



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2025 – 07:27 pm BST

PDB ID : 9HG0 / pdb\_00009hg0  
Title : Crystal structure of M. smegmatis GMP reductase with XMP\* intermediate in complex with NADP+ and IMP.  
Authors : Dolezal, M.; Pichova, I.  
Deposited on : 2024-11-18  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

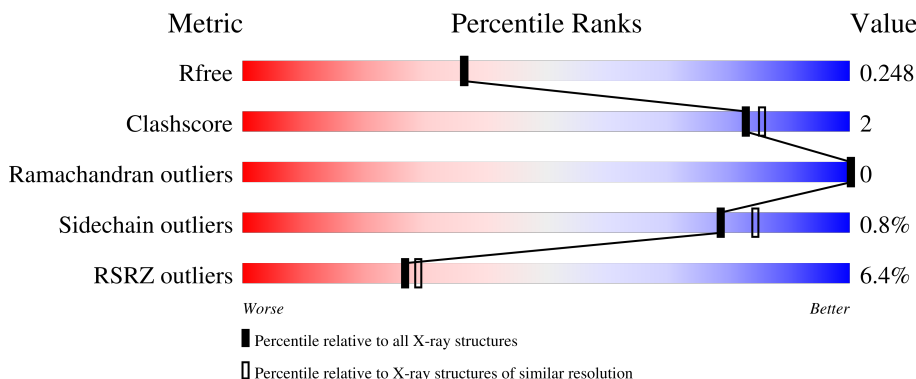
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



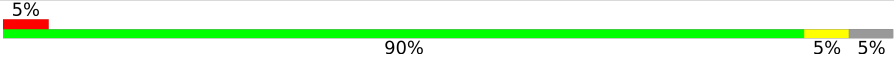
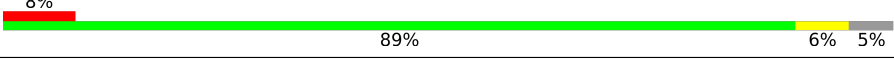

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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>5%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	496	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>•</div> <div>5%</div> </div> </div>
1	C	496	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	D	496	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	E	496	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	496	 5% 90% 5% 5%
1	G	496	 8% 89% 6% 5%
1	H	496	 8% 88% 7% 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28877 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	0	0
			3422	2132	613	663	14			
1	B	473	Total	C	N	O	S	0	0	0
			3425	2133	613	665	14			
1	C	473	Total	C	N	O	S	0	0	0
			3426	2135	614	663	14			
1	D	473	Total	C	N	O	S	0	0	0
			3423	2133	613	663	14			
1	E	473	Total	C	N	O	S	0	0	0
			3423	2133	613	663	14			
1	F	473	Total	C	N	O	S	0	0	0
			3426	2136	615	661	14			
1	G	473	Total	C	N	O	S	0	0	0
			3422	2133	614	661	14			
1	H	473	Total	C	N	O	S	0	0	0
			3417	2129	613	661	14			

There are 144 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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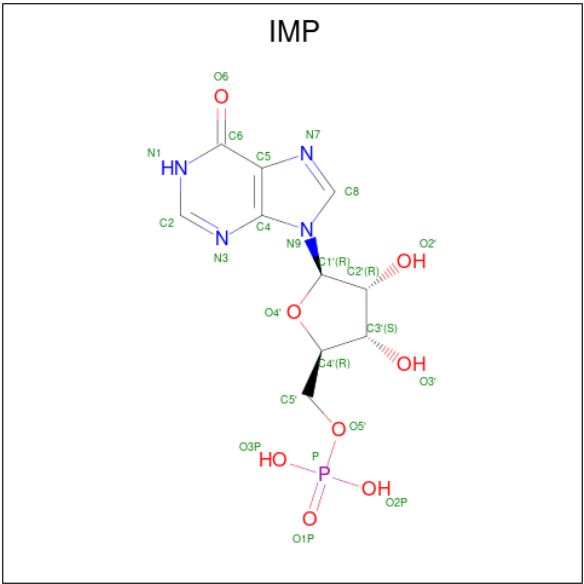
Chain	Residue	Modelled	Actual	Comment	Reference
F	486	ASP	-	expression tag	UNP A0QYE8
F	487	LEU	-	expression tag	UNP A0QYE8
F	488	GLU	-	expression tag	UNP A0QYE8
F	489	HIS	-	expression tag	UNP A0QYE8
F	490	HIS	-	expression tag	UNP A0QYE8
F	491	HIS	-	expression tag	UNP A0QYE8
F	492	HIS	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is INOSINIC ACID (CCD ID: 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	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	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	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	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

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

- # NAP
- 
- Chemical structure of Naproxen (NAP) is shown, featuring a naphthalene ring system with a carboxylic acid group and a 2-(6-methoxy-2-naphthyl)propyl side chain. The structure is labeled with atom numbers (1-14 for the naphthalene rings, 15-20 for the propyl group) and stereochemistry (wedges and dashes).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

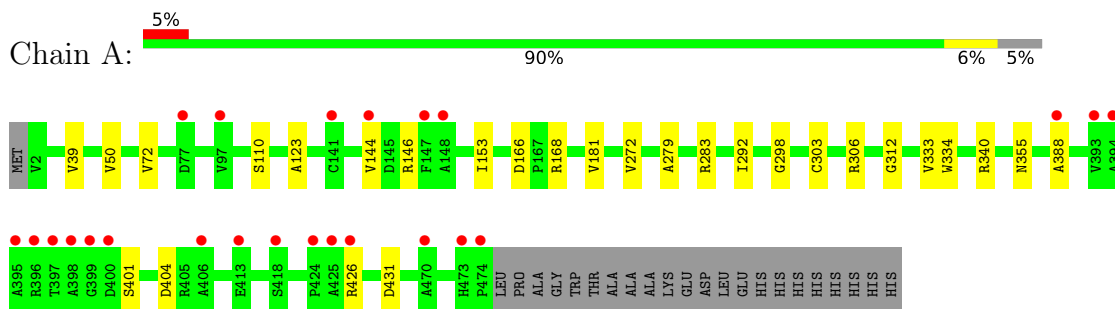
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	100	Total	O	0	0
			100	100		
4	C	117	Total	O	0	0
			117	117		
4	D	119	Total	O	0	0
			119	119		
4	E	68	Total	O	0	0
			68	68		
4	F	83	Total	O	0	0
			83	83		
4	G	72	Total	O	0	0
			72	72		
4	H	60	Total	O	0	0
			60	60		

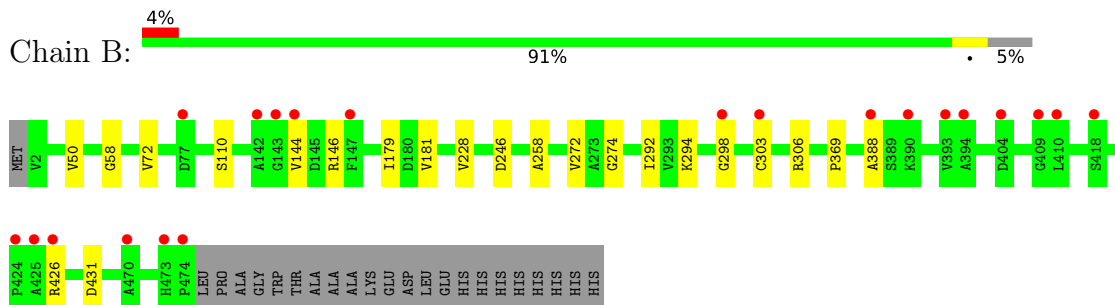
### 3 Residue-property plots [i](#)

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

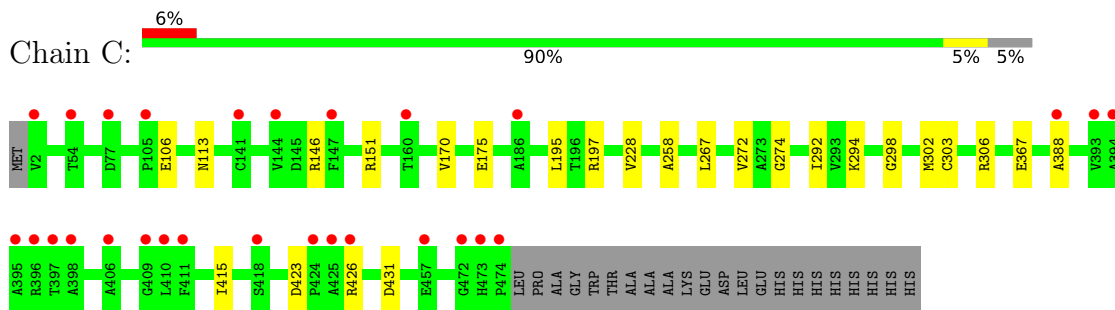
- Molecule 1: GMP reductase



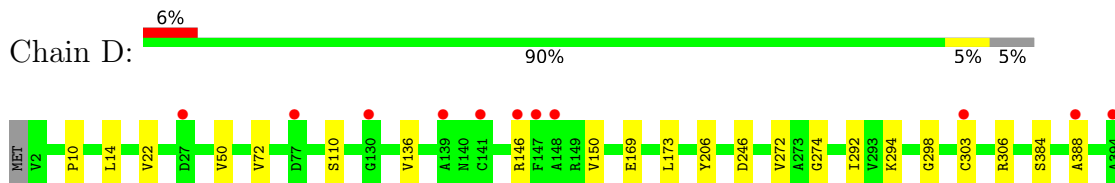
- Molecule 1: GMP reductase



- Molecule 1: GMP reductase

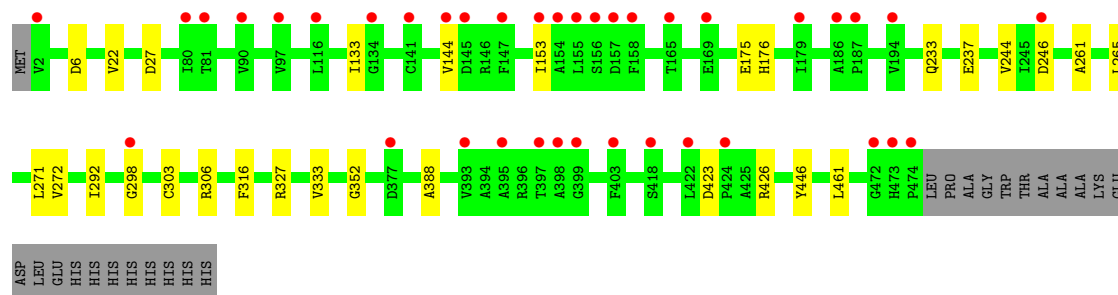
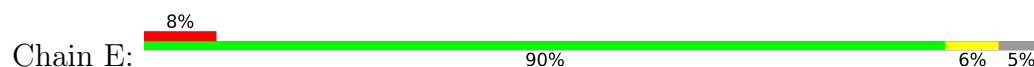


- Molecule 1: GMP reductase

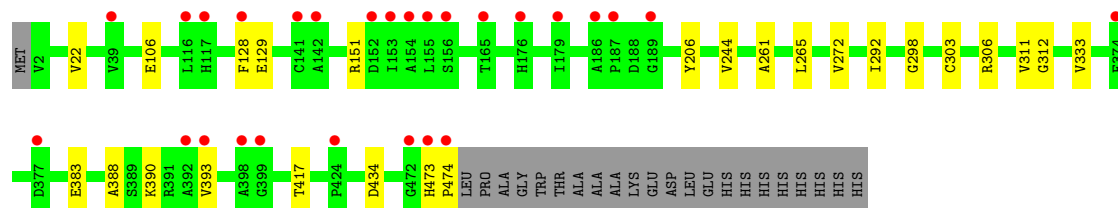




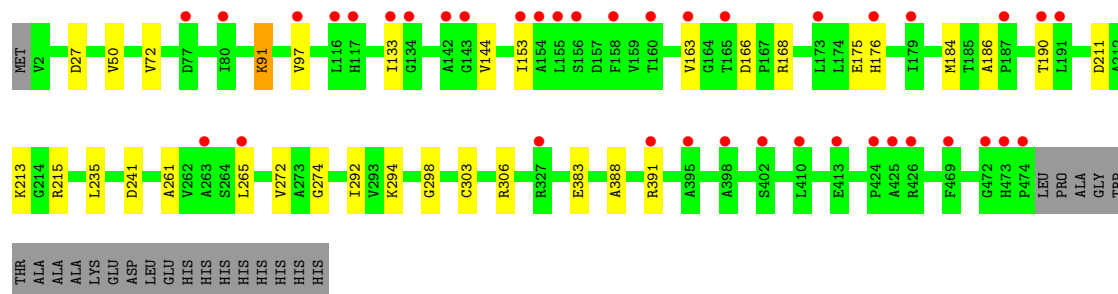
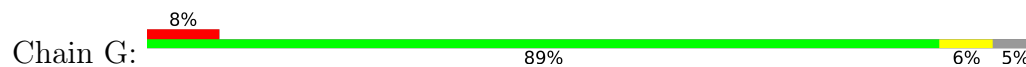
• Molecule 1: GMP reductase



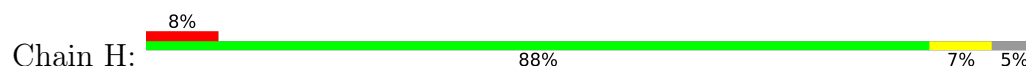
• Molecule 1: GMP reductase



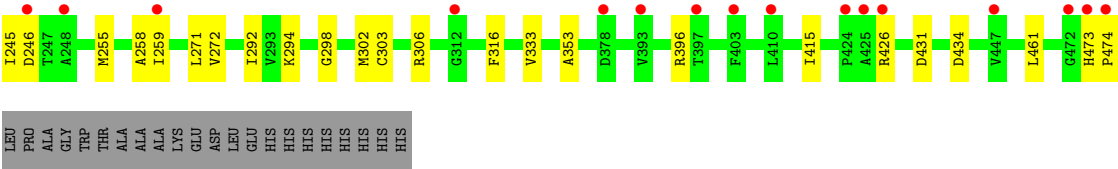
• Molecule 1: GMP reductase



• Molecule 1: GMP reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.80Å 204.91Å 116.15Å 90.00° 102.31° 90.00°	Depositor
Resolution (Å)	42.55 – 2.10 42.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.55-2.10) 99.4 (42.55-2.10)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21_5204	Depositor
R, $R_{free}$	0.218 , 0.248 0.218 , 0.248	Depositor DCC
$R_{free}$ test set	13482 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9187e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NAP, IMP

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	0.11	0/3479	0.27	0/4741
1	B	0.11	0/3482	0.28	0/4745
1	C	0.11	0/3483	0.28	0/4745
1	D	0.11	0/3480	0.27	0/4742
1	E	0.11	0/3480	0.27	0/4742
1	F	0.10	0/3483	0.27	0/4744
1	G	0.10	0/3479	0.28	0/4740
1	H	0.10	0/3474	0.26	0/4735
All	All	0.11	0/27840	0.27	0/37934

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	3422	0	3394	17	0
1	B	3425	0	3396	14	0
1	C	3426	0	3405	15	0
1	D	3423	0	3396	14	0
1	E	3423	0	3396	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3426	0	3412	13	0
1	G	3422	0	3401	18	0
1	H	3417	0	3388	22	0
2	A	46	0	21	1	0
2	B	46	0	21	0	0
2	C	46	0	21	0	0
2	D	46	0	21	0	0
2	E	46	0	21	0	0
2	F	46	0	21	0	0
2	G	46	0	21	0	0
2	H	46	0	21	0	0
3	A	48	0	25	1	0
3	B	48	0	25	2	0
3	C	48	0	25	1	0
3	D	48	0	25	1	0
3	E	48	0	25	4	0
3	F	48	0	25	2	0
3	G	96	0	50	1	0
4	A	122	0	0	0	0
4	B	100	0	0	0	0
4	C	117	0	0	0	0
4	D	119	0	0	0	0
4	E	68	0	0	0	0
4	F	83	0	0	0	0
4	G	72	0	0	0	0
4	H	60	0	0	1	0
All	All	28877	0	27556	130	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.

The worst 5 of 130 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:C:298:GLY:HA3	1:C:306:ARG:HE	1.43	0.83
1:D:110:SER:HB2	1:D:146:ARG:HB3	1.76	0.65
1:D:298:GLY:HA3	1:D:306:ARG:HE	1.62	0.64
1:B:272:VAL:HG22	1:B:292:ILE:HB	1.82	0.61
1:A:340:ARG:NH2	2:A:501:IMP:O2P	2.33	0.61

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	471/496 (95%)	463 (98%)	8 (2%)	0	100	100
1	B	471/496 (95%)	461 (98%)	10 (2%)	0	100	100
1	C	471/496 (95%)	461 (98%)	10 (2%)	0	100	100
1	D	471/496 (95%)	461 (98%)	10 (2%)	0	100	100
1	E	471/496 (95%)	463 (98%)	8 (2%)	0	100	100
1	F	471/496 (95%)	461 (98%)	10 (2%)	0	100	100
1	G	471/496 (95%)	458 (97%)	13 (3%)	0	100	100
1	H	471/496 (95%)	458 (97%)	13 (3%)	0	100	100
All	All	3768/3968 (95%)	3686 (98%)	82 (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	349/372 (94%)	346 (99%)	3 (1%)	75	82
1	B	350/372 (94%)	349 (100%)	1 (0%)	91	94
1	C	350/372 (94%)	348 (99%)	2 (1%)	84	89
1	D	349/372 (94%)	347 (99%)	2 (1%)	84	89
1	E	349/372 (94%)	344 (99%)	5 (1%)	62	70
1	F	350/372 (94%)	347 (99%)	3 (1%)	75	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	349/372 (94%)	345 (99%)	4 (1%)	70	77
1	H	348/372 (94%)	346 (99%)	2 (1%)	84	89
All	All	2794/2976 (94%)	2772 (99%)	22 (1%)	79	84

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	303	CYS
1	G	133	ILE
1	G	91	LYS
1	G	235	LEU
1	D	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	328	GLN
1	G	341	HIS
1	H	473	HIS
1	G	176	HIS
1	H	113	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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	IMP	C	501	1	21,25,25	0.68	0	24,38,38	0.81	0
2	IMP	G	503	-	21,25,25	0.62	0	24,38,38	0.76	0
3	NAP	B	502	-	45,52,52	0.64	0	56,80,80	0.60	1 (1%)
2	IMP	C	503	-	21,25,25	0.61	0	24,38,38	0.77	0
3	NAP	F	502	-	45,52,52	0.65	0	56,80,80	0.62	1 (1%)
3	NAP	E	502	-	45,52,52	0.64	1 (2%)	56,80,80	0.63	1 (1%)
3	NAP	D	502	-	45,52,52	0.64	1 (2%)	56,80,80	0.62	1 (1%)
2	IMP	G	501	1	21,25,25	0.67	0	24,38,38	0.80	0
2	IMP	F	501	1	21,25,25	0.69	0	24,38,38	0.82	0
2	IMP	E	501	1	21,25,25	0.68	0	24,38,38	0.80	0
2	IMP	D	501	1	21,25,25	0.67	0	24,38,38	0.81	0
2	IMP	A	501	1	21,25,25	0.67	0	24,38,38	0.83	0
2	IMP	E	503	-	21,25,25	0.61	0	24,38,38	0.78	0
2	IMP	H	502	-	21,25,25	0.62	0	24,38,38	0.76	0
2	IMP	D	503	-	21,25,25	0.60	0	24,38,38	0.76	0
2	IMP	B	503	-	21,25,25	0.63	0	24,38,38	0.78	0
3	NAP	G	504	-	45,52,52	0.64	0	56,80,80	0.61	1 (1%)
2	IMP	F	503	-	21,25,25	0.63	0	24,38,38	0.76	0
3	NAP	C	502	-	45,52,52	0.64	0	56,80,80	0.64	1 (1%)
3	NAP	G	502	-	45,52,52	0.65	1 (2%)	56,80,80	0.61	1 (1%)
2	IMP	A	503	-	21,25,25	0.63	0	24,38,38	0.76	0
2	IMP	B	501	1	21,25,25	0.70	0	24,38,38	0.81	0
3	NAP	A	502	-	45,52,52	0.64	1 (2%)	56,80,80	0.61	1 (1%)
2	IMP	H	501	1	21,25,25	0.67	0	24,38,38	0.81	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	IMP	C	501	1	-	0/6/26/26	0/3/3/3
2	IMP	G	503	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	502	-	-	9/31/67/67	0/5/5/5
2	IMP	C	503	-	-	0/6/26/26	0/3/3/3
3	NAP	F	502	-	-	10/31/67/67	0/5/5/5
3	NAP	E	502	-	-	11/31/67/67	0/5/5/5
3	NAP	D	502	-	-	12/31/67/67	0/5/5/5
2	IMP	G	501	1	-	0/6/26/26	0/3/3/3
2	IMP	F	501	1	-	0/6/26/26	0/3/3/3
2	IMP	E	501	1	-	0/6/26/26	0/3/3/3
2	IMP	D	501	1	-	0/6/26/26	0/3/3/3
2	IMP	A	501	1	-	0/6/26/26	0/3/3/3
2	IMP	E	503	-	-	0/6/26/26	0/3/3/3
2	IMP	H	502	-	-	0/6/26/26	0/3/3/3
2	IMP	D	503	-	-	0/6/26/26	0/3/3/3
2	IMP	B	503	-	-	0/6/26/26	0/3/3/3
3	NAP	G	504	-	-	10/31/67/67	0/5/5/5
2	IMP	F	503	-	-	0/6/26/26	0/3/3/3
3	NAP	C	502	-	-	11/31/67/67	0/5/5/5
3	NAP	G	502	-	-	10/31/67/67	0/5/5/5
2	IMP	A	503	-	-	0/6/26/26	0/3/3/3
2	IMP	B	501	1	-	0/6/26/26	0/3/3/3
3	NAP	A	502	-	-	10/31/67/67	0/5/5/5
2	IMP	H	501	1	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAP	P2B-O2B	2.02	1.63	1.59
3	E	502	NAP	P2B-O2B	2.01	1.63	1.59
3	G	502	NAP	P2B-O2B	2.00	1.63	1.59
3	D	502	NAP	P2B-O2B	2.00	1.63	1.59

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAP	C5A-C6A-N6A	2.36	123.94	120.35
3	G	504	NAP	C5A-C6A-N6A	2.35	123.92	120.35
3	E	502	NAP	C5A-C6A-N6A	2.33	123.89	120.35
3	F	502	NAP	C5A-C6A-N6A	2.33	123.89	120.35
3	C	502	NAP	C5A-C6A-N6A	2.32	123.87	120.35



There are no chirality outliers.

5 of 83 torsion outliers are listed below:

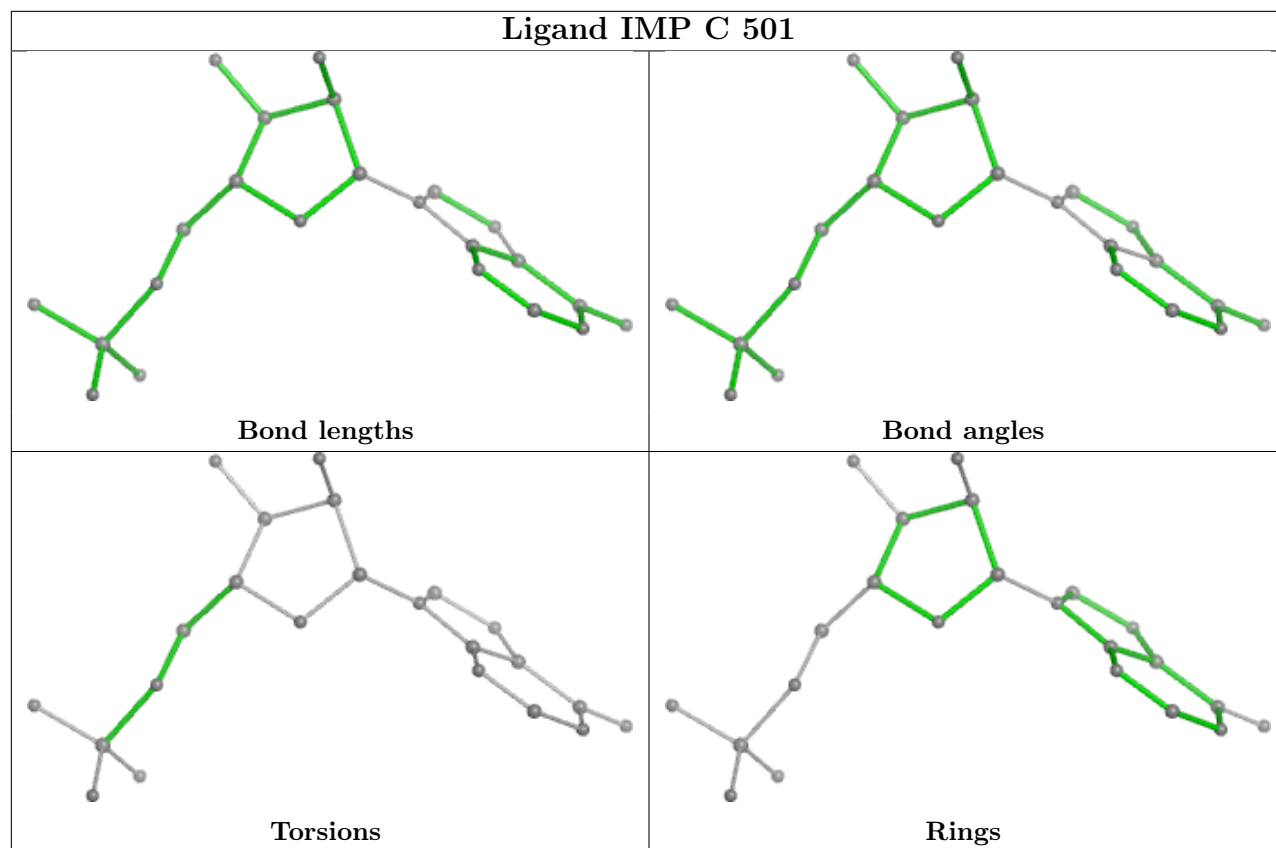
Mol	Chain	Res	Type	Atoms
3	A	502	NAP	C5B-O5B-PA-O1A
3	A	502	NAP	C2D-C1D-N1N-C2N
3	A	502	NAP	C2D-C1D-N1N-C6N
3	B	502	NAP	C5B-O5B-PA-O1A
3	B	502	NAP	C2D-C1D-N1N-C2N

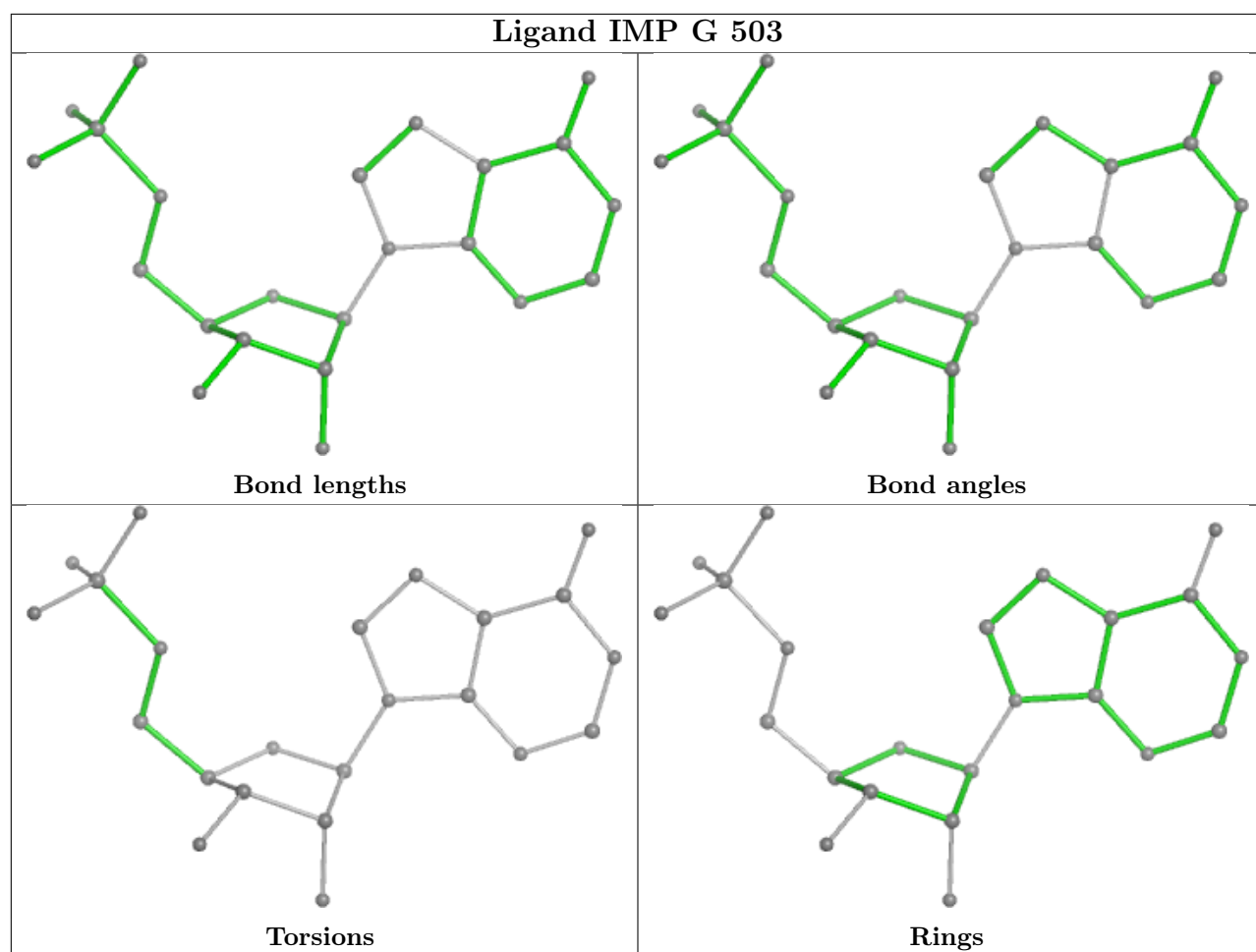
There are no ring outliers.

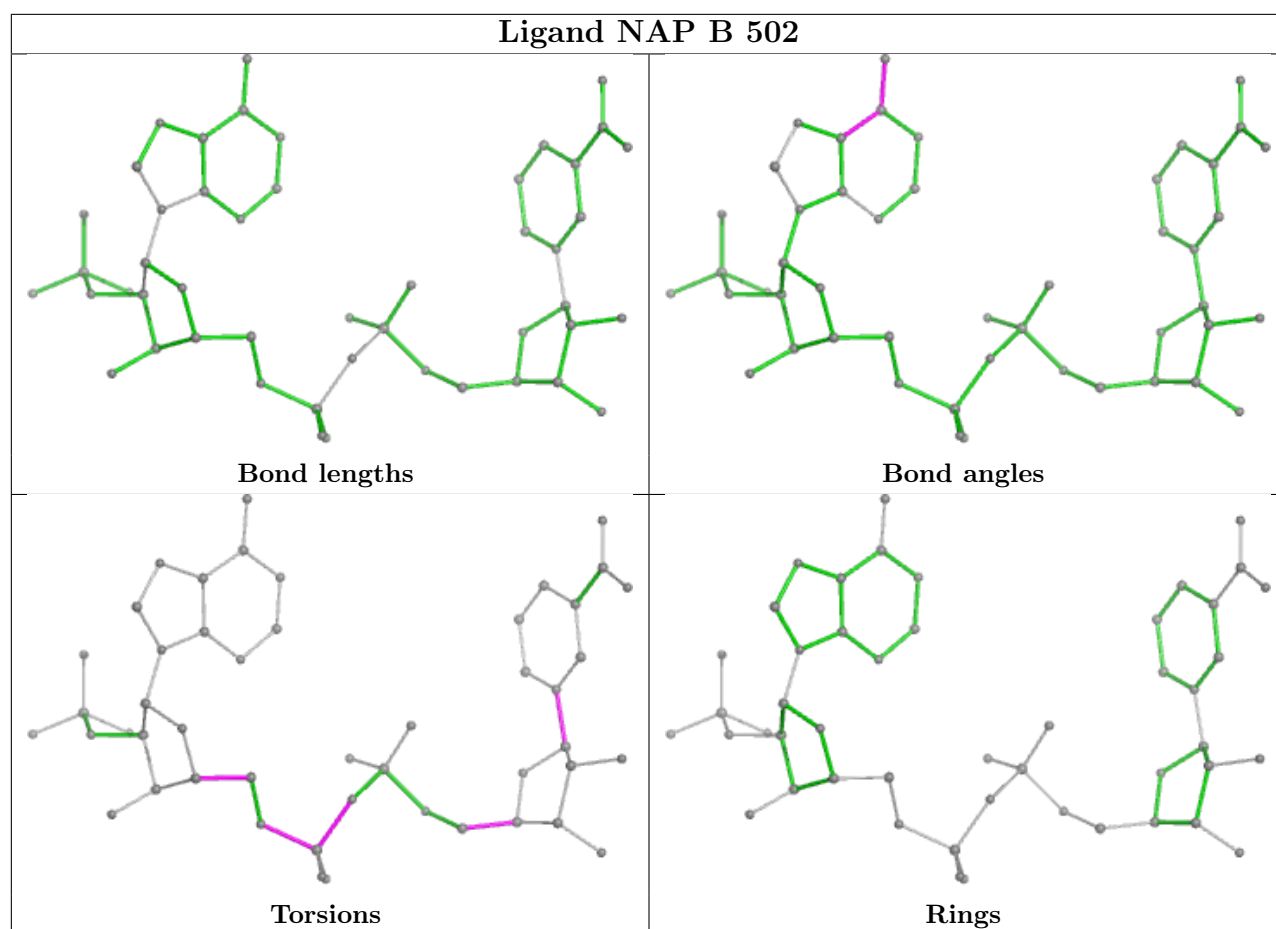
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	NAP	2	0
3	F	502	NAP	2	0
3	E	502	NAP	4	0
3	D	502	NAP	1	0
2	A	501	IMP	1	0
3	C	502	NAP	1	0
3	G	502	NAP	1	0
3	A	502	NAP	1	0

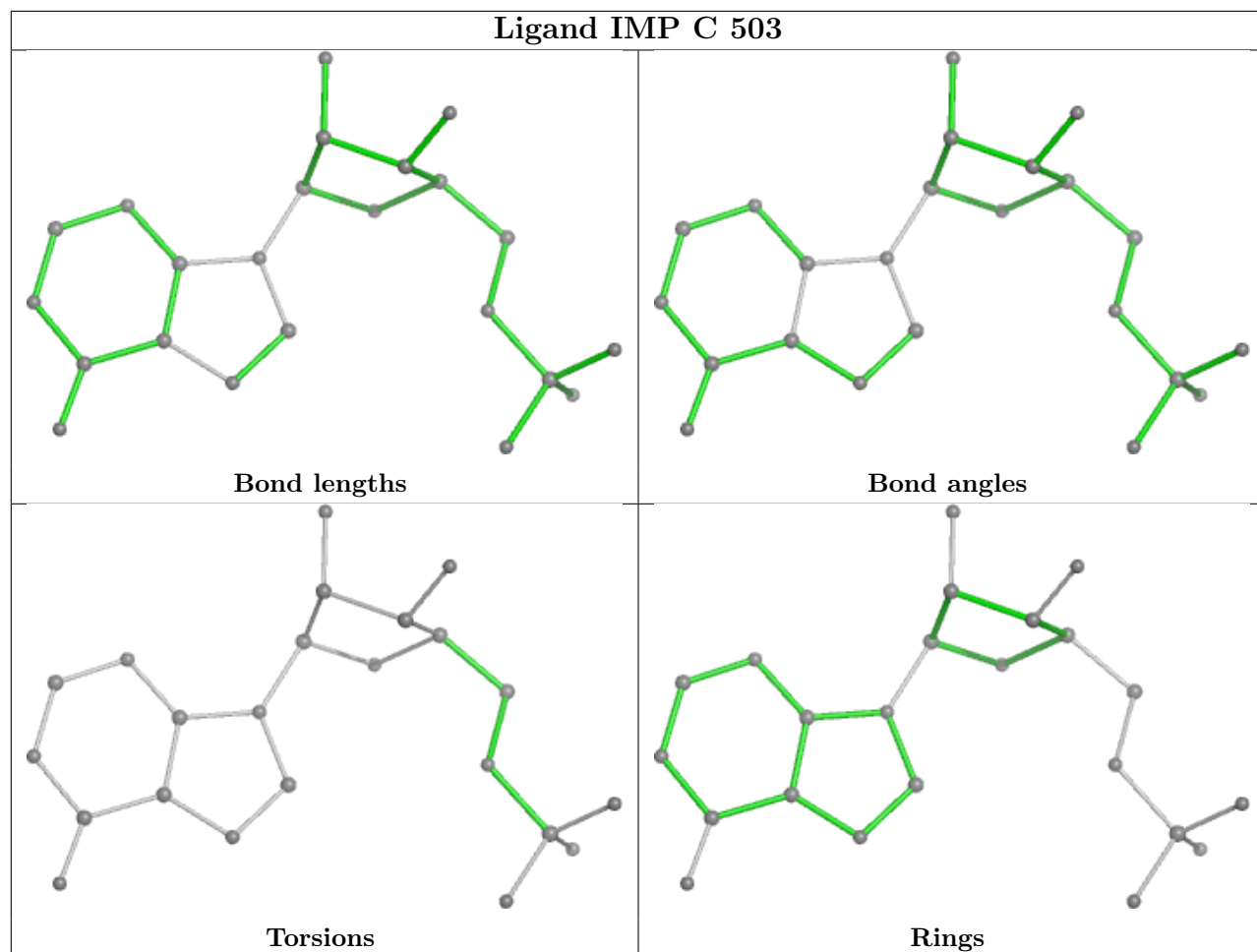
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

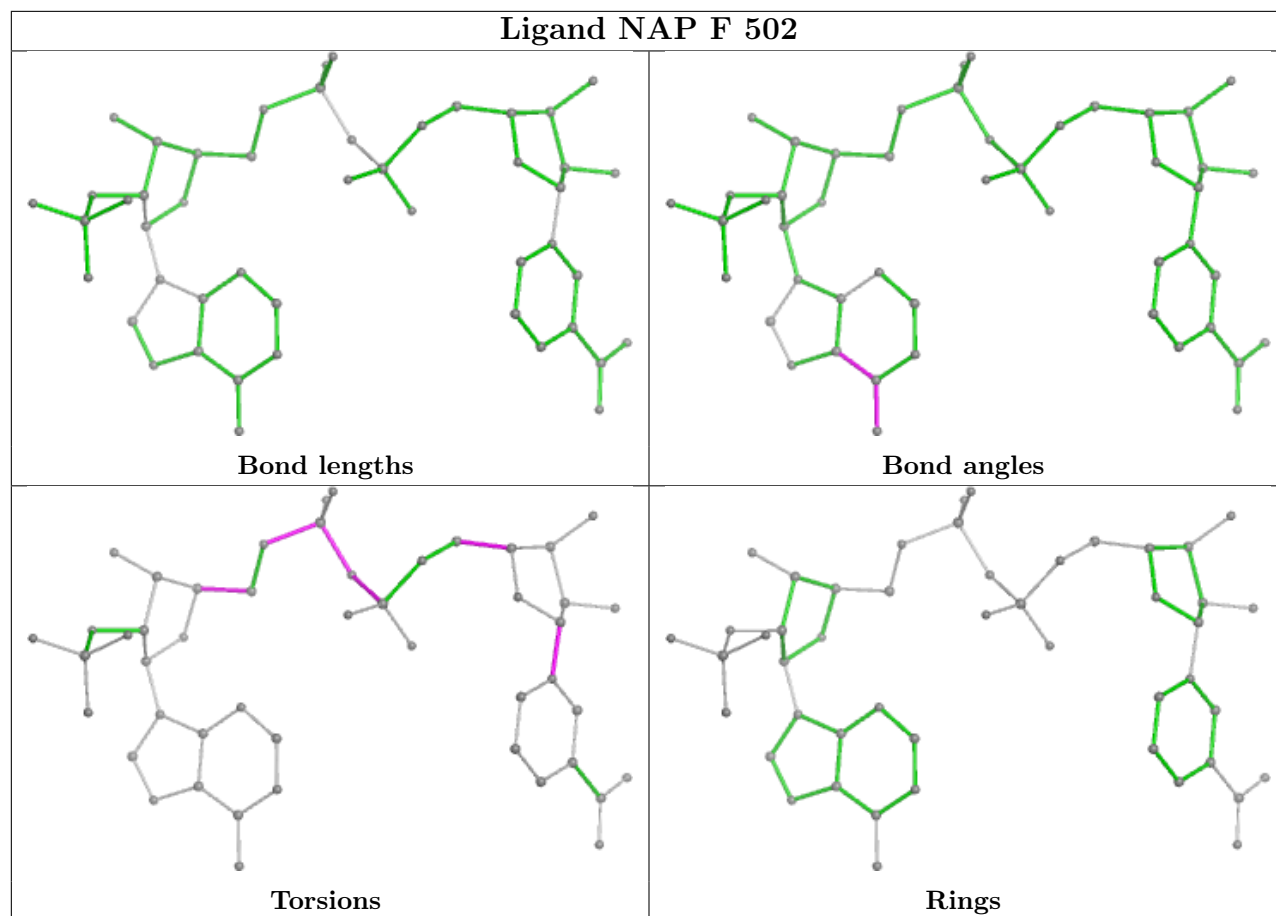


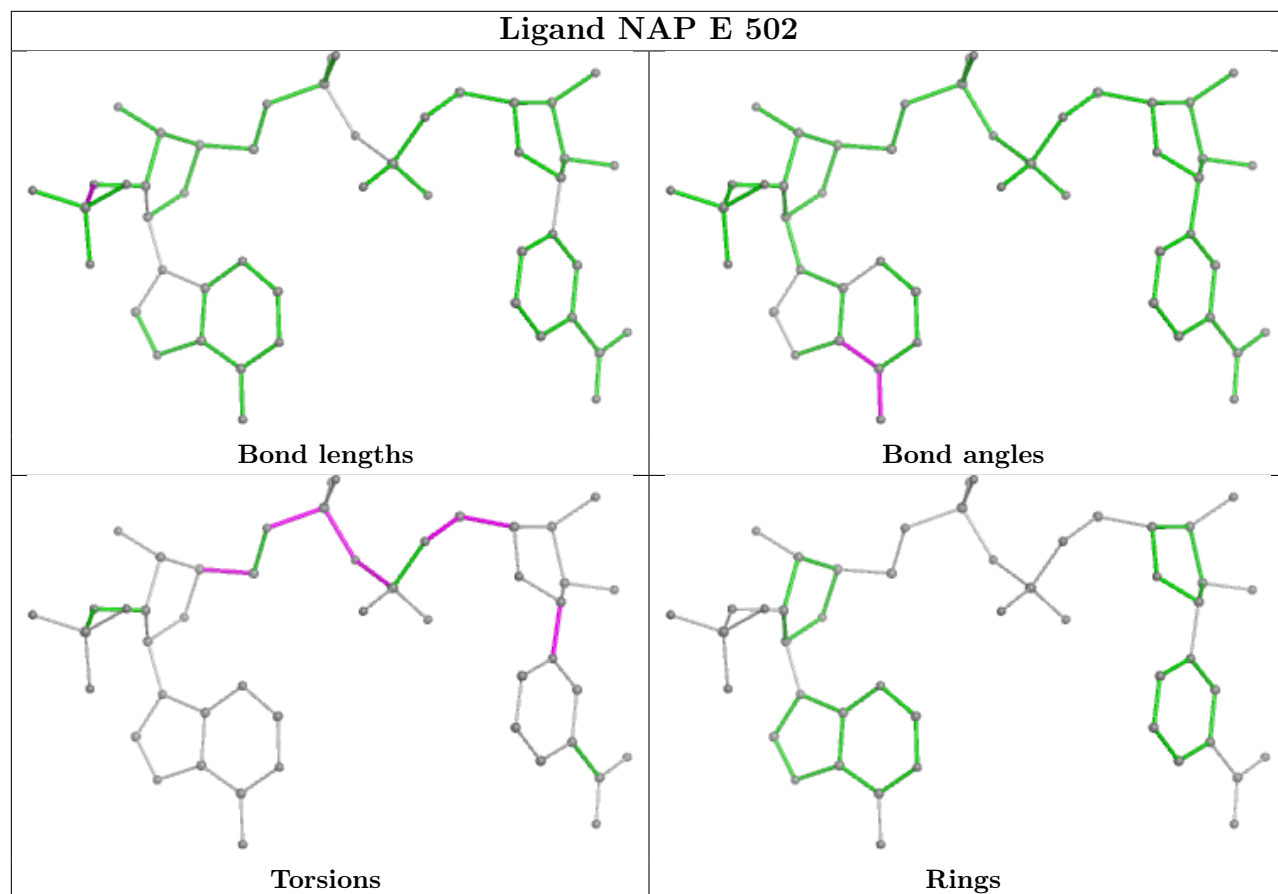


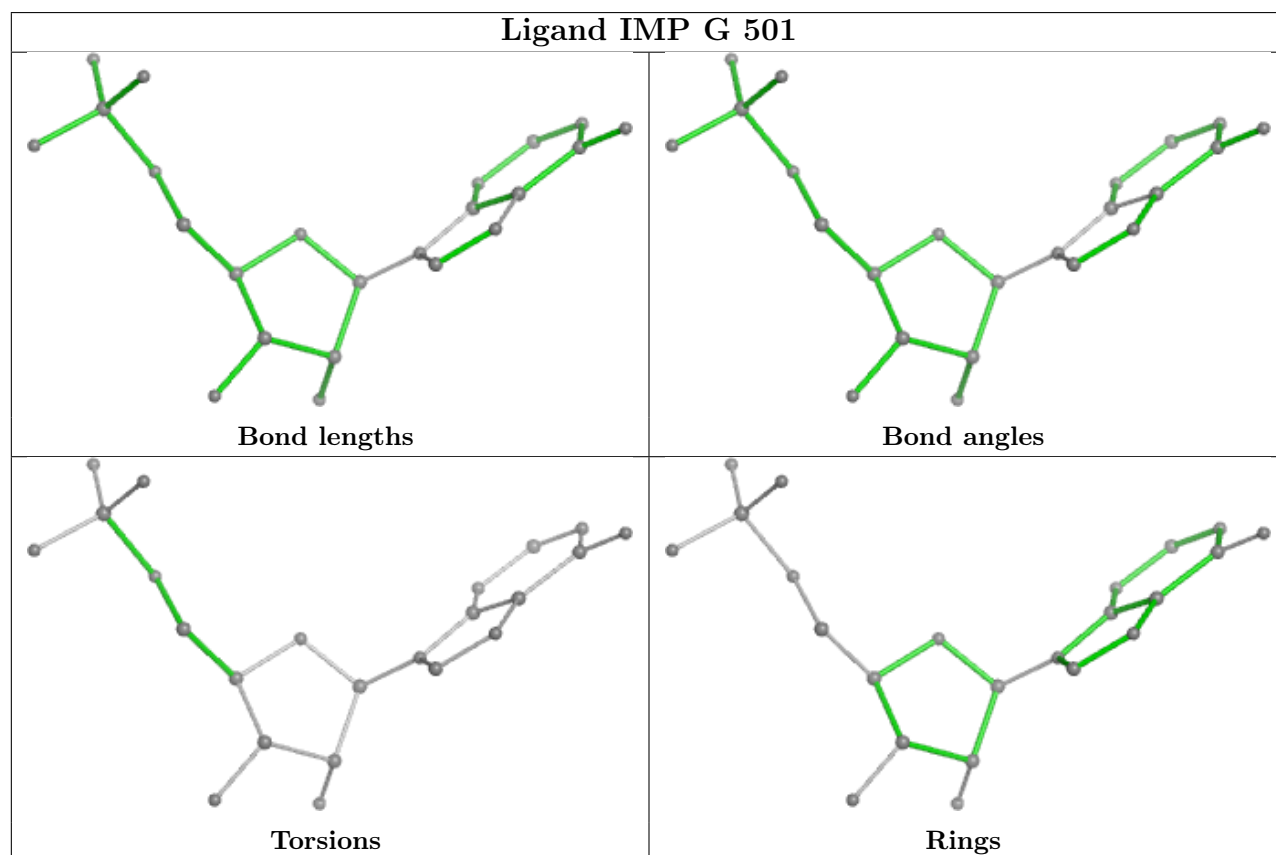
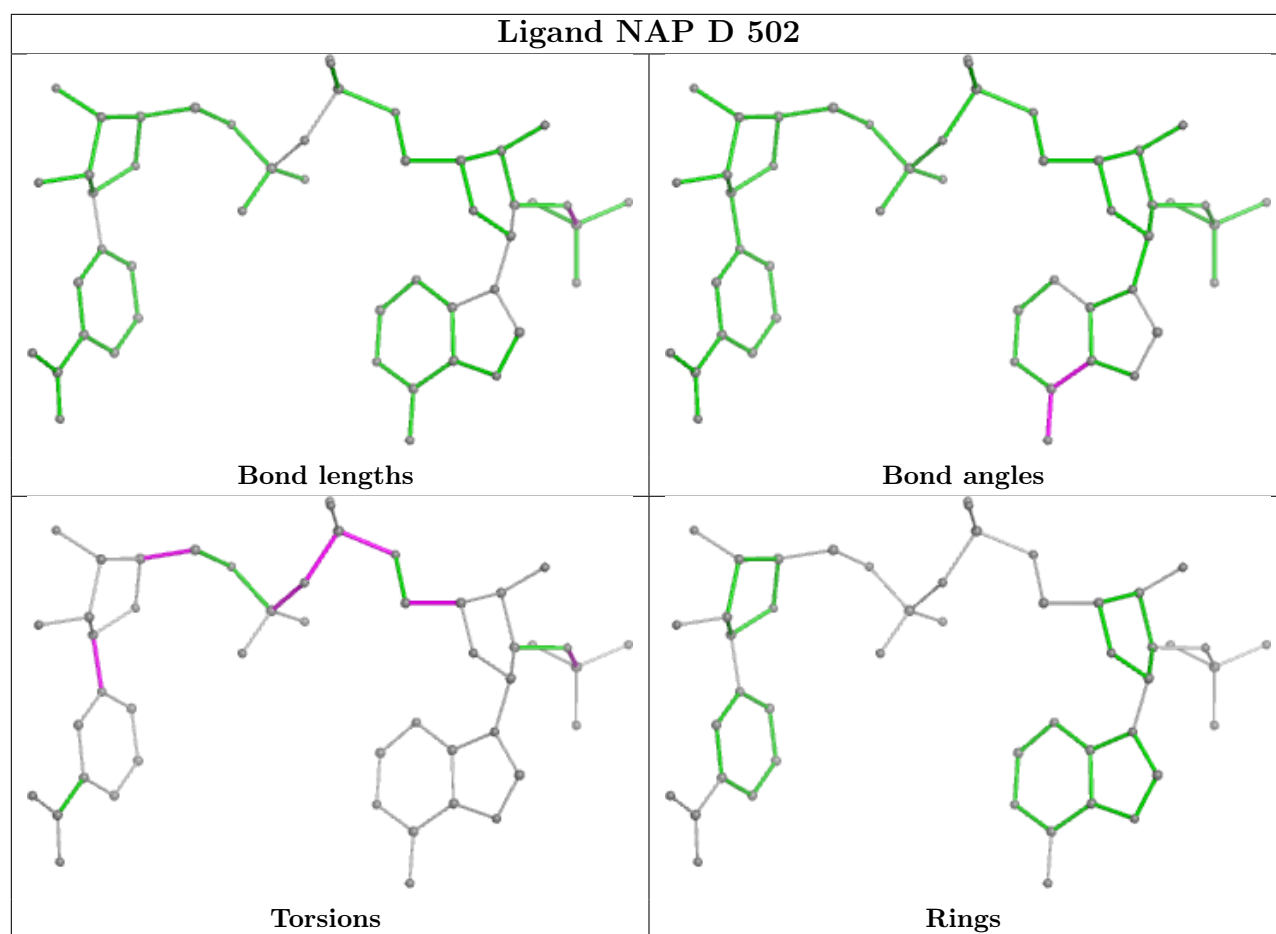


## Ligand IMP C 503



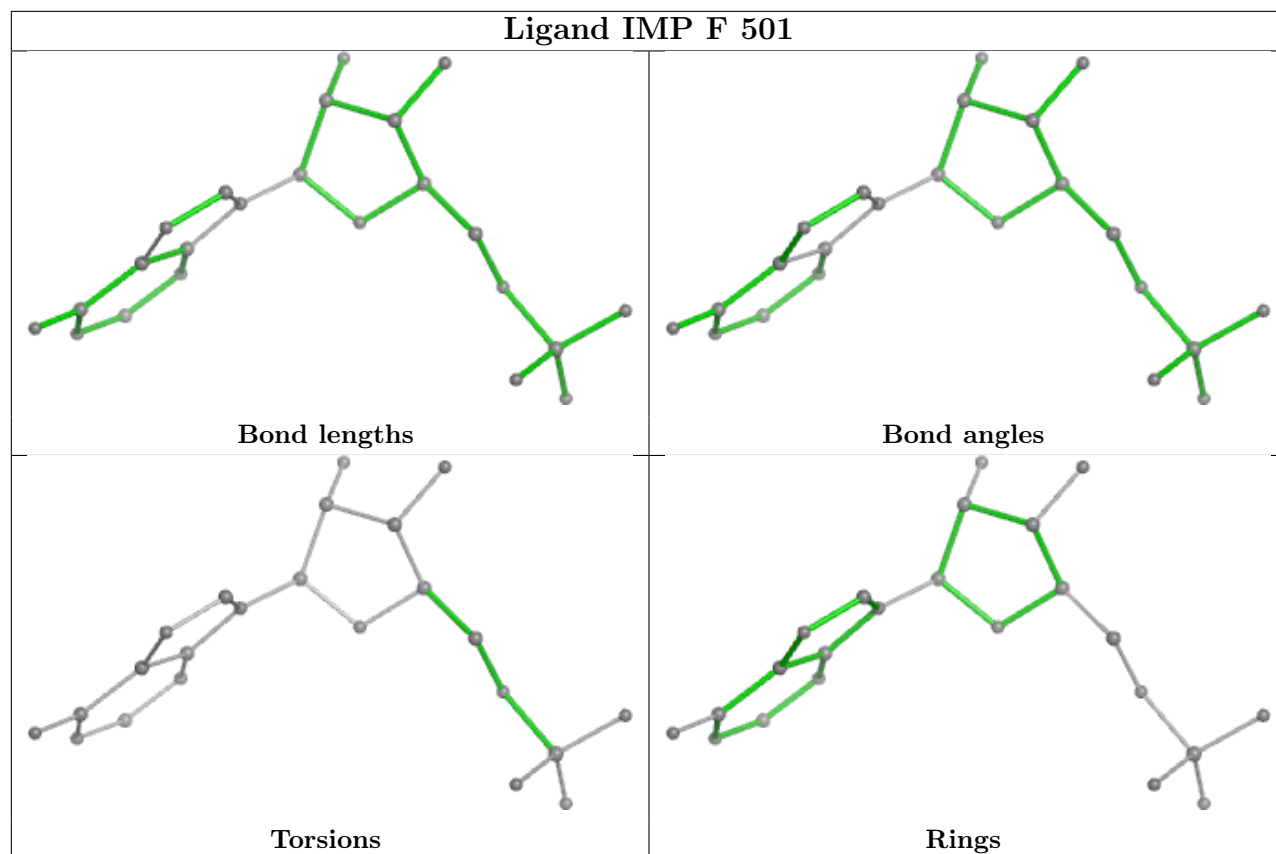




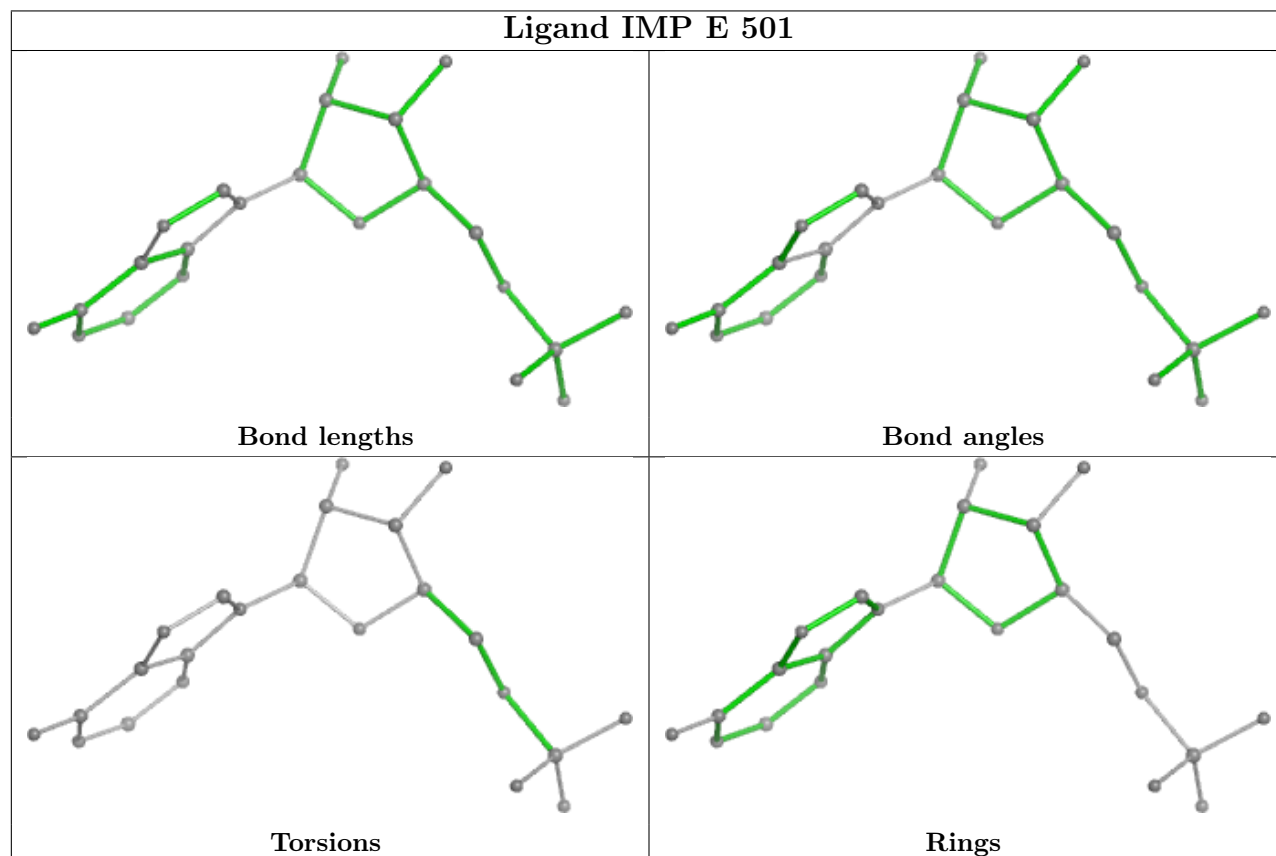




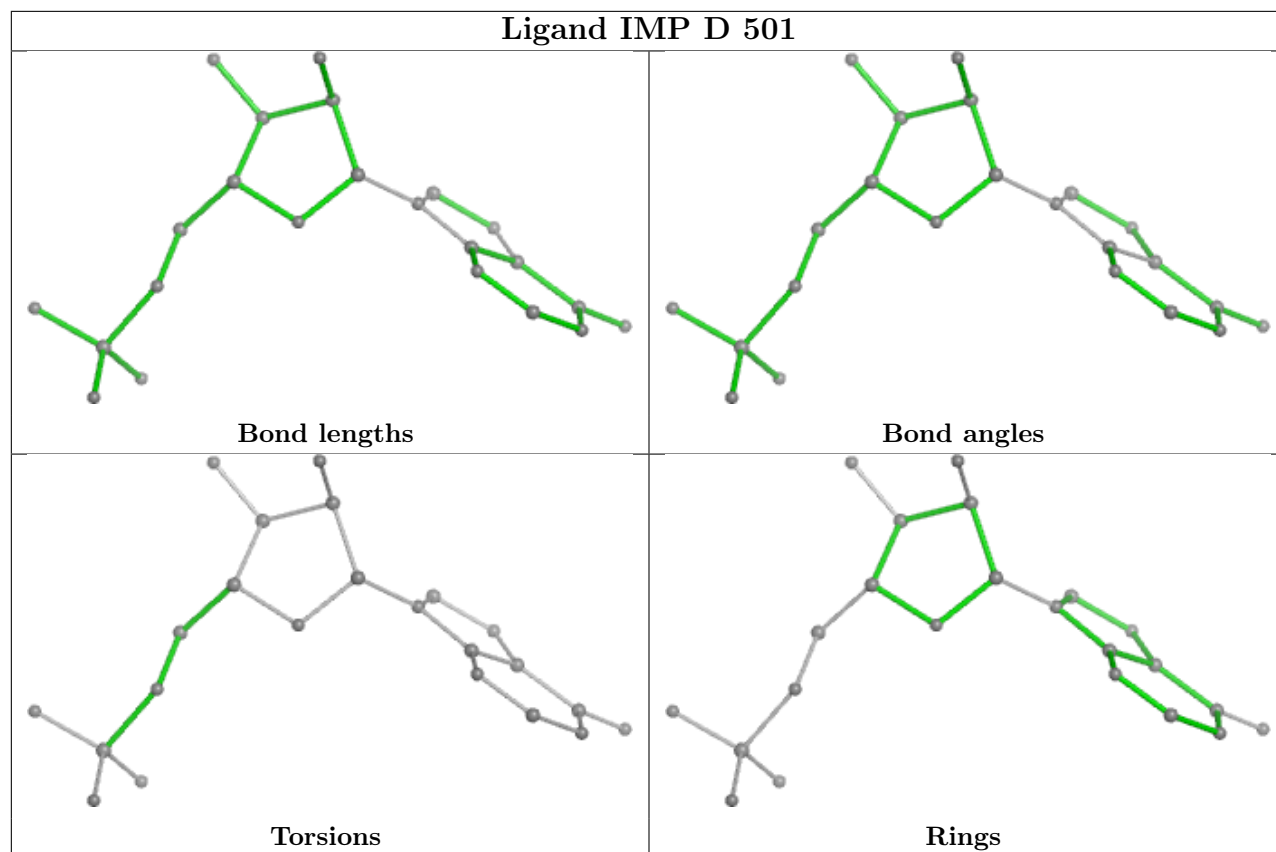
## Ligand IMP F 501



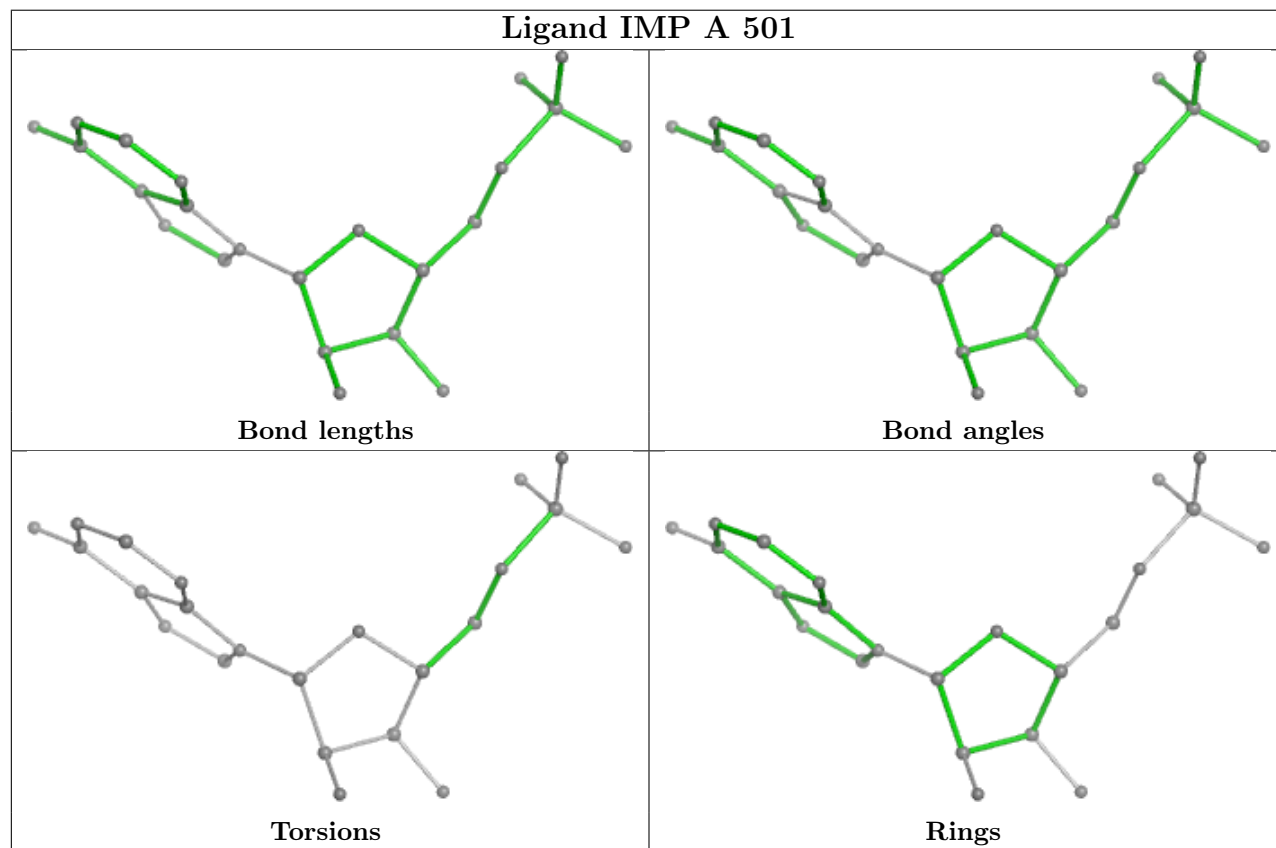
## Ligand IMP E 501



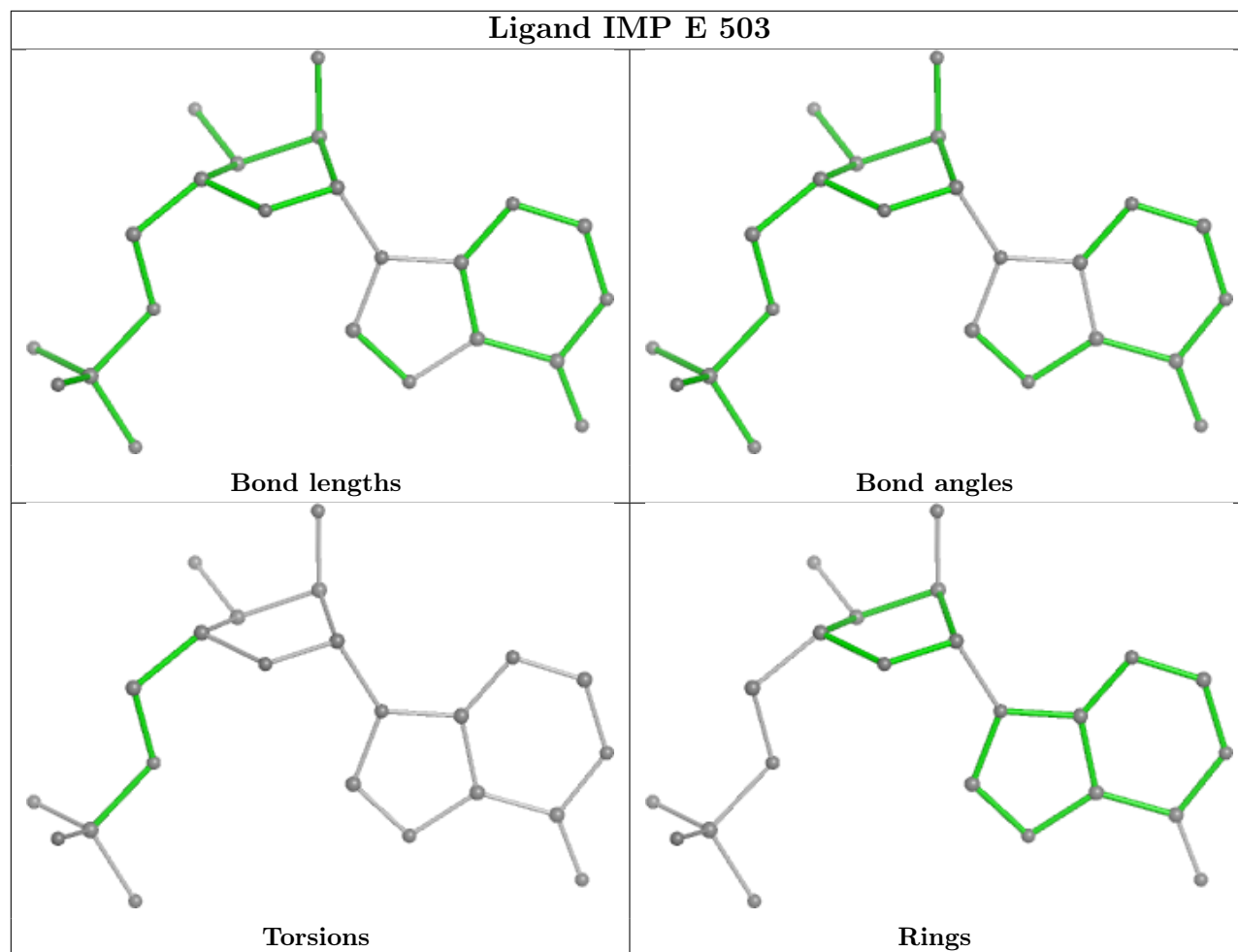
## Ligand IMP D 501



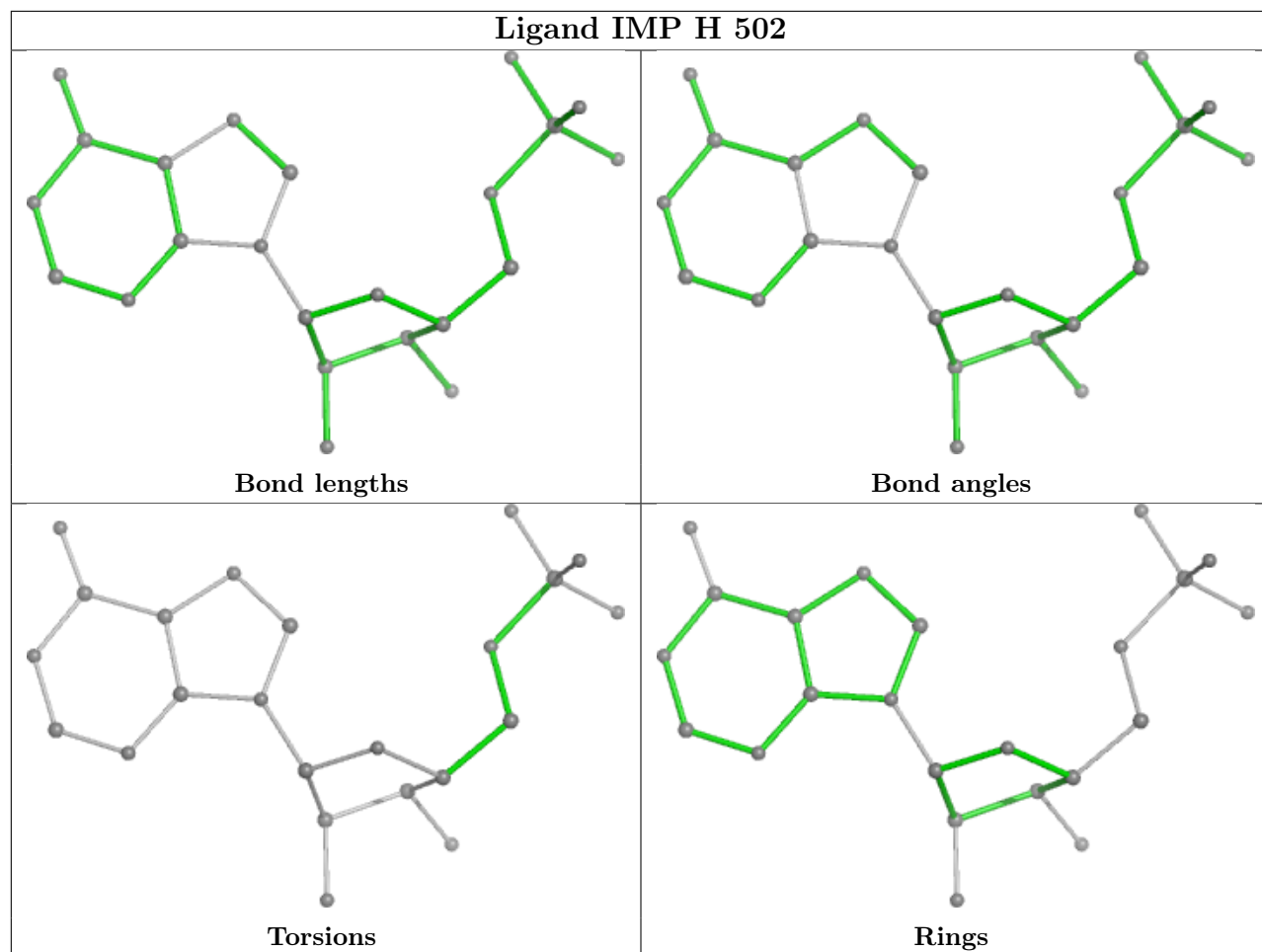
## Ligand IMP A 501



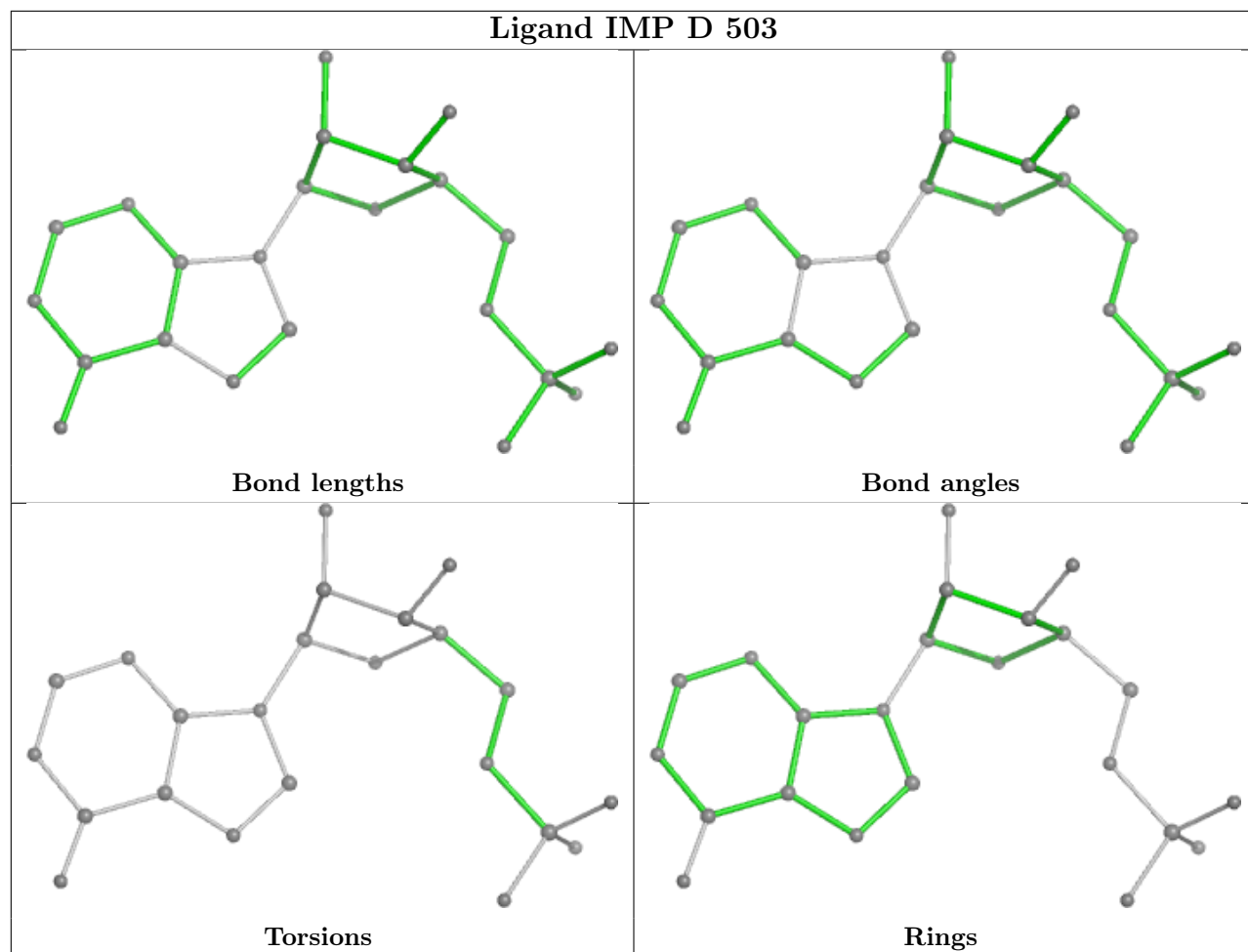
## Ligand IMP E 503

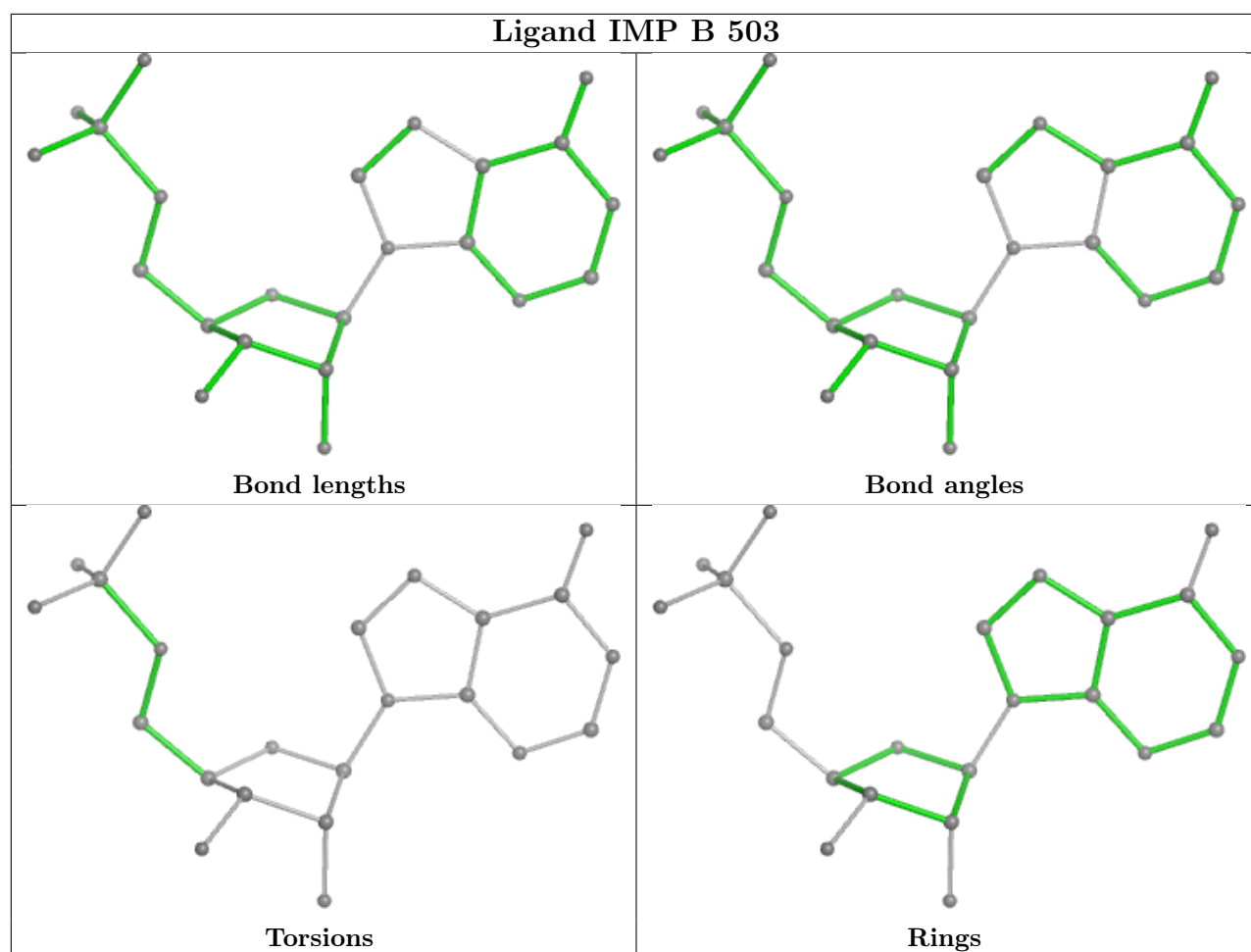


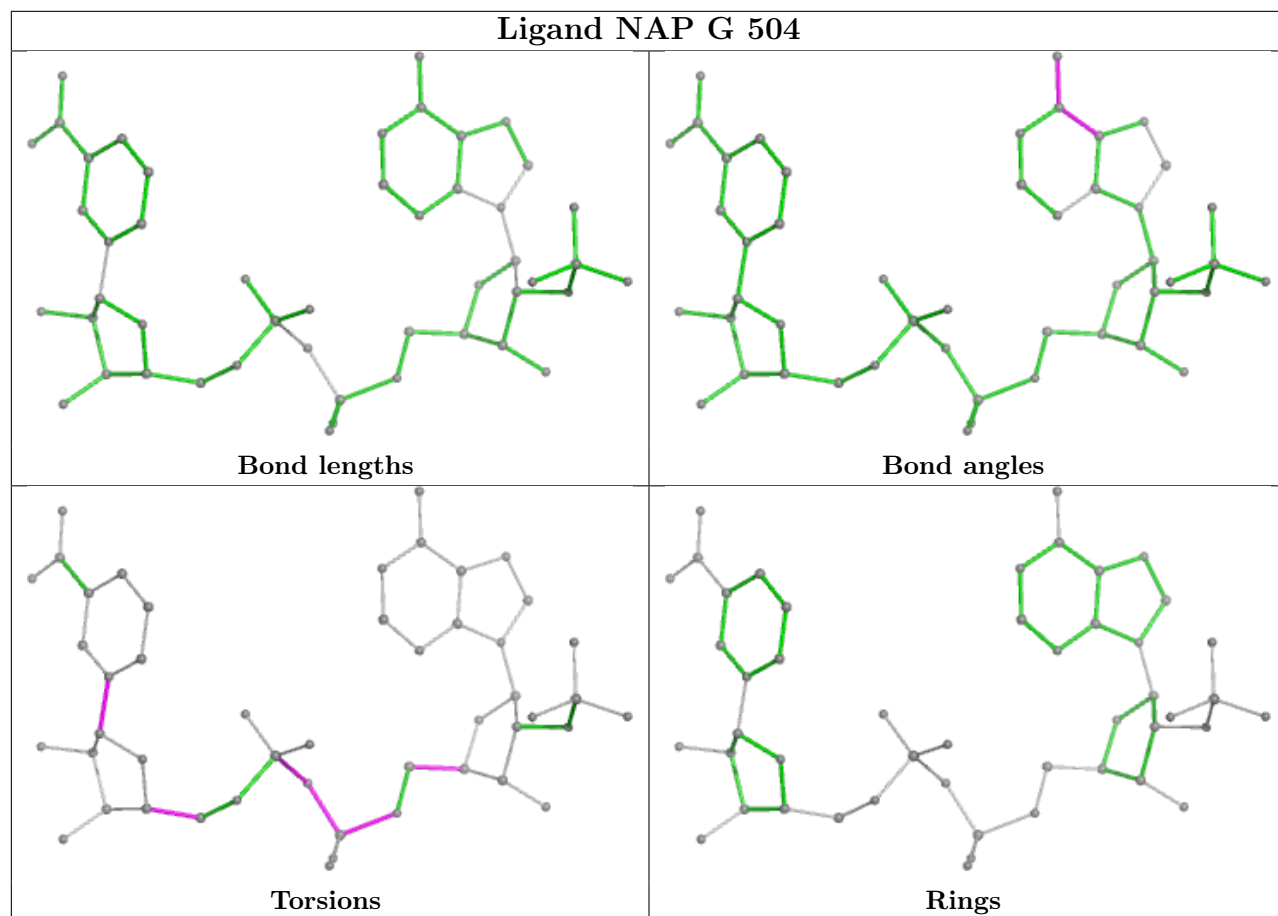
## Ligand IMP H 502



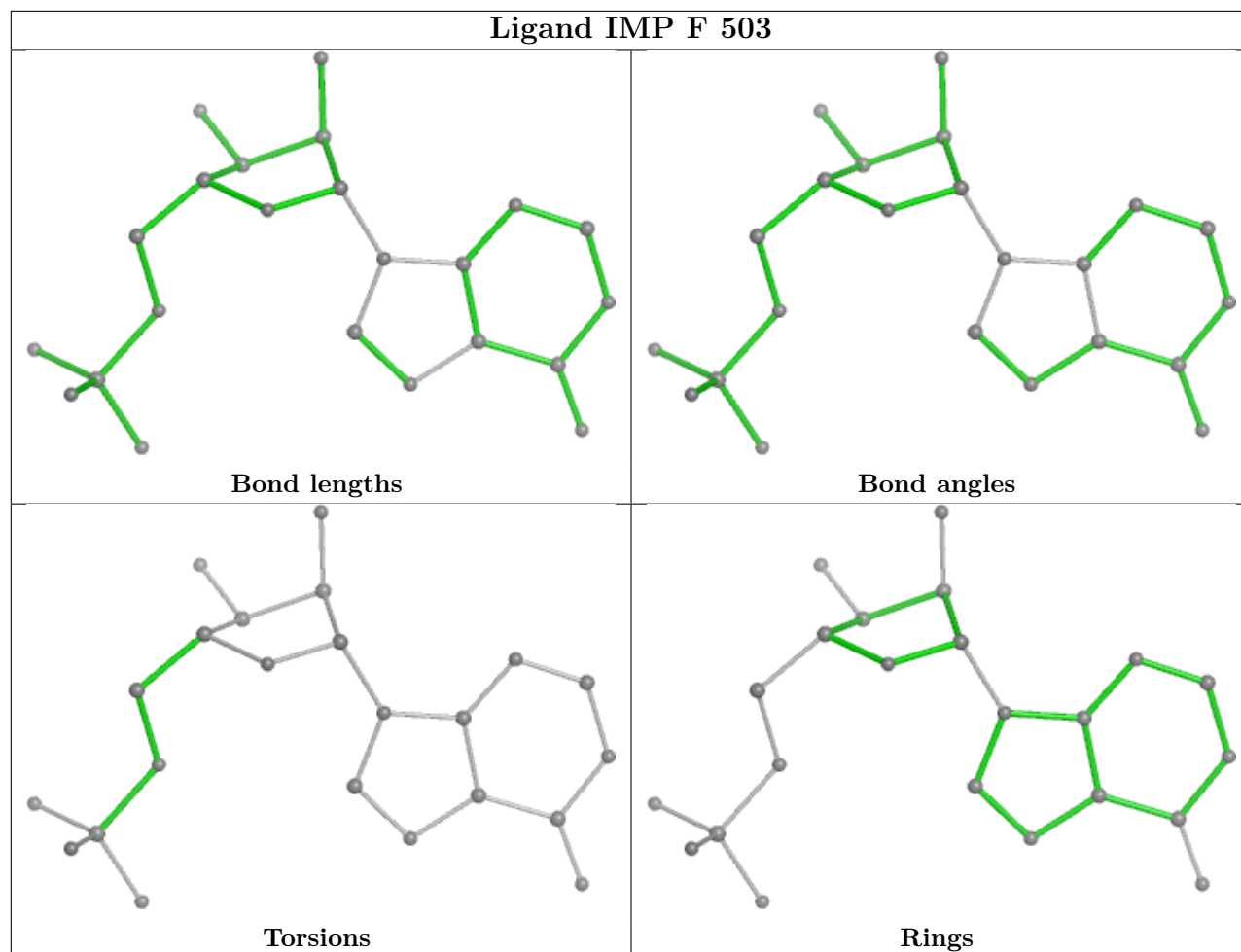
## Ligand IMP D 503



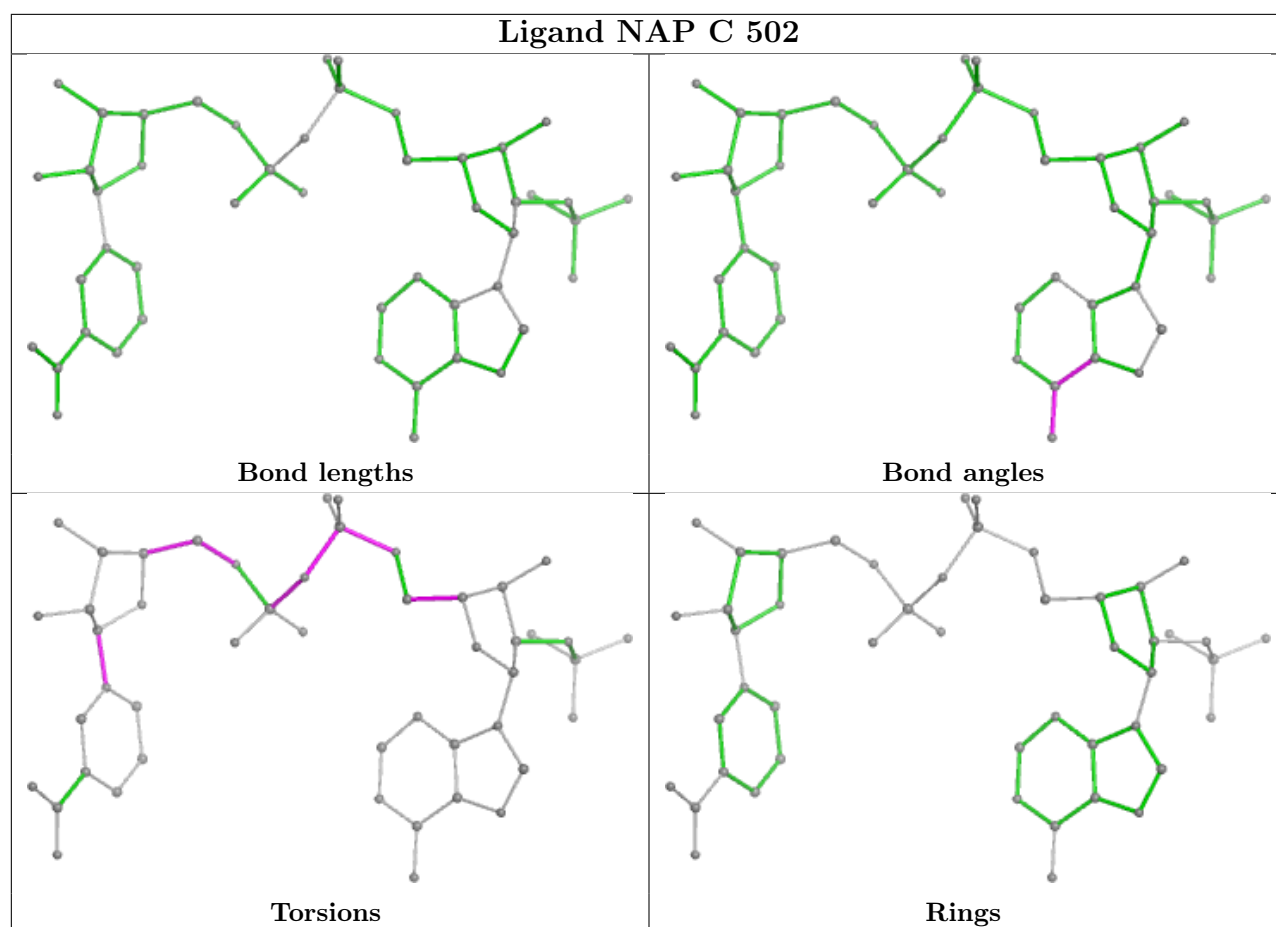


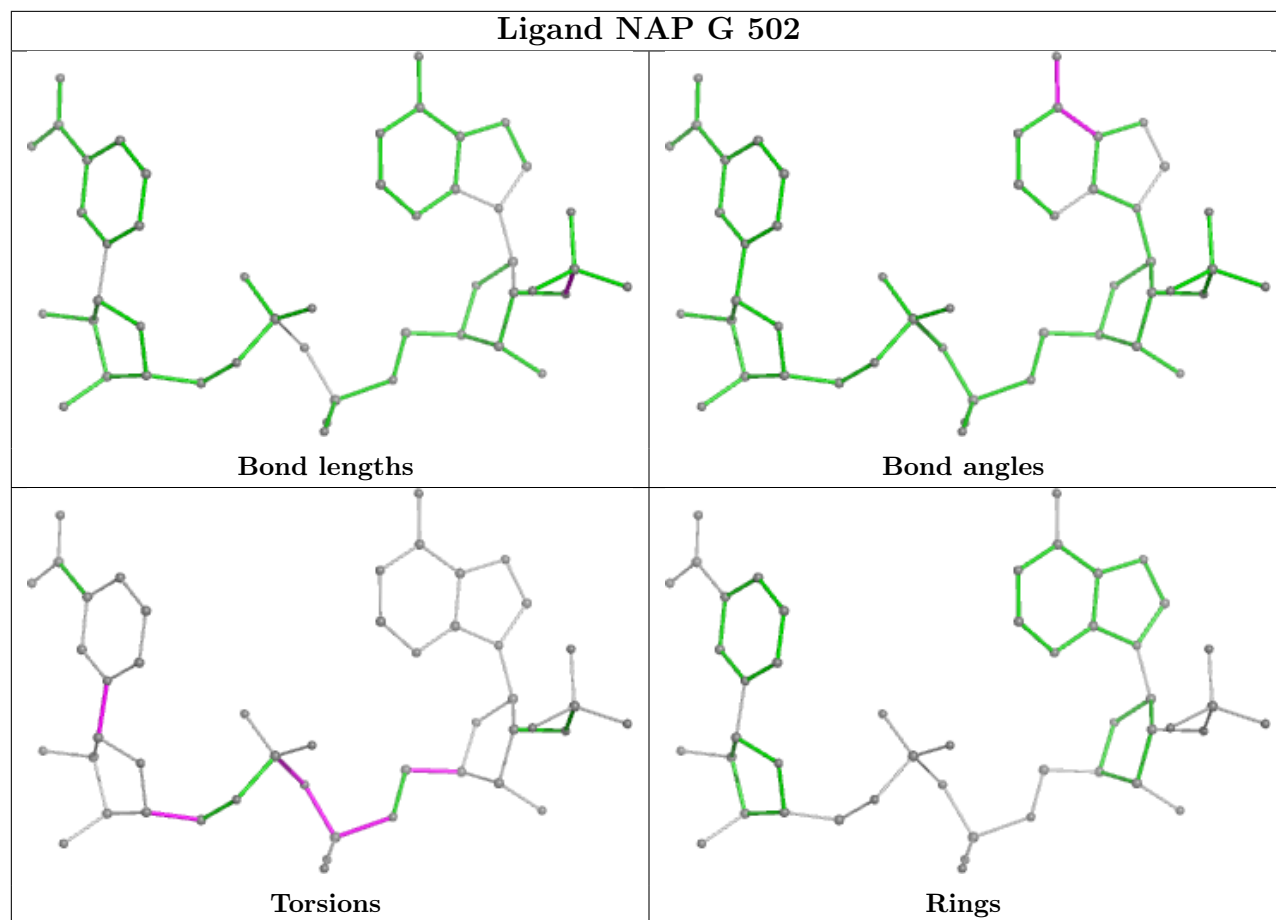


## Ligand IMP F 503

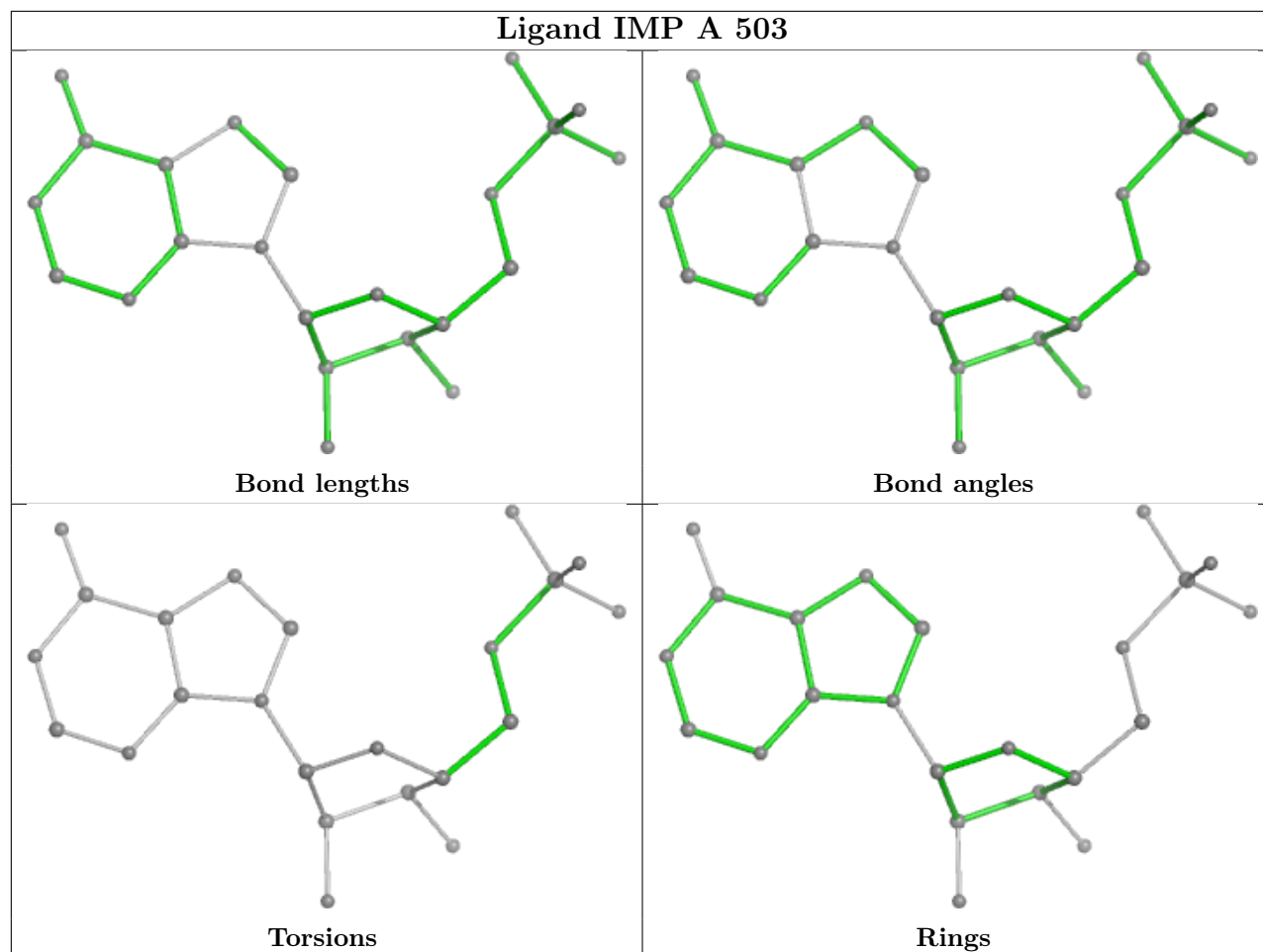




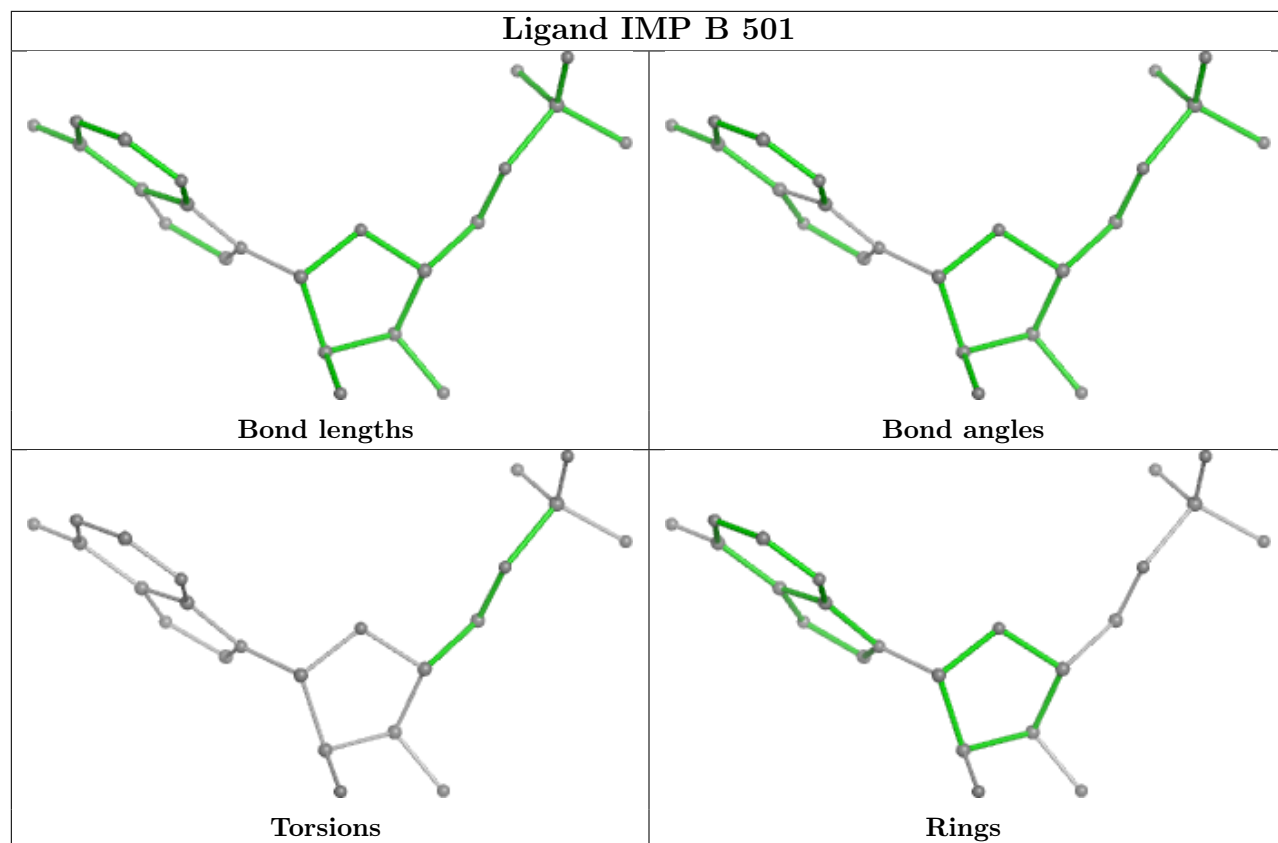




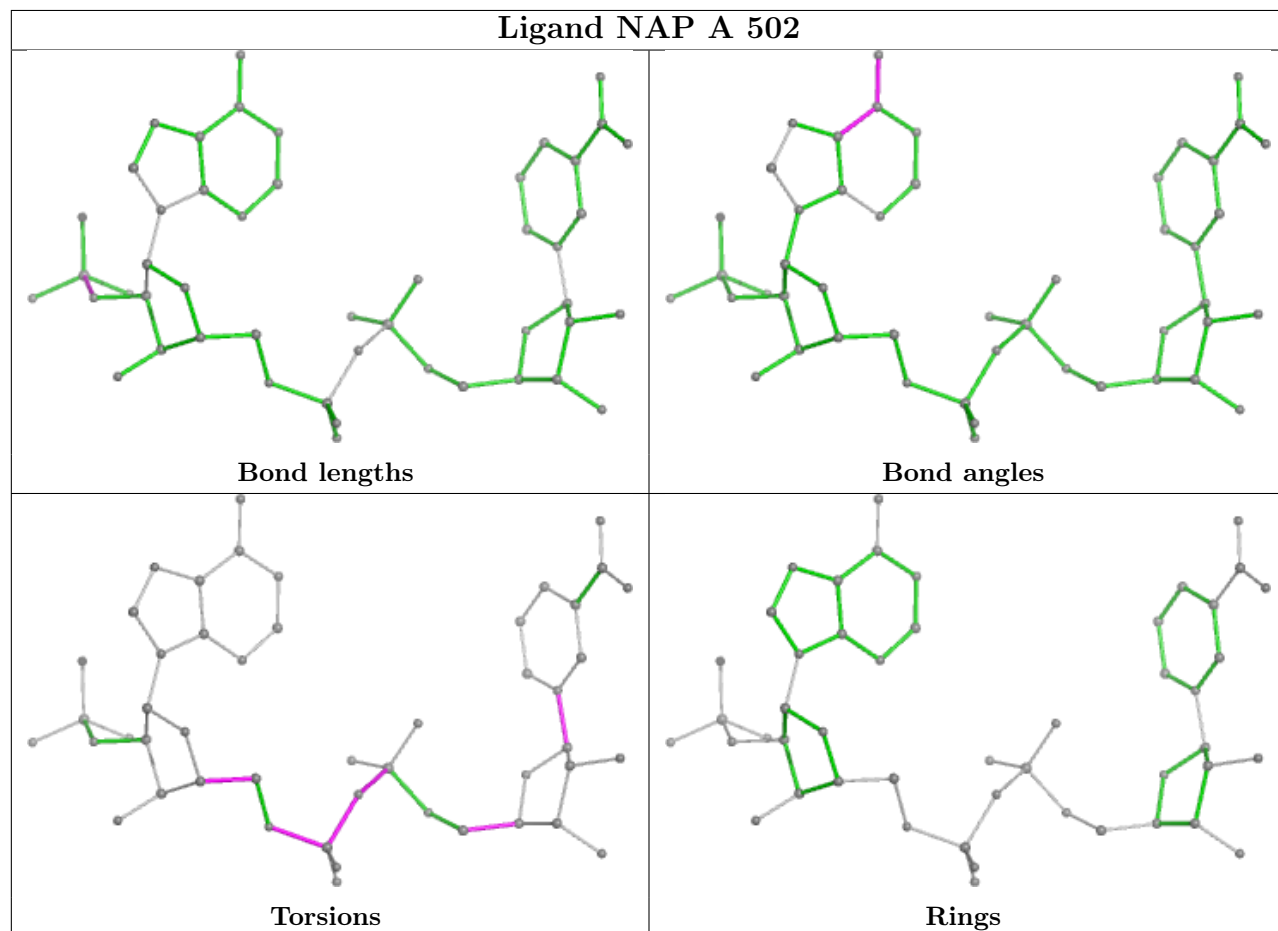
## Ligand IMP A 503

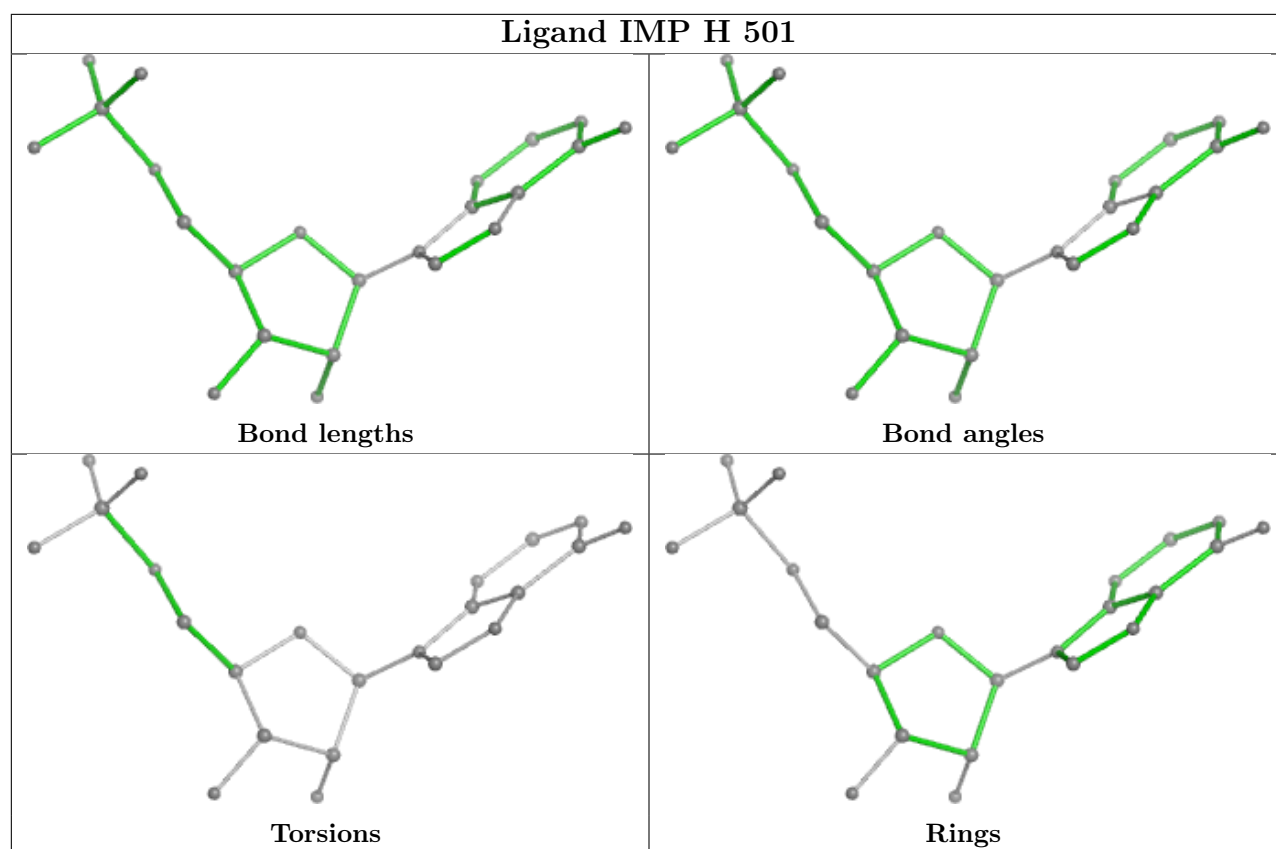


## Ligand IMP B 501



## Ligand NAP A 502





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	473/496 (95%)	0.47	24 (5%) 34 36	32, 44, 69, 83	0
1	B	473/496 (95%)	0.46	21 (4%) 39 42	33, 45, 68, 83	0
1	C	473/496 (95%)	0.52	28 (5%) 29 31	33, 45, 71, 84	0
1	D	473/496 (95%)	0.43	28 (5%) 29 31	31, 43, 67, 87	0
1	E	473/496 (95%)	0.79	38 (8%) 20 21	37, 53, 73, 90	0
1	F	473/496 (95%)	0.72	27 (5%) 30 33	37, 49, 73, 89	0
1	G	473/496 (95%)	0.83	39 (8%) 19 21	38, 52, 74, 89	0
1	H	473/496 (95%)	0.83	38 (8%) 20 21	40, 54, 73, 87	0
All	All	3784/3968 (95%)	0.63	243 (6%) 27 29	31, 48, 72, 90	0

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	474	PRO	5.9
1	C	147	PHE	5.7
1	D	147	PHE	5.5
1	H	155	LEU	5.4
1	A	474	PRO	5.4

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

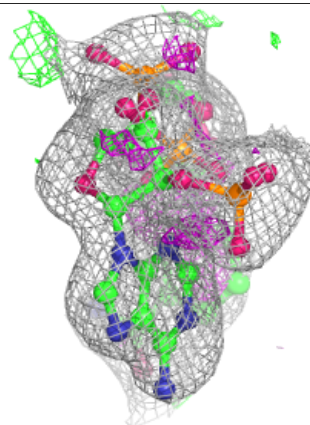
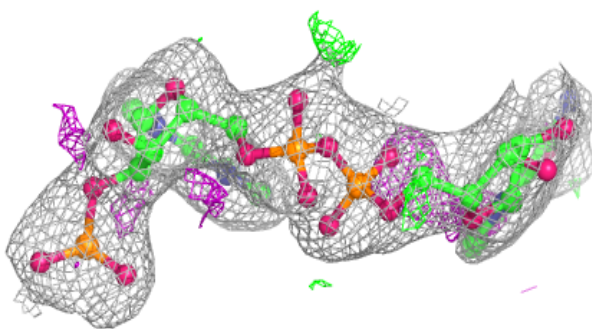
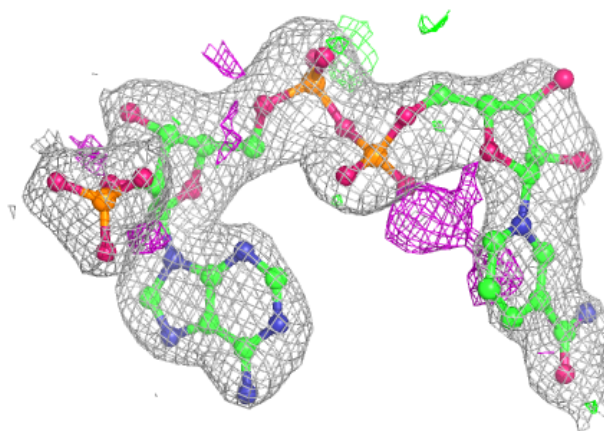
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	NAP	C	502	48/48	0.89	0.12	46,54,73,80	0
3	NAP	E	502	48/48	0.89	0.11	53,59,72,82	0
3	NAP	G	502	48/48	0.89	0.12	47,53,72,79	0
3	NAP	B	502	48/48	0.90	0.11	39,51,69,75	0
2	IMP	F	503	23/23	0.90	0.10	45,54,63,69	0
3	NAP	D	502	48/48	0.90	0.11	40,52,72,74	0
2	IMP	H	502	23/23	0.90	0.09	49,56,59,64	0
3	NAP	A	502	48/48	0.90	0.11	43,50,65,71	0
3	NAP	G	504	48/48	0.90	0.11	52,61,73,77	0
3	NAP	F	502	48/48	0.91	0.10	44,54,72,80	0
2	IMP	G	503	23/23	0.92	0.09	50,54,59,62	0
2	IMP	E	503	23/23	0.92	0.09	49,55,60,64	0
2	IMP	E	501	23/23	0.94	0.10	39,47,53,56	0
2	IMP	H	501	23/23	0.95	0.09	41,49,53,53	0
2	IMP	F	501	23/23	0.95	0.09	39,42,47,49	0
2	IMP	C	503	23/23	0.95	0.07	41,48,52,54	0
2	IMP	G	501	23/23	0.95	0.08	39,43,53,55	0
2	IMP	D	503	23/23	0.95	0.06	40,45,48,55	0
2	IMP	D	501	23/23	0.96	0.08	32,39,46,52	0
2	IMP	A	503	23/23	0.96	0.07	42,45,50,52	0
2	IMP	B	501	23/23	0.96	0.08	32,37,46,48	0
2	IMP	B	503	23/23	0.96	0.07	41,46,51,54	0
2	IMP	C	501	23/23	0.96	0.08	34,40,46,50	0
2	IMP	A	501	23/23	0.96	0.07	33,37,44,50	0

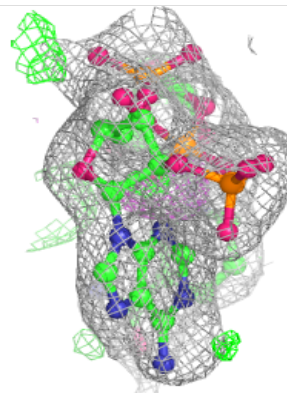
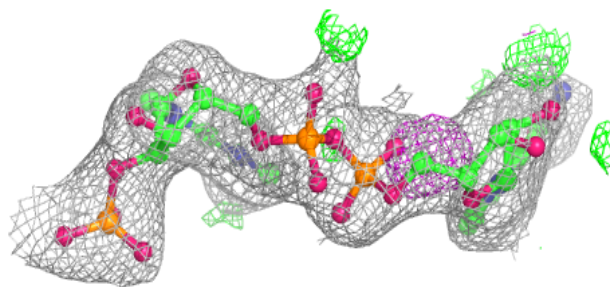
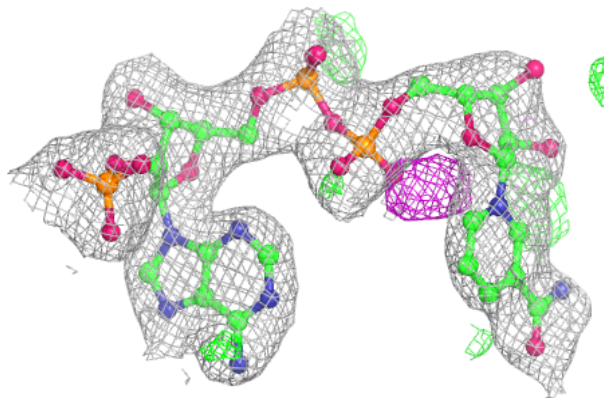
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP C 502:**

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

**Electron density around NAP E 502:**

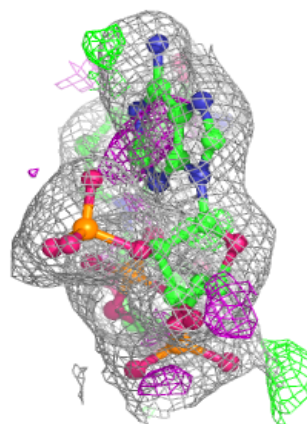
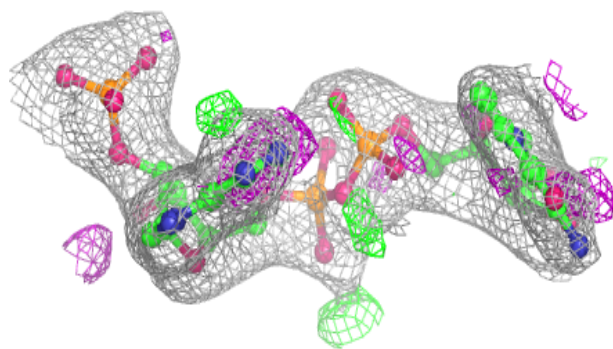
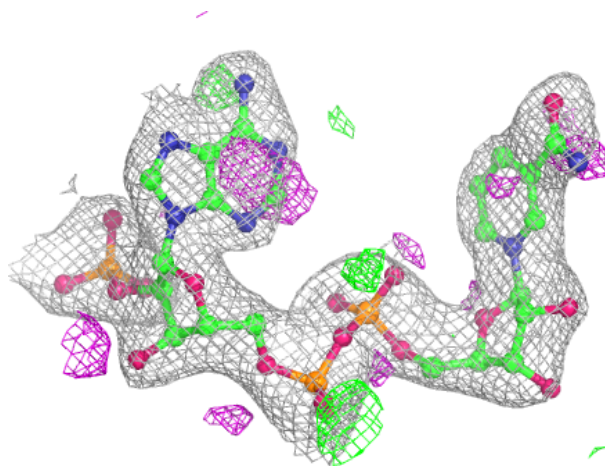
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





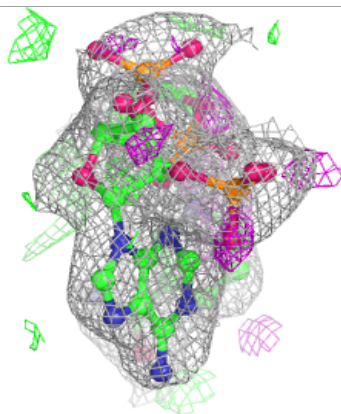
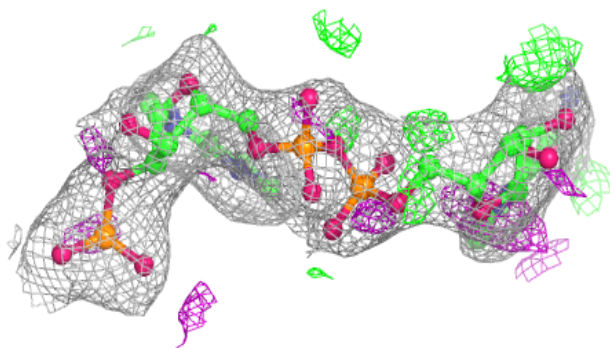
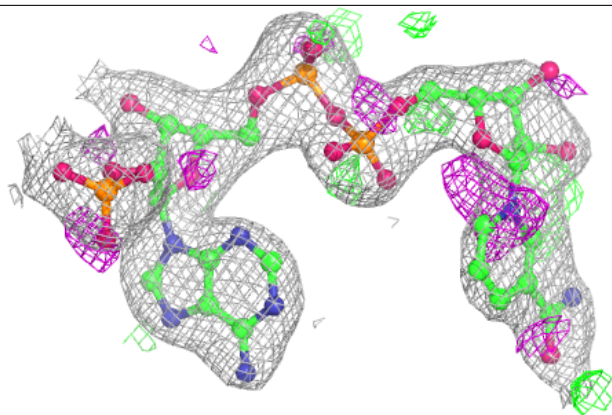
**Electron density around NAP G 502:**

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and green (positive)

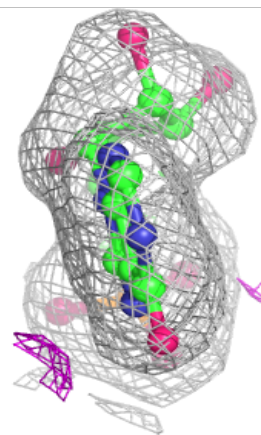
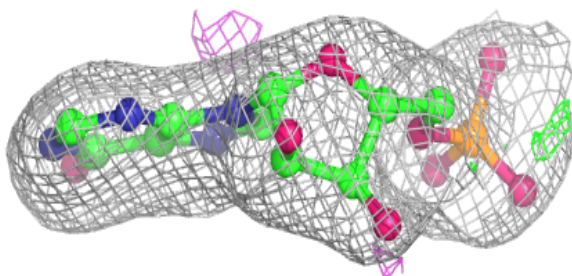
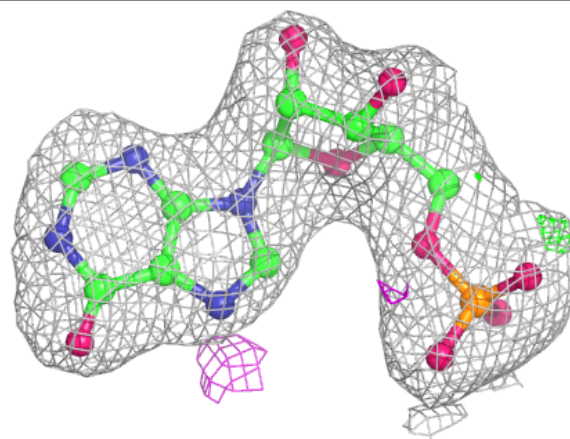


**Electron density around NAP B 502:**

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and green (positive)

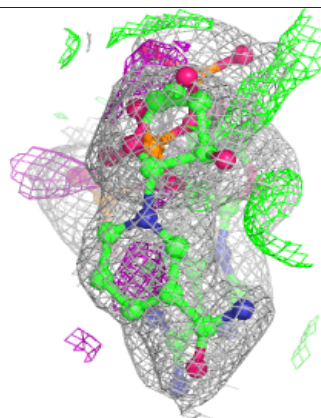
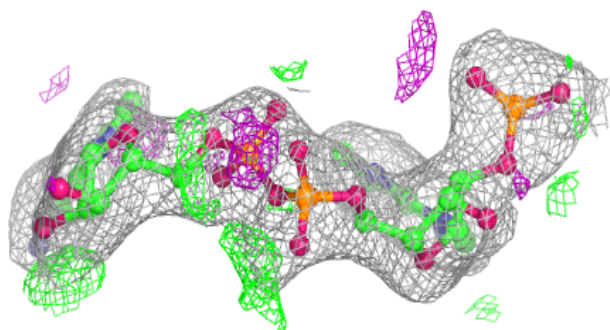
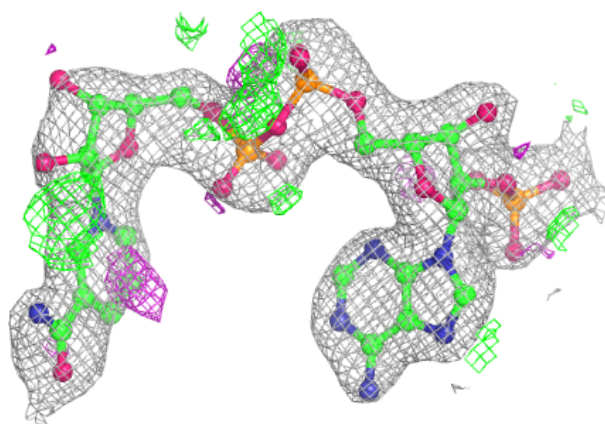
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and green (positive)

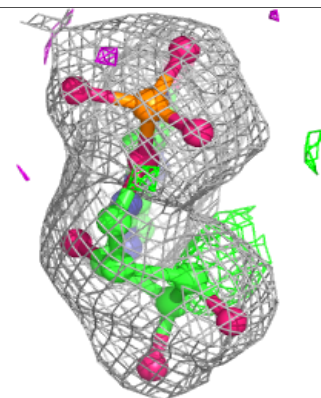
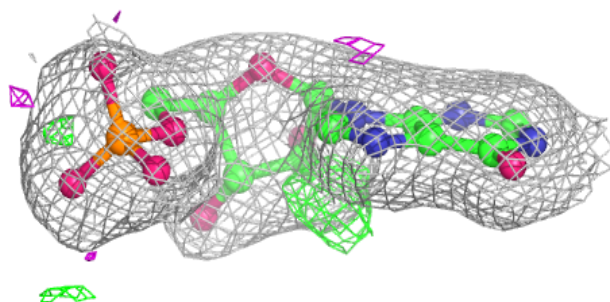
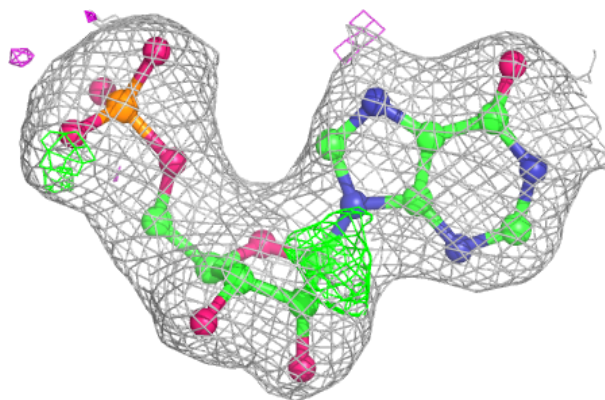


**Electron density around NAP D 502:**

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and green (positive)

**Electron density around IMP H 502:**

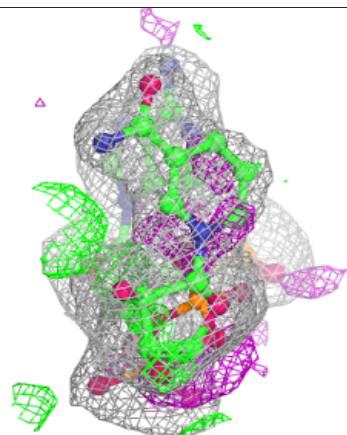
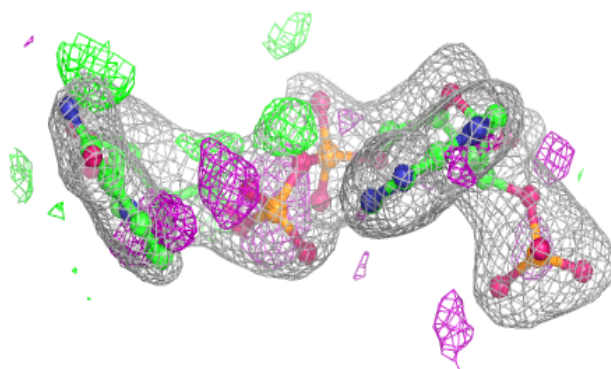
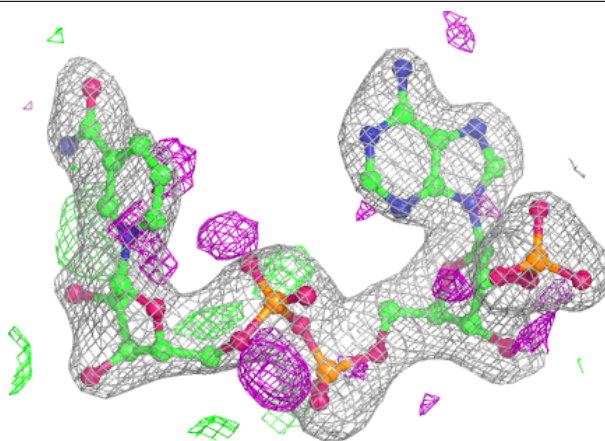
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



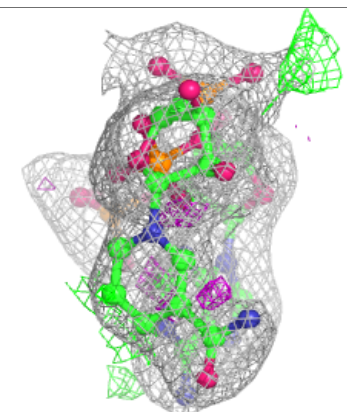
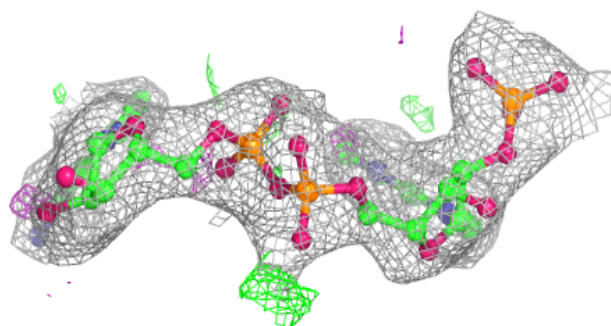
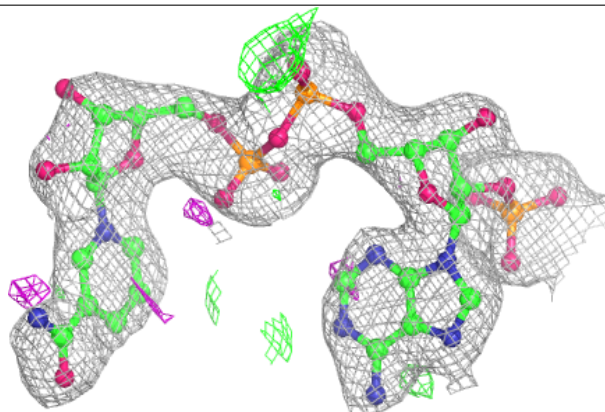


**Electron density around NAP A 502:**

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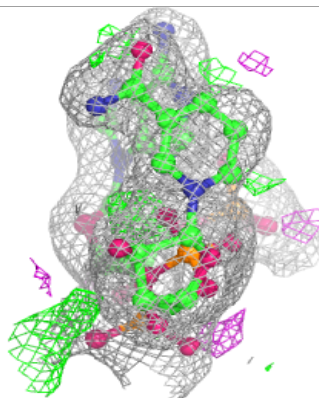
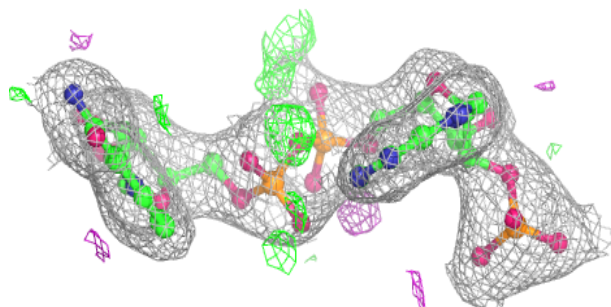
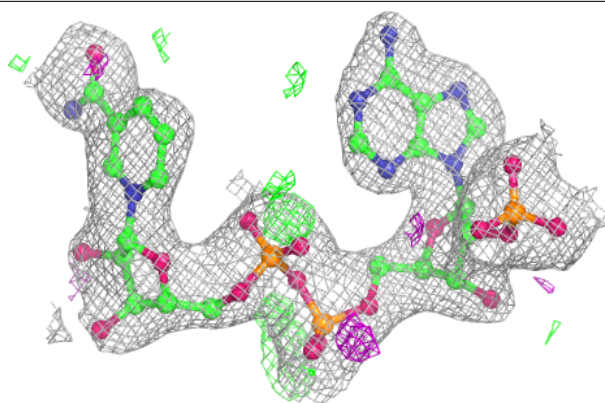
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and green (positive)

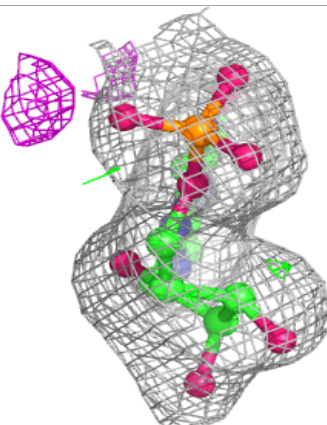
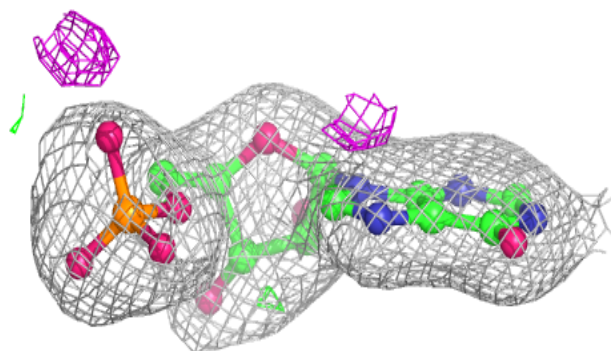
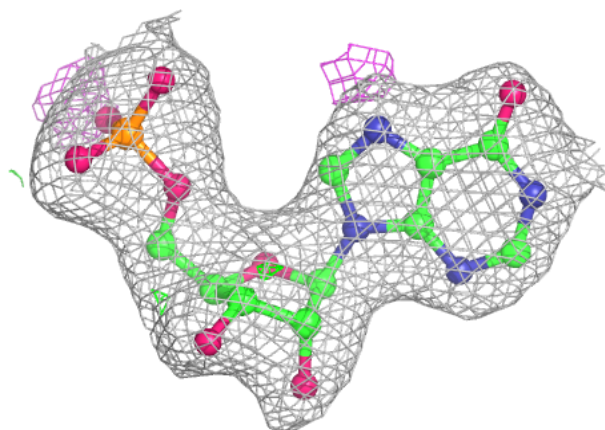


**Electron density around NAP F 502:**

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and green (positive)

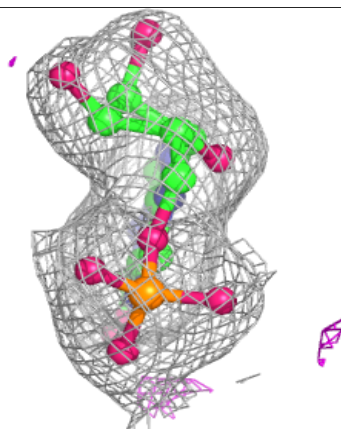
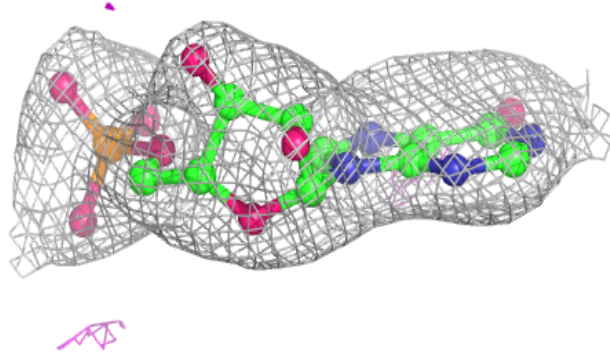
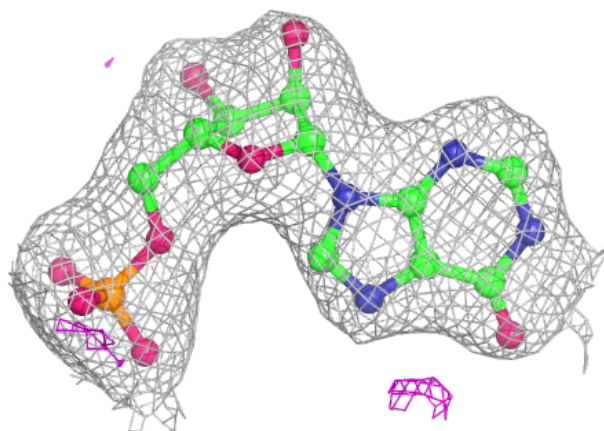
**Electron density around IMP G 503:**

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and green (positive)



**Electron density around IMP E 503:**

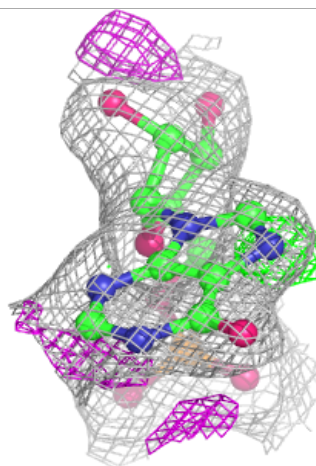
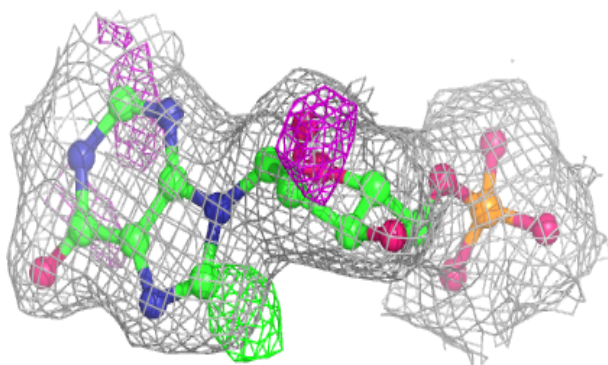
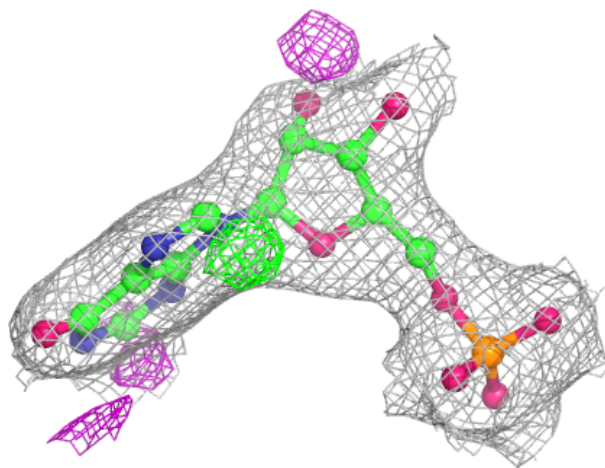
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





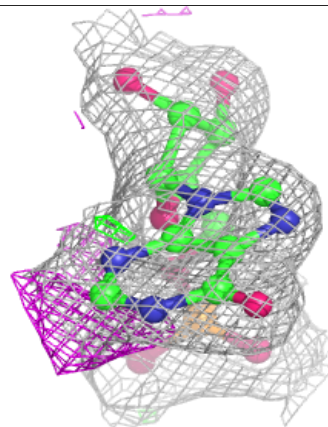
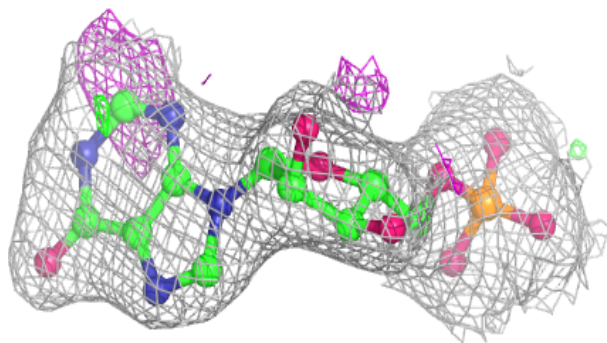
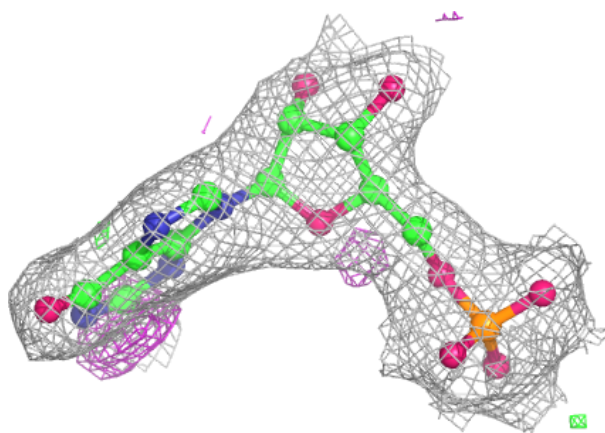
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and green (positive)



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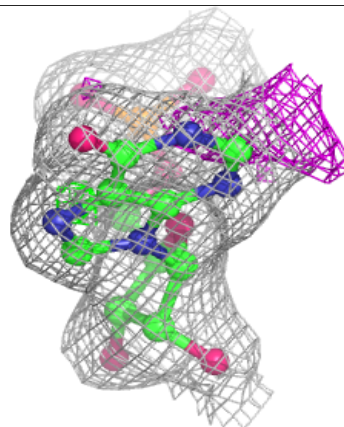
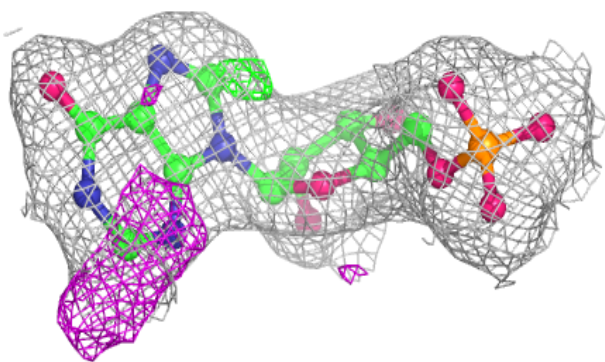
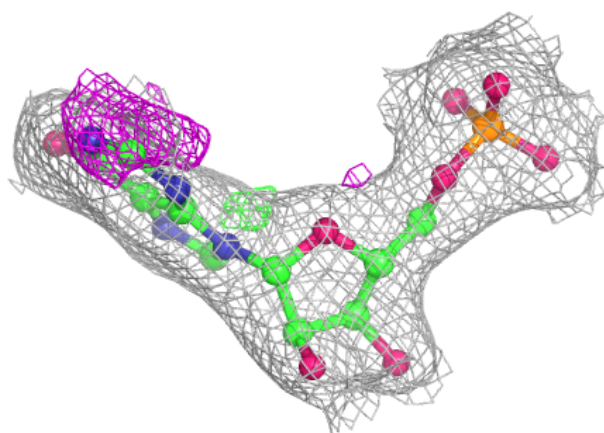
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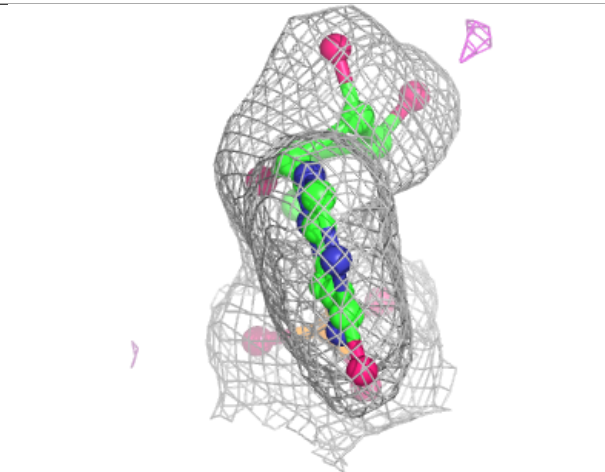
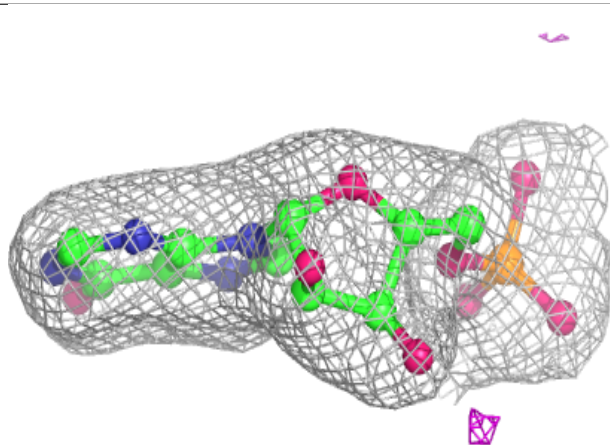
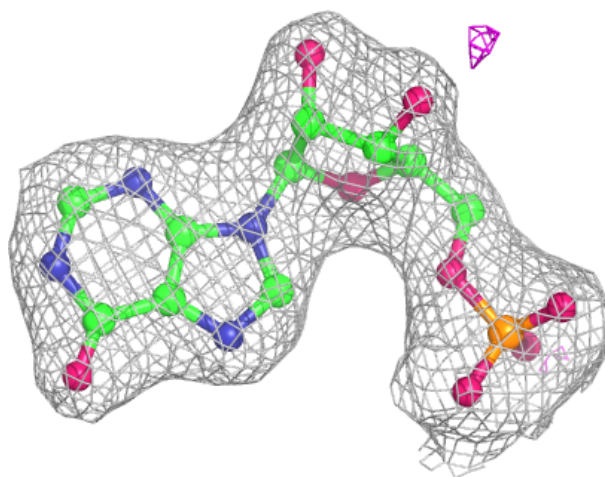
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and green (positive)



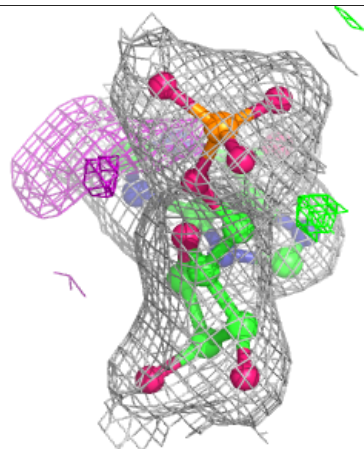
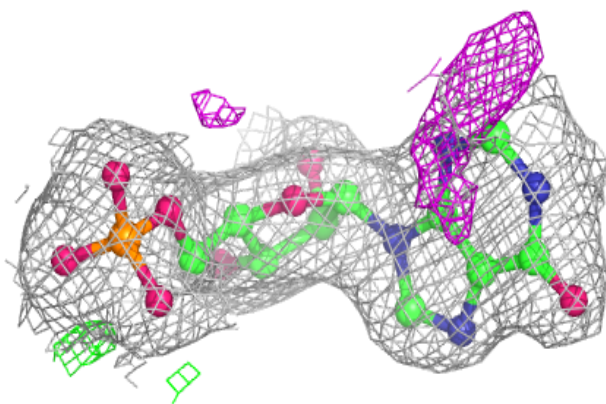
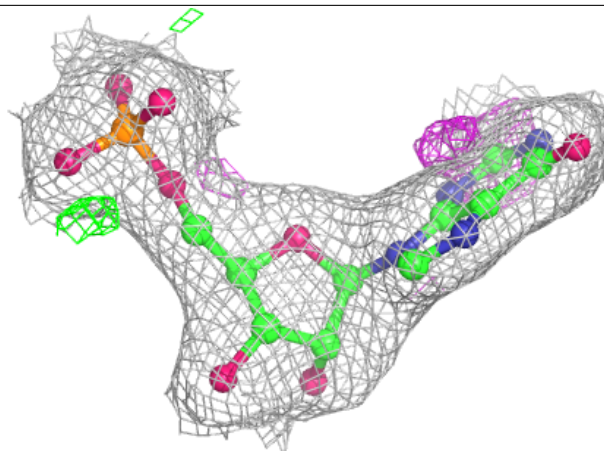
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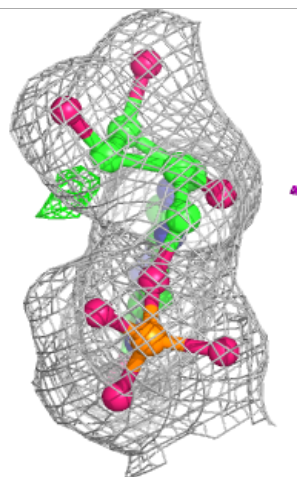
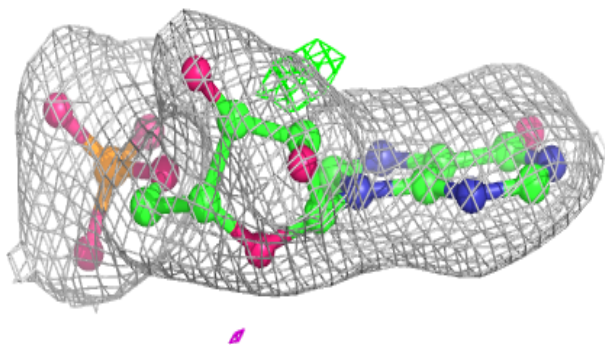
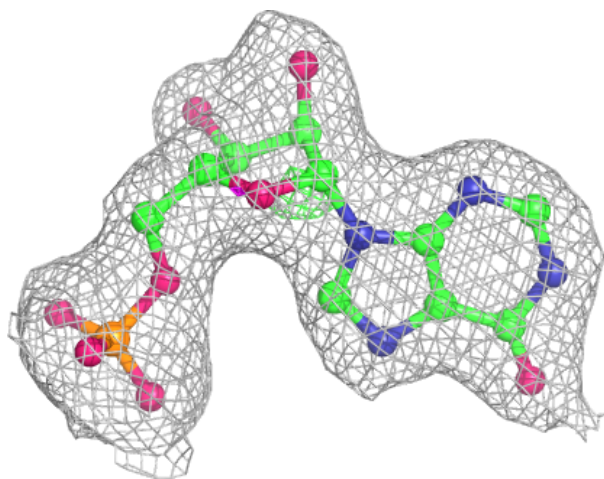
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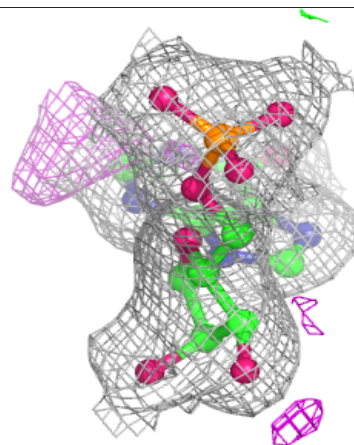
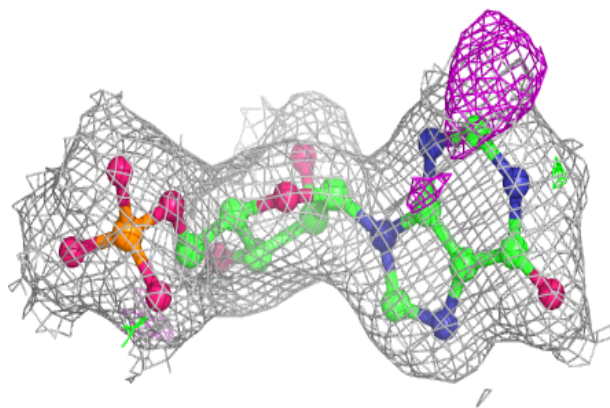
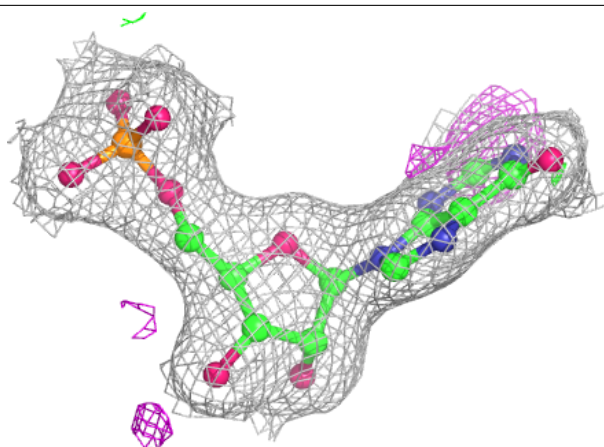
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and green (positive)



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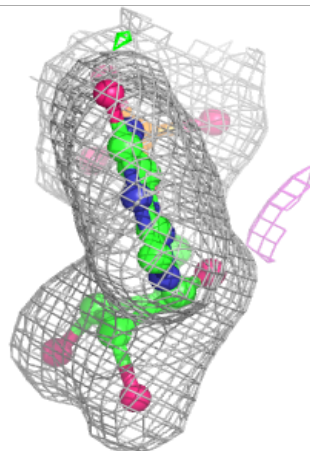
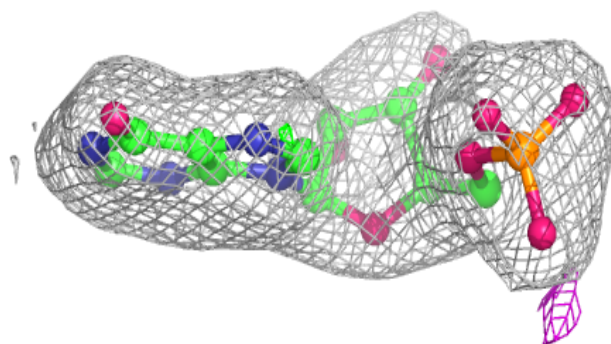
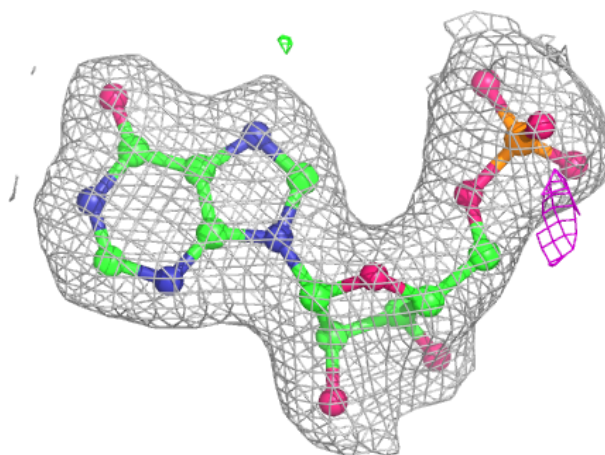
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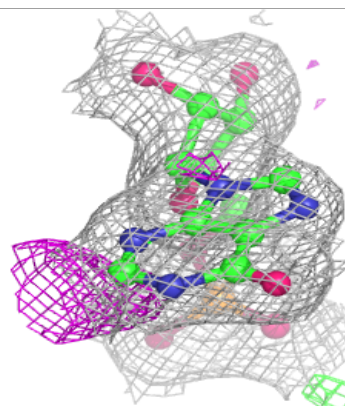
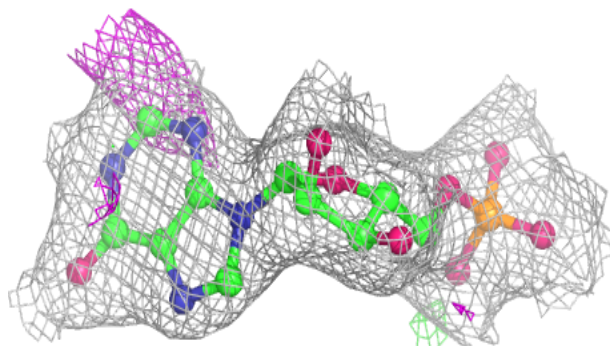
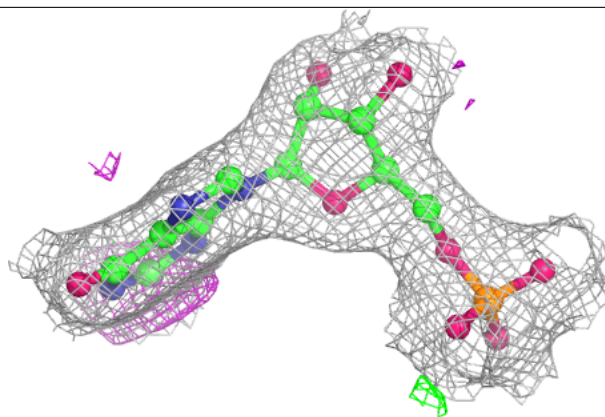
**Electron density around IMP A 503:**

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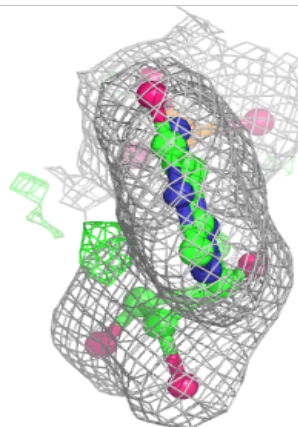
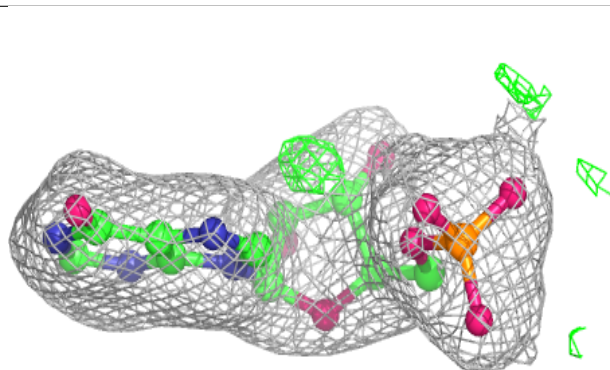
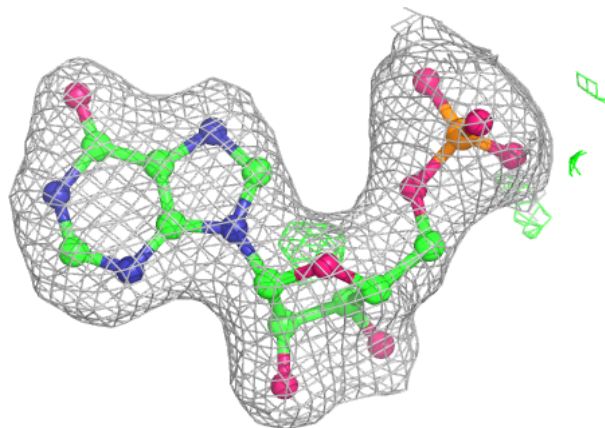


**Electron density around IMP B 501:**

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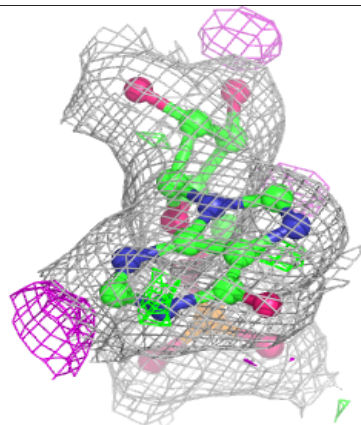
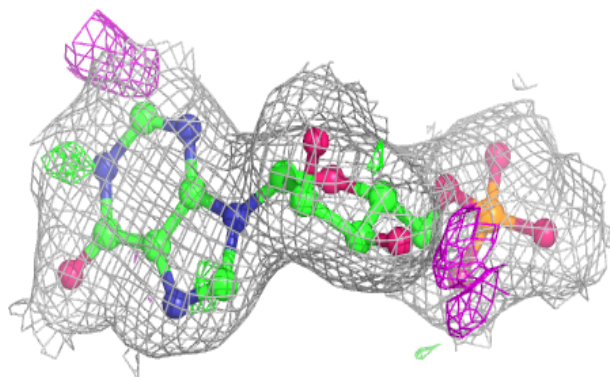
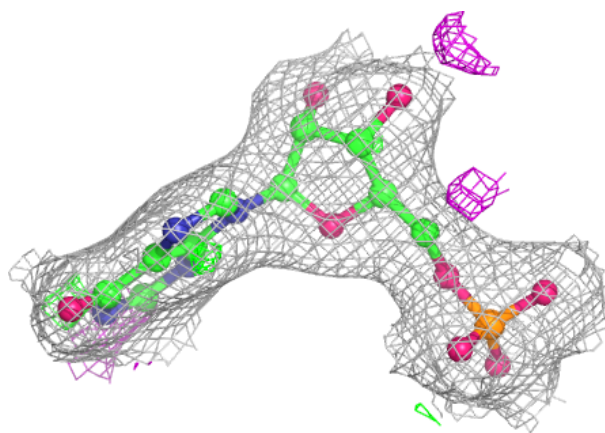
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and green (positive)

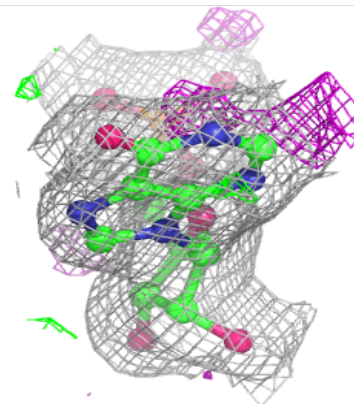
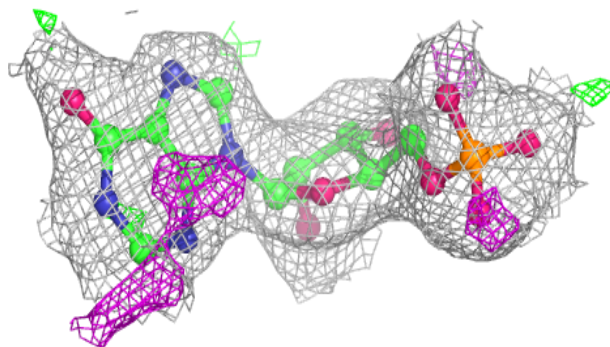
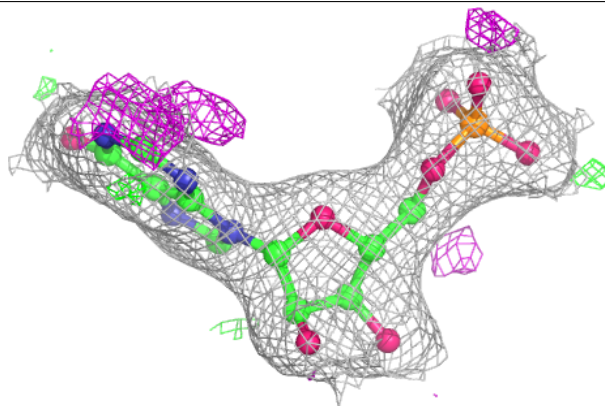


**Electron density around IMP C 501:**

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

**Electron density around IMP A 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.