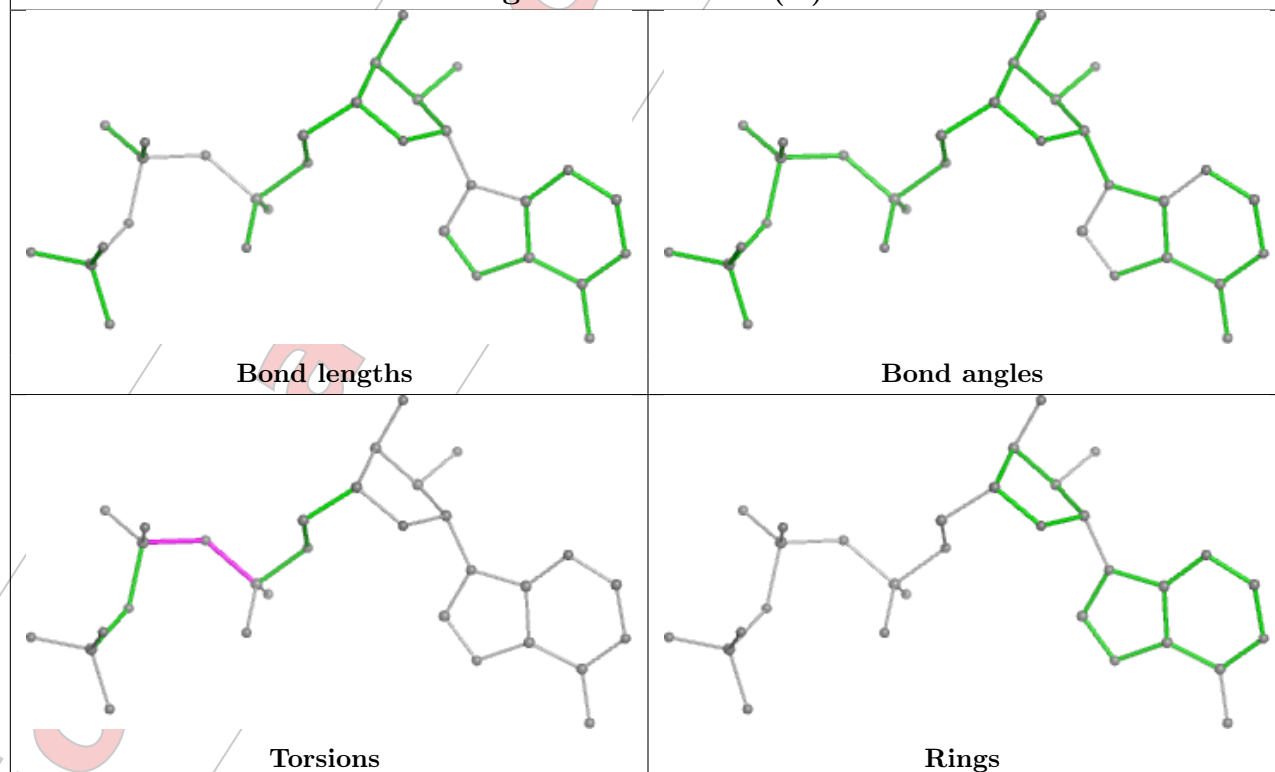




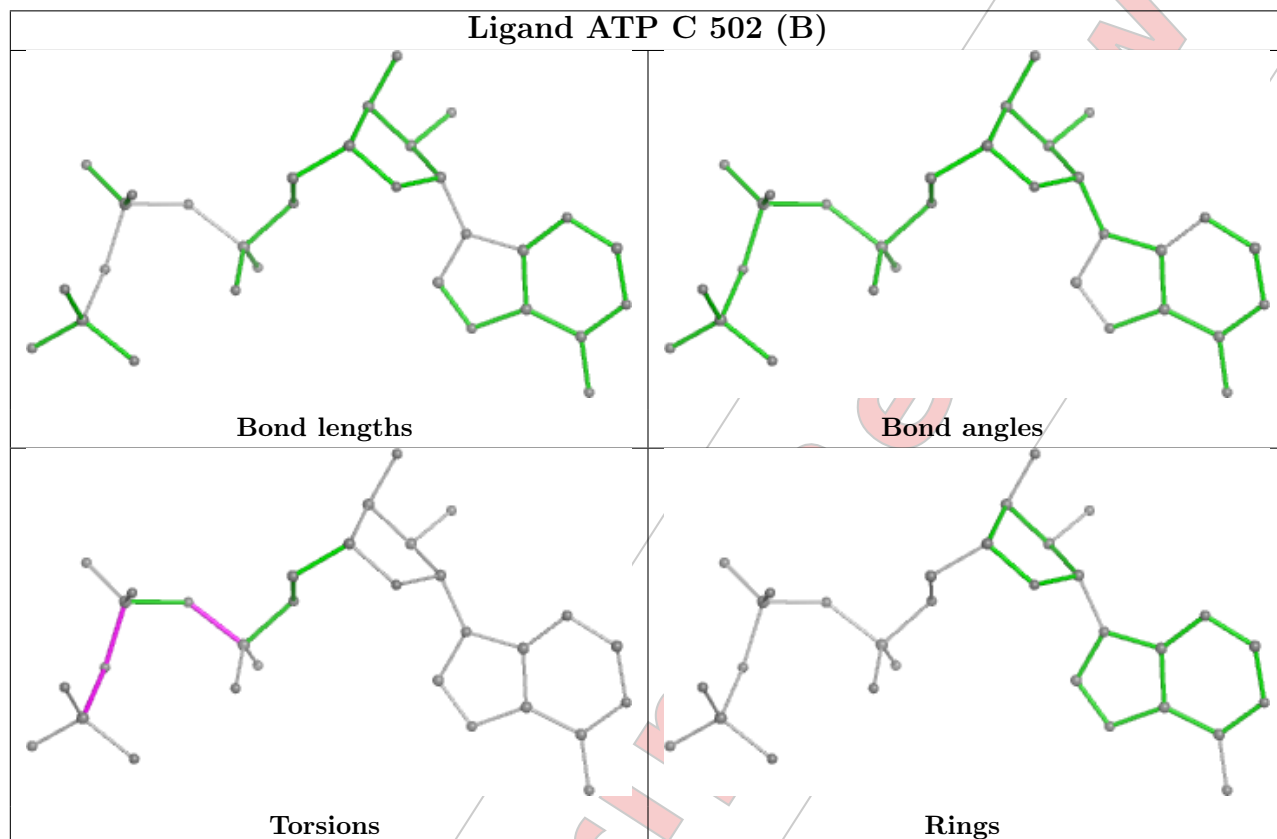
Ligand ATP A 502 (A)



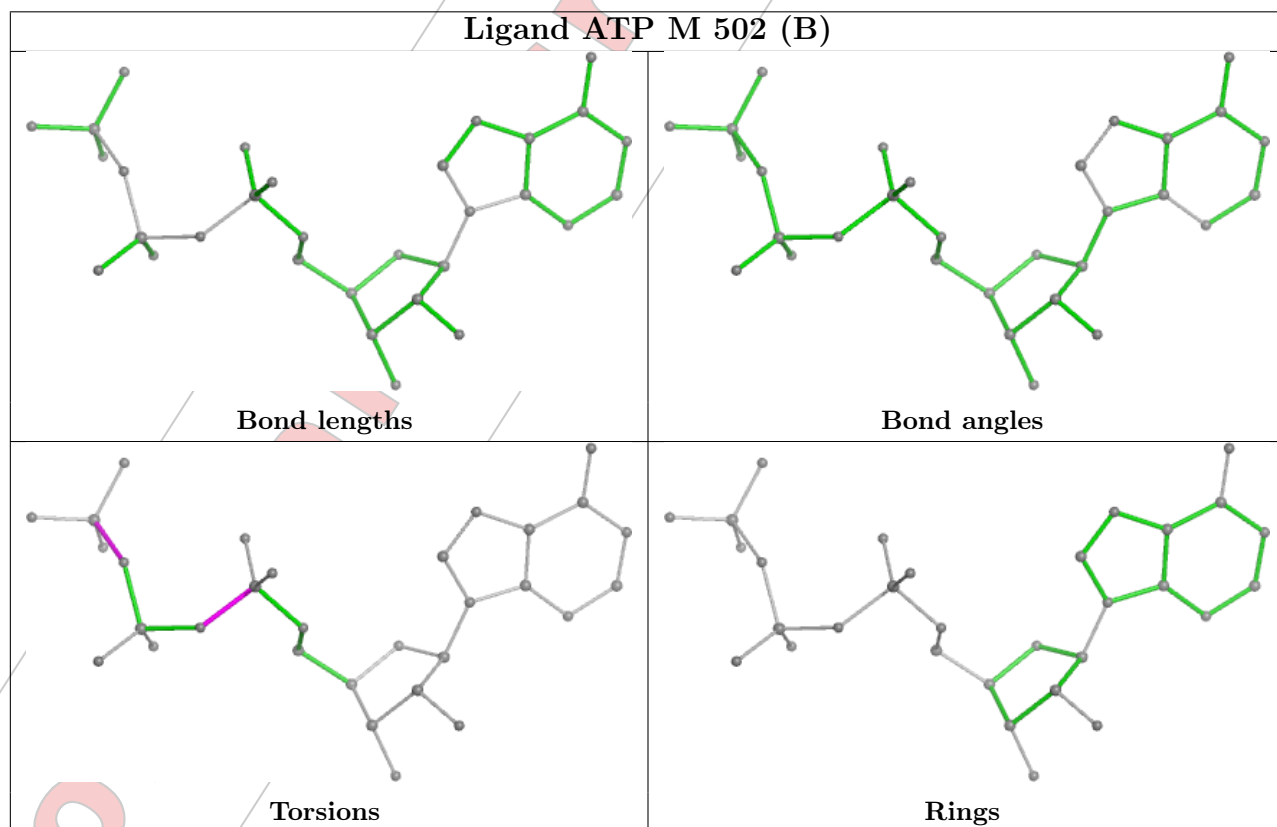
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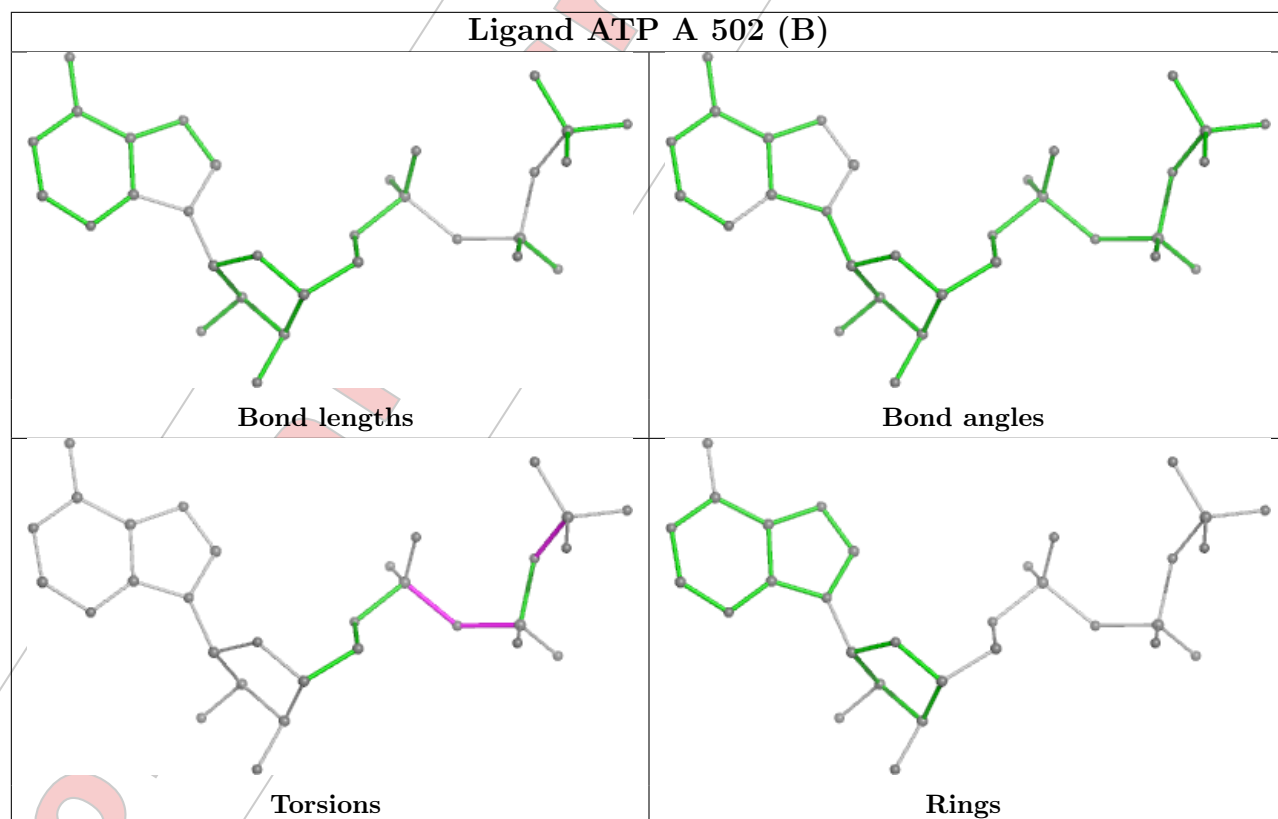
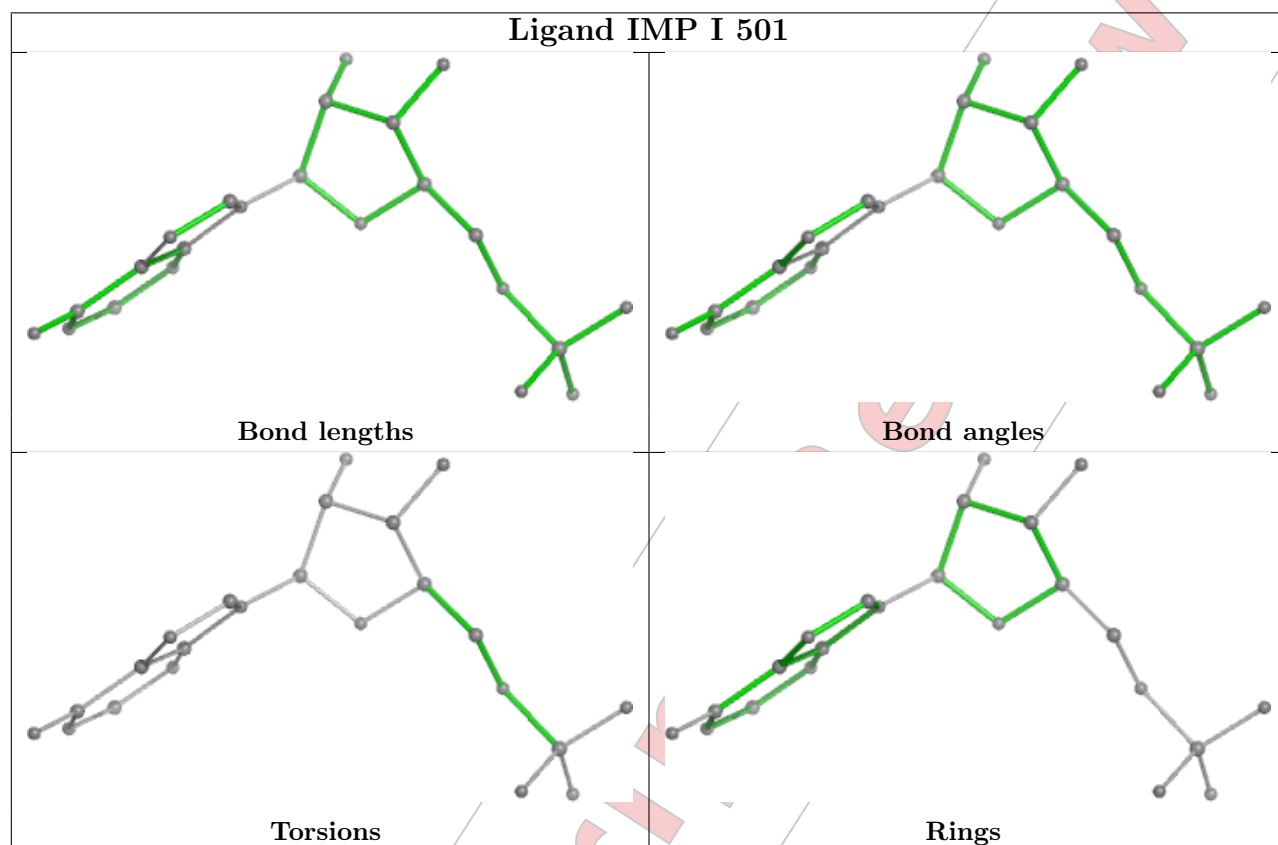


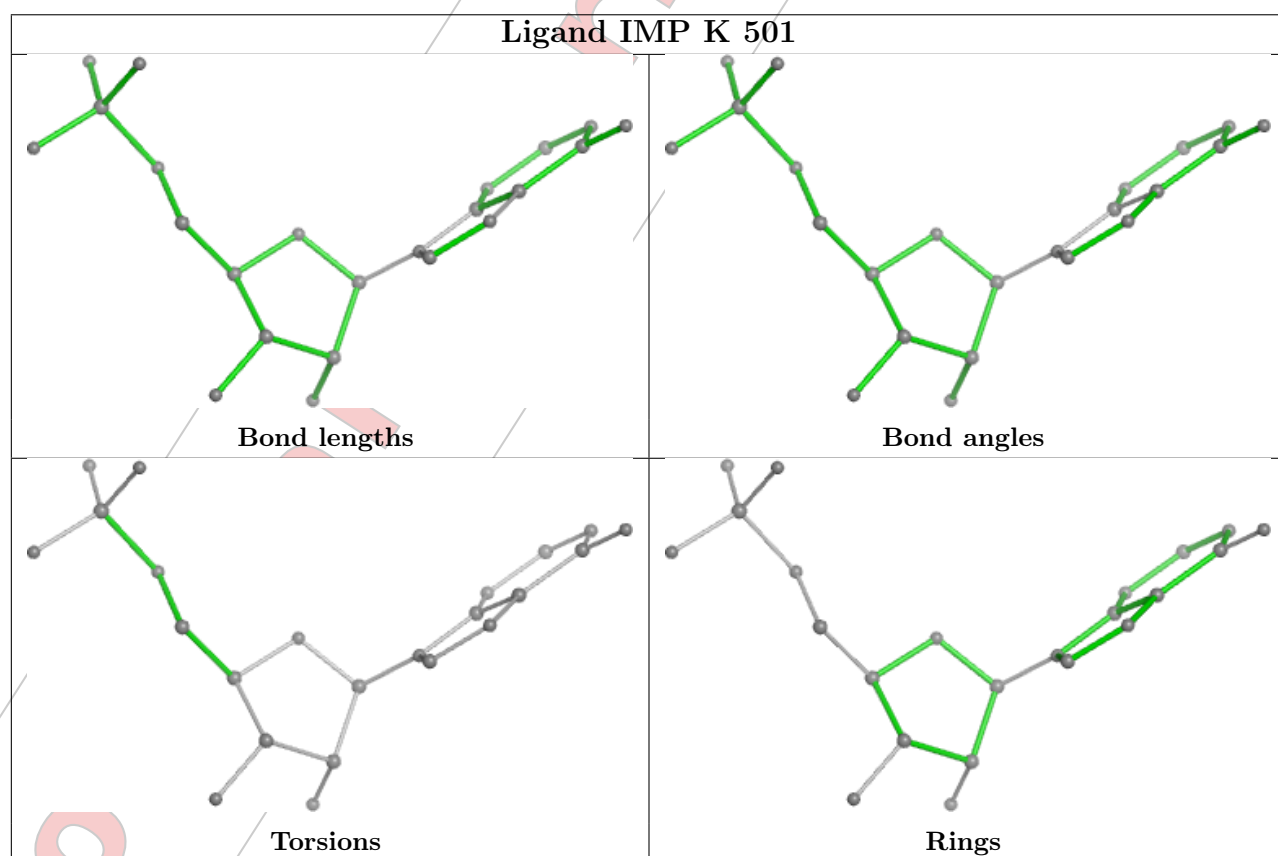
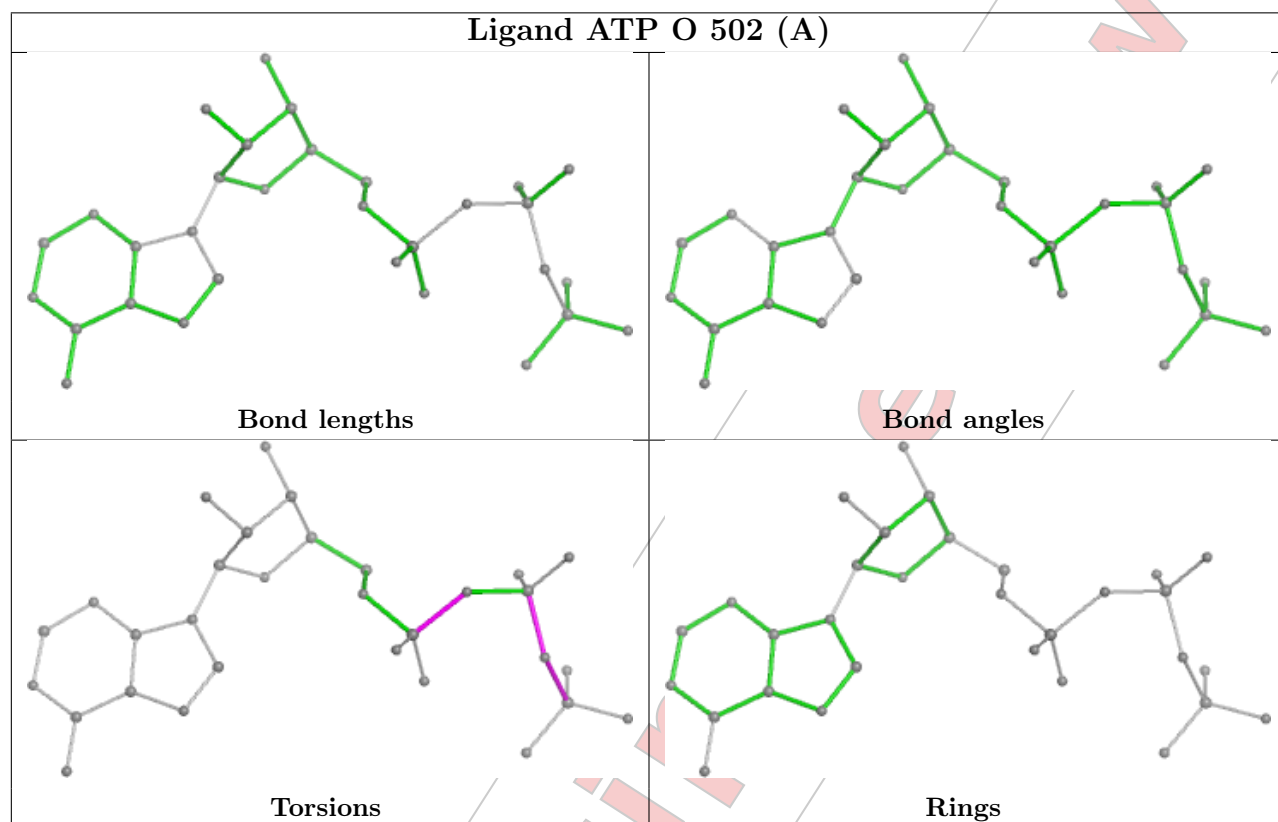
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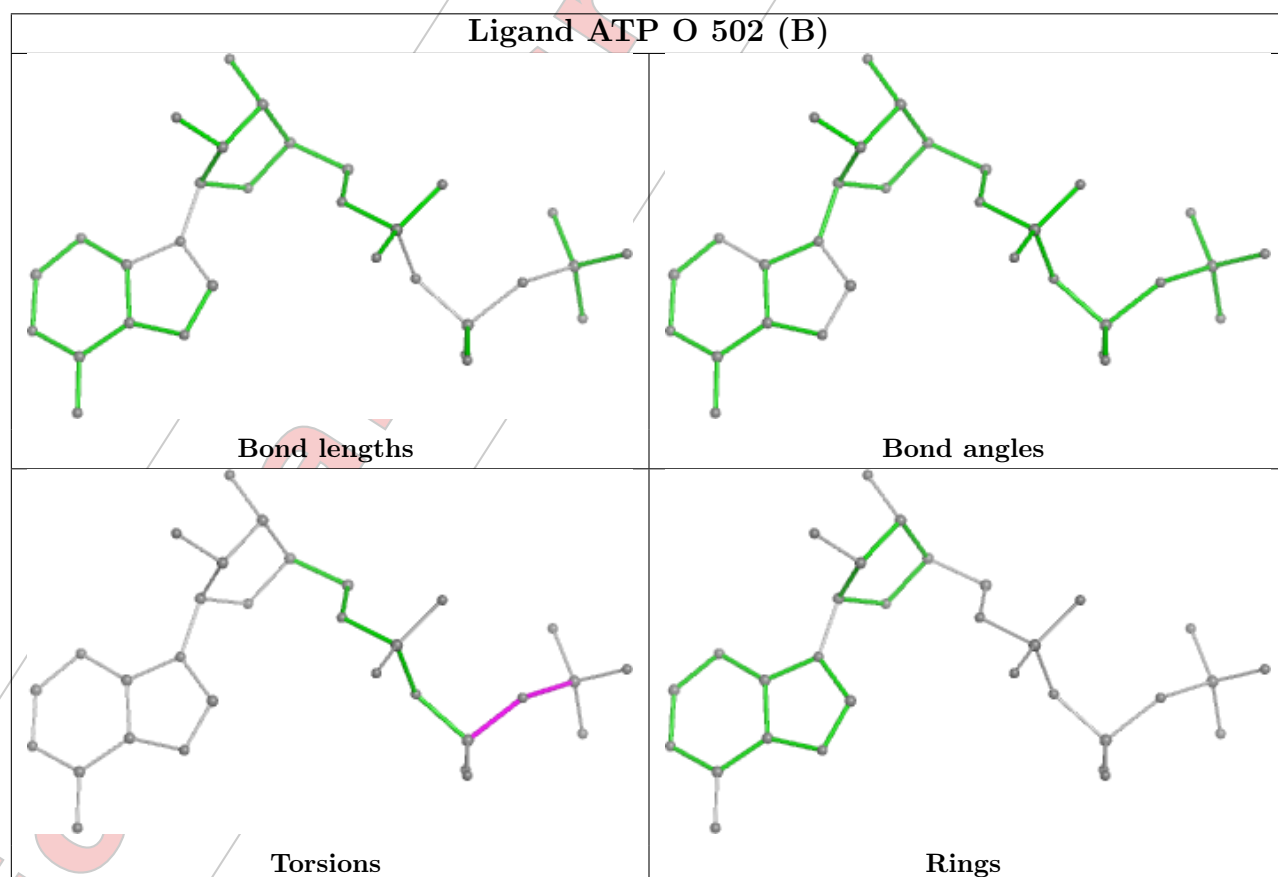
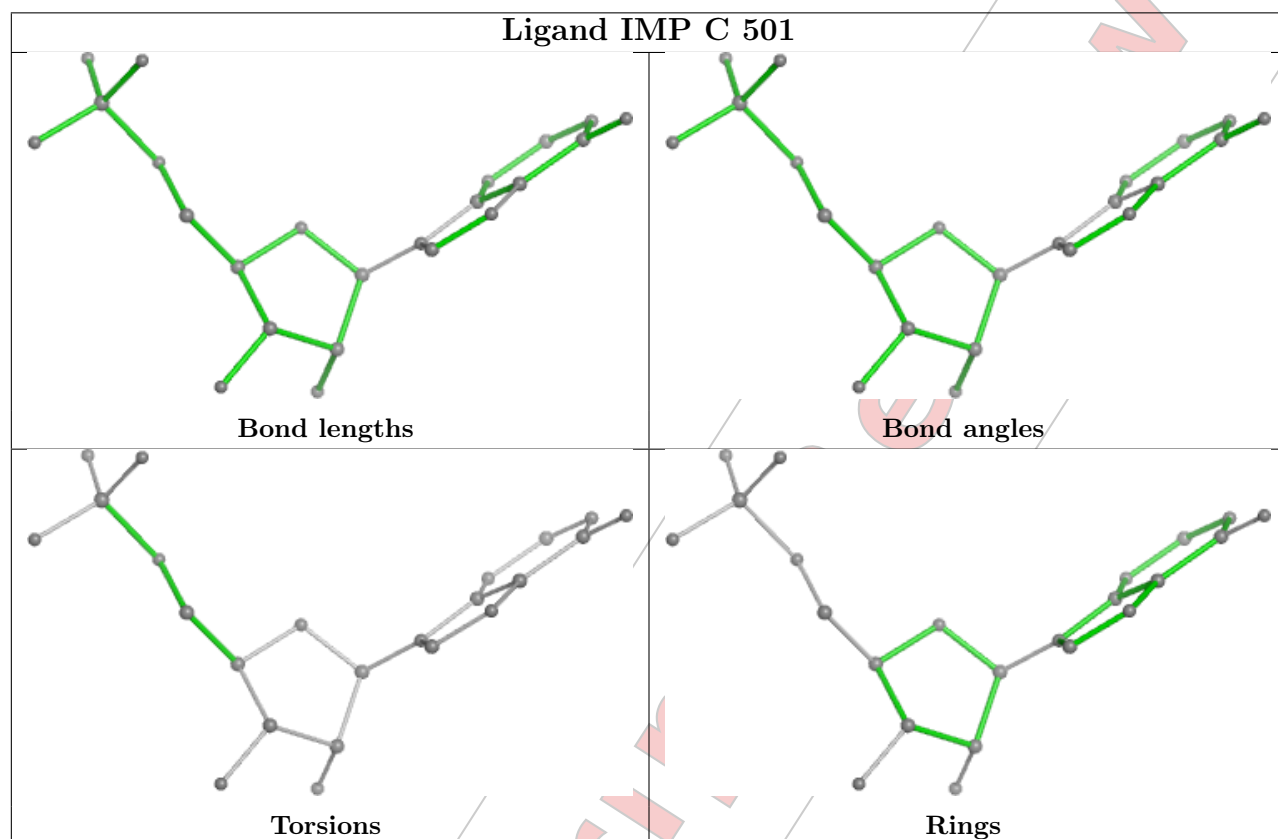
Ligand ATP M 502 (B)

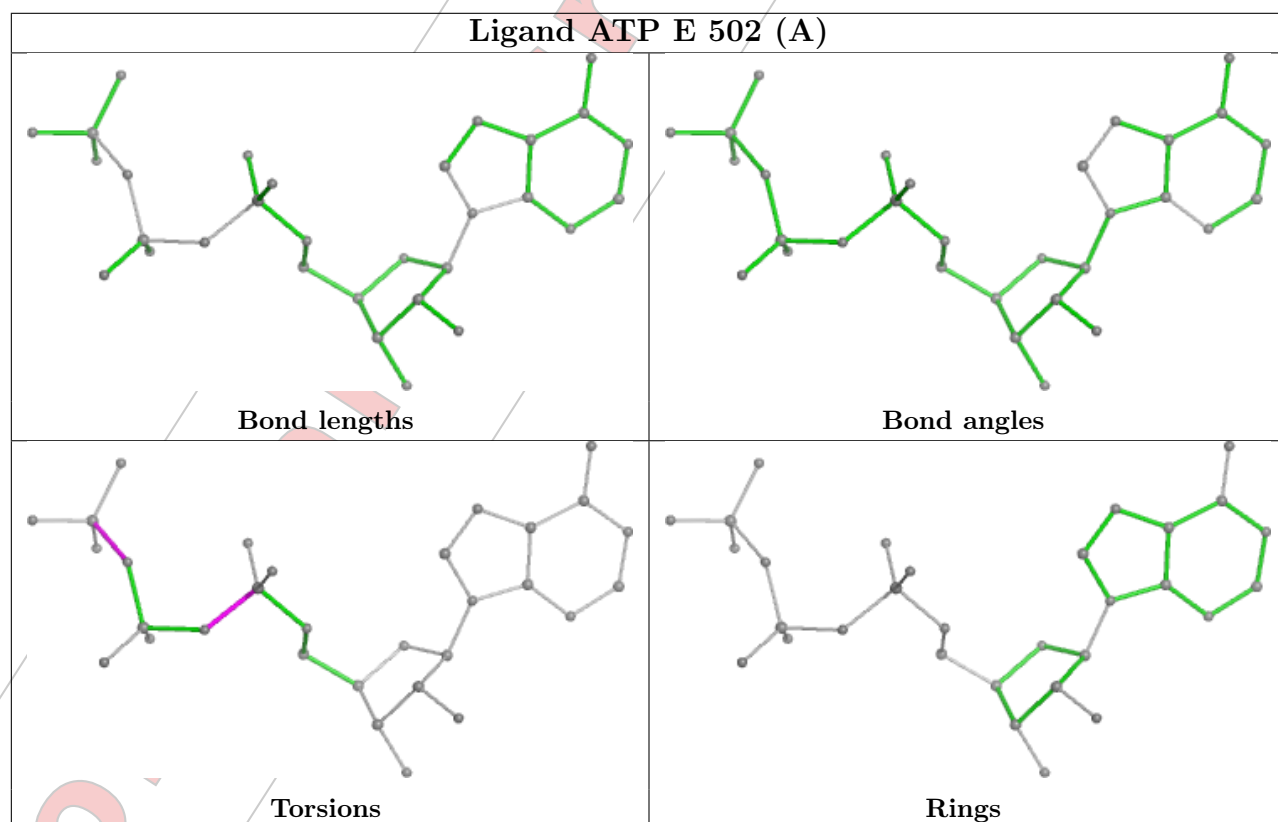
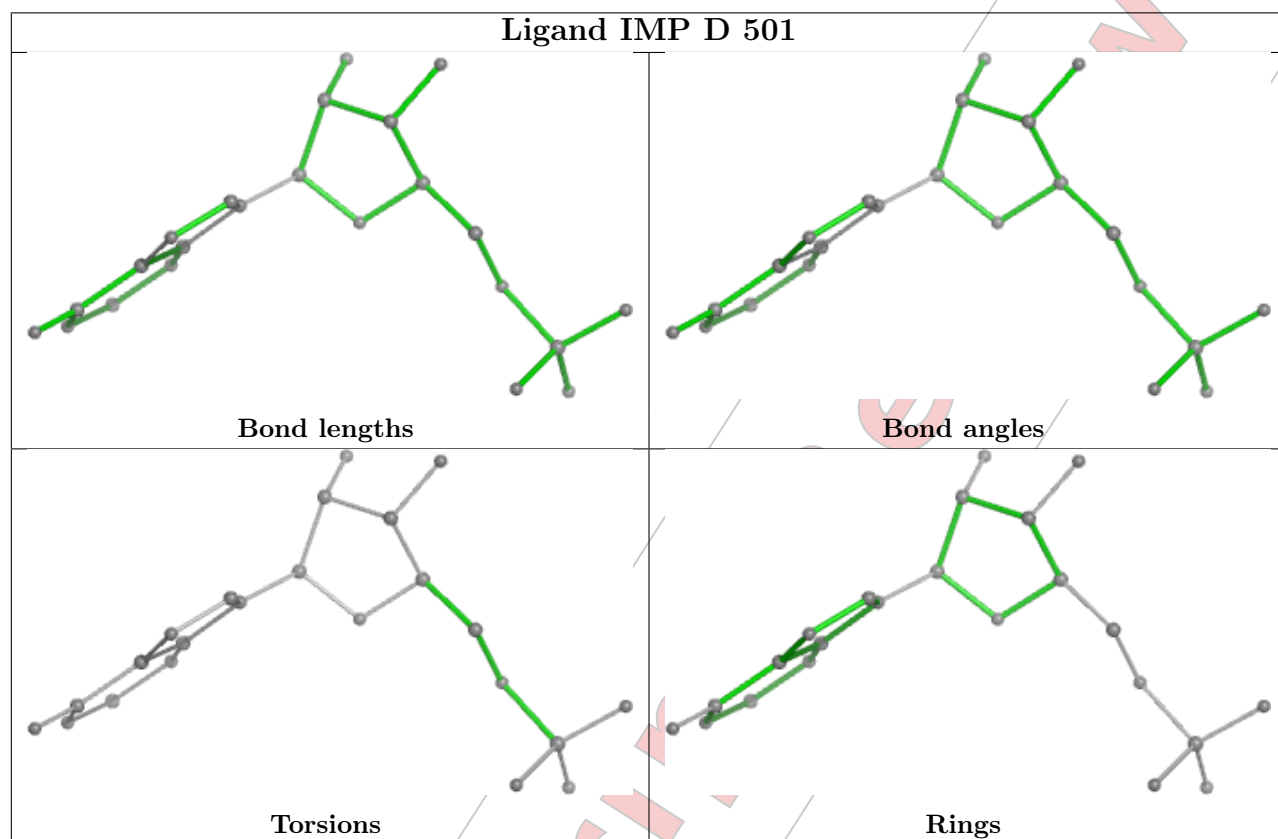


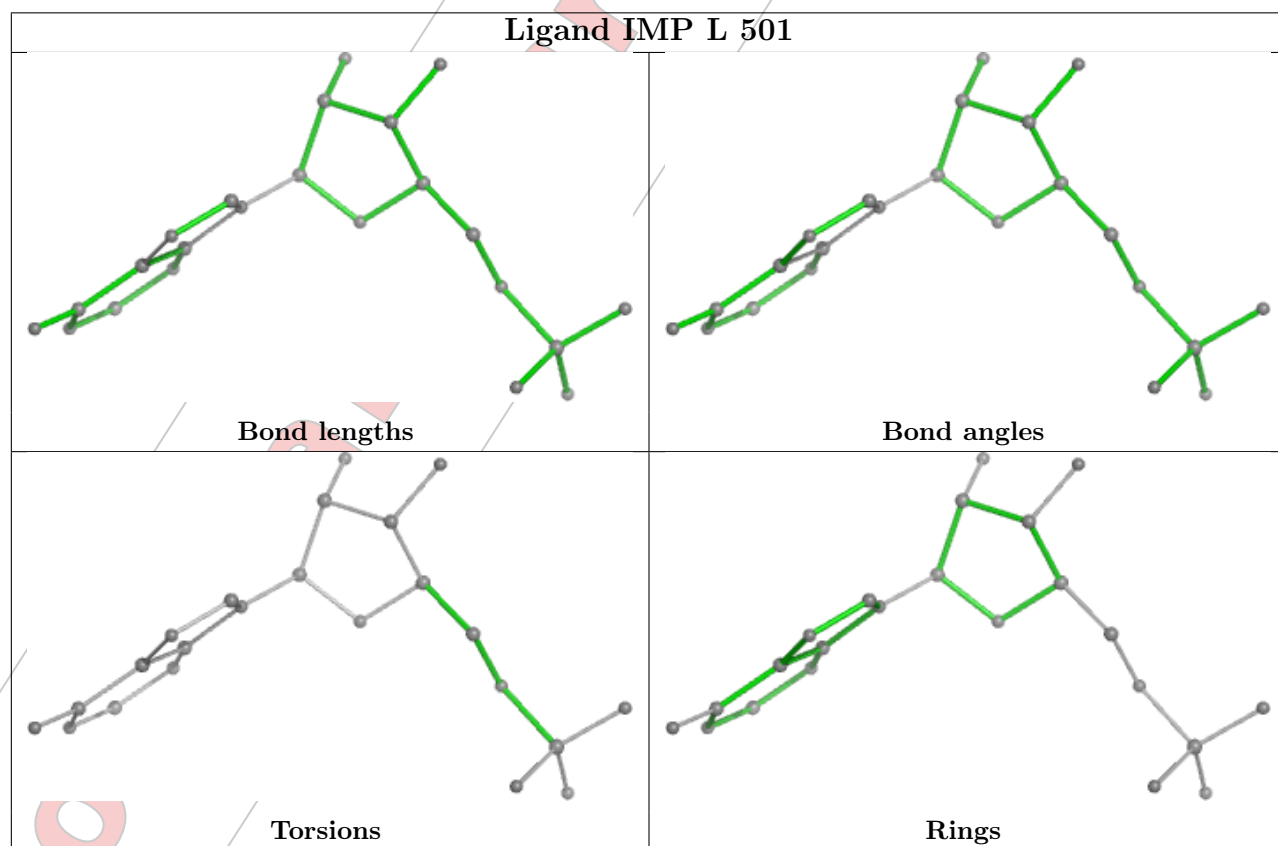
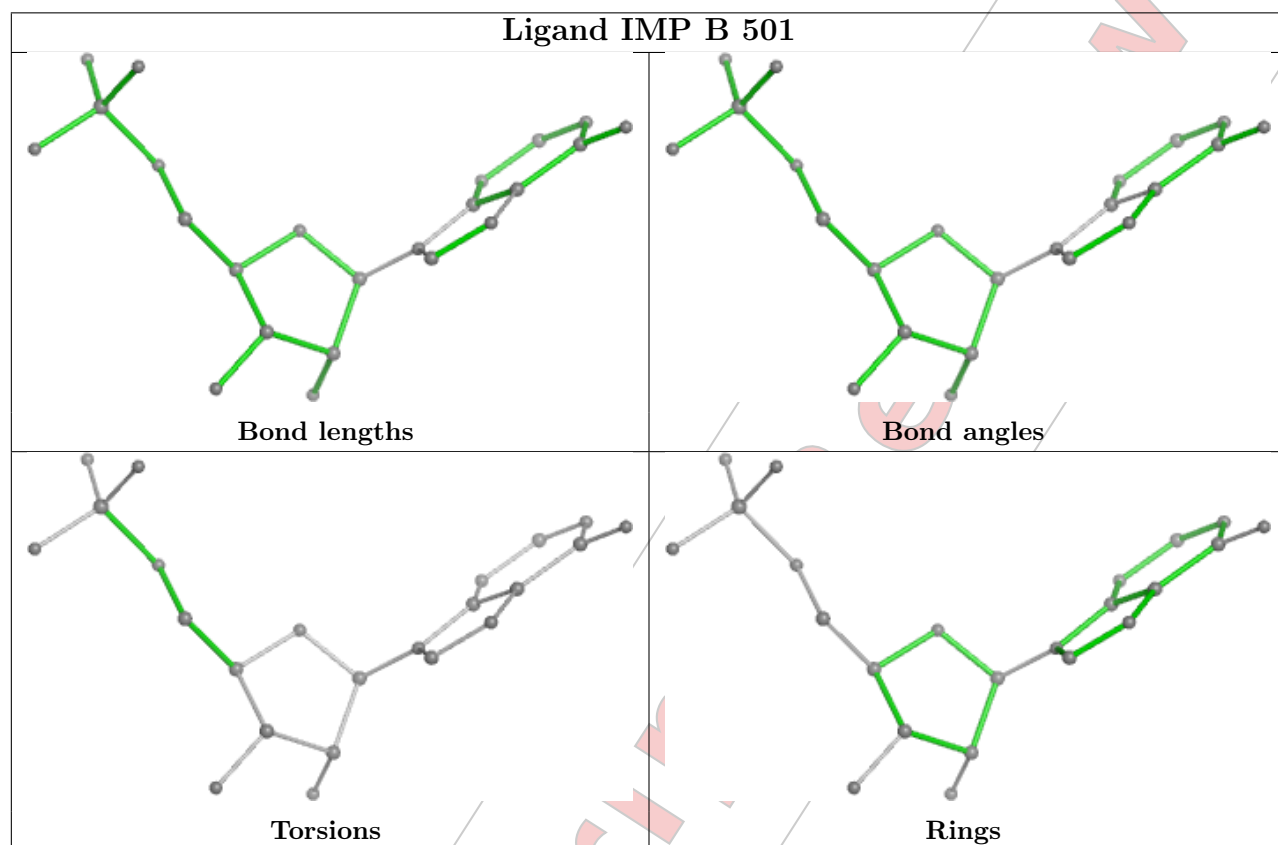


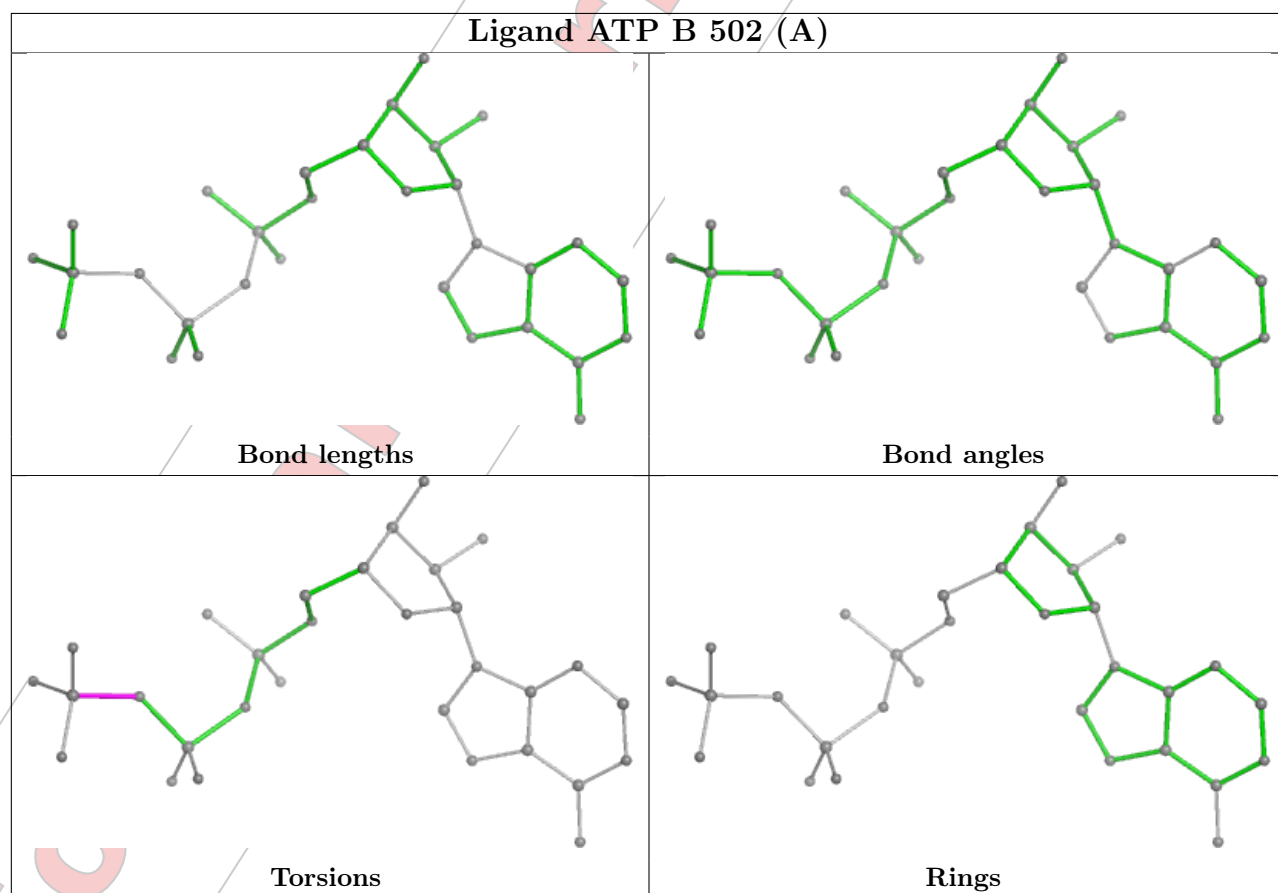
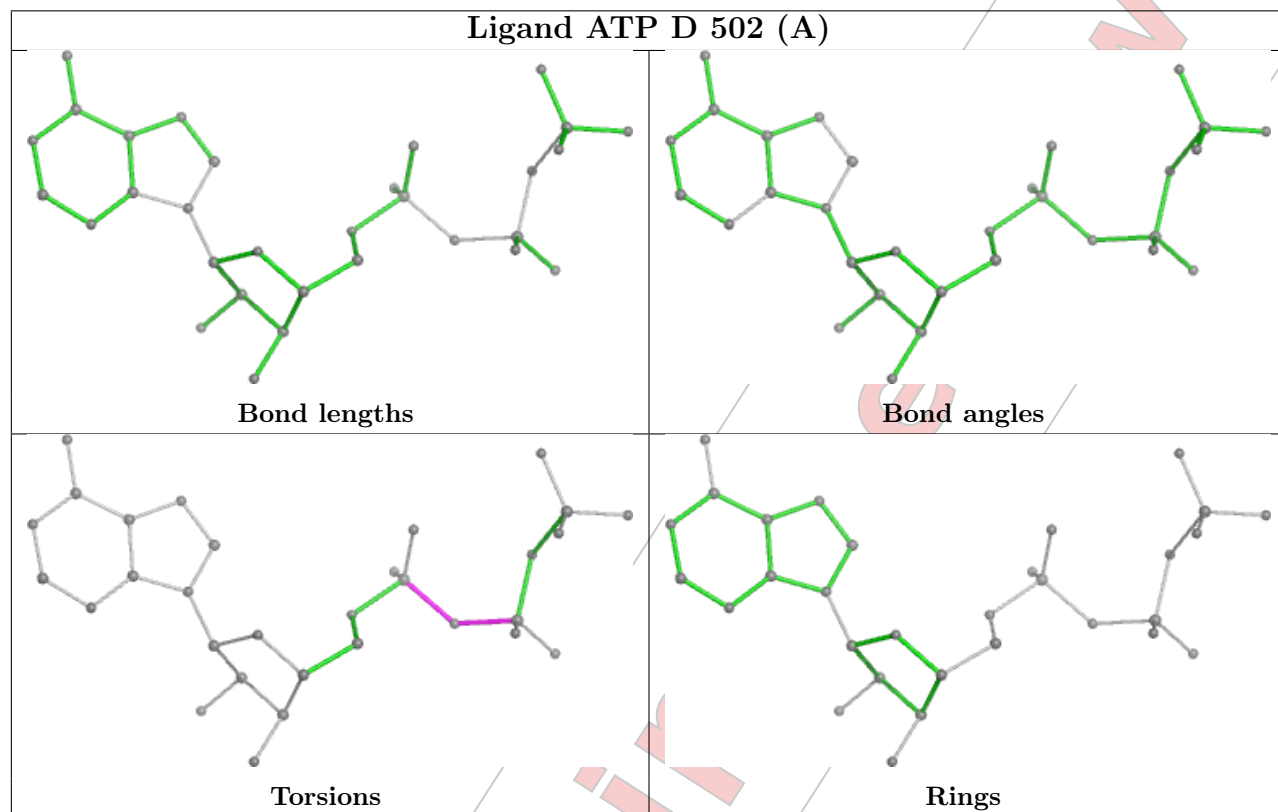


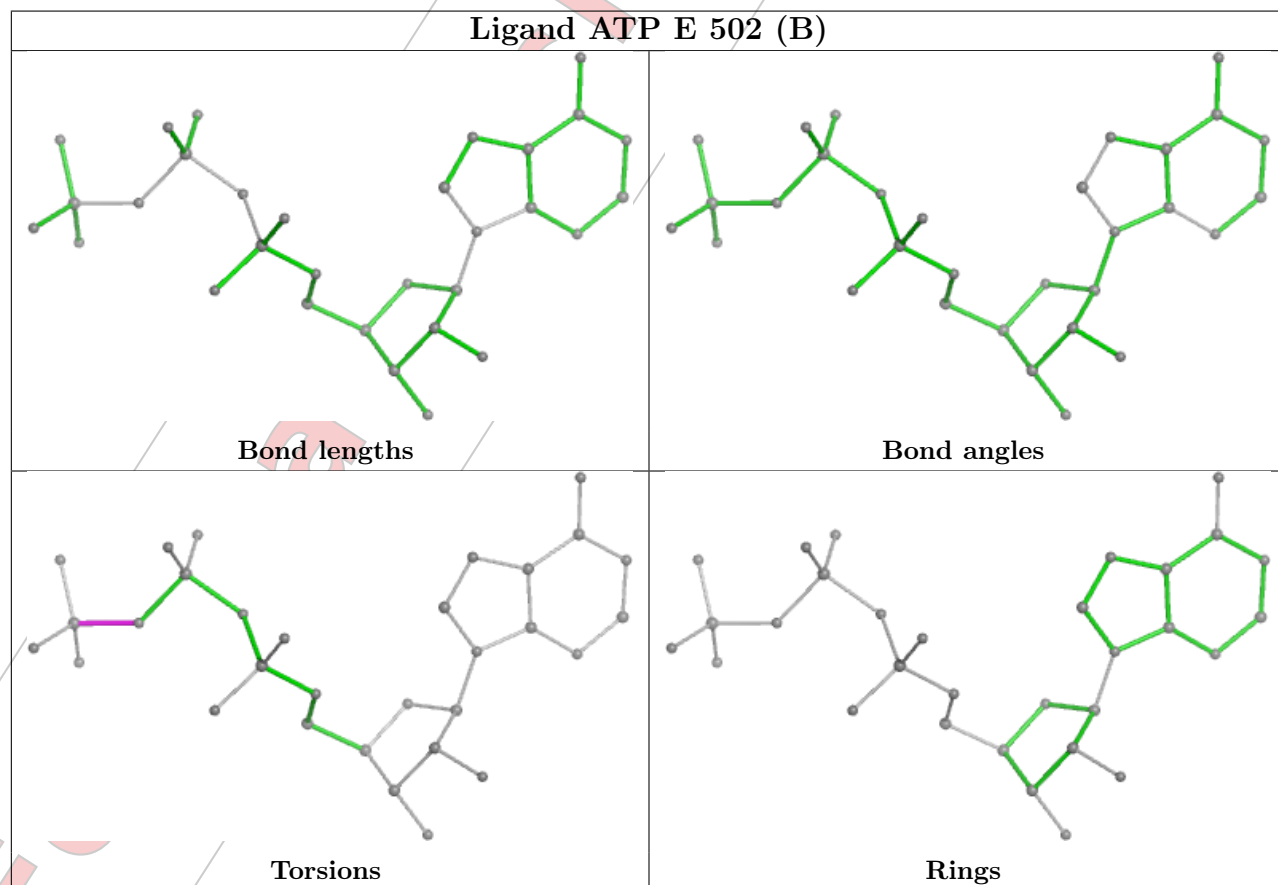
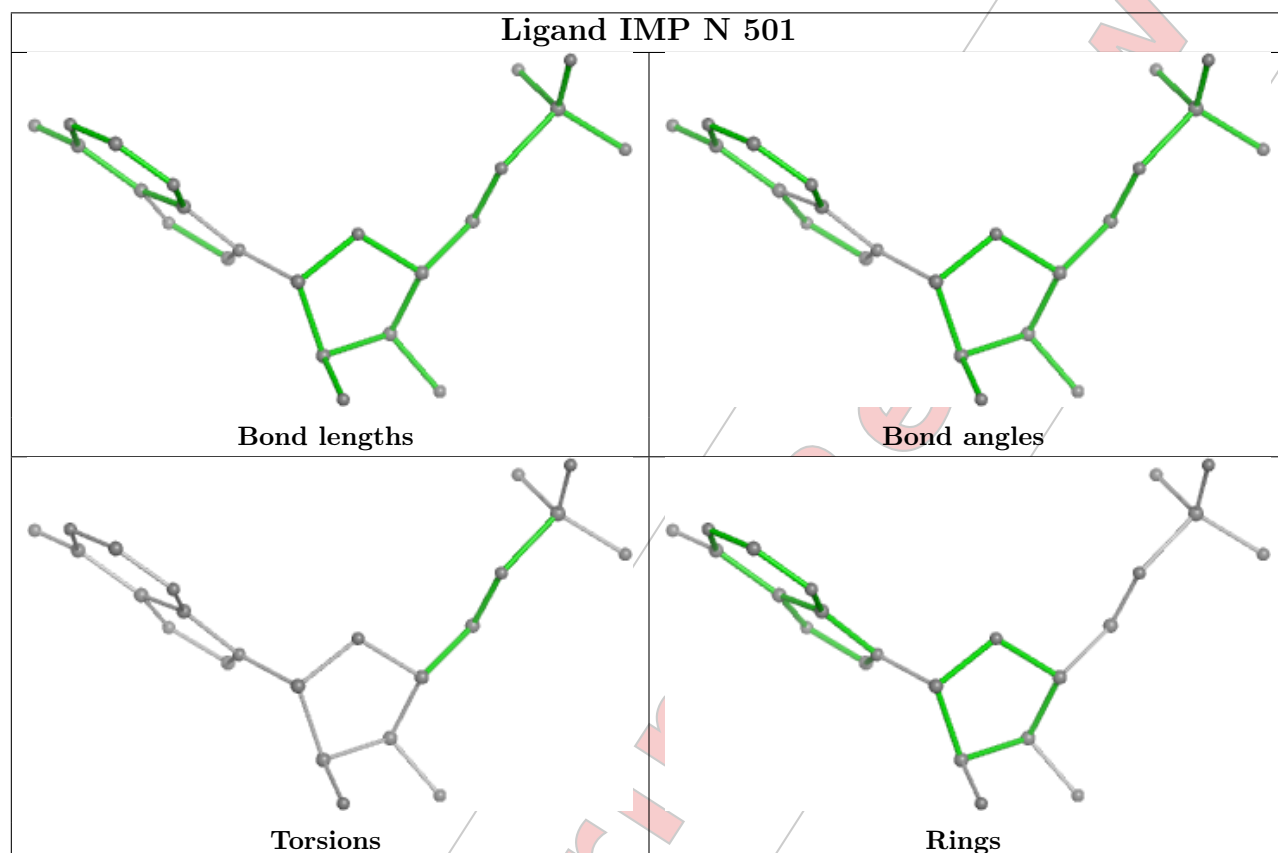




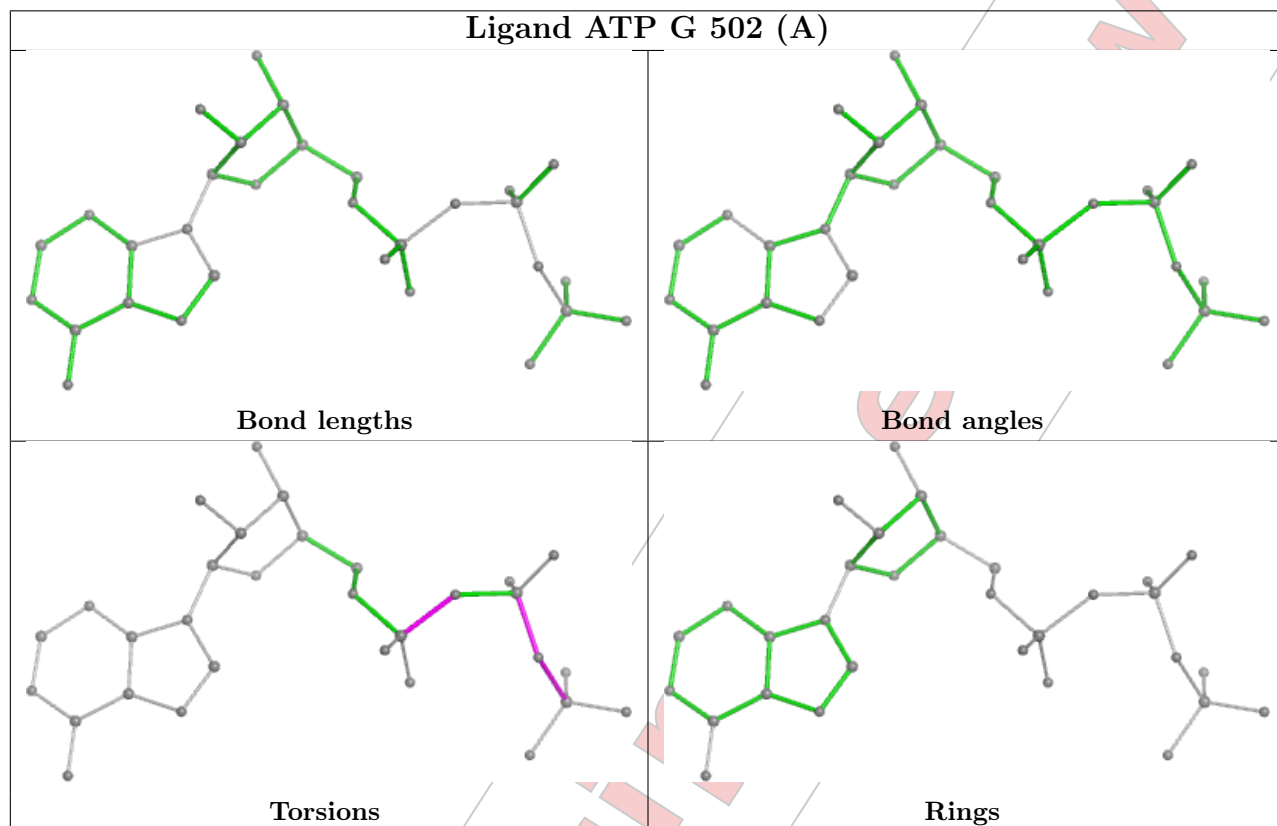




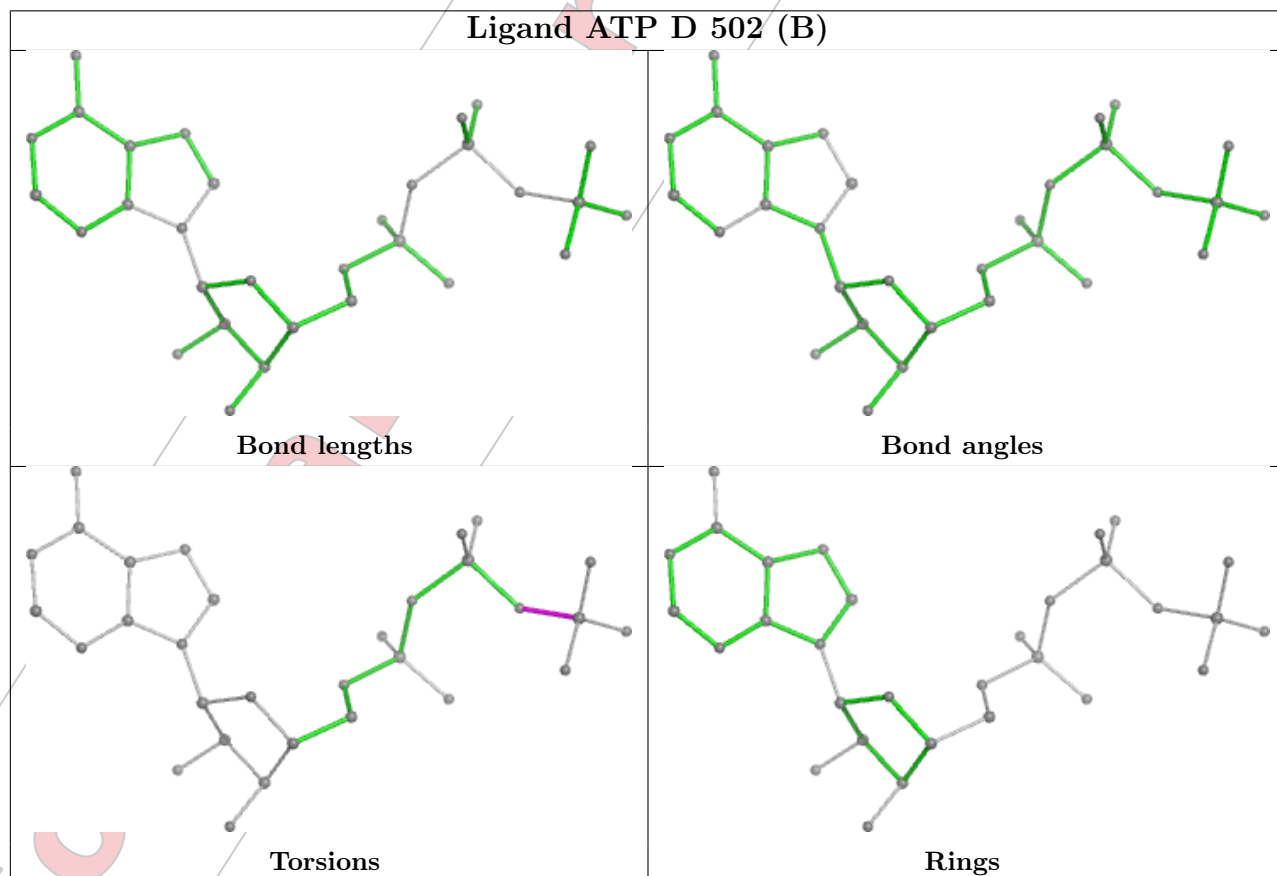


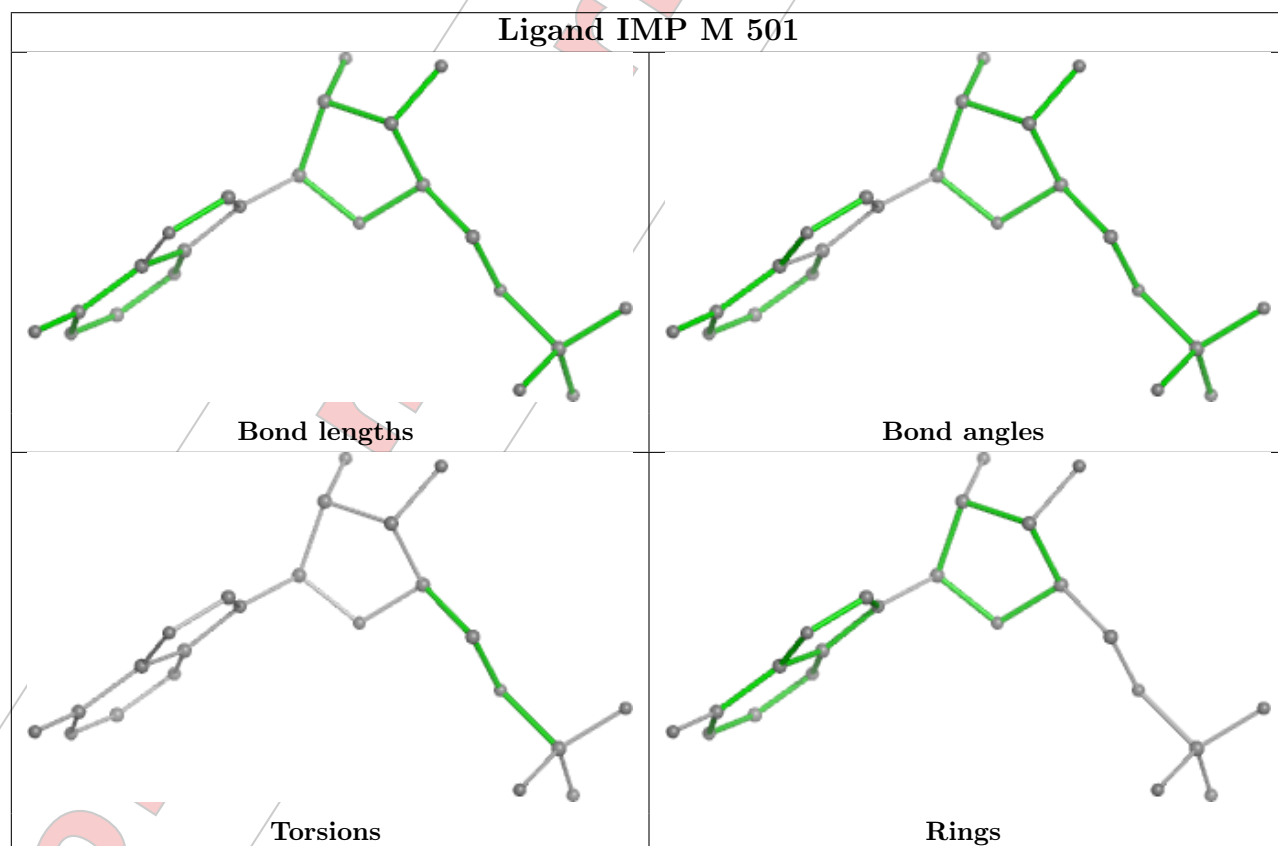
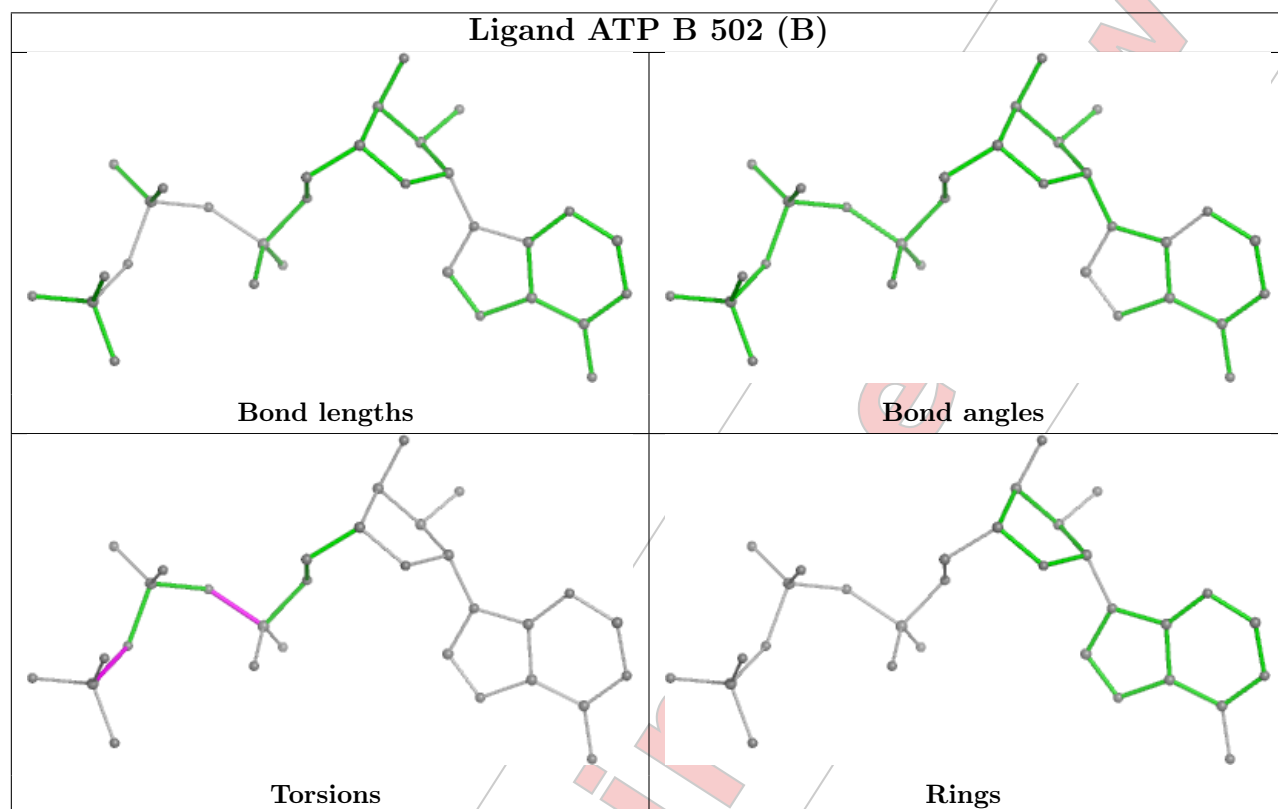


Ligand ATP G 502 (A)



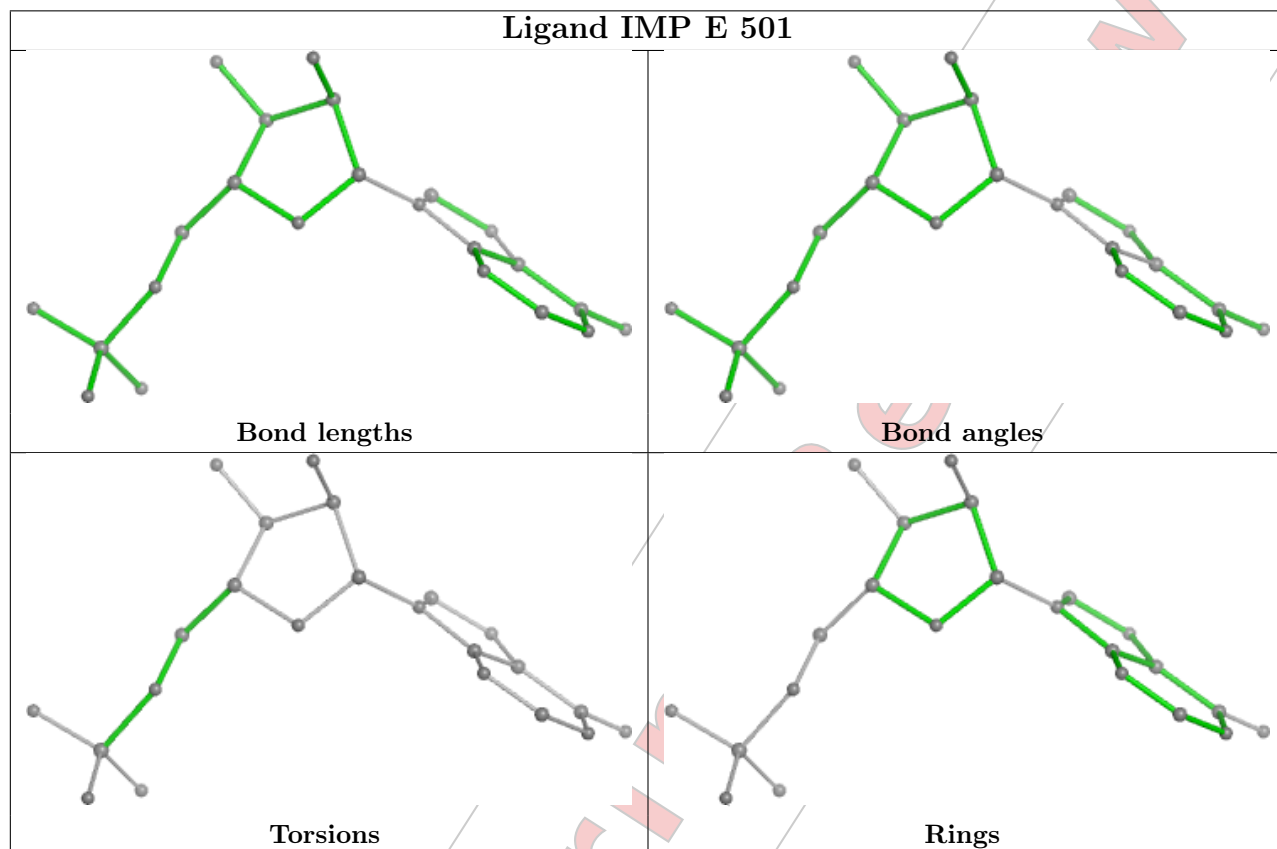
Ligand ATP D 502 (B)



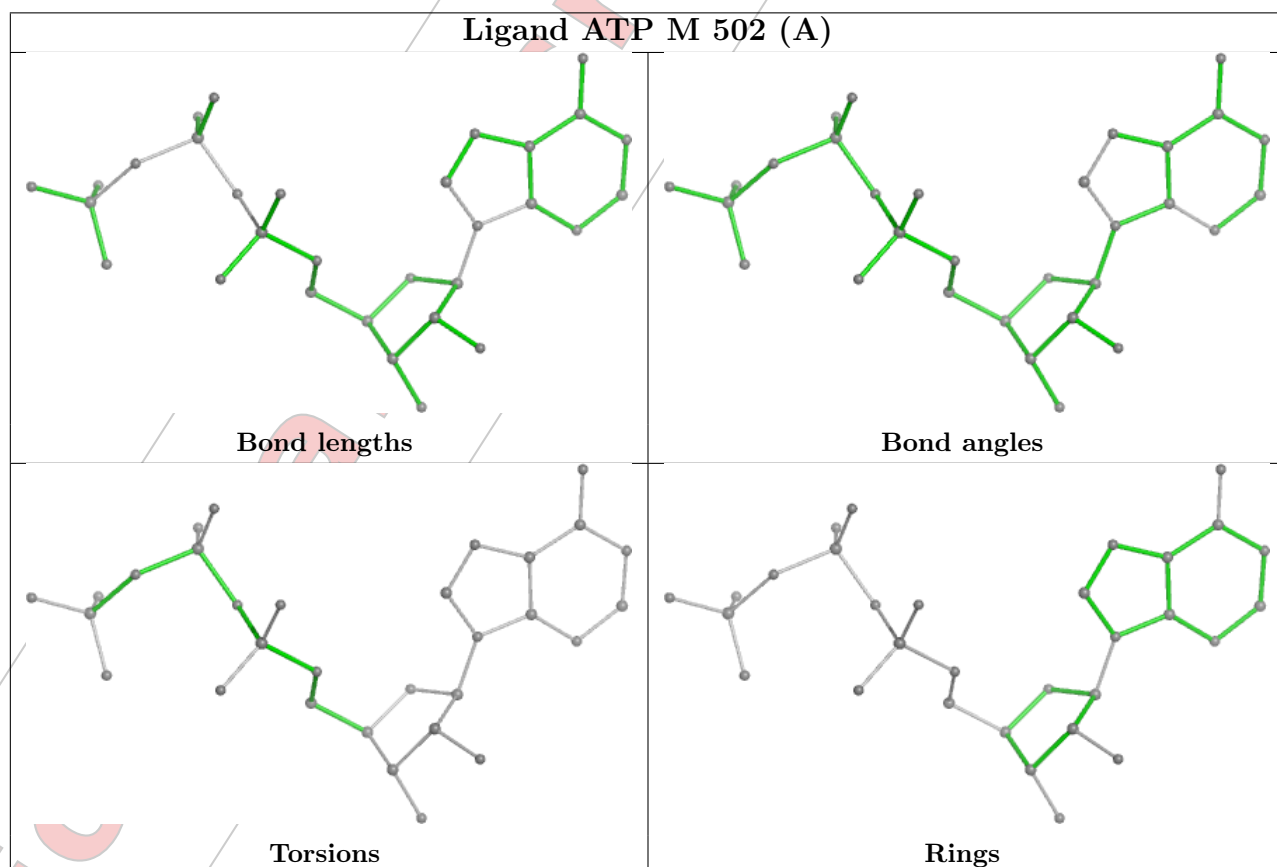


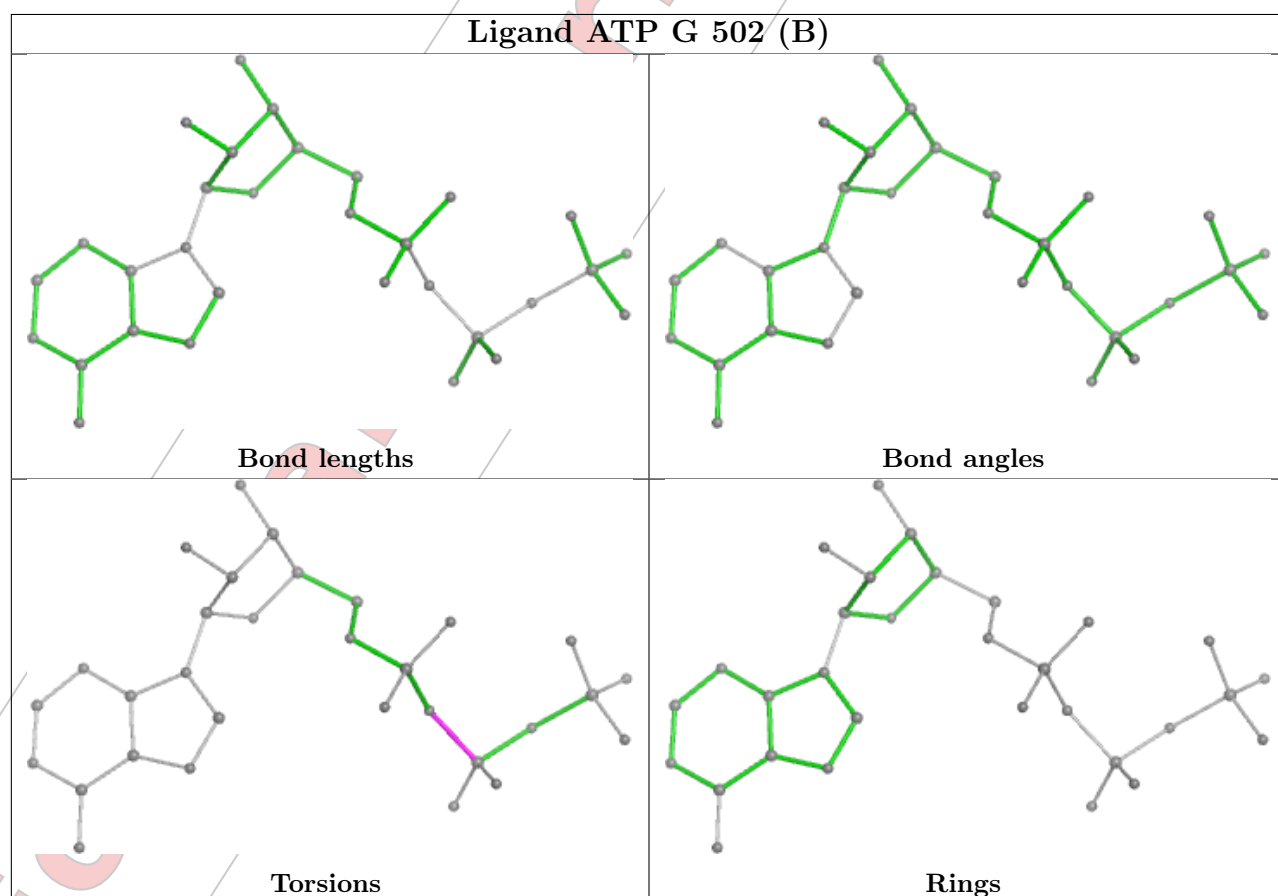
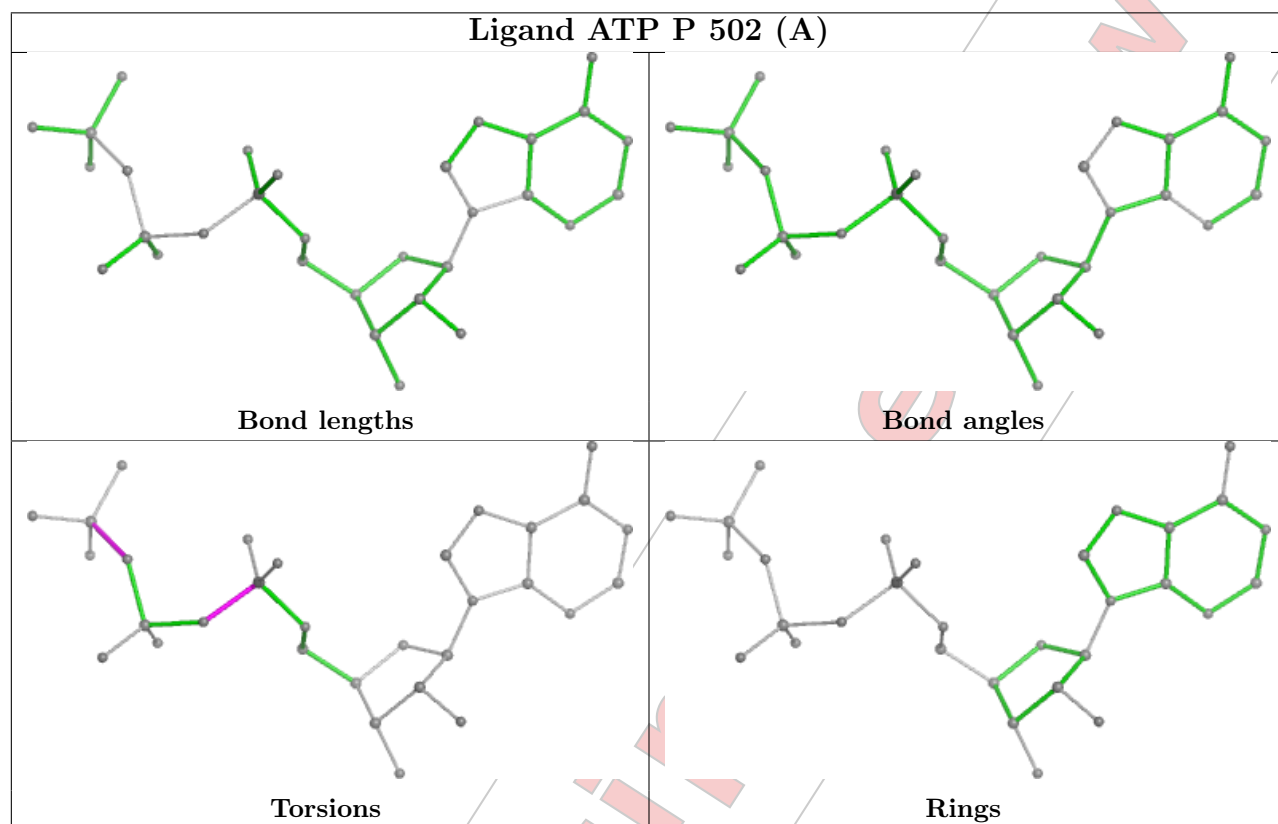


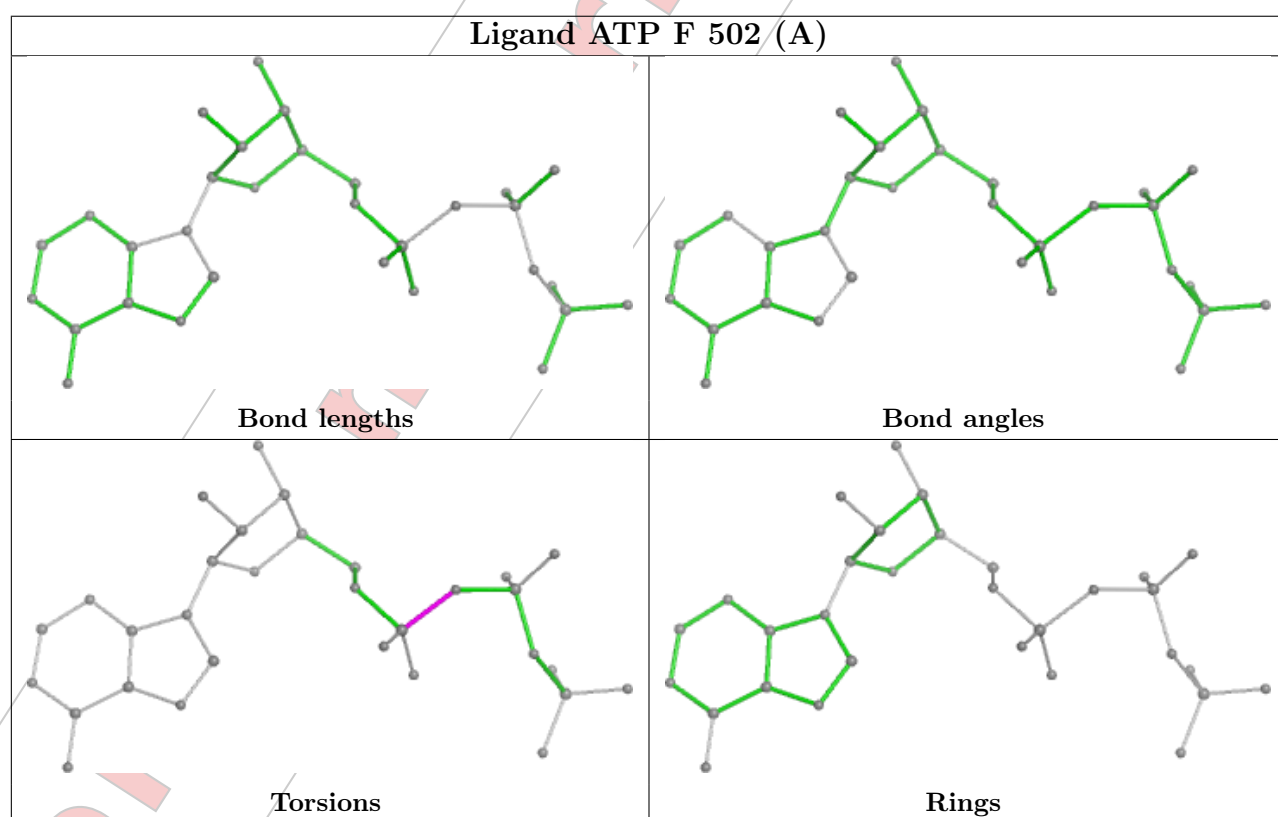
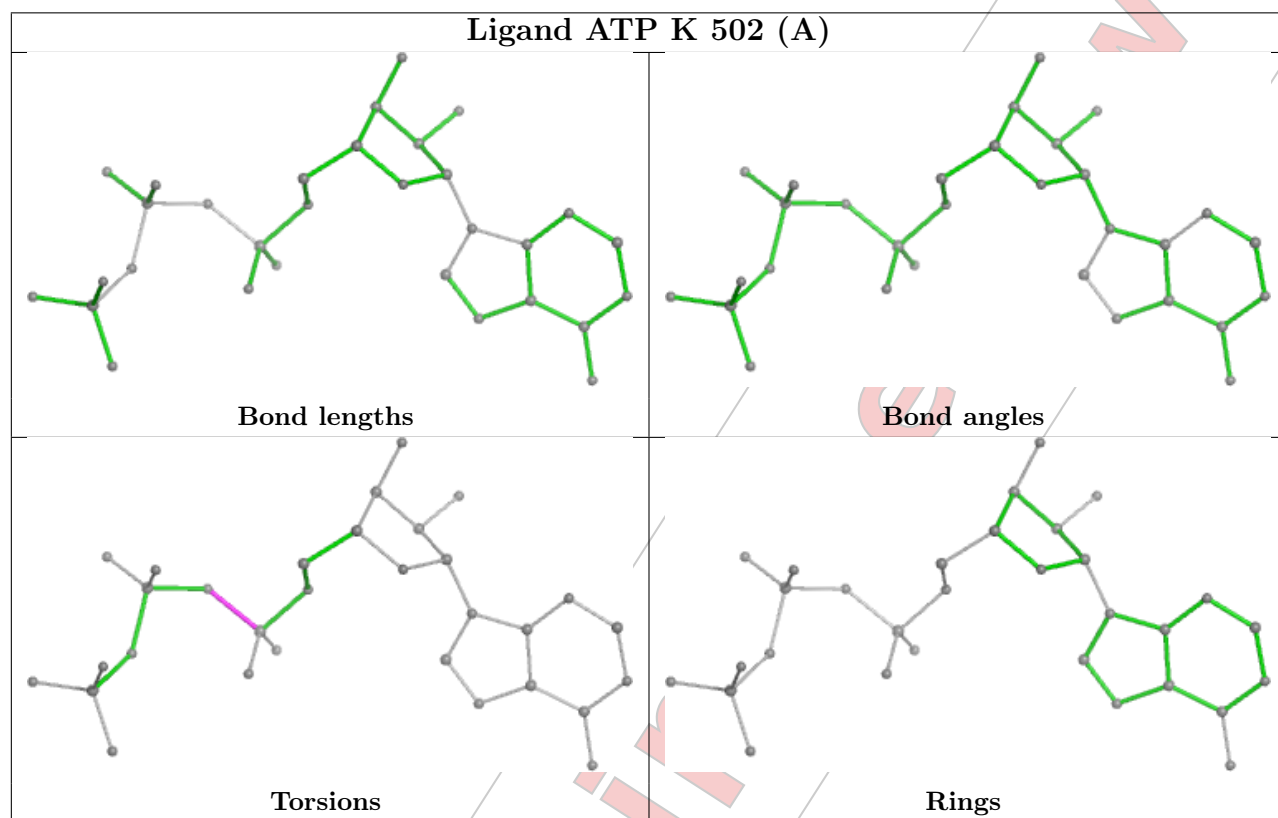
## Ligand IMP E 501

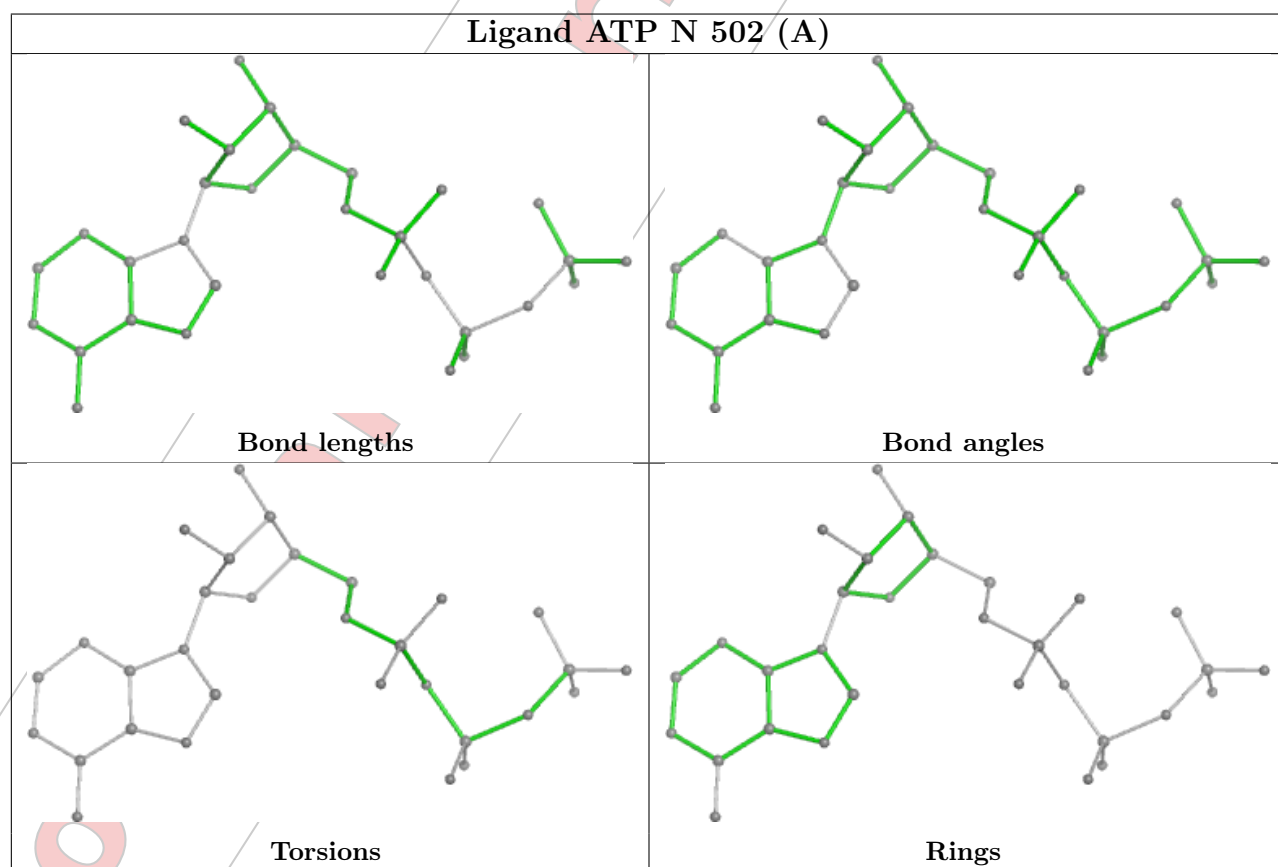
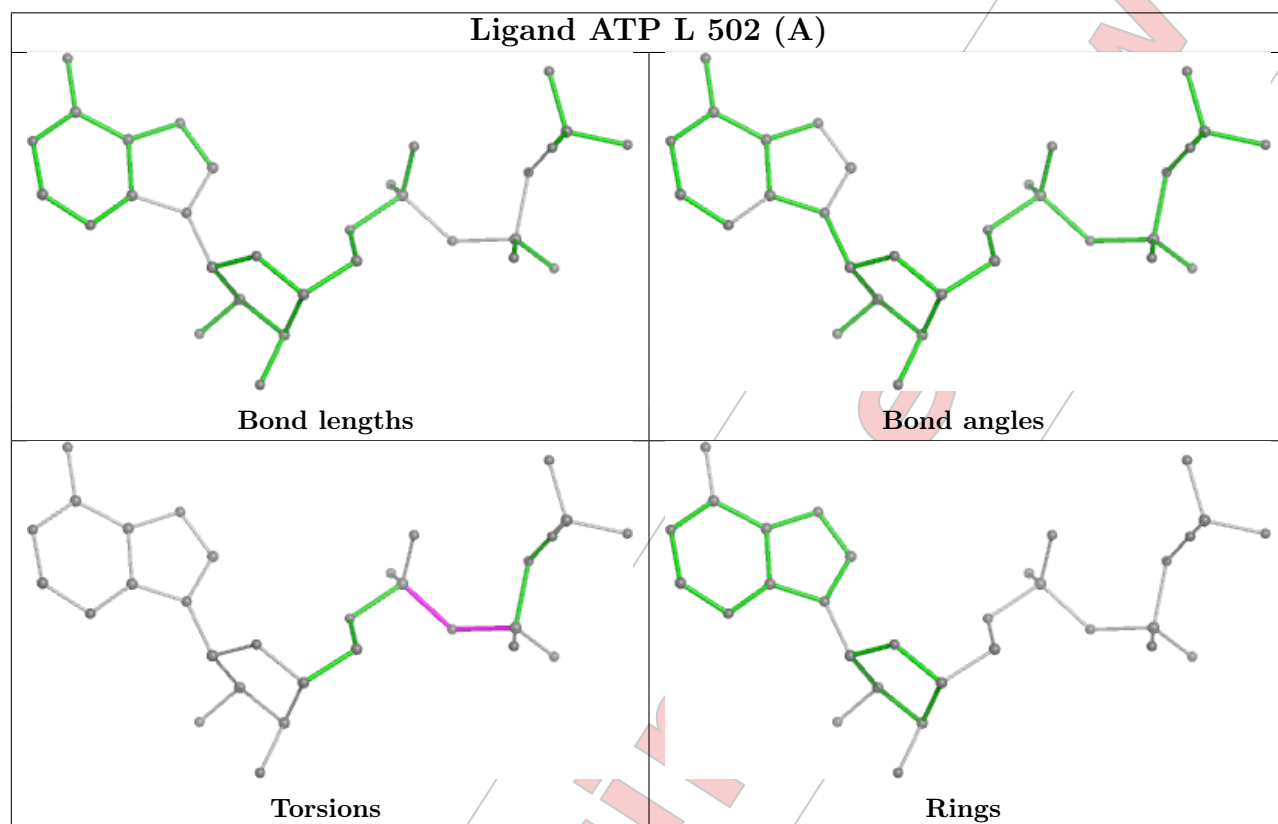


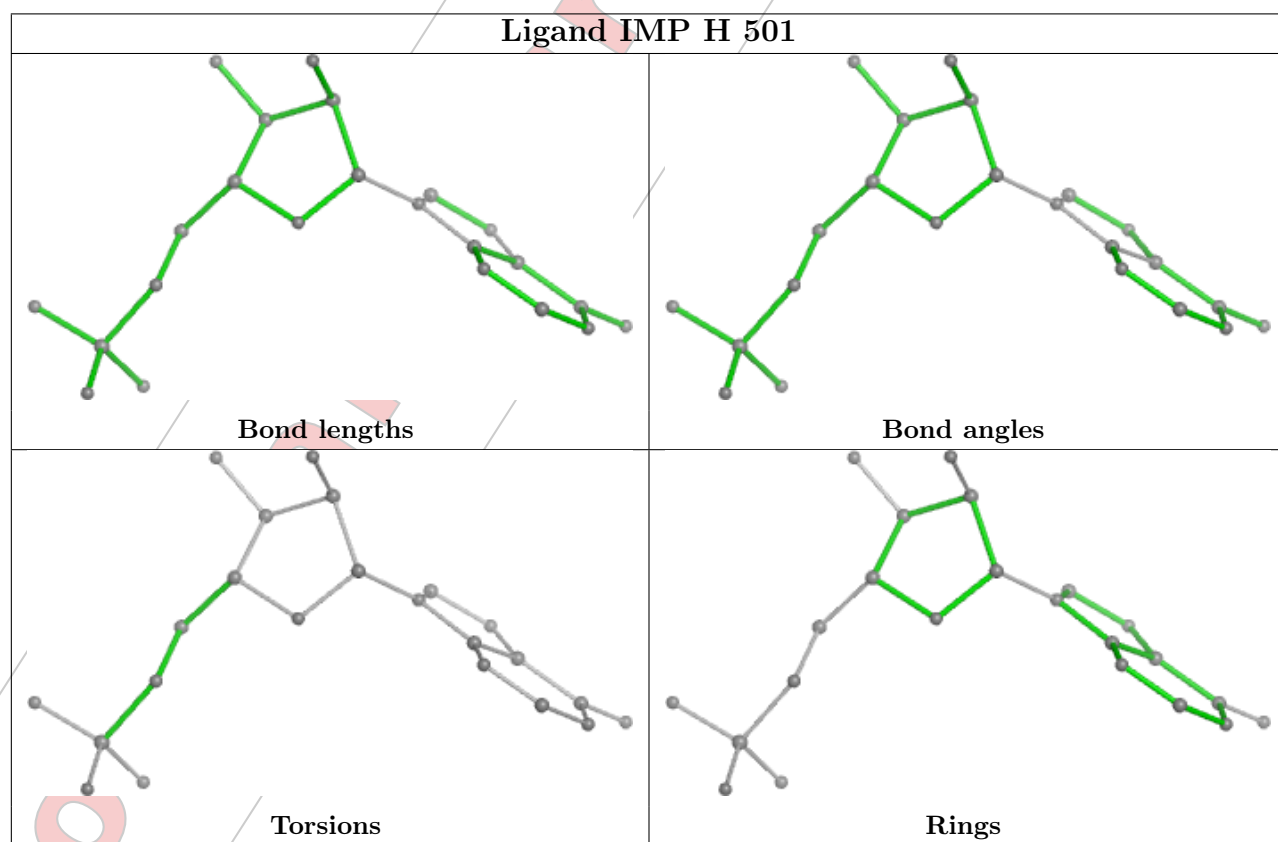
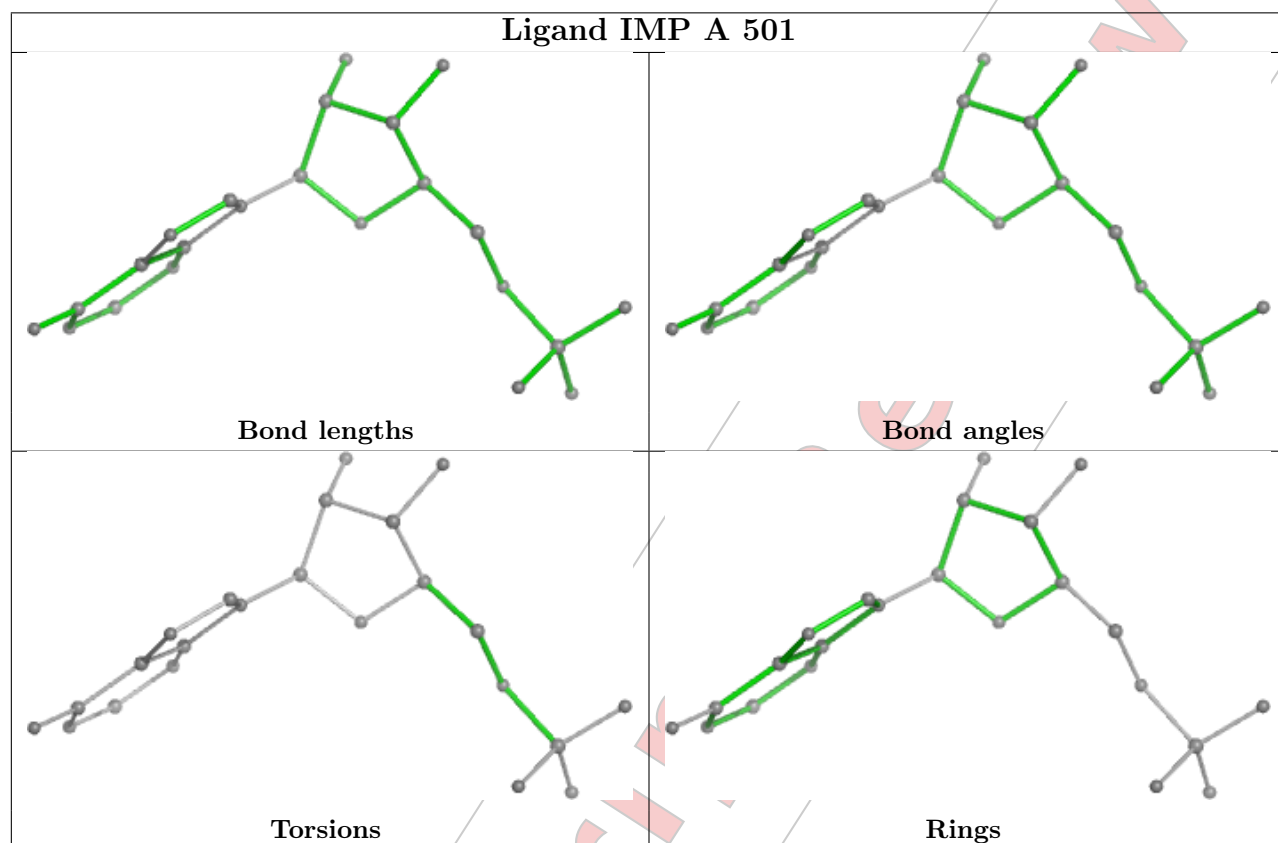
## Ligand ATP M 502 (A)

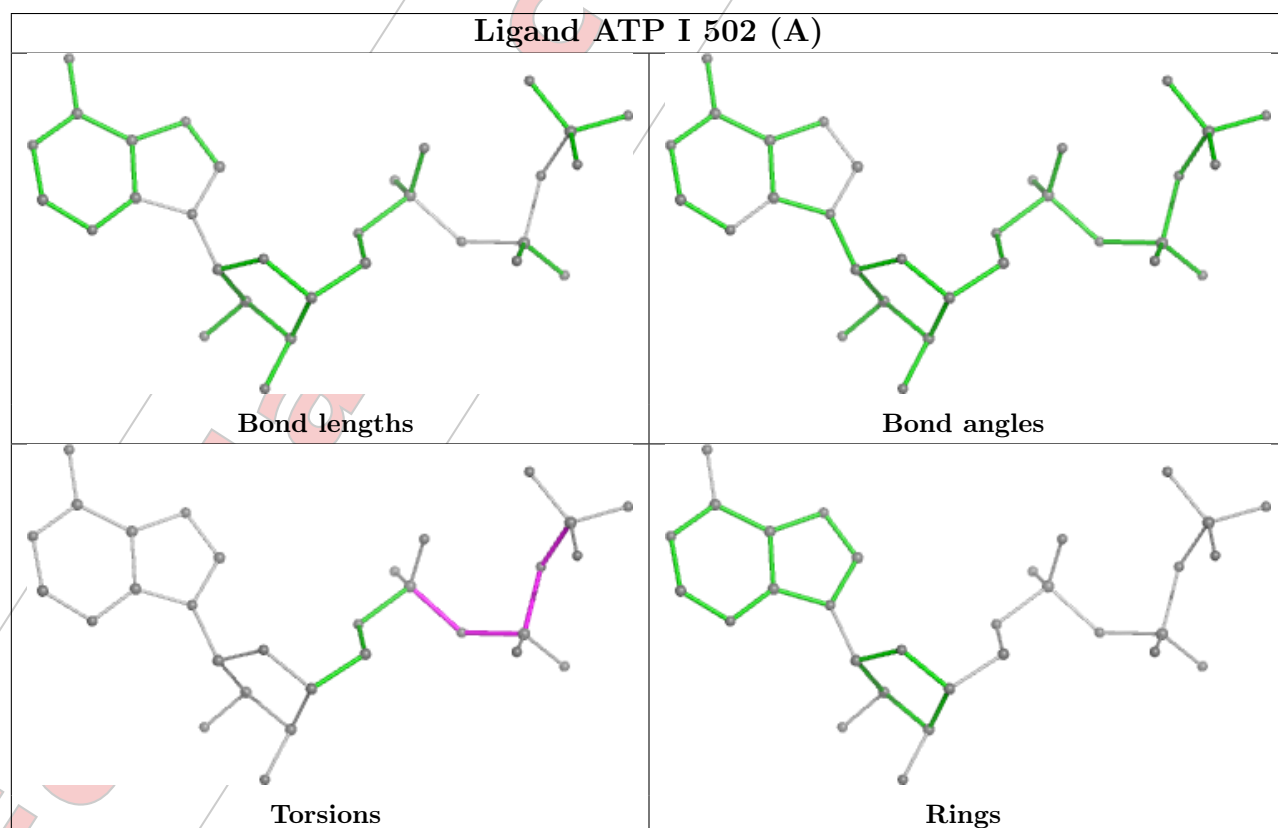
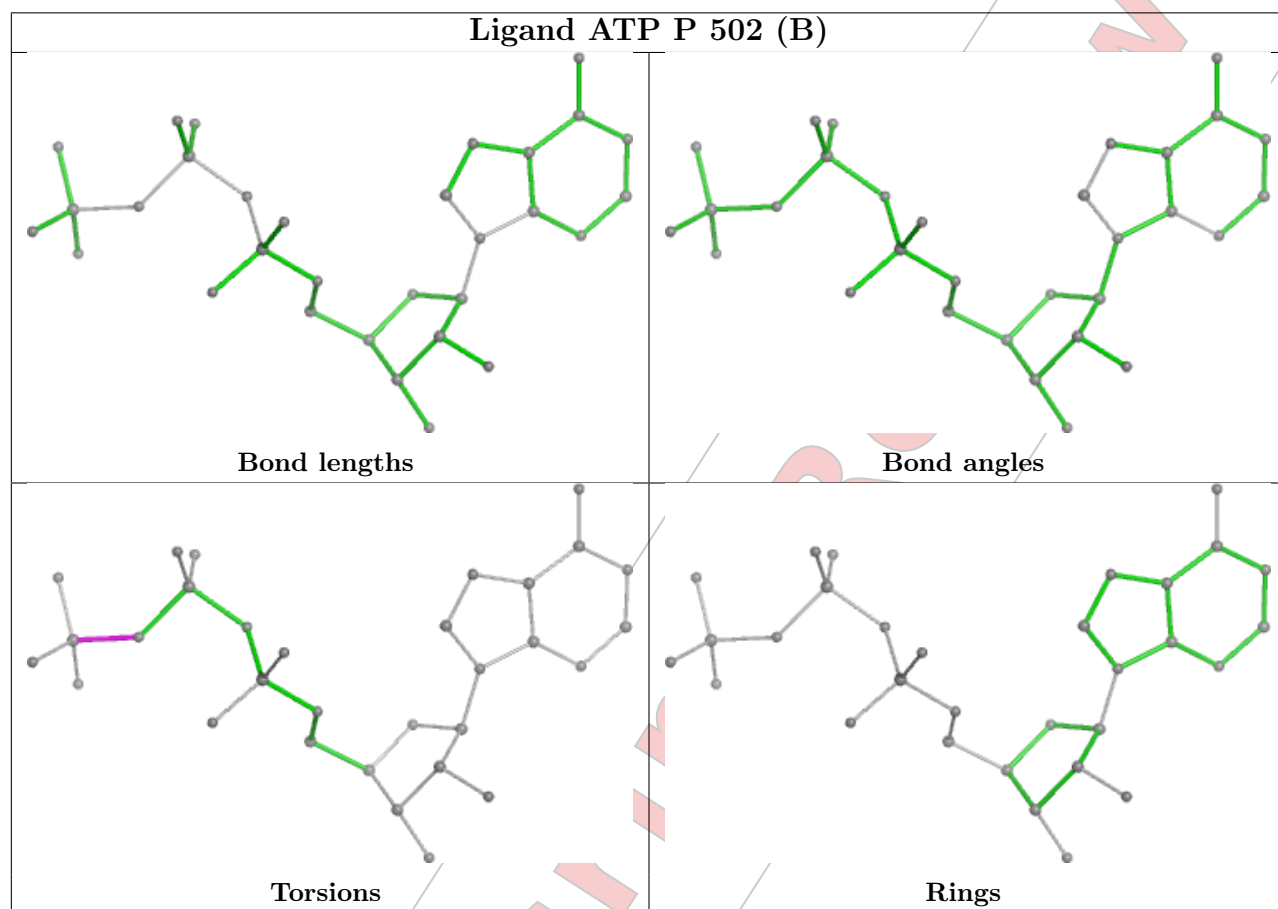


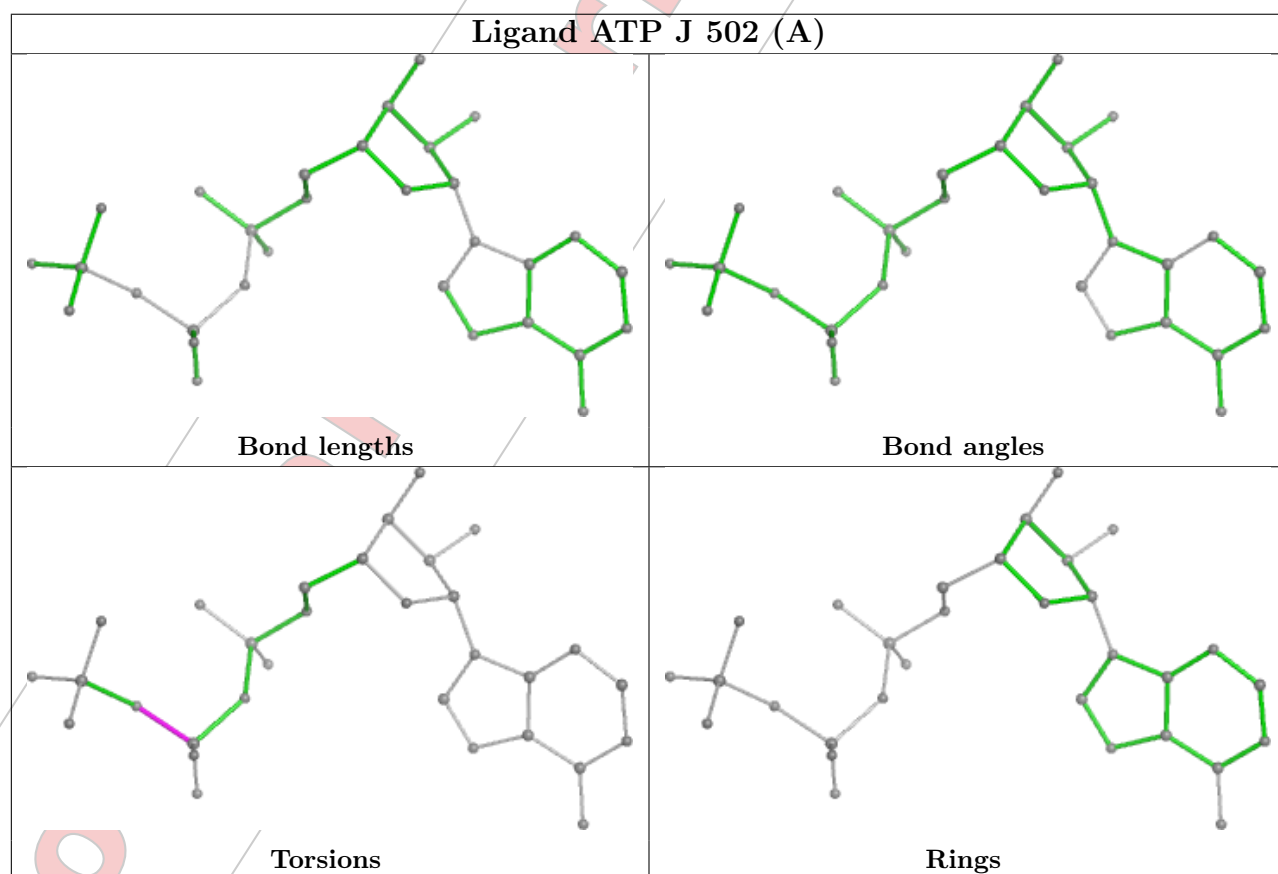
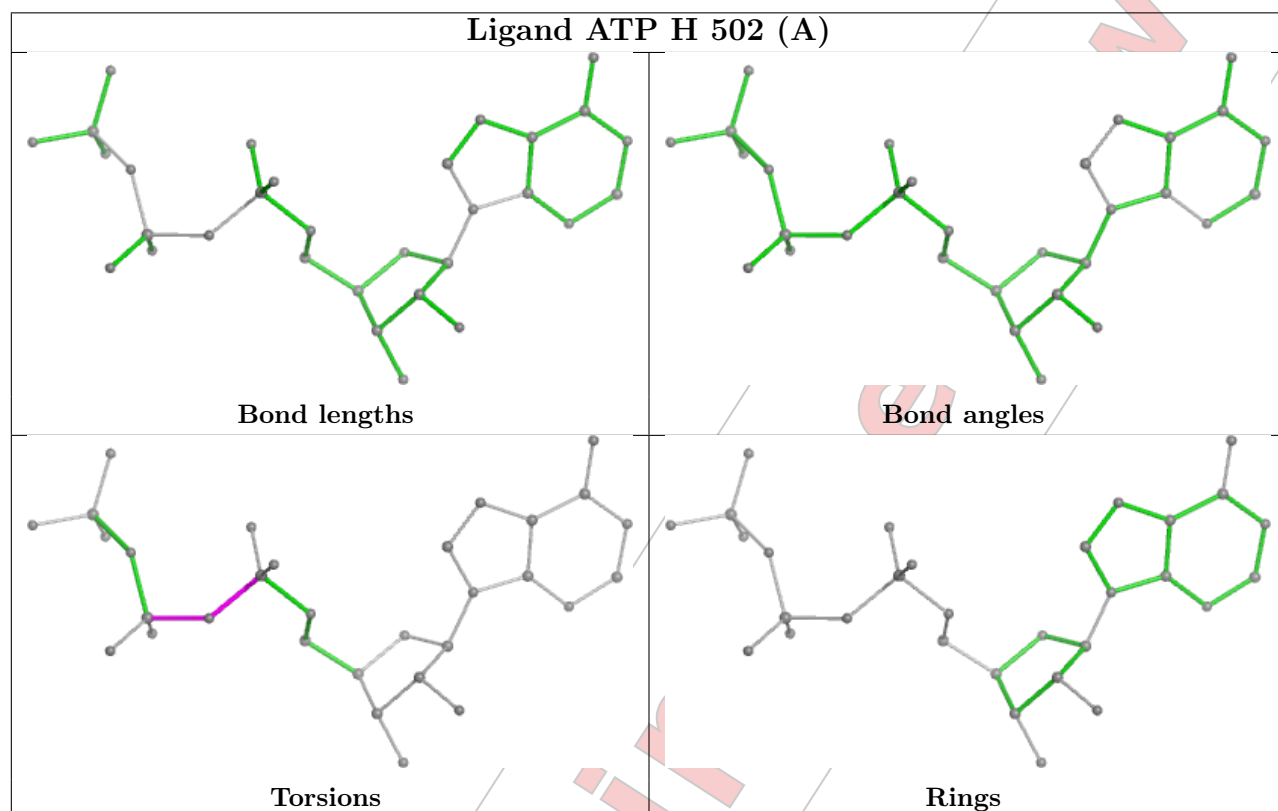














## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

For Manuscript Review

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	461/496 (92%)	0.25	18 (3%)	44	44	13, 28, 45, 63	4 (0%)
1	B	460/496 (92%)	0.25	21 (4%)	38	38	14, 29, 50, 67	3 (0%)
1	C	461/496 (92%)	0.21	26 (5%)	31	30	13, 26, 46, 66	4 (0%)
1	D	460/496 (92%)	0.05	19 (4%)	42	42	12, 25, 43, 59	3 (0%)
1	E	460/496 (92%)	0.09	18 (3%)	44	44	13, 25, 45, 62	4 (0%)
1	F	461/496 (92%)	0.13	21 (4%)	38	38	12, 25, 45, 64	3 (0%)
1	G	461/496 (92%)	0.08	22 (4%)	36	36	12, 25, 44, 63	3 (0%)
1	H	461/496 (92%)	0.07	16 (3%)	47	48	13, 25, 43, 64	3 (0%)
1	I	461/496 (92%)	0.72	43 (9%)	16	14	17, 36, 57, 74	3 (0%)
1	J	461/496 (92%)	0.20	28 (6%)	28	28	14, 27, 49, 66	3 (0%)
1	K	460/496 (92%)	0.31	24 (5%)	34	33	14, 28, 49, 66	3 (0%)
1	L	461/496 (92%)	0.62	35 (7%)	21	20	16, 33, 53, 67	3 (0%)
1	M	461/496 (92%)	0.79	31 (6%)	25	24	18, 38, 56, 73	3 (0%)
1	N	460/496 (92%)	0.58	26 (5%)	30	30	17, 34, 52, 71	3 (0%)
1	O	461/496 (92%)	0.74	30 (6%)	26	25	17, 36, 54, 72	3 (0%)
1	P	460/496 (92%)	0.78	34 (7%)	22	21	20, 38, 56, 73	3 (0%)
All	All	7370/7936 (92%)	0.37	412 (5%)	31	30	12, 30, 51, 74	51 (0%)

All (412) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ALA	6.2
1	H	29	ALA	5.4
1	N	425	ALA	5.2
1	L	424	PRO	5.1
1	J	467	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	128	PHE	4.7
1	A	425	ALA	4.7
1	E	29	ALA	4.6
1	E	425	ALA	4.6
1	J	425	ALA	4.6
1	D	29	ALA	4.5
1	G	425	ALA	4.5
1	M	467	ALA	4.5
1	H	467	ALA	4.4
1	P	29	ALA	4.4
1	K	424	PRO	4.4
1	B	424	PRO	4.3
1	P	425	ALA	4.3
1	A	467	ALA	4.3
1	C	29	ALA	4.3
1	N	466	ALA	4.3
1	G	376	ARG	4.3
1	I	128	PHE	4.3
1	B	425	ALA	4.3
1	B	467	ALA	4.3
1	C	467	ALA	4.3
1	L	394	ALA	4.3
1	L	374	PHE	4.2
1	I	467	ALA	4.2
1	O	467	ALA	4.2
1	M	466	ALA	4.1
1	C	424	PRO	4.1
1	O	425	ALA	4.1
1	K	466	ALA	4.0
1	K	467	ALA	4.0
1	N	29	ALA	4.0
1	G	29	ALA	4.0
1	D	424	PRO	4.0
1	F	424	PRO	4.0
1	I	425	ALA	4.0
1	M	424	PRO	3.9
1	L	467	ALA	3.9
1	F	29	ALA	3.9
1	F	466	ALA	3.9
1	K	425	ALA	3.9
1	G	424	PRO	3.8
1	E	424	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	467	ALA	3.8
1	F	425	ALA	3.8
1	P	128	PHE	3.7
1	D	467	ALA	3.7
1	O	300	GLY	3.7
1	E	467	ALA	3.6
1	C	403	PHE	3.6
1	C	425	ALA	3.6
1	J	376	ARG	3.6
1	C	410	LEU	3.6
1	C	401	SER	3.6
1	L	2	VAL	3.5
1	L	425	ALA	3.5
1	O	424	PRO	3.5
1	G	378	ASP	3.5
1	M	403	PHE	3.5
1	N	467	ALA	3.5
1	O	394	ALA	3.5
1	M	29	ALA	3.5
1	O	128	PHE	3.5
1	C	466	ALA	3.4
1	F	467	ALA	3.4
1	M	425	ALA	3.4
1	H	424	PRO	3.4
1	I	424	PRO	3.4
1	E	426	ARG	3.4
1	O	410	LEU	3.4
1	N	401	SER	3.4
1	G	377	ASP	3.4
1	N	424	PRO	3.4
1	I	394	ALA	3.4
1	G	401	SER	3.3
1	M	376	ARG	3.3
1	C	1	MET	3.3
1	I	186	ALA	3.3
1	I	403	PHE	3.3
1	H	466	ALA	3.3
1	M	394	ALA	3.3
1	P	142	ALA	3.3
1	D	426	ARG	3.2
1	F	128	PHE	3.2
1	M	411	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.2
1	I	302	MET	3.2
1	B	394	ALA	3.2
1	I	29	ALA	3.2
1	P	394	ALA	3.2
1	P	467	ALA	3.2
1	G	302	MET	3.2
1	D	410	LEU	3.2
1	P	402	SER	3.2
1	D	466	ALA	3.2
1	I	466	ALA	3.2
1	J	394	ALA	3.2
1	J	2	VAL	3.2
1	P	144	VAL	3.2
1	B	29	ALA	3.2
1	F	374	PHE	3.2
1	O	29	ALA	3.2
1	J	424	PRO	3.2
1	G	416	SER	3.1
1	K	377	ASP	3.1
1	P	378	ASP	3.1
1	N	411	PHE	3.1
1	P	403	PHE	3.1
1	A	417	THR	3.1
1	A	376	ARG	3.1
1	N	404	ASP	3.1
1	P	376	ARG	3.1
1	I	410	LEU	3.1
1	N	410	LEU	3.1
1	J	378	ASP	3.1
1	B	144	VAL	3.1
1	I	426	ARG	3.1
1	M	426	ARG	3.1
1	M	402	SER	3.1
1	E	466	ALA	3.0
1	B	403	PHE	3.0
1	L	376	ARG	3.0
1	P	401	SER	3.0
1	M	329	LEU	3.0
1	H	1	MET	3.0
1	O	374	PHE	3.0
1	J	29	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	424	PRO	3.0
1	P	424	PRO	2.9
1	P	374	PHE	2.9
1	B	376	ARG	2.9
1	C	376	ARG	2.9
1	G	394	ALA	2.9
1	K	394	ALA	2.9
1	L	411	PHE	2.9
1	C	408	LYS	2.9
1	C	378	ASP	2.9
1	P	155	LEU	2.8
1	I	201	ILE	2.8
1	K	2	VAL	2.8
1	B	466	ALA	2.8
1	I	416	SER	2.8
1	P	416	SER	2.8
1	I	155	LEU	2.8
1	D	302	MET	2.8
1	P	302	MET	2.8
1	E	401	SER	2.8
1	J	466	ALA	2.8
1	O	466	ALA	2.8
1	C	128	PHE	2.8
1	J	411	PHE	2.8
1	N	426	ARG	2.8
1	D	2	VAL	2.8
1	I	187	PRO	2.8
1	D	394	ALA	2.8
1	A	378	ASP	2.7
1	M	378	ASP	2.7
1	K	410	LEU	2.7
1	O	271	LEU	2.7
1	D	401	SER	2.7
1	I	153	ILE	2.7
1	L	29	ALA	2.7
1	E	302	MET	2.7
1	O	378	ASP	2.7
1	K	413	GLU	2.7
1	I	271	LEU	2.7
1	K	376	ARG	2.7
1	O	376	ARG	2.7
1	O	1	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	128	PHE	2.7
1	D	402	SER	2.7
1	K	302	MET	2.7
1	I	417	THR	2.7
1	I	378	ASP	2.7
1	B	143	GLY	2.7
1	C	405	ARG	2.7
1	L	1	MET	2.7
1	E	404	ASP	2.6
1	G	404	ASP	2.6
1	N	377	ASP	2.6
1	I	185	THR	2.6
1	P	466	ALA	2.6
1	J	379	ARG	2.6
1	J	416	SER	2.6
1	N	416	SER	2.6
1	C	302	MET	2.6
1	M	408	LYS	2.6
1	O	377	ASP	2.6
1	M	374	PHE	2.6
1	N	403	PHE	2.6
1	E	402	SER	2.6
1	I	142	ALA	2.6
1	G	1	MET	2.6
1	E	2	VAL	2.6
1	P	27	ASP	2.6
1	L	409	GLY	2.6
1	G	403	PHE	2.5
1	K	416	SER	2.6
1	L	466	ALA	2.5
1	B	378	ASP	2.5
1	N	376	ARG	2.5
1	M	409	GLY	2.5
1	A	29	ALA	2.5
1	F	114	ALA	2.5
1	H	374	PHE	2.5
1	I	411	PHE	2.5
1	L	403	PHE	2.5
1	M	373	LEU	2.5
1	N	128	PHE	2.5
1	P	411	PHE	2.5
1	B	404	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	376	ARG	2.5
1	A	402	SER	2.5
1	N	402	SER	2.5
1	A	466	ALA	2.5
1	H	376	ARG	2.5
1	J	426	ARG	2.5
1	N	394	ALA	2.5
1	P	114	ALA	2.5
1	E	378	ASP	2.5
1	E	128	PHE	2.5
1	K	374	PHE	2.5
1	P	271	LEU	2.5
1	H	401	SER	2.5
1	D	409	GLY	2.5
1	I	189	GLY	2.5
1	I	300	GLY	2.5
1	H	425	ALA	2.5
1	L	116	LEU	2.4
1	P	408	LYS	2.4
1	H	128	PHE	2.4
1	I	374	PHE	2.4
1	J	374	PHE	2.4
1	K	403	PHE	2.4
1	F	402	SER	2.4
1	I	133	ILE	2.4
1	K	153	ILE	2.4
1	F	143	GLY	2.4
1	I	81	THR	2.4
1	I	376	ARG	2.4
1	O	56	VAL	2.4
1	E	394	ALA	2.4
1	F	394	ALA	2.4
1	J	1	MET	2.4
1	J	142	ALA	2.4
1	L	410	LEU	2.4
1	B	156	SER	2.4
1	K	401	SER	2.4
1	E	374	PHE	2.4
1	G	374	PHE	2.4
1	K	128	PHE	2.4
1	M	128	PHE	2.4
1	C	414	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	408	LYS	2.4
1	N	2	VAL	2.4
1	C	394	ALA	2.4
1	O	114	ALA	2.4
1	O	301	ALA	2.4
1	B	401	SER	2.4
1	I	413	GLU	2.4
1	H	377	ASP	2.4
1	L	128	PHE	2.4
1	L	133	ILE	2.4
1	K	408	LYS	2.4
1	B	114	ALA	2.4
1	F	155	LEU	2.4
1	J	377	ASP	2.4
1	L	377	ASP	2.4
1	M	410	LEU	2.4
1	F	302	MET	2.3
1	L	187	PRO	2.3
1	O	299	PRO	2.3
1	P	187	PRO	2.3
1	I	301	ALA	2.3
1	K	114	ALA	2.3
1	C	404	ASP	2.3
1	I	144	VAL	2.3
1	L	417	THR	2.3
1	F	413	GLU	2.3
1	H	402	SER	2.3
1	M	401	SER	2.3
1	I	1	MET	2.3
1	O	302	MET	2.3
1	I	2	VAL	2.3
1	L	163	VAL	2.3
1	A	426	ARG	2.3
1	I	116	LEU	2.3
1	B	402	SER	2.3
1	F	403	PHE	2.3
1	N	374	PHE	2.3
1	K	404	ASP	2.3
1	N	408	LYS	2.3
1	H	394	ALA	2.3
1	P	212	ALA	2.3
1	B	405	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	426	ARG	2.3
1	L	3	ARG	2.3
1	L	414	GLY	2.3
1	N	414	GLY	2.3
1	J	413	GLU	2.3
1	L	115	LEU	2.3
1	M	115	LEU	2.3
1	A	377	ASP	2.2
1	G	27	ASP	2.2
1	N	157	ASP	2.2
1	C	411	PHE	2.2
1	I	147	PHE	2.2
1	O	32	PHE	2.2
1	E	413	GLU	2.2
1	L	117	HIS	2.2
1	O	144	VAL	2.2
1	M	422	LEU	2.2
1	P	116	LEU	2.2
1	H	426	ARG	2.2
1	A	328	GLN	2.2
1	K	133	ILE	2.2
1	M	117	HIS	2.2
1	L	32	PHE	2.2
1	A	139	ALA	2.2
1	G	466	ALA	2.2
1	H	417	THR	2.2
1	O	402	SER	2.2
1	O	417	THR	2.2
1	I	150	VAL	2.2
1	M	155	LEU	2.2
1	M	173	LEU	2.2
1	P	179	ILE	2.2
1	A	403	PHE	2.2
1	D	403	PHE	2.2
1	G	411	PHE	2.2
1	L	416	SER	2.2
1	F	426	ARG	2.2
1	J	405	ARG	2.2
1	B	423	ASP	2.2
1	C	412	GLU	2.2
1	F	2	VAL	2.2
1	O	2	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	2	VAL	2.2
1	G	410	LEU	2.2
1	L	173	LEU	2.2
1	J	143	GLY	2.2
1	O	130	GLY	2.2
1	I	192	ALA	2.1
1	M	142	ALA	2.1
1	M	418	SER	2.1
1	D	412	GLU	2.1
1	D	113	ASN	2.1
1	G	128	PHE	2.1
1	P	380	PRO	2.1
1	J	409	GLY	2.1
1	M	163	VAL	2.1
1	P	410	LEU	2.1
1	N	302	MET	2.1
1	P	3	ARG	2.1
1	J	401	SER	2.1
1	L	408	LYS	2.1
1	D	413	GLU	2.1
1	M	377	ASP	2.1
1	F	113	ASN	2.1
1	K	29	ALA	2.1
1	L	406	ALA	2.1
1	N	415	ILE	2.1
1	D	411	PHE	2.1
1	J	147	PHE	2.1
1	J	403	PHE	2.1
1	O	403	PHE	2.1
1	F	1	MET	2.1
1	L	302	MET	2.1
1	P	129	GLU	2.1
1	I	173	LEU	2.1
1	J	155	LEU	2.1
1	K	28	VAL	2.1
1	D	378	ASP	2.1
1	F	377	ASP	2.1
1	J	417	THR	2.1
1	L	153	ILE	2.1
1	O	133	ILE	2.1
1	C	215	ARG	2.1
1	C	426	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	379	ARG	2.1
1	C	374	PHE	2.1
1	G	32	PHE	2.1
1	A	413	GLU	2.1
1	C	413	GLU	2.1
1	B	375	ASP	2.1
1	I	377	ASP	2.1
1	L	155	LEU	2.1
1	P	109	VAL	2.1
1	A	394	ALA	2.0
1	K	139	ALA	2.0
1	B	302	MET	2.0
1	J	302	MET	2.0
1	M	302	MET	2.0
1	C	409	GLY	2.0
1	I	414	GLY	2.0
1	E	377	ASP	2.0
1	F	411	PHE	2.0
1	H	378	ASP	2.0
1	O	327	ARG	2.0
1	M	2	VAL	2.0
1	N	144	VAL	2.0
1	I	212	ALA	2.0
1	L	412	GLU	2.0
1	B	377	ASP	2.0
1	C	143	GLY	2.0
1	I	401	SER	2.0
1	P	377	ASP	2.0
1	N	113	ASN	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	M	502[A]	31/31	0.85	0.12	39,41,49,50	31
3	ATP	M	502[B]	31/31	0.85	0.12	38,41,49,51	31
3	ATP	O	502[A]	31/31	0.87	0.11	31,33,46,48	31
3	ATP	O	502[B]	31/31	0.87	0.11	31,34,46,47	31
3	ATP	N	502[A]	31/31	0.88	0.11	32,34,43,47	31
3	ATP	N	502[B]	31/31	0.88	0.11	32,34,42,44	31
3	ATP	L	502[A]	31/31	0.88	0.11	34,37,46,49	31
3	ATP	L	502[B]	31/31	0.88	0.11	35,37,46,49	31
3	ATP	I	502[A]	31/31	0.89	0.11	35,40,49,50	31
3	ATP	I	502[B]	31/31	0.89	0.11	35,40,49,51	31
3	ATP	J	502[A]	31/31	0.89	0.10	28,32,39,39	31
3	ATP	J	502[B]	31/31	0.89	0.10	28,32,38,38	31
3	ATP	P	502[A]	31/31	0.89	0.12	36,39,48,50	31
3	ATP	P	502[B]	31/31	0.89	0.12	38,40,48,51	31
3	ATP	C	502[A]	31/31	0.92	0.09	26,28,35,36	31
3	ATP	C	502[B]	31/31	0.92	0.09	24,28,35,36	31
3	ATP	G	502[A]	31/31	0.92	0.09	21,27,38,39	31
3	ATP	G	502[B]	31/31	0.92	0.09	23,27,38,39	31
3	ATP	A	502[A]	31/31	0.92	0.09	26,29,39,41	31
3	ATP	A	502[B]	31/31	0.92	0.09	24,29,41,41	31
3	ATP	B	502[A]	31/31	0.92	0.10	26,29,38,40	31
3	ATP	B	502[B]	31/31	0.92	0.10	23,29,38,40	31
3	ATP	K	502[A]	31/31	0.92	0.09	24,29,39,39	31
3	ATP	K	502[B]	31/31	0.92	0.09	27,30,39,39	31
3	ATP	D	502[A]	31/31	0.93	0.08	20,25,36,38	31
3	ATP	D	502[B]	31/31	0.93	0.08	22,25,37,38	31
3	ATP	H	502[A]	31/31	0.93	0.09	19,28,35,37	31
3	ATP	H	502[B]	31/31	0.93	0.09	24,28,35,37	31
3	ATP	E	502[A]	31/31	0.94	0.08	17,25,32,36	31
3	ATP	E	502[B]	31/31	0.94	0.08	23,25,32,35	31
3	ATP	F	502[A]	31/31	0.94	0.09	17,26,38,39	31
3	ATP	F	502[B]	31/31	0.94	0.09	24,27,37,38	31
2	IMP	N	501	23/23	0.97	0.07	26,29,32,32	0
2	IMP	O	501	23/23	0.97	0.07	26,31,34,38	0
2	IMP	P	501	23/23	0.97	0.06	27,32,37,38	0
2	IMP	I	501	23/23	0.97	0.07	27,31,34,35	0
2	IMP	L	501	23/23	0.97	0.06	23,27,30,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IMP	M	501	23/23	0.98	0.06	29,33,38,41	0
2	IMP	C	501	23/23	0.98	0.05	19,22,27,29	0
2	IMP	F	501	23/23	0.98	0.05	17,21,23,27	0
2	IMP	G	501	23/23	0.98	0.05	19,21,24,27	0
2	IMP	H	501	23/23	0.98	0.05	19,21,24,26	0
2	IMP	A	501	23/23	0.98	0.05	18,23,27,28	0
2	IMP	J	501	23/23	0.98	0.05	21,25,30,32	0
2	IMP	K	501	23/23	0.98	0.05	21,23,26,28	0
2	IMP	B	501	23/23	0.98	0.06	20,23,28,30	0
2	IMP	E	501	23/23	0.99	0.04	18,20,22,26	0
2	IMP	D	501	23/23	0.99	0.04	20,22,26,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.