



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:37 AM UTC

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

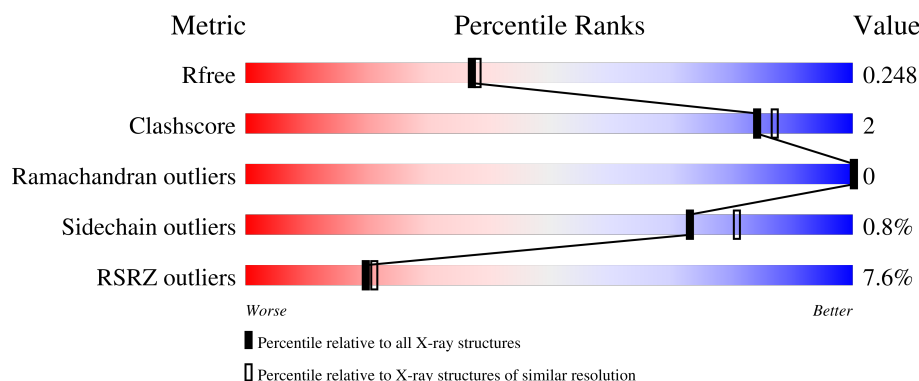
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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	6% 90% 6% 5%
1	B	496	5% 91% • 5%
1	C	496	7% 90% 5% 5%
1	D	496	6% 90% 5% 5%
1	E	496	10% 90% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	496	7% 90% 5% 5%
1	G	496	9% 89% 6% 5%
1	H	496	9% 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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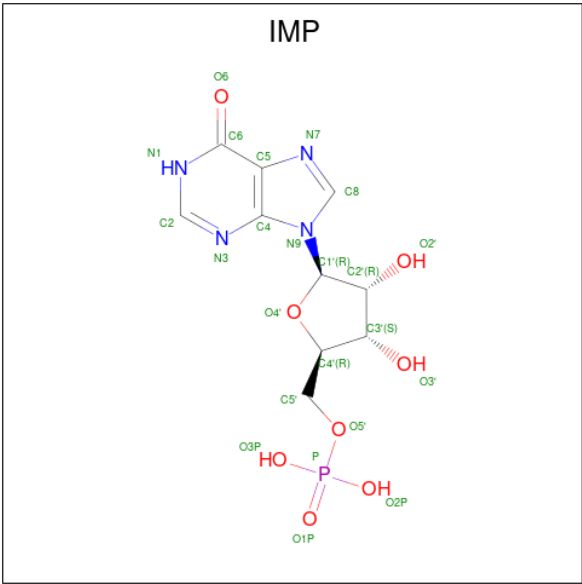
Chain	Residue	Modelled	Actual	Comment	Reference
F	486	ASP	-	expression tag	UNP A0QYE8
F	487	LEU	-	expression tag	UNP A0QYE8
F	488	GLU	-	expression tag	UNP A0QYE8
F	489	HIS	-	expression tag	UNP A0QYE8
F	490	HIS	-	expression tag	UNP A0QYE8
F	491	HIS	-	expression tag	UNP A0QYE8
F	492	HIS	-	expression tag	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: C₁₀H₁₃N₄O₈P) (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

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



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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		

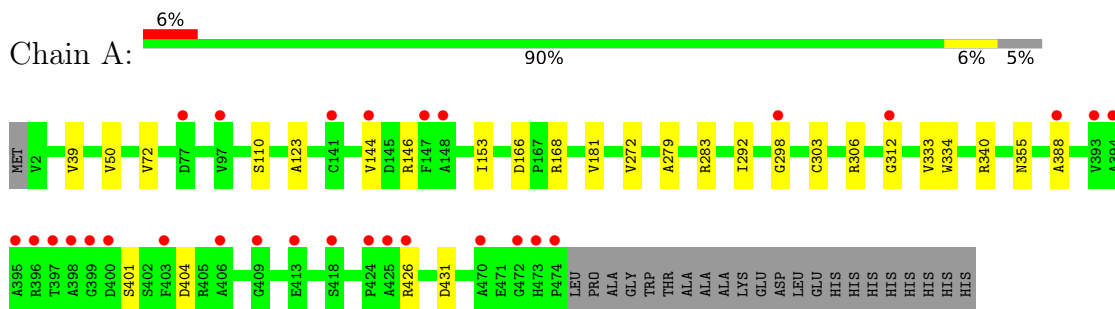
- Molecule 4 is water.

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		

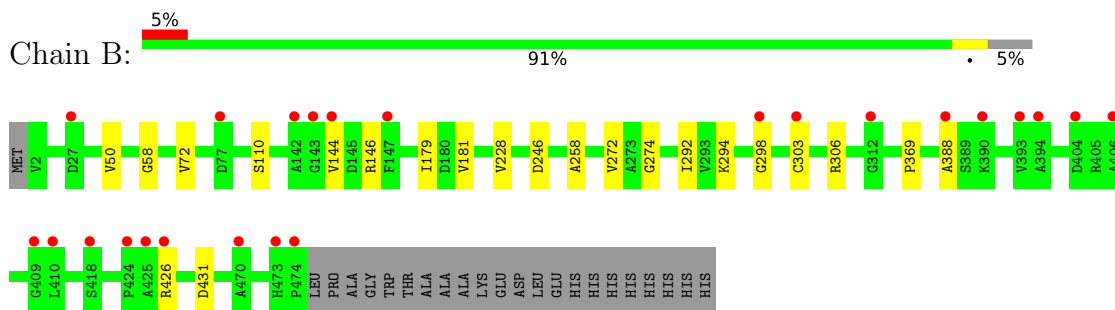
3 Residue-property plots [i](#)

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.

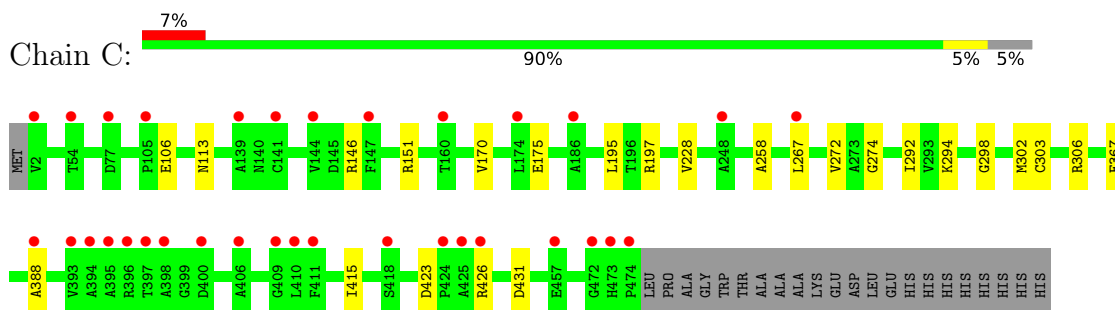
- Molecule 1: GMP reductase



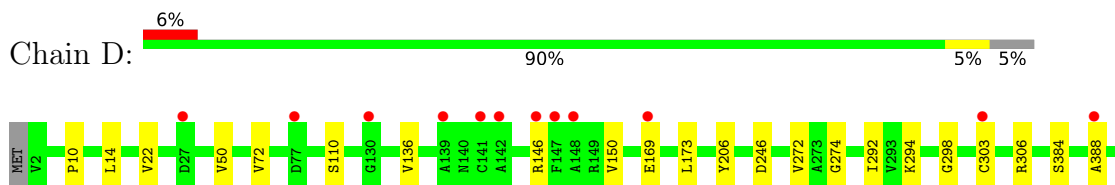
- Molecule 1: GMP reductase



- Molecule 1: GMP reductase

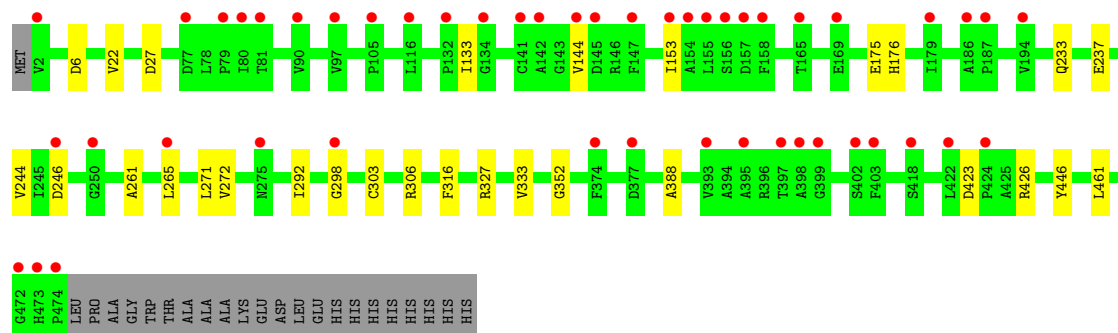
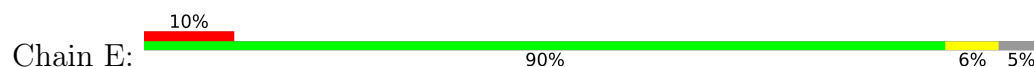


- Molecule 1: GMP reductase

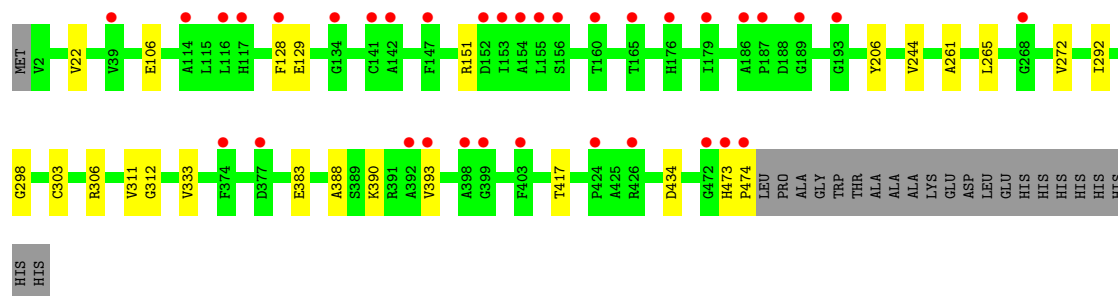
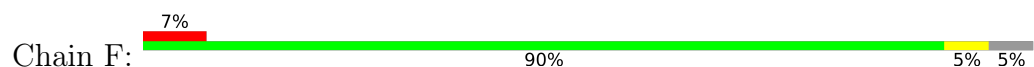




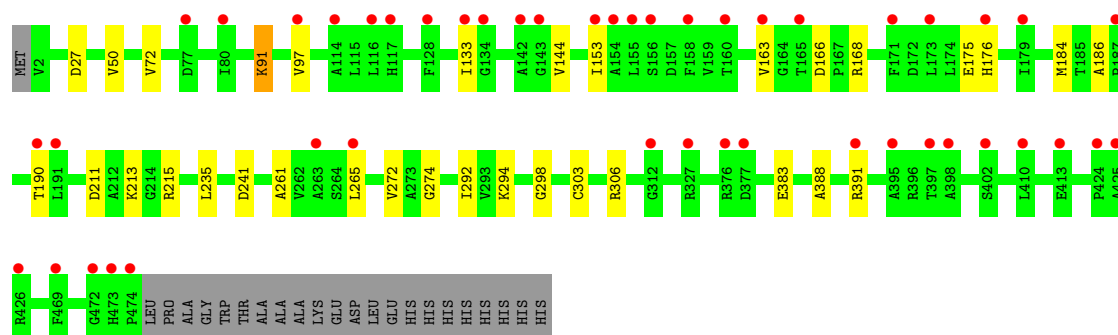
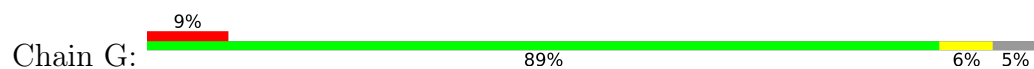
• Molecule 1: GMP reductase



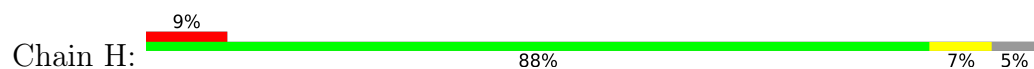
• Molecule 1: GMP reductase

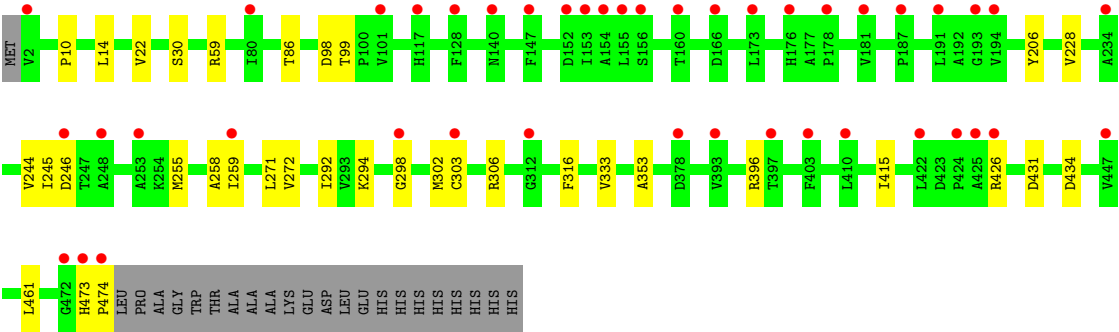


• Molecule 1: GMP reductase



• Molecule 1: GMP reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.10Å)	Xtrriage
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 ²)	49.5	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28877	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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.

All (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
1:A:110:SER:HB2	1:A:146:ARG:HB3	1.84	0.59
1:C:175:GLU:OE1	1:C:197:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ARG:N	1:C:146:ARG:HD2	2.17	0.58
1:A:298:GLY:HA3	1:A:306:ARG:HE	1.69	0.57
1:D:272:VAL:HG22	1:D:292:ILE:HB	1.87	0.57
1:G:166:ASP:OD2	1:G:168:ARG:HB3	2.05	0.56
1:F:272:VAL:HG22	1:F:292:ILE:HB	1.86	0.56
1:E:272:VAL:HG22	1:E:292:ILE:HB	1.88	0.56
1:G:272:VAL:HG22	1:G:292:ILE:HB	1.87	0.55
1:G:144:VAL:HG21	1:G:153:ILE:HG21	1.89	0.55
1:H:272:VAL:HG22	1:H:292:ILE:HB	1.88	0.55
1:D:426:ARG:HB2	1:D:431:ASP:HB3	1.89	0.55
1:E:423:ASP:OD2	1:E:426:ARG:HB2	2.07	0.54
1:H:298:GLY:HA3	1:H:306:ARG:HE	1.72	0.54
1:C:272:VAL:HG22	1:C:292:ILE:HB	1.88	0.53
1:A:123:ALA:HB3	1:A:181:VAL:HG21	1.91	0.52
1:A:272:VAL:HG22	1:A:292:ILE:HB	1.92	0.52
1:B:426:ARG:HB2	1:B:431:ASP:HB3	1.91	0.52
1:H:98:ASP:OD2	1:H:99:THR:N	2.43	0.51
1:H:426:ARG:HB2	1:H:431:ASP:HB3	1.92	0.51
1:E:388:ALA:HB2	3:E:502:NAP:H6N	1.93	0.51
1:G:213:LYS:HE3	1:G:215:ARG:NH2	2.26	0.50
1:G:298:GLY:HA3	1:G:306:ARG:HE	1.76	0.50
1:H:59:ARG:HB2	1:H:86:THR:HG23	1.94	0.50
1:A:144:VAL:HG21	1:A:153:ILE:HG21	1.93	0.50
1:B:388:ALA:HB2	3:B:502:NAP:H6N	1.93	0.50
1:B:298:GLY:HA3	1:B:306:ARG:HE	1.76	0.50
1:A:144:VAL:O	1:A:146:ARG:NH2	2.45	0.50
1:A:426:ARG:HB2	1:A:431:ASP:HB3	1.94	0.50
1:D:10:PRO:HG3	1:D:14:LEU:HD21	1.93	0.50
1:B:50:VAL:HB	1:B:72:VAL:HG22	1.94	0.50
1:F:388:ALA:HB2	3:F:502:NAP:H6N	1.95	0.49
1:H:426:ARG:HB2	1:H:431:ASP:CB	2.43	0.49
1:E:298:GLY:HA3	1:E:306:ARG:HE	1.78	0.48
1:G:388:ALA:HB2	3:G:502:NAP:H6N	1.95	0.48
1:H:255:MET:O	1:H:258:ALA:N	2.44	0.48
1:C:388:ALA:HB2	3:C:502:NAP:H6N	1.96	0.48
1:A:401:SER:OG	1:A:404:ASP:OD1	2.32	0.48
3:E:502:NAP:N3A	3:E:502:NAP:H51A	2.29	0.48
1:G:50:VAL:HB	1:G:72:VAL:HG22	1.96	0.48
1:H:246:ASP:OD1	1:H:294:LYS:NZ	2.34	0.48
1:B:144:VAL:O	1:B:146:ARG:NH2	2.45	0.47
1:E:175:GLU:HG2	1:E:176:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:ARG:NH2	1:E:352:GLY:O	2.47	0.47
1:C:274:GLY:HA3	1:C:294:LYS:HB3	1.96	0.47
1:D:50:VAL:HB	1:D:72:VAL:HG22	1.95	0.47
1:D:136:VAL:HG21	1:D:150:VAL:HG13	1.97	0.47
1:H:298:GLY:HA3	1:H:306:ARG:NE	2.29	0.47
1:G:97:VAL:HG21	1:G:163:VAL:HG23	1.97	0.47
1:G:97:VAL:HG22	1:G:184:MET:HG3	1.96	0.47
1:A:279:ALA:O	1:A:283:ARG:HG3	2.15	0.47
1:D:388:ALA:HB2	3:D:502:NAP:H6N	1.97	0.47
1:A:388:ALA:HB2	3:A:502:NAP:H6N	1.97	0.47
1:A:298:GLY:HA3	1:A:306:ARG:NE	2.28	0.47
1:H:255:MET:SD	1:H:259:ILE:HD11	2.55	0.47
1:G:186:ALA:HB3	1:G:190:THR:HG22	1.97	0.46
1:C:228:VAL:HG11	1:C:258:ALA:HB1	1.98	0.46
1:B:228:VAL:HG11	1:B:258:ALA:HB1	1.98	0.45
1:H:244:VAL:HG22	1:H:272:VAL:HB	1.99	0.45
1:D:298:GLY:HA3	1:D:306:ARG:NE	2.29	0.45
1:C:106:GLU:OE1	1:C:151:ARG:NH2	2.45	0.45
1:B:426:ARG:HB2	1:B:431:ASP:CB	2.46	0.45
1:E:244:VAL:HG22	1:E:272:VAL:HB	1.98	0.45
1:G:298:GLY:HA3	1:G:306:ARG:NE	2.31	0.45
1:D:169:GLU:O	1:D:173:LEU:HG	2.17	0.45
1:G:261:ALA:O	1:G:265:LEU:HD13	2.16	0.45
1:E:246:ASP:OD2	3:E:502:NAP:H3D	2.17	0.45
1:B:246:ASP:OD2	3:B:502:NAP:H3D	2.16	0.44
1:G:27:ASP:OD1	1:G:27:ASP:N	2.50	0.44
1:D:206:TYR:OH	1:D:434:ASP:OD1	2.28	0.44
1:F:473:HIS:CG	1:F:474:PRO:HD2	2.52	0.44
1:B:179:ILE:HG22	1:B:181:VAL:HG12	2.00	0.44
1:H:206:TYR:OH	1:H:434:ASP:OD1	2.31	0.44
1:C:302:MET:SD	1:C:415:ILE:HD11	2.58	0.44
1:F:244:VAL:HG22	1:F:272:VAL:HB	1.99	0.44
1:H:302:MET:SD	1:H:415:ILE:HD11	2.58	0.44
1:C:426:ARG:HB2	1:C:431:ASP:HB3	2.00	0.43
1:D:384:SER:HB3	1:D:420:MET:HE3	2.00	0.43
1:F:128:PHE:CE1	1:F:129:GLU:HG3	2.53	0.43
1:H:333:VAL:HG23	1:H:353:ALA:HA	2.00	0.43
1:H:316:PHE:HZ	1:H:461:LEU:HD13	1.83	0.43
1:C:113:ASN:HD22	1:C:146:ARG:NH2	2.17	0.43
1:B:298:GLY:HA3	1:B:306:ARG:NE	2.33	0.43
1:E:261:ALA:O	1:E:265:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:GLY:HA3	1:E:306:ARG:NE	2.33	0.43
1:H:245:ILE:HD11	1:H:271:LEU:HD22	2.00	0.43
1:B:274:GLY:HA3	1:B:294:LYS:HB3	2.00	0.43
1:G:383:GLU:OE2	1:G:391:ARG:NH2	2.47	0.43
1:H:10:PRO:HG3	1:H:14:LEU:HD21	2.01	0.43
1:C:367:GLU:N	1:C:367:GLU:OE1	2.52	0.43
1:C:423:ASP:OD2	1:C:426:ARG:HG2	2.19	0.43
1:G:274:GLY:HA3	1:G:294:LYS:HB3	2.01	0.43
1:A:50:VAL:HB	1:A:72:VAL:HG22	2.01	0.42
1:E:27:ASP:OD1	1:E:27:ASP:N	2.53	0.42
1:H:396:ARG:NH1	4:H:601:HOH:O	2.36	0.42
1:G:91:LYS:NZ	1:G:241:ASP:OD2	2.53	0.42
1:E:446:TYR:CG	1:F:311:VAL:HG11	2.55	0.42
1:E:271:LEU:HD12	1:E:271:LEU:HA	1.90	0.42
1:G:91:LYS:HE2	1:G:211:ASP:OD2	2.20	0.42
1:H:255:MET:HG3	1:H:259:ILE:HD11	2.02	0.42
1:B:58:GLY:HA3	1:B:369:PRO:HG3	2.01	0.42
1:C:426:ARG:HB2	1:C:431:ASP:CB	2.50	0.42
1:E:233:GLN:O	1:E:237:GLU:HG3	2.20	0.41
1:C:170:VAL:HG11	1:C:195:LEU:HD23	2.02	0.41
1:F:306:ARG:NE	1:F:312:GLY:HA3	2.36	0.41
1:H:228:VAL:HG11	1:H:258:ALA:HB1	2.03	0.41
1:A:334:TRP:CD1	1:A:355:ASN:HB2	2.55	0.41
1:F:383:GLU:OE2	1:F:417:THR:HG23	2.20	0.41
1:D:274:GLY:HA3	1:D:294:LYS:HB3	2.03	0.41
1:F:261:ALA:O	1:F:265:LEU:HG	2.20	0.41
1:F:298:GLY:HA3	1:F:306:ARG:NE	2.35	0.41
1:E:144:VAL:HG21	1:E:153:ILE:HG21	2.03	0.41
1:F:106:GLU:OE1	1:F:151:ARG:NH1	2.52	0.41
1:F:390:LYS:HA	1:F:393:VAL:HG22	2.03	0.41
3:E:502:NAP:O2X	1:H:30:SER:OG	2.36	0.41
1:F:206:TYR:OH	1:F:434:ASP:OD1	2.30	0.40
1:A:306:ARG:NE	1:A:312:GLY:HA3	2.36	0.40
1:A:426:ARG:HB2	1:A:431:ASP:CB	2.51	0.40
1:A:166:ASP:OD2	1:A:168:ARG:N	2.47	0.40
1:D:246:ASP:OD1	1:D:294:LYS:NZ	2.48	0.40
1:E:316:PHE:HZ	1:E:461:LEU:HD13	1.85	0.40
1:G:175:GLU:HG2	1:G:176:HIS:CE1	2.56	0.40
1:B:110:SER:HB2	1:B:146:ARG:HB3	2.03	0.40
3:F:502:NAP:N3A	3:F:502:NAP:H51A	2.36	0.40
1:H:473:HIS:CG	1:H:474:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/372 (94%)	346 (99%)	3 (1%)	70	78
1	B	350/372 (94%)	349 (100%)	1 (0%)	86	91
1	C	350/372 (94%)	348 (99%)	2 (1%)	78	86
1	D	349/372 (94%)	347 (99%)	2 (1%)	78	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	349/372 (94%)	344 (99%)	5 (1%)	59	67
1	F	350/372 (94%)	347 (99%)	3 (1%)	70	78
1	G	349/372 (94%)	345 (99%)	4 (1%)	65	74
1	H	348/372 (94%)	346 (99%)	2 (1%)	78	86
All	All	2794/2976 (94%)	2772 (99%)	22 (1%)	73	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	303	CYS
1	A	333	VAL
1	B	303	CYS
1	C	267	LEU
1	C	303	CYS
1	D	22	VAL
1	D	303	CYS
1	E	6	ASP
1	E	22	VAL
1	E	133	ILE
1	E	303	CYS
1	E	333	VAL
1	F	22	VAL
1	F	303	CYS
1	F	333	VAL
1	G	91	LYS
1	G	133	ILE
1	G	235	LEU
1	G	303	CYS
1	H	22	VAL
1	H	303	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	HIS
1	A	473	HIS
1	B	121	HIS
1	B	252	GLN
1	B	341	HIS

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Mol	Chain	Res	Type
1	B	456	HIS
1	B	473	HIS
1	C	113	ASN
1	C	176	HIS
1	C	456	HIS
1	D	341	HIS
1	E	249	HIS
1	E	341	HIS
1	F	113	ASN
1	F	328	GLN
1	G	121	HIS
1	G	176	HIS
1	G	341	HIS
1	H	113	ASN
1	H	121	HIS
1	H	176	HIS
1	H	249	HIS
1	H	341	HIS
1	H	456	HIS
1	H	473	HIS

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 ⓘ

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	E	501	1	25,25,25	0.37	0	37,38,38	0.66	0
2	IMP	B	503	-	25,25,25	0.34	0	37,38,38	0.49	0
2	IMP	C	503	-	25,25,25	0.34	0	37,38,38	0.48	0
3	NAP	C	502	-	50,52,52	0.51	1 (2%)	71,80,80	0.55	1 (1%)
2	IMP	G	501	1	25,25,25	0.37	0	37,38,38	0.66	0
2	IMP	H	501	1	25,25,25	0.38	0	37,38,38	0.67	0
2	IMP	F	501	1	25,25,25	0.38	0	37,38,38	0.68	0
3	NAP	E	502	-	50,52,52	0.51	1 (2%)	71,80,80	0.57	1 (1%)
3	NAP	G	502	-	50,52,52	0.51	1 (2%)	71,80,80	0.54	1 (1%)
2	IMP	D	503	-	25,25,25	0.34	0	37,38,38	0.47	0
2	IMP	B	501	1	25,25,25	0.39	0	37,38,38	0.68	0
2	IMP	F	503	-	25,25,25	0.34	0	37,38,38	0.47	0
2	IMP	A	503	-	25,25,25	0.34	0	37,38,38	0.48	0
2	IMP	G	503	-	25,25,25	0.35	0	37,38,38	0.48	0
3	NAP	A	502	-	50,52,52	0.51	1 (2%)	71,80,80	0.53	1 (1%)
2	IMP	H	502	-	25,25,25	0.34	0	37,38,38	0.48	0
3	NAP	B	502	-	50,52,52	0.50	1 (2%)	71,80,80	0.55	1 (1%)
2	IMP	E	503	-	25,25,25	0.34	0	37,38,38	0.49	0
2	IMP	C	501	1	25,25,25	0.39	0	37,38,38	0.69	0
2	IMP	A	501	1	25,25,25	0.39	0	37,38,38	0.69	0
2	IMP	D	501	1	25,25,25	0.38	0	37,38,38	0.68	0
3	NAP	F	502	-	50,52,52	0.51	1 (2%)	71,80,80	0.56	1 (1%)
3	NAP	G	504	-	50,52,52	0.51	1 (2%)	71,80,80	0.57	1 (1%)
3	NAP	D	502	-	50,52,52	0.51	1 (2%)	71,80,80	0.54	1 (1%)

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	E	501	1	-	0/10/26/26	0/3/3/3
2	IMP	B	503	-	-	0/10/26/26	0/3/3/3
2	IMP	C	503	-	-	0/10/26/26	0/3/3/3
3	NAP	C	502	-	-	10/35/67/67	0/5/5/5
2	IMP	G	501	1	-	0/10/26/26	0/3/3/3
2	IMP	H	501	1	-	0/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	F	501	1	-	0/10/26/26	0/3/3/3
3	NAP	E	502	-	-	10/35/67/67	0/5/5/5
3	NAP	G	502	-	-	9/35/67/67	0/5/5/5
2	IMP	D	503	-	-	0/10/26/26	0/3/3/3
2	IMP	B	501	1	-	0/10/26/26	0/3/3/3
2	IMP	F	503	-	-	0/10/26/26	0/3/3/3
2	IMP	A	503	-	-	0/10/26/26	0/3/3/3
2	IMP	G	503	-	-	0/10/26/26	0/3/3/3
3	NAP	A	502	-	-	8/35/67/67	0/5/5/5
2	IMP	H	502	-	-	0/10/26/26	0/3/3/3
3	NAP	B	502	-	-	9/35/67/67	0/5/5/5
2	IMP	E	503	-	-	0/10/26/26	0/3/3/3
2	IMP	C	501	1	-	0/10/26/26	0/3/3/3
2	IMP	A	501	1	-	0/10/26/26	0/3/3/3
2	IMP	D	501	1	-	0/10/26/26	0/3/3/3
3	NAP	F	502	-	-	9/35/67/67	0/5/5/5
3	NAP	G	504	-	-	8/35/67/67	0/5/5/5
3	NAP	D	502	-	-	10/35/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAP	P2B-O2B	2.05	1.63	1.59
3	E	502	NAP	P2B-O2B	2.04	1.63	1.59
3	G	502	NAP	P2B-O2B	2.03	1.63	1.59
3	D	502	NAP	P2B-O2B	2.03	1.63	1.59
3	B	502	NAP	P2B-O2B	2.02	1.63	1.59
3	C	502	NAP	P2B-O2B	2.02	1.63	1.59
3	G	504	NAP	P2B-O2B	2.02	1.63	1.59
3	F	502	NAP	P2B-O2B	2.01	1.63	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	504	NAP	P2B-O2B-C2B	-3.05	115.30	123.43
3	E	502	NAP	P2B-O2B-C2B	-2.91	115.67	123.43
3	F	502	NAP	P2B-O2B-C2B	-2.88	115.74	123.43
3	B	502	NAP	P2B-O2B-C2B	-2.77	116.03	123.43
3	C	502	NAP	P2B-O2B-C2B	-2.71	116.19	123.43
3	G	502	NAP	P2B-O2B-C2B	-2.66	116.32	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NAP	P2B-O2B-C2B	-2.55	116.61	123.43
3	A	502	NAP	P2B-O2B-C2B	-2.33	117.21	123.43

There are no chirality outliers.

All (73) 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
3	B	502	NAP	C2D-C1D-N1N-C6N
3	C	502	NAP	C5B-O5B-PA-O1A
3	C	502	NAP	C5B-O5B-PA-O3
3	C	502	NAP	PA-O3-PN-O5D
3	C	502	NAP	C2D-C1D-N1N-C2N
3	C	502	NAP	C2D-C1D-N1N-C6N
3	D	502	NAP	C5B-O5B-PA-O1A
3	D	502	NAP	C5B-O5B-PA-O3
3	D	502	NAP	C2D-C1D-N1N-C2N
3	D	502	NAP	C2D-C1D-N1N-C6N
3	E	502	NAP	C5B-O5B-PA-O1A
3	E	502	NAP	C2D-C1D-N1N-C2N
3	E	502	NAP	C2D-C1D-N1N-C6N
3	F	502	NAP	C5B-O5B-PA-O1A
3	F	502	NAP	C2D-C1D-N1N-C2N
3	F	502	NAP	C2D-C1D-N1N-C6N
3	G	502	NAP	C5B-O5B-PA-O1A
3	G	502	NAP	C2D-C1D-N1N-C2N
3	G	502	NAP	C2D-C1D-N1N-C6N
3	G	504	NAP	C5B-O5B-PA-O1A
3	G	504	NAP	C2D-C1D-N1N-C2N
3	G	504	NAP	C2D-C1D-N1N-C6N
3	E	502	NAP	O4D-C4D-C5D-O5D
3	E	502	NAP	C3D-C4D-C5D-O5D
3	C	502	NAP	O4D-C4D-C5D-O5D
3	C	502	NAP	C3D-C4D-C5D-O5D
3	D	502	NAP	PN-O3-PA-O1A
3	G	504	NAP	PN-O3-PA-O1A
3	A	502	NAP	PA-O3-PN-O5D
3	D	502	NAP	PA-O3-PN-O5D

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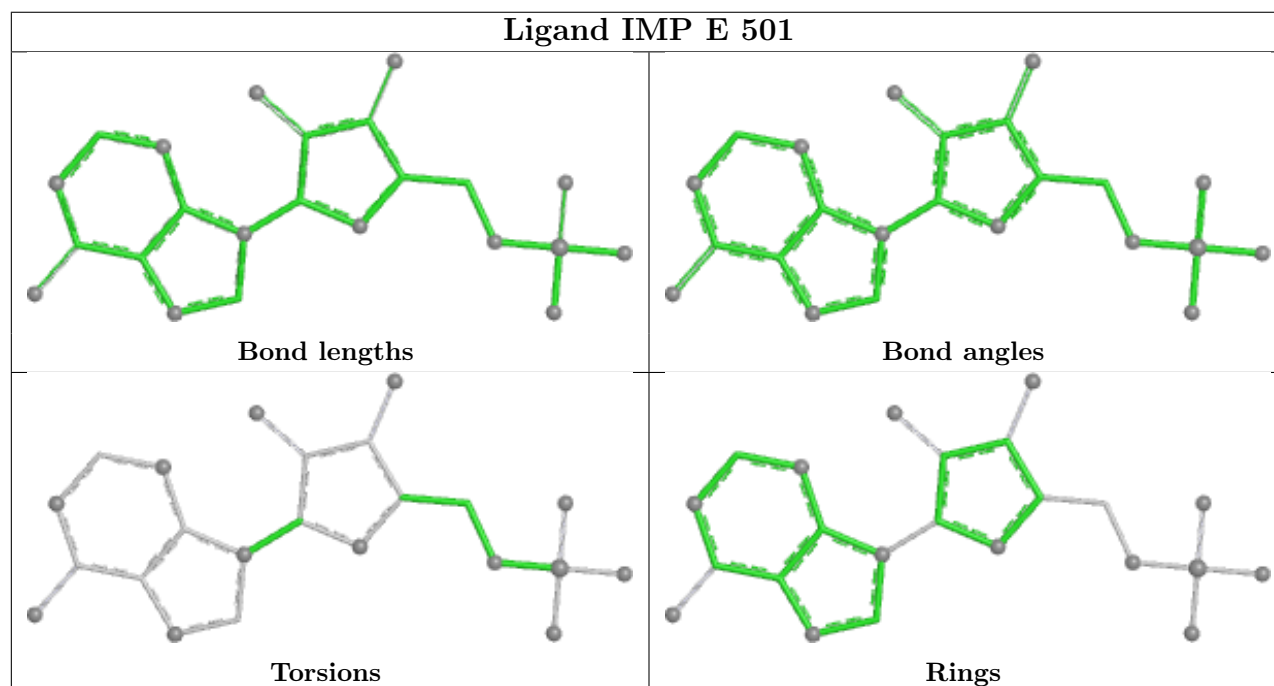
Mol	Chain	Res	Type	Atoms
3	E	502	NAP	PA-O3-PN-O5D
3	F	502	NAP	PA-O3-PN-O5D
3	G	502	NAP	PA-O3-PN-O5D
3	G	504	NAP	PA-O3-PN-O5D
3	G	502	NAP	O4D-C4D-C5D-O5D
3	G	502	NAP	C3D-C4D-C5D-O5D
3	A	502	NAP	PN-O3-PA-O1A
3	E	502	NAP	PN-O3-PA-O2A
3	A	502	NAP	C3D-C4D-C5D-O5D
3	F	502	NAP	C3D-C4D-C5D-O5D
3	F	502	NAP	O4D-C4D-C5D-O5D
3	B	502	NAP	C5B-O5B-PA-O3
3	E	502	NAP	C5B-O5B-PA-O3
3	F	502	NAP	C5B-O5B-PA-O3
3	G	502	NAP	C5B-O5B-PA-O3
3	A	502	NAP	O4D-C4D-C5D-O5D
3	D	502	NAP	PN-O3-PA-O2A
3	F	502	NAP	PN-O3-PA-O1A
3	G	502	NAP	PN-O3-PA-O1A
3	G	504	NAP	PN-O3-PA-O2A
3	D	502	NAP	C3D-C4D-C5D-O5D
3	G	504	NAP	C3D-C4D-C5D-O5D
3	C	502	NAP	C4D-C5D-O5D-PN
3	D	502	NAP	O4D-C4D-C5D-O5D
3	G	504	NAP	O4D-C4D-C5D-O5D
3	B	502	NAP	PN-O3-PA-O1A
3	C	502	NAP	PN-O3-PA-O1A
3	E	502	NAP	PN-O3-PA-O1A
3	F	502	NAP	PN-O3-PA-O2A
3	G	502	NAP	PN-O3-PA-O2A
3	E	502	NAP	C4D-C5D-O5D-PN
3	B	502	NAP	C3D-C4D-C5D-O5D
3	B	502	NAP	O4D-C4D-C5D-O5D
3	A	502	NAP	PN-O3-PA-O2A
3	B	502	NAP	PN-O3-PA-O2A
3	C	502	NAP	PN-O3-PA-O2A
3	B	502	NAP	C2B-O2B-P2B-O3X
3	D	502	NAP	C2B-O2B-P2B-O3X

There are no ring outliers.

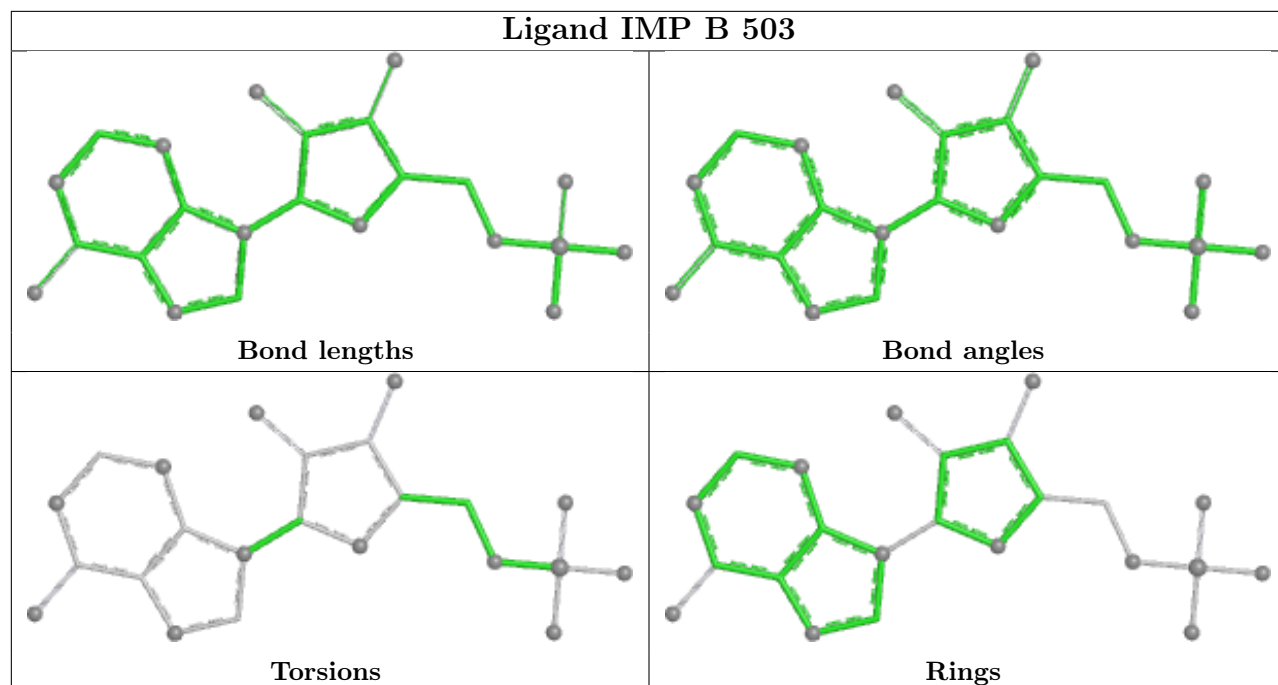
8 monomers are involved in 13 short contacts:

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

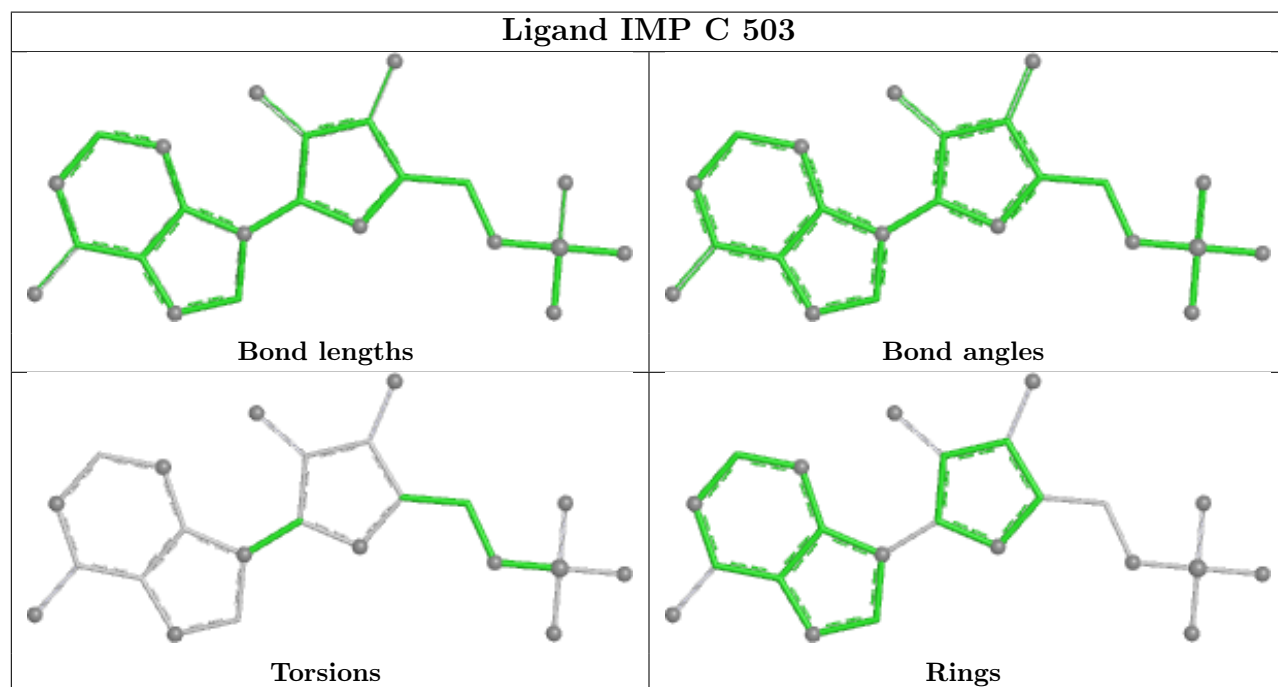
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



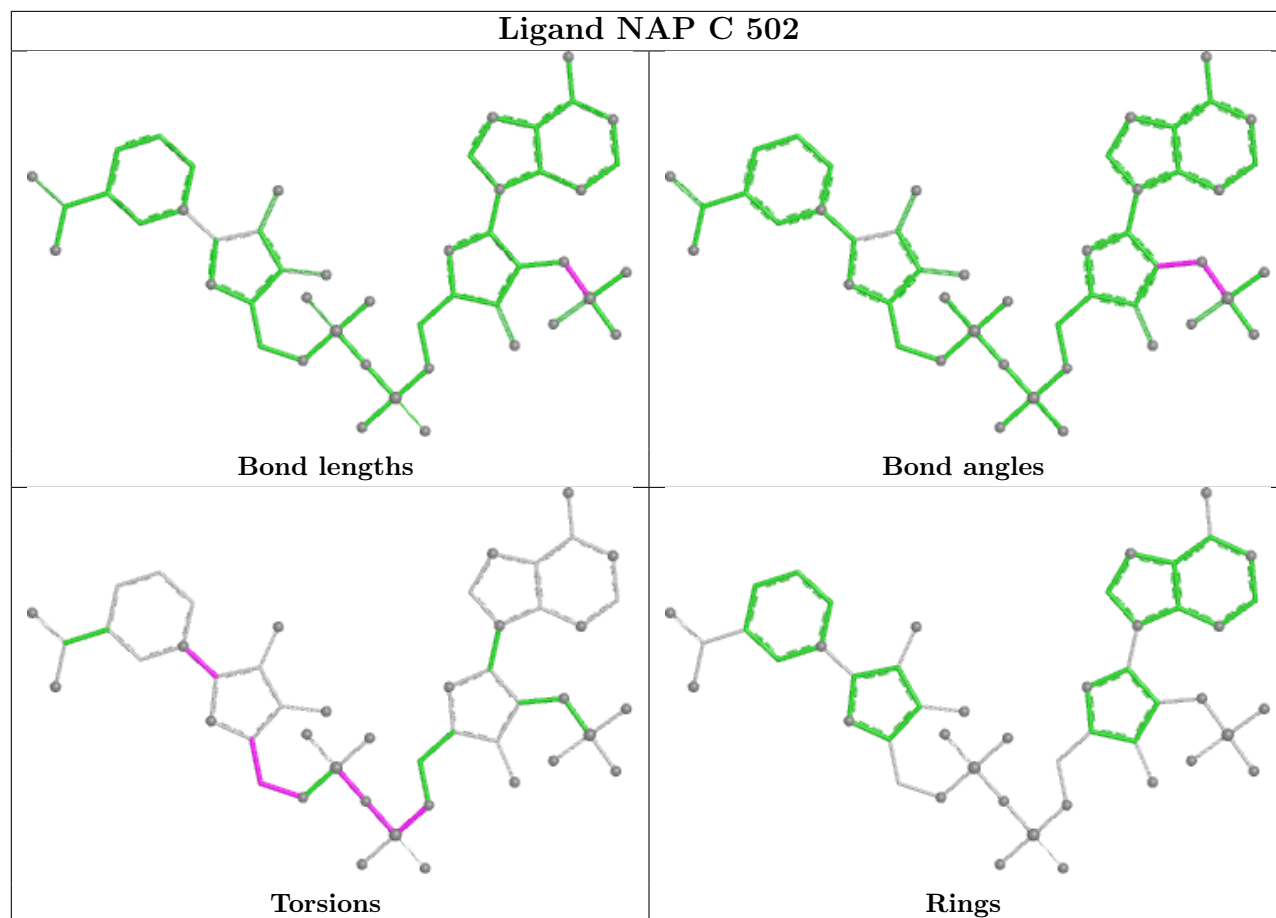
Ligand IMP B 503



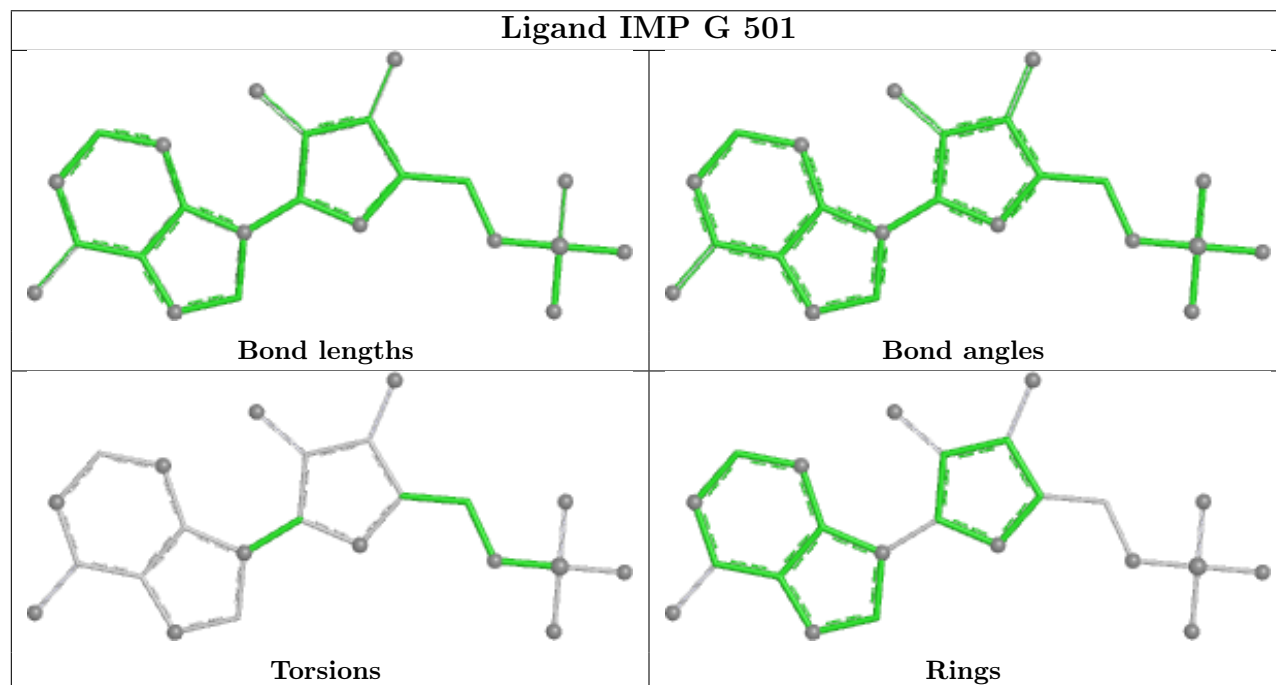
Ligand IMP C 503



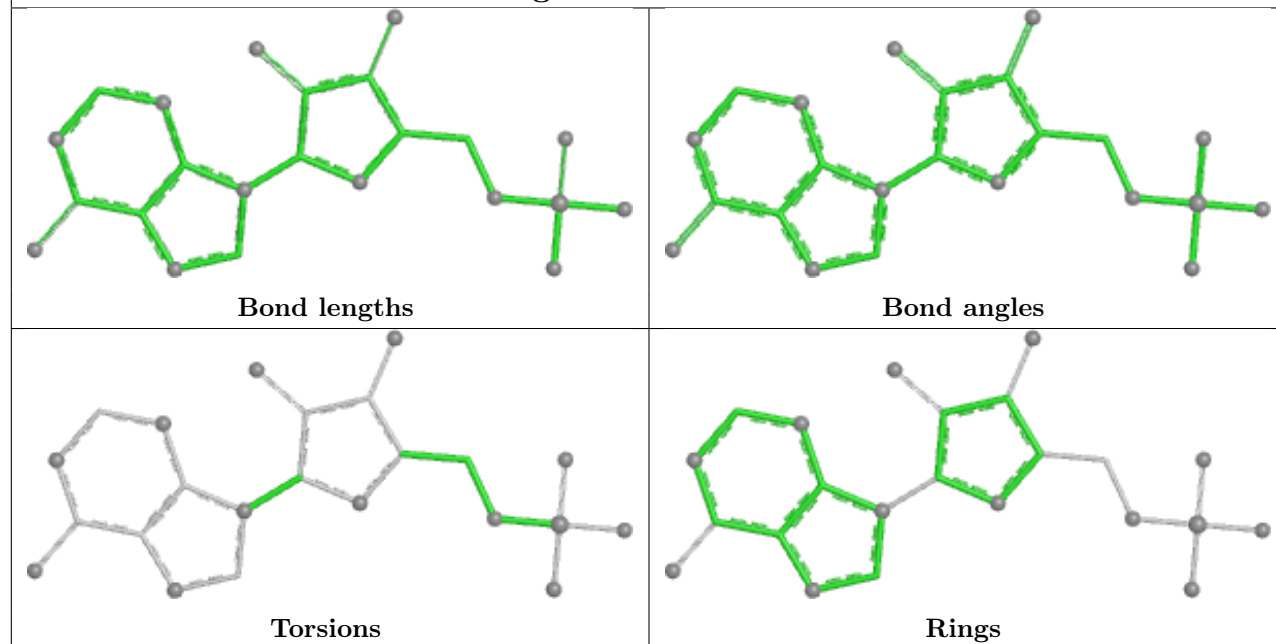
Ligand NAP C 502



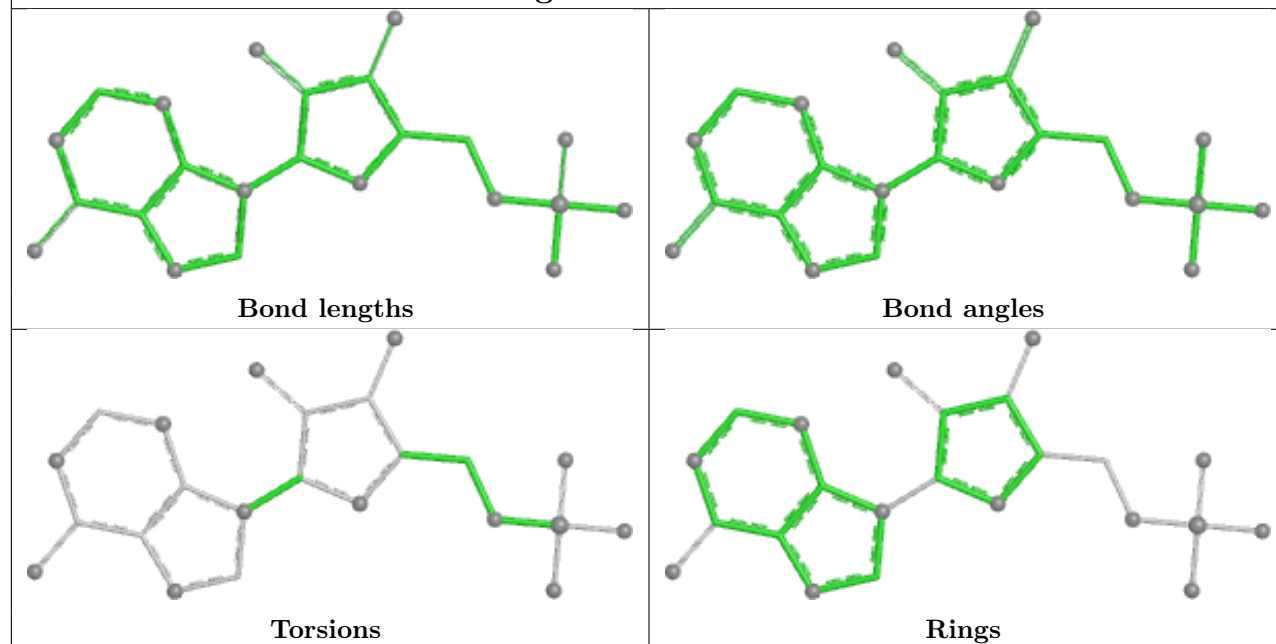
Ligand IMP G 501

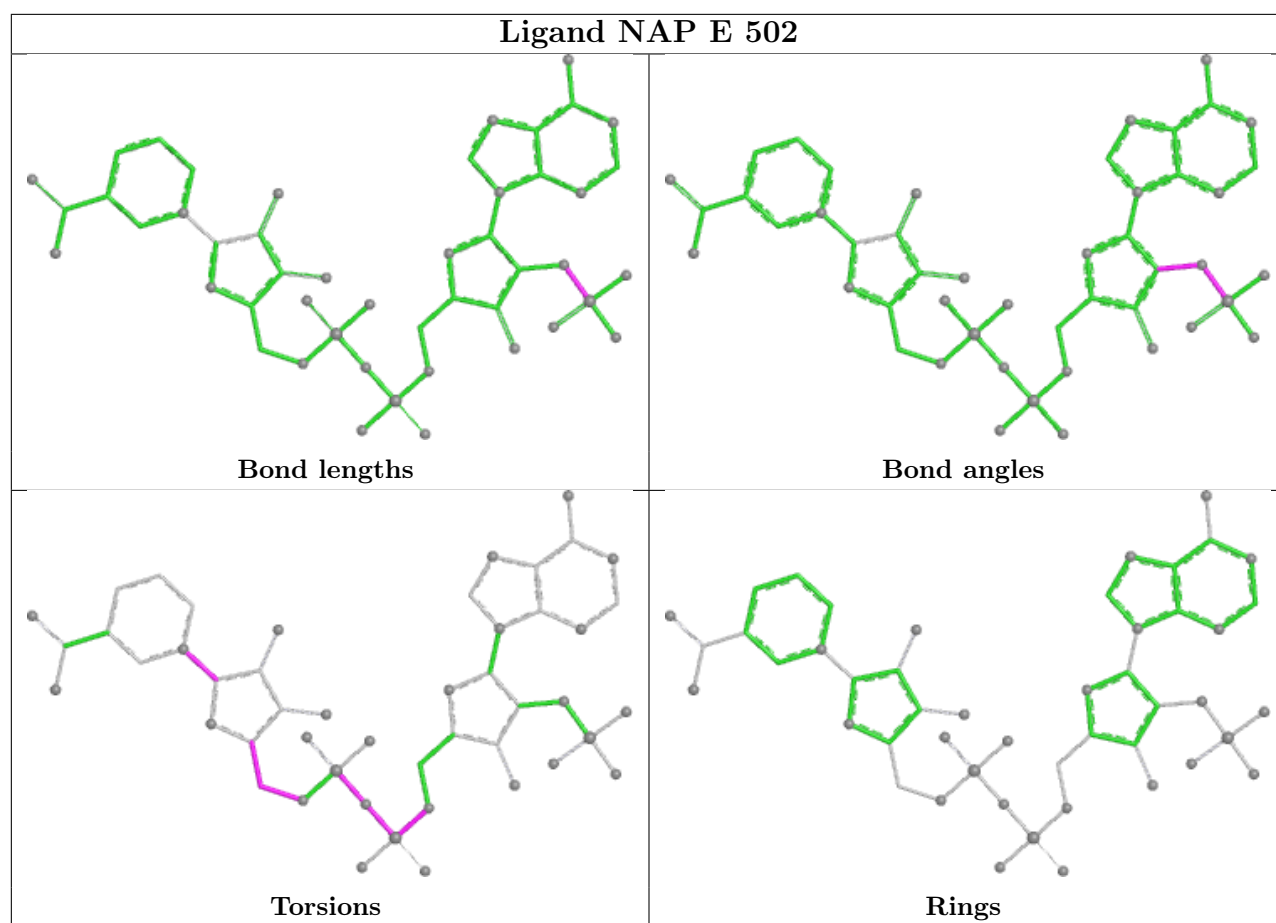


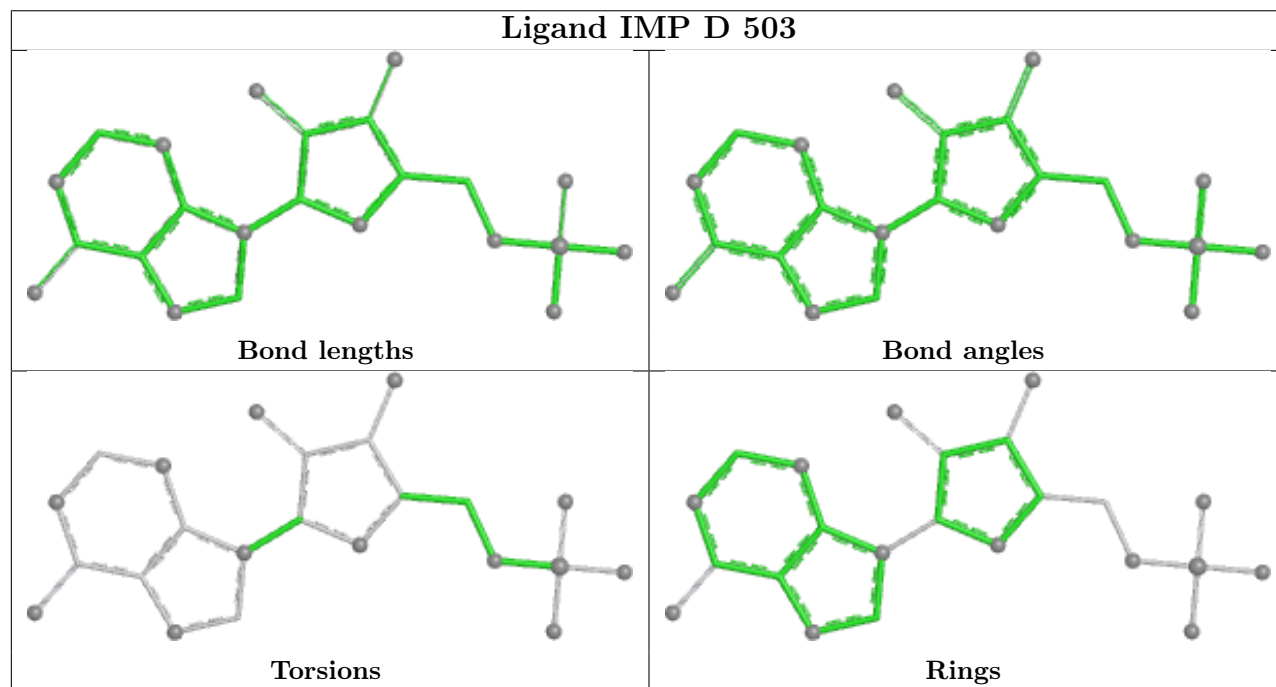
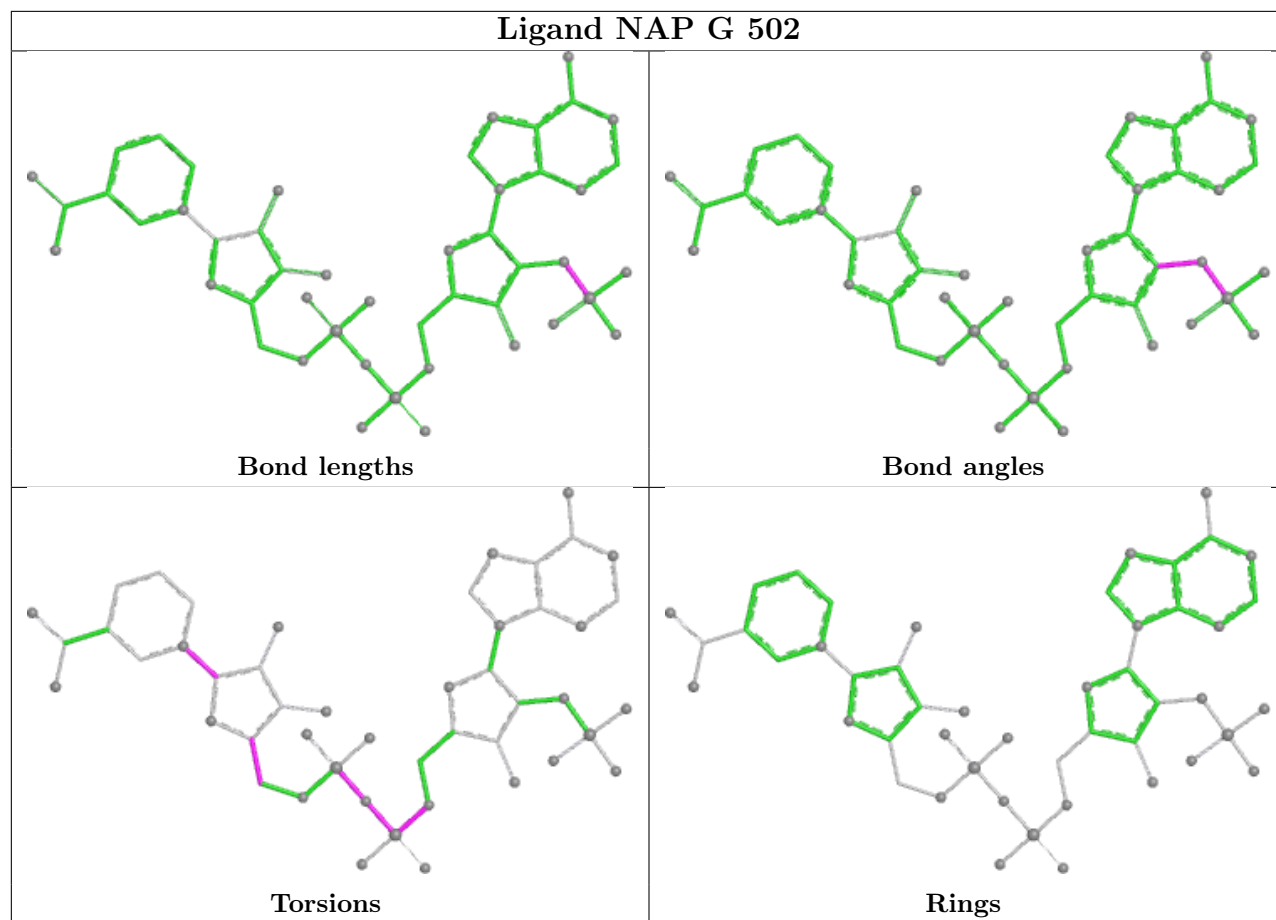
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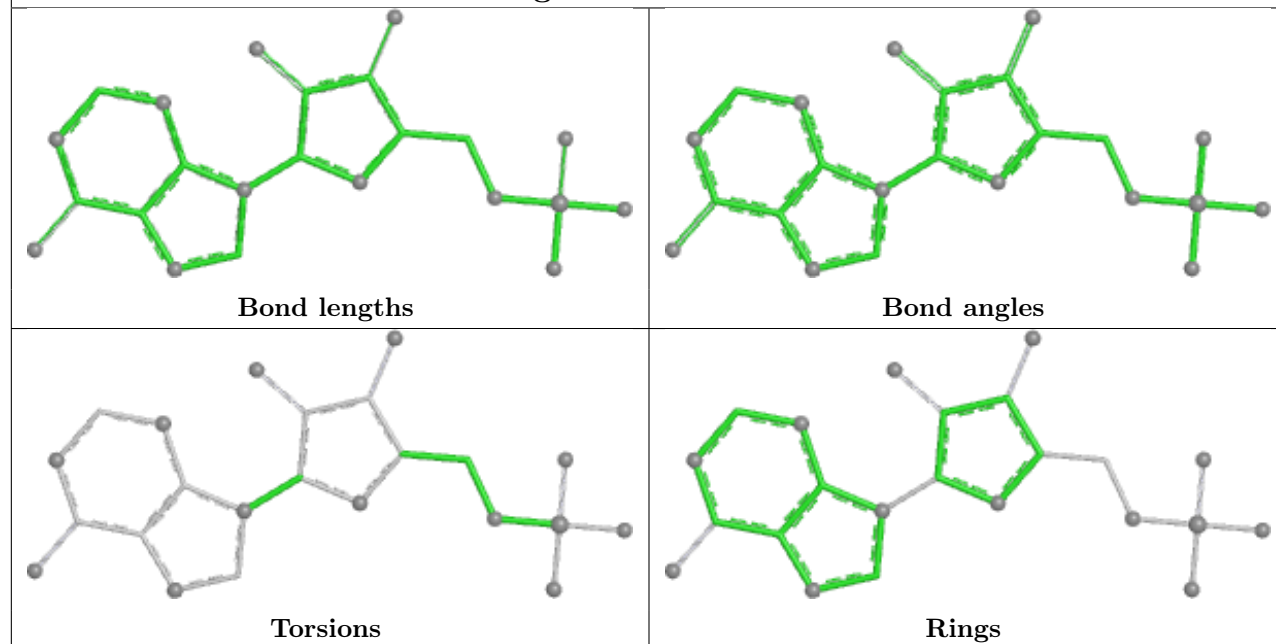
Ligand IMP F 501



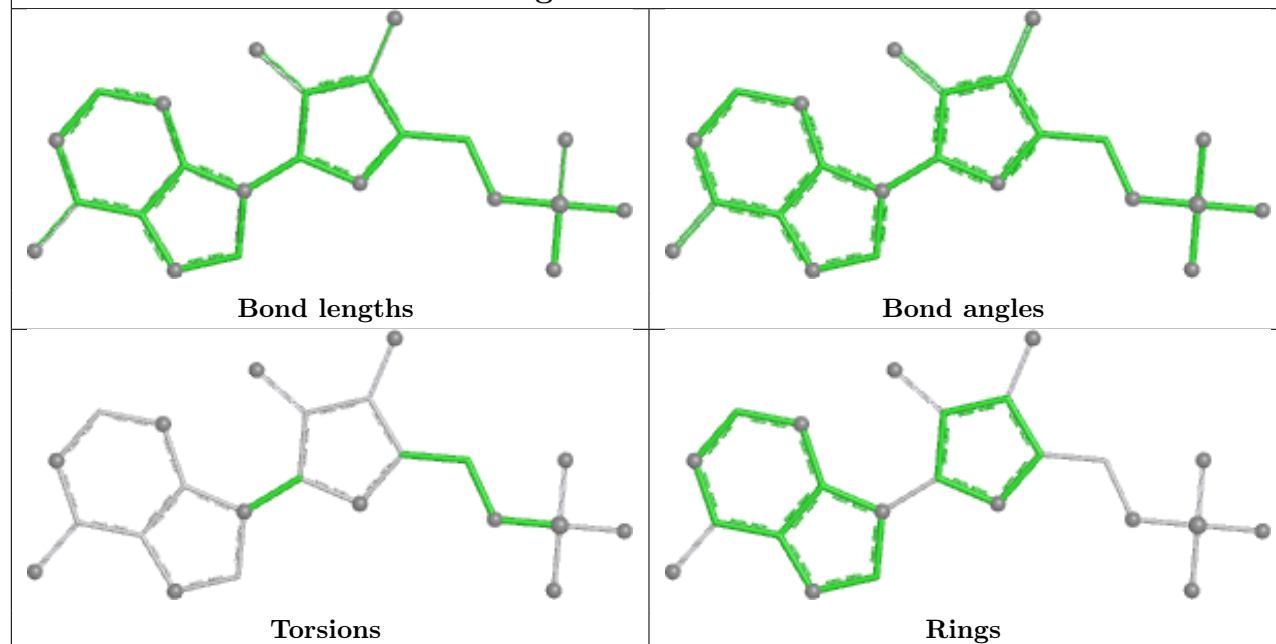




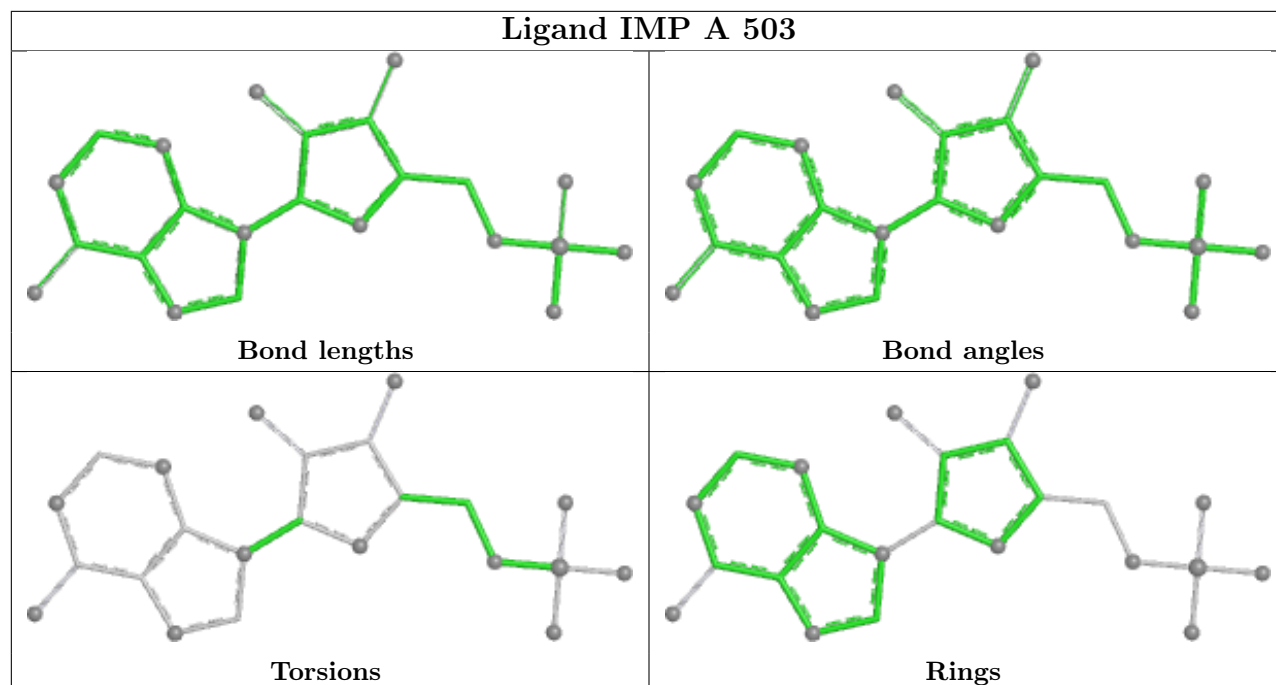
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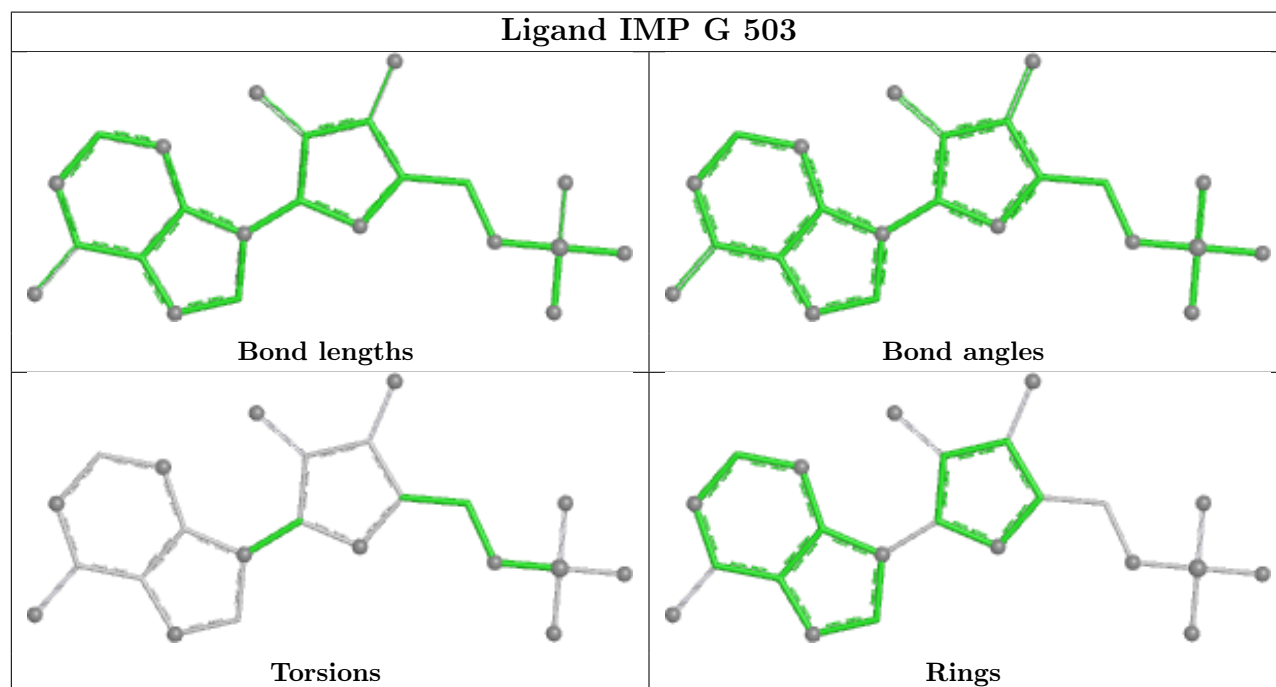
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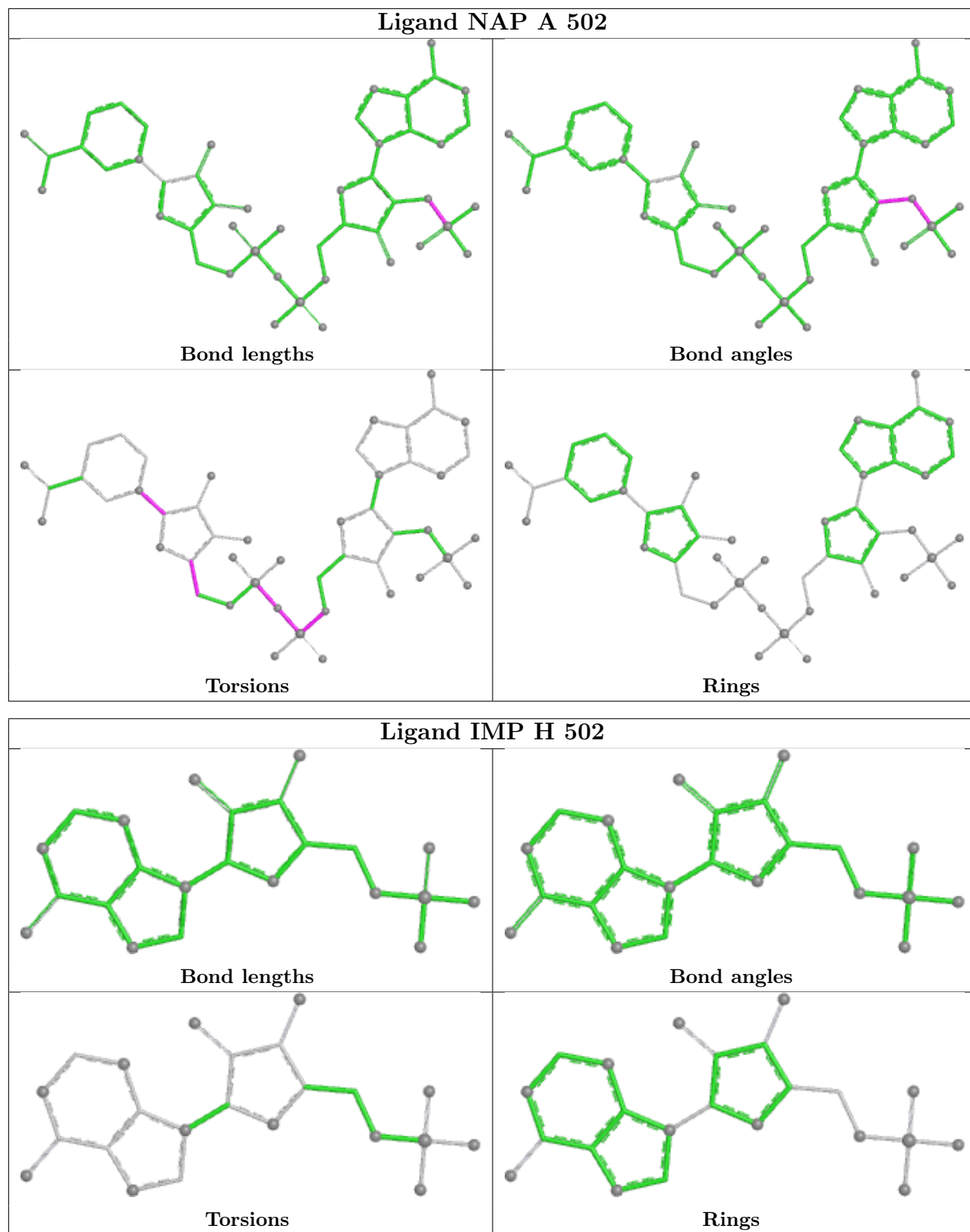


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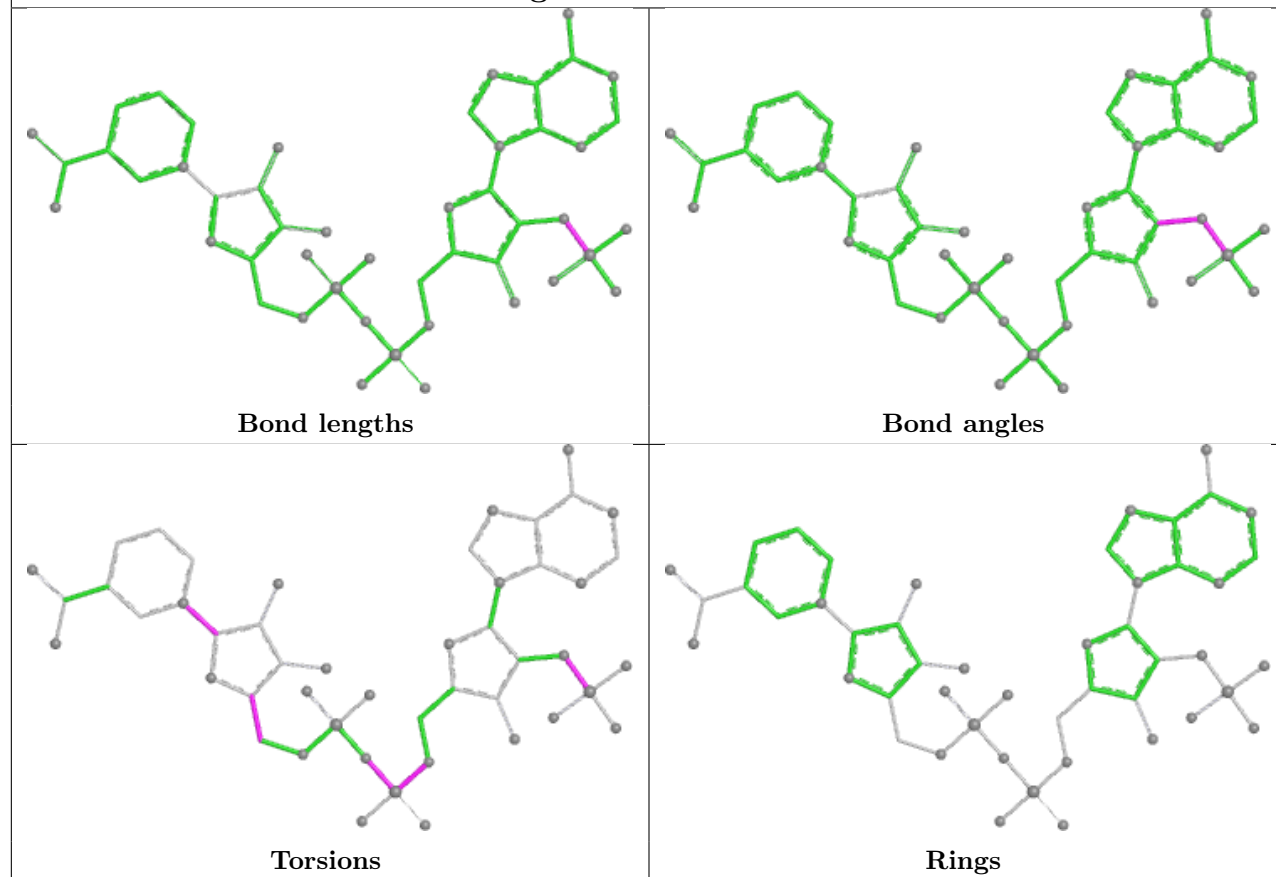


Ligand IMP G 503

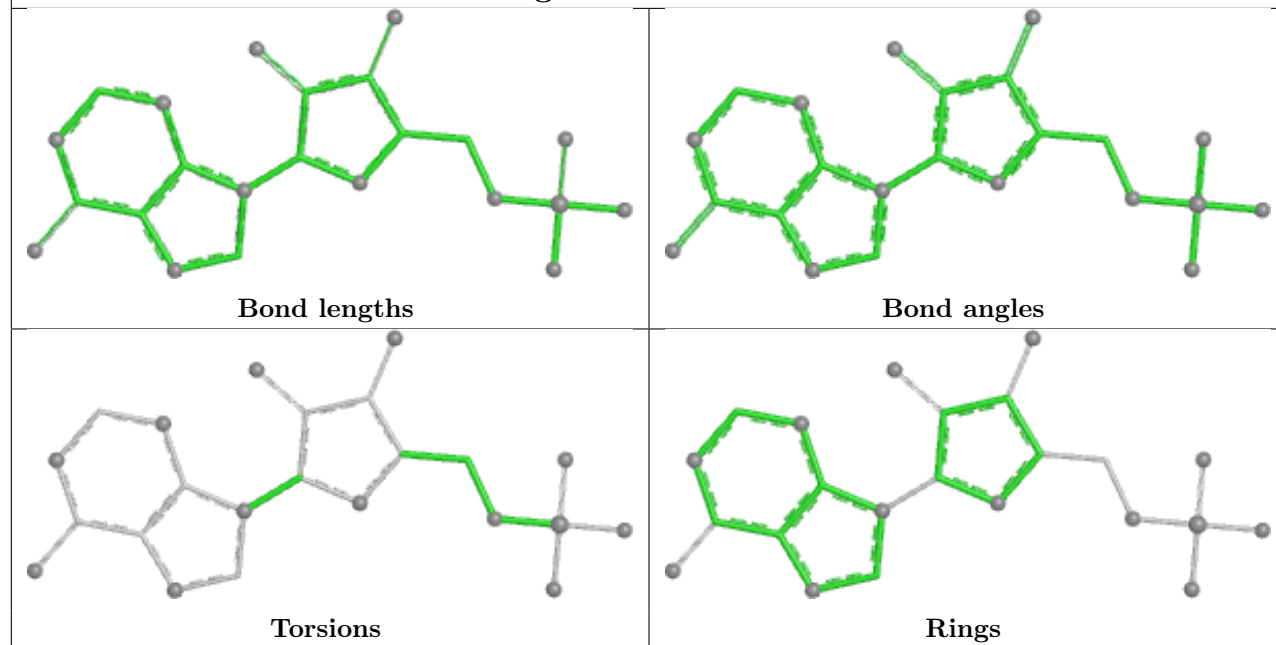




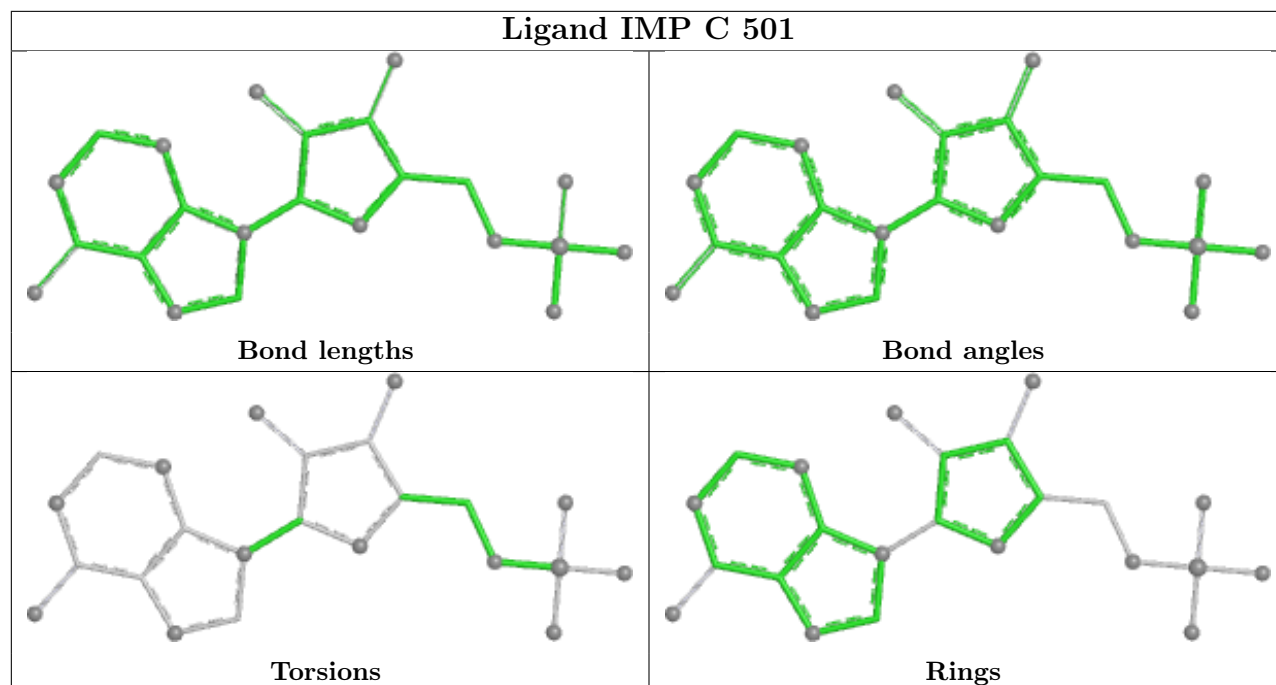
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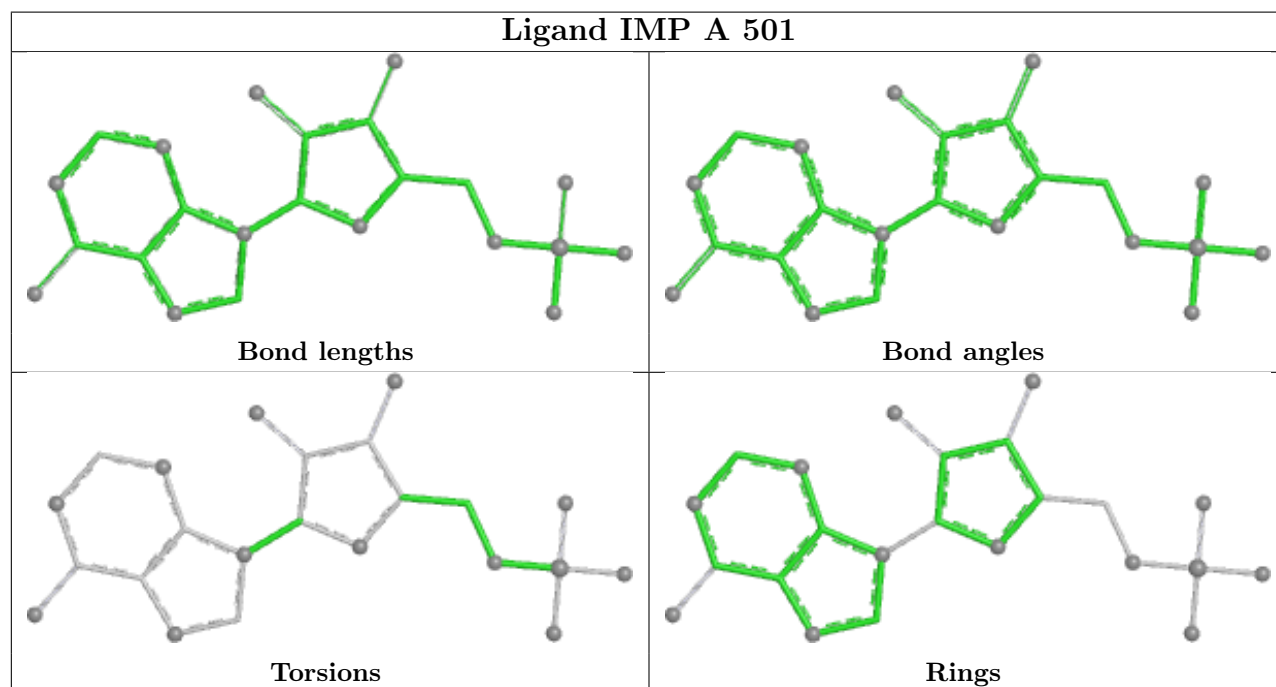
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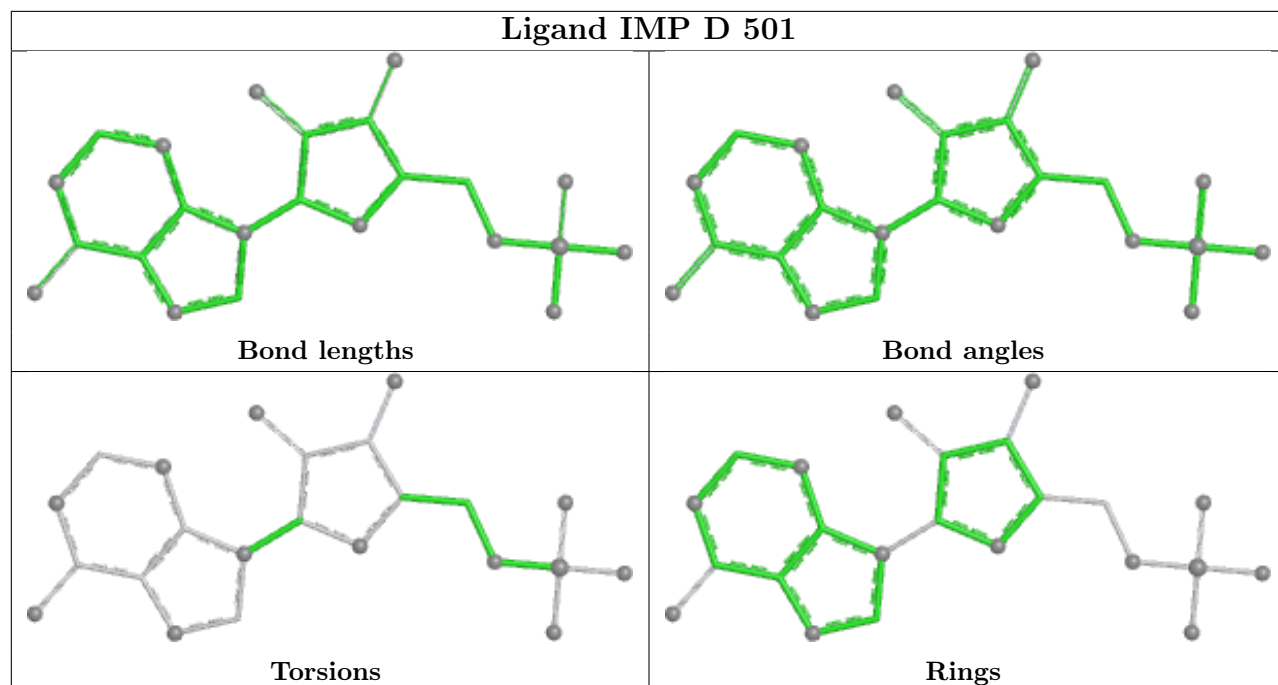
Ligand IMP C 501



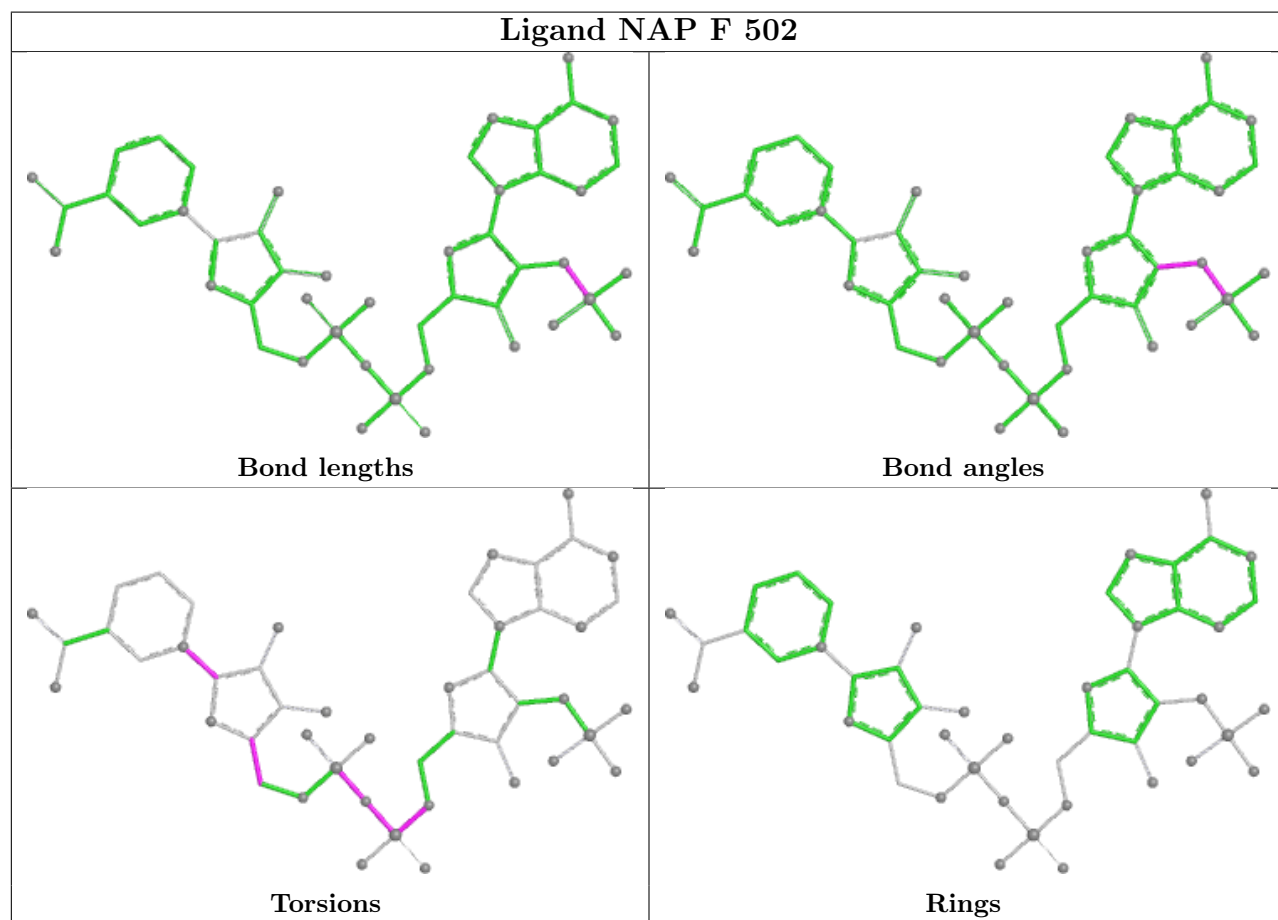
Ligand IMP A 501

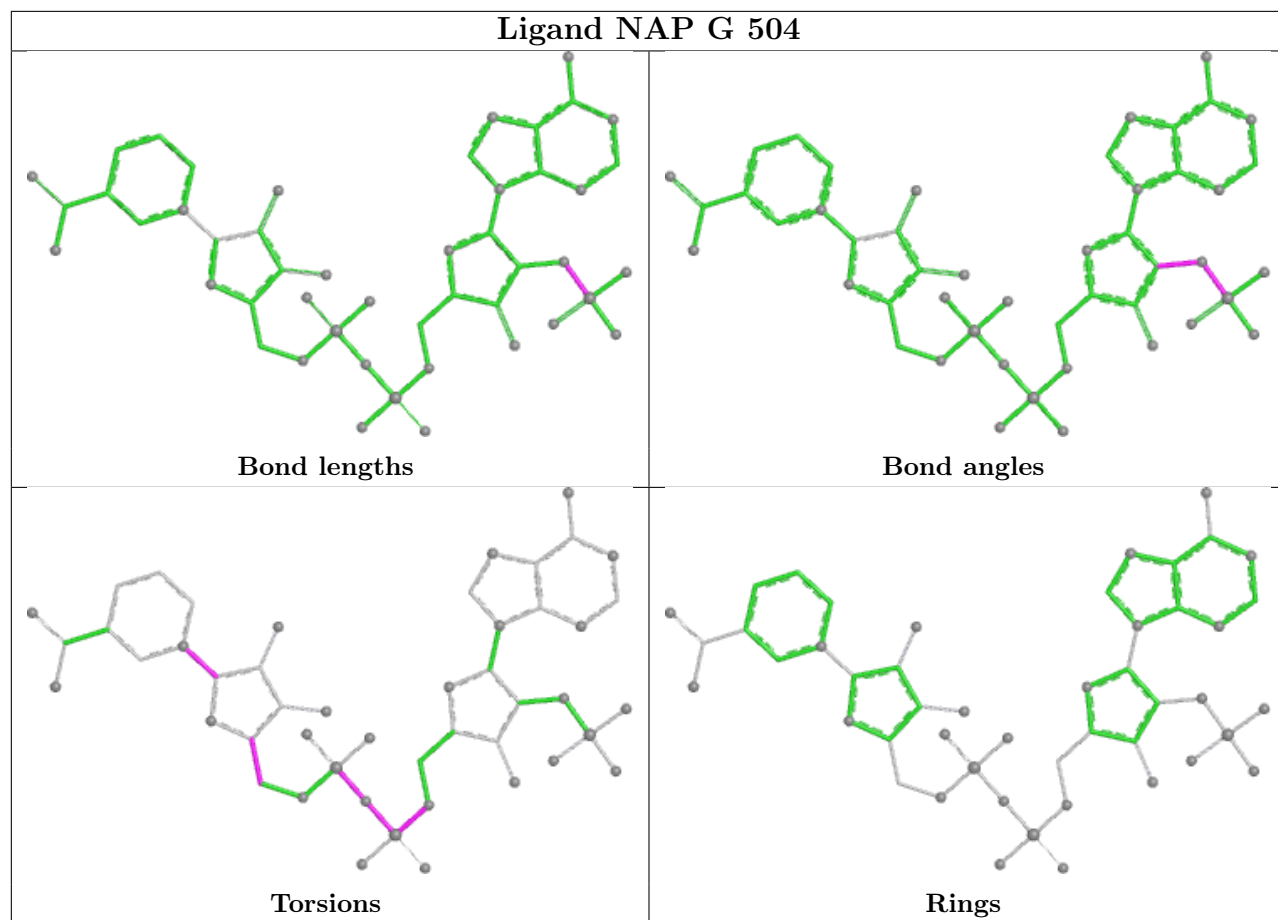


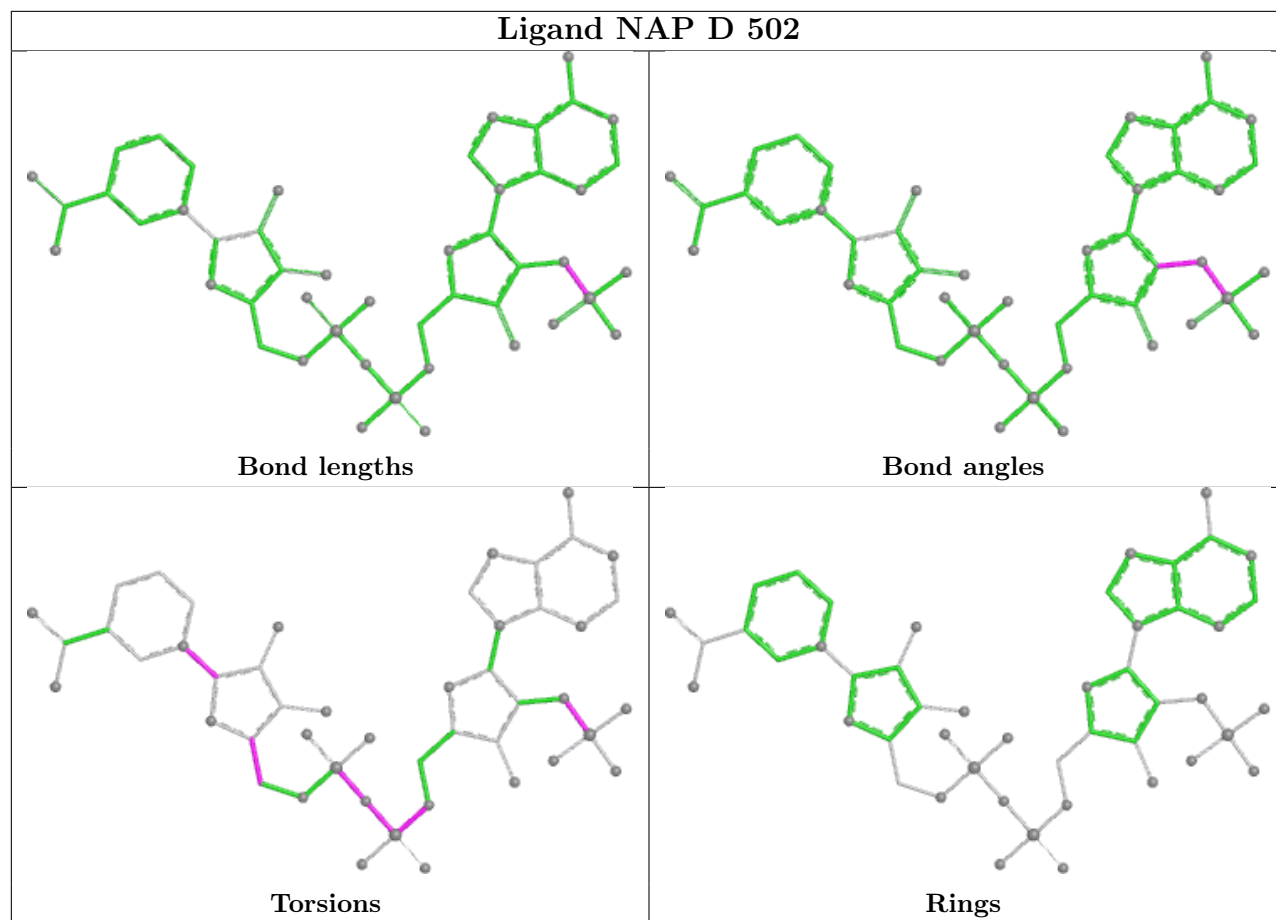
Ligand IMP D 501



Ligand NAP F 502







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	473/496 (95%)	0.58	29 (6%)	27	29	32, 44, 69, 83	0
1	B	473/496 (95%)	0.57	24 (5%)	33	35	33, 45, 68, 83	0
1	C	473/496 (95%)	0.63	33 (6%)	22	24	33, 45, 71, 84	0
1	D	473/496 (95%)	0.54	31 (6%)	24	26	31, 43, 67, 87	0
1	E	473/496 (95%)	0.91	48 (10%)	12	13	37, 53, 73, 90	0
1	F	473/496 (95%)	0.83	35 (7%)	20	22	37, 49, 73, 89	0
1	G	473/496 (95%)	0.94	46 (9%)	13	14	38, 52, 74, 89	0
1	H	473/496 (95%)	0.95	43 (9%)	15	15	40, 54, 73, 87	0
All	All	3784/3968 (95%)	0.74	289 (7%)	20	21	31, 48, 72, 90	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	474	PRO	6.0
1	C	147	PHE	5.9
1	D	147	PHE	5.8
1	H	155	LEU	5.6
1	A	474	PRO	5.6
1	F	155	LEU	5.2
1	G	155	LEU	5.0
1	G	474	PRO	4.9
1	D	474	PRO	4.8
1	E	473	HIS	4.7
1	G	473	HIS	4.6
1	H	473	HIS	4.6
1	E	474	PRO	4.4
1	F	473	HIS	4.4
1	H	153	ILE	4.3
1	A	147	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	154	ALA	4.2
1	H	424	PRO	4.2
1	C	397	THR	4.2
1	G	133	ILE	4.1
1	H	154	ALA	4.1
1	F	474	PRO	4.0
1	B	147	PHE	4.0
1	E	155	LEU	3.9
1	H	474	PRO	3.9
1	E	153	ILE	3.9
1	D	397	THR	3.8
1	F	153	ILE	3.8
1	C	426	ARG	3.8
1	D	426	ARG	3.8
1	C	473	HIS	3.7
1	H	156	SER	3.7
1	H	472	GLY	3.7
1	B	470	ALA	3.7
1	B	474	PRO	3.6
1	H	426	ARG	3.6
1	E	194	VAL	3.6
1	H	403	PHE	3.6
1	E	403	PHE	3.5
1	G	154	ALA	3.5
1	D	398	ALA	3.4
1	D	141	CYS	3.4
1	E	424	PRO	3.4
1	H	2	VAL	3.4
1	E	154	ALA	3.4
1	G	158	PHE	3.3
1	C	141	CYS	3.3
1	D	473	HIS	3.3
1	A	144	VAL	3.3
1	H	447	VAL	3.3
1	F	472	GLY	3.2
1	A	473	HIS	3.2
1	H	259	ILE	3.2
1	E	156	SER	3.2
1	H	166	ASP	3.2
1	A	413	GLU	3.2
1	E	393	VAL	3.1
1	D	400	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	473	HIS	3.1
1	C	425	ALA	3.1
1	A	426	ARG	3.1
1	E	116	LEU	3.1
1	B	77	ASP	3.1
1	C	393	VAL	3.1
1	F	398	ALA	3.1
1	G	153	ILE	3.1
1	A	399	GLY	3.0
1	A	470	ALA	3.0
1	F	399	GLY	3.0
1	F	424	PRO	3.0
1	A	388	ALA	3.0
1	D	409	GLY	3.0
1	F	187	PRO	3.0
1	C	394	ALA	3.0
1	G	163	VAL	3.0
1	A	394	ALA	2.9
1	D	27	ASP	2.9
1	B	388	ALA	2.9
1	E	398	ALA	2.9
1	F	116	LEU	2.9
1	A	397	THR	2.9
1	D	396	ARG	2.9
1	B	425	ALA	2.9
1	C	406	ALA	2.9
1	H	173	LEU	2.9
1	A	77	ASP	2.9
1	B	426	ARG	2.9
1	G	165	THR	2.9
1	A	395	ALA	2.9
1	E	80	ILE	2.8
1	E	169	GLU	2.8
1	B	418	SER	2.8
1	C	388	ALA	2.8
1	D	406	ALA	2.8
1	E	134	GLY	2.8
1	E	395	ALA	2.8
1	G	134	GLY	2.8
1	G	187	PRO	2.8
1	E	158	PHE	2.8
1	G	191	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	148	ALA	2.7
1	F	142	ALA	2.7
1	H	248	ALA	2.7
1	H	410	LEU	2.7
1	F	179	ILE	2.7
1	C	418	SER	2.7
1	C	409	GLY	2.7
1	H	193	GLY	2.7
1	G	426	ARG	2.7
1	C	160	THR	2.7
1	E	165	THR	2.7
1	E	187	PRO	2.7
1	F	156	SER	2.7
1	G	156	SER	2.7
1	B	298	GLY	2.7
1	G	398	ALA	2.7
1	G	265	LEU	2.7
1	H	187	PRO	2.7
1	B	393	VAL	2.7
1	E	90	VAL	2.7
1	C	472	GLY	2.7
1	D	472	GLY	2.7
1	A	424	PRO	2.6
1	E	377	ASP	2.6
1	E	144	VAL	2.6
1	G	80	ILE	2.6
1	H	393	VAL	2.6
1	E	399	GLY	2.6
1	E	472	GLY	2.6
1	G	413	GLU	2.6
1	C	186	ALA	2.6
1	F	186	ALA	2.6
1	D	130	GLY	2.6
1	D	410	LEU	2.6
1	B	409	GLY	2.6
1	F	141	CYS	2.6
1	A	425	ALA	2.6
1	G	116	LEU	2.6
1	H	425	ALA	2.5
1	G	402	SER	2.5
1	E	147	PHE	2.5
1	G	97	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	117	HIS	2.5
1	F	152	ASP	2.5
1	F	165	THR	2.5
1	G	425	ALA	2.5
1	G	176	HIS	2.5
1	C	396	ARG	2.5
1	E	97	VAL	2.5
1	F	392	ALA	2.5
1	G	117	HIS	2.5
1	H	128	PHE	2.5
1	D	77	ASP	2.4
1	E	157	ASP	2.4
1	F	377	ASP	2.4
1	G	160	THR	2.4
1	H	397	THR	2.4
1	C	398	ALA	2.4
1	C	457	GLU	2.4
1	F	393	VAL	2.4
1	E	418	SER	2.4
1	E	81	THR	2.4
1	E	397	THR	2.4
1	G	424	PRO	2.4
1	D	388	ALA	2.4
1	G	395	ALA	2.4
1	G	173	LEU	2.4
1	H	176	HIS	2.4
1	G	472	GLY	2.4
1	H	194	VAL	2.4
1	A	396	ARG	2.4
1	D	146	ARG	2.4
1	B	424	PRO	2.4
1	H	178	PRO	2.4
1	F	176	HIS	2.4
1	E	186	ALA	2.4
1	C	410	LEU	2.4
1	G	469	PHE	2.4
1	H	80	ILE	2.4
1	H	101	VAL	2.4
1	B	303	CYS	2.4
1	C	54	THR	2.4
1	A	398	ALA	2.3
1	B	394	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	394	ALA	2.3
1	G	410	LEU	2.3
1	E	298	GLY	2.3
1	B	404	ASP	2.3
1	H	246	ASP	2.3
1	F	374	PHE	2.3
1	A	418	SER	2.3
1	G	179	ILE	2.3
1	G	190	THR	2.3
1	B	410	LEU	2.3
1	C	411	PHE	2.3
1	A	393	VAL	2.3
1	F	39	VAL	2.3
1	D	303	CYS	2.3
1	D	425	ALA	2.3
1	H	234	ALA	2.3
1	D	399	GLY	2.3
1	E	145	ASP	2.3
1	E	422	LEU	2.3
1	D	469	PHE	2.3
1	H	181	VAL	2.3
1	A	141	CYS	2.3
1	A	406	ALA	2.3
1	G	142	ALA	2.3
1	G	263	ALA	2.3
1	H	378	ASP	2.3
1	H	312	GLY	2.3
1	A	97	VAL	2.2
1	B	144	VAL	2.2
1	C	2	VAL	2.2
1	C	105	PRO	2.2
1	E	2	VAL	2.2
1	A	148	ALA	2.2
1	H	117	HIS	2.2
1	F	128	PHE	2.2
1	C	144	VAL	2.2
1	C	424	PRO	2.2
1	E	179	ILE	2.2
1	H	160	THR	2.2
1	H	152	ASP	2.2
1	B	143	GLY	2.2
1	F	189	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	2.2
1	D	401	SER	2.2
1	D	418	SER	2.2
1	G	327	ARG	2.2
1	G	391	ARG	2.2
1	H	147	PHE	2.2
1	G	143	GLY	2.2
1	C	395	ALA	2.2
1	D	139	ALA	2.2
1	D	470	ALA	2.2
1	E	141	CYS	2.2
1	H	140	ASN	2.2
1	E	374	PHE	2.1
1	G	171	PHE	2.1
1	E	250	GLY	2.1
1	E	142	ALA	2.1
1	G	114	ALA	2.1
1	H	191	LEU	2.1
1	F	160	THR	2.1
1	G	397	THR	2.1
1	F	403	PHE	2.1
1	G	128	PHE	2.1
1	D	142	ALA	2.1
1	F	114	ALA	2.1
1	H	253	ALA	2.1
1	E	265	LEU	2.1
1	A	400	ASP	2.1
1	C	77	ASP	2.1
1	E	246	ASP	2.1
1	G	77	ASP	2.1
1	A	472	GLY	2.1
1	F	193	GLY	2.1
1	F	147	PHE	2.1
1	B	390	LYS	2.1
1	C	139	ALA	2.1
1	C	174	LEU	2.1
1	E	402	SER	2.1
1	C	400	ASP	2.1
1	E	132	PRO	2.1
1	A	409	GLY	2.1
1	B	312	GLY	2.1
1	F	268	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	312	GLY	2.1
1	H	298	GLY	2.1
1	D	393	VAL	2.1
1	B	406	ALA	2.1
1	C	248	ALA	2.1
1	C	267	LEU	2.0
1	H	422	LEU	2.0
1	E	275	ASN	2.0
1	E	77	ASP	2.0
1	G	377	ASP	2.0
1	H	303	CYS	2.0
1	E	79	PRO	2.0
1	E	105	PRO	2.0
1	A	298	GLY	2.0
1	A	403	PHE	2.0
1	D	169	GLU	2.0
1	B	27	ASP	2.0
1	F	426	ARG	2.0
1	G	376	ARG	2.0
1	A	312	GLY	2.0
1	F	134	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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

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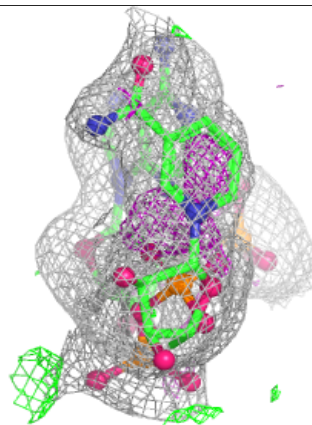
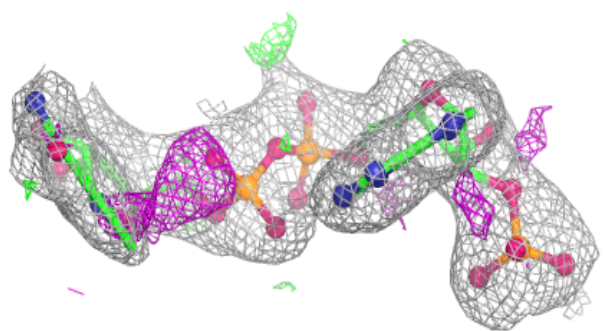
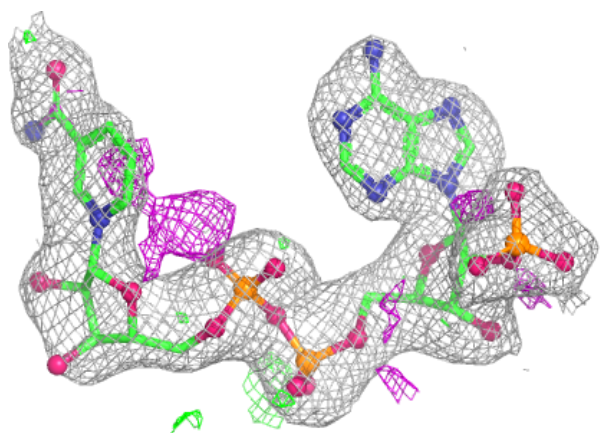
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	G	502	48/48	0.89	0.12	47,53,72,79	0
3	NAP	B	502	48/48	0.90	0.11	39,51,69,75	0
2	IMP	F	503	23/23	0.90	0.10	45,54,63,69	0
3	NAP	D	502	48/48	0.90	0.11	40,52,72,74	0
2	IMP	H	502	23/23	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

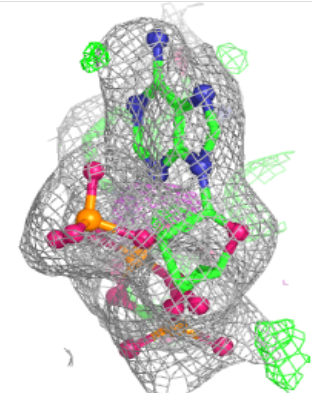
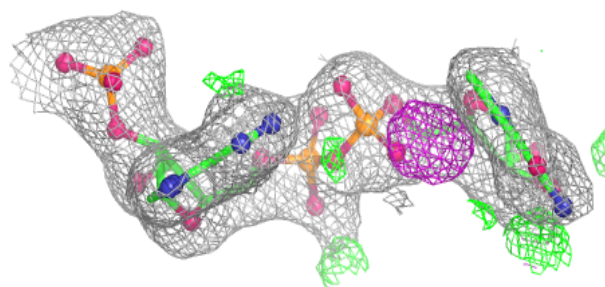
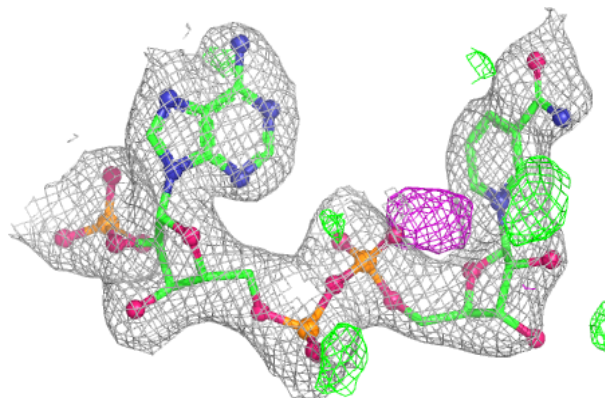
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

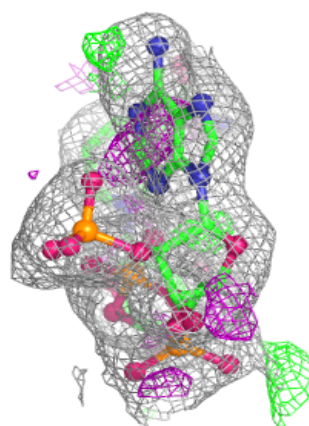
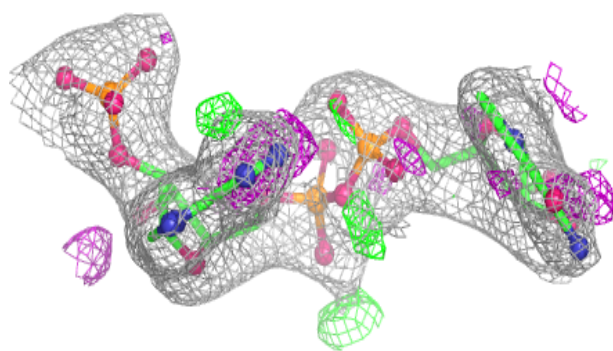
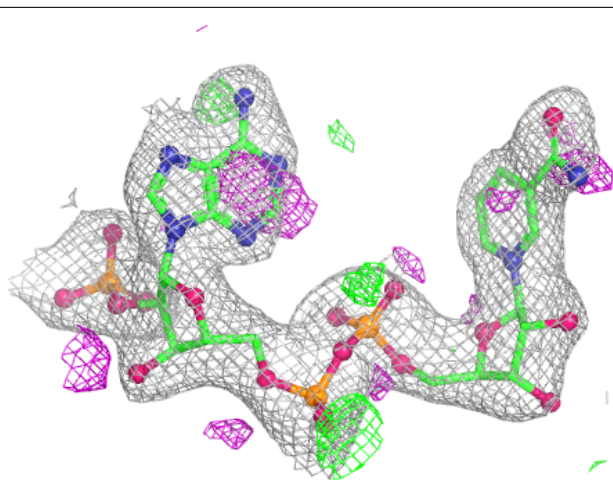
**Electron density around NAP E 502:**

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



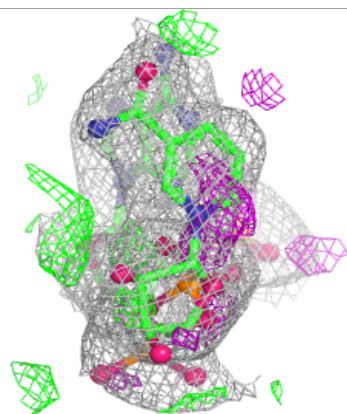
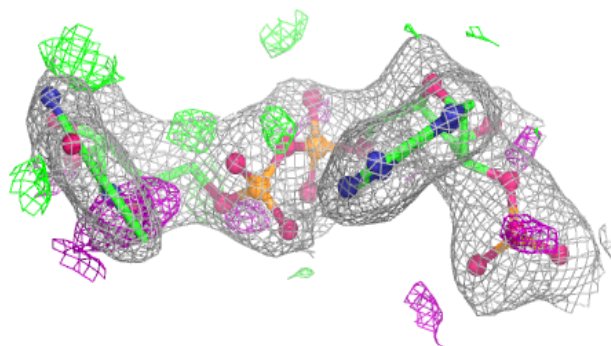
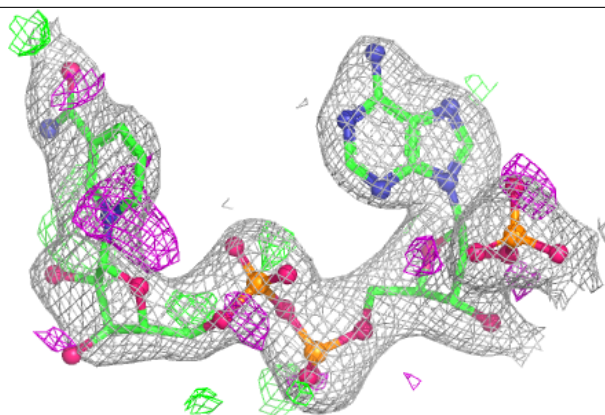
Electron density around NAP G 502:

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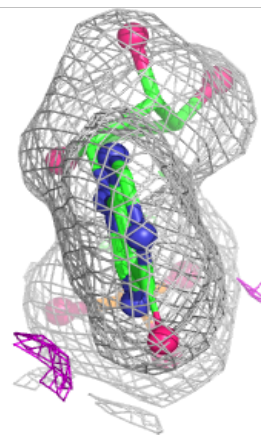
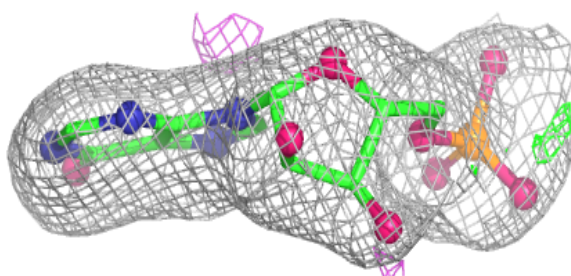
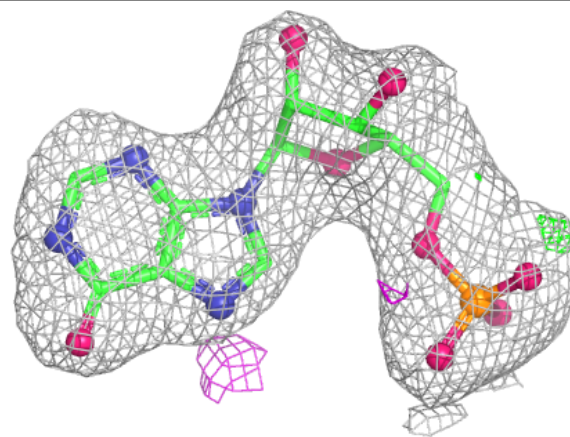


Electron density around NAP B 502:

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and green (positive)

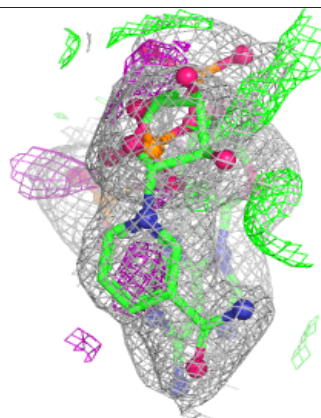
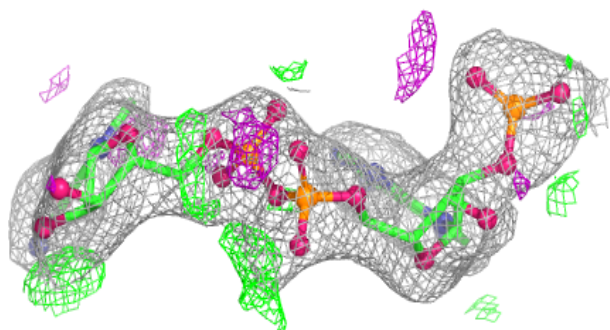
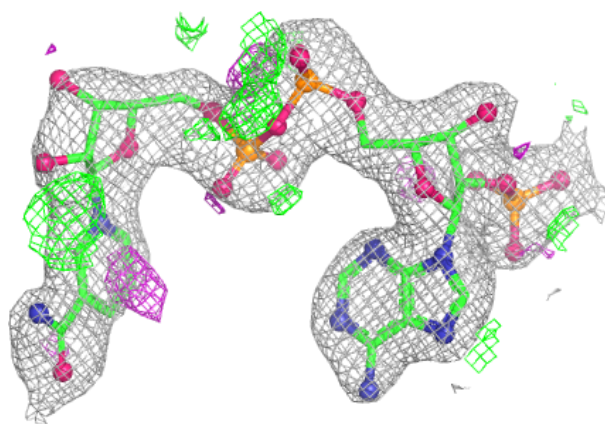
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

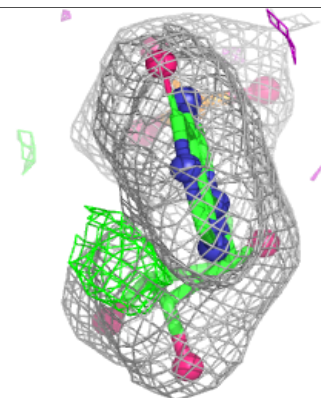
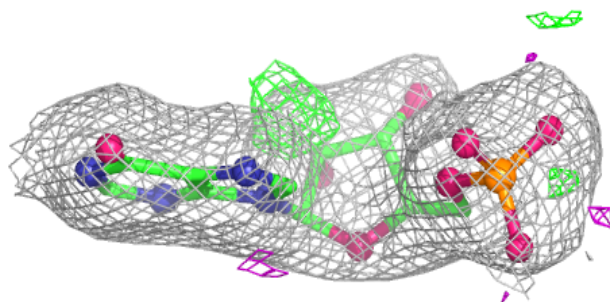
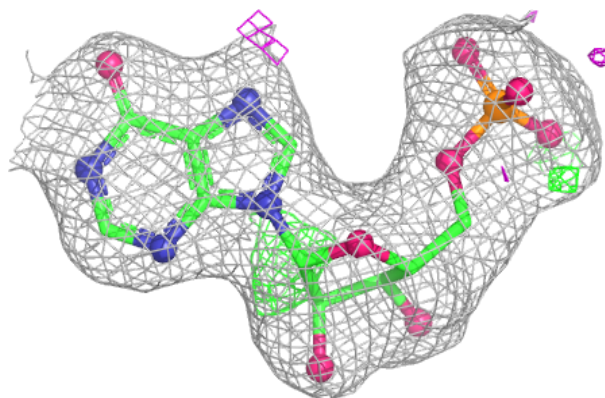


Electron density around NAP D 502:

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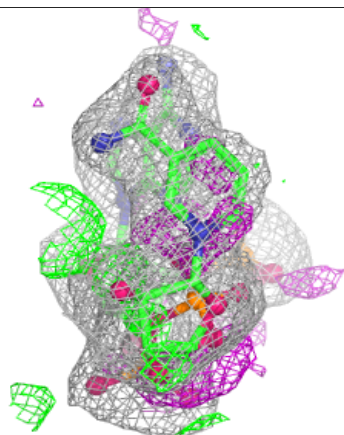
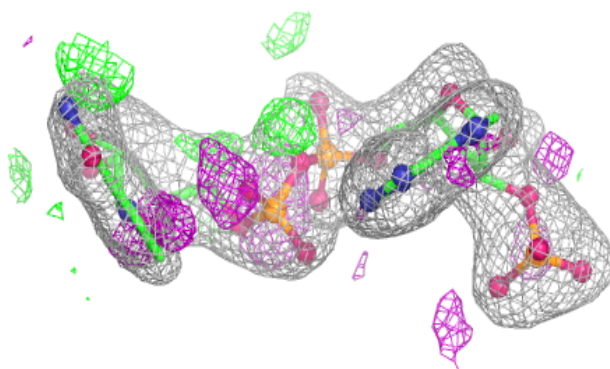
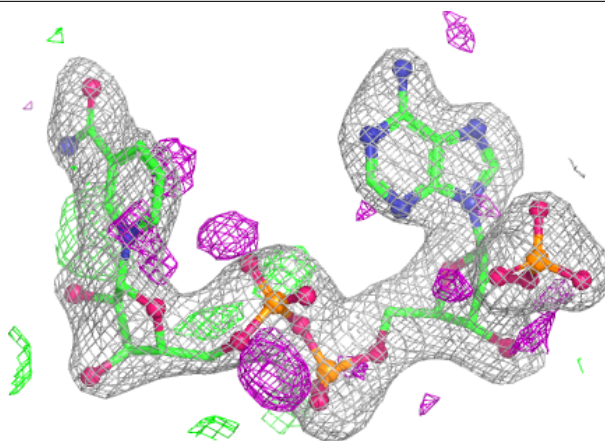
**Electron density around IMP H 502:**

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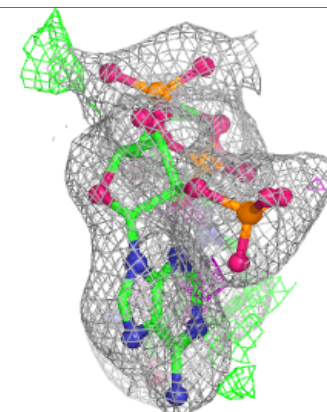
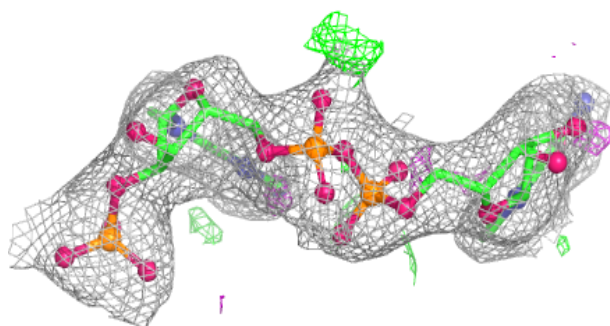
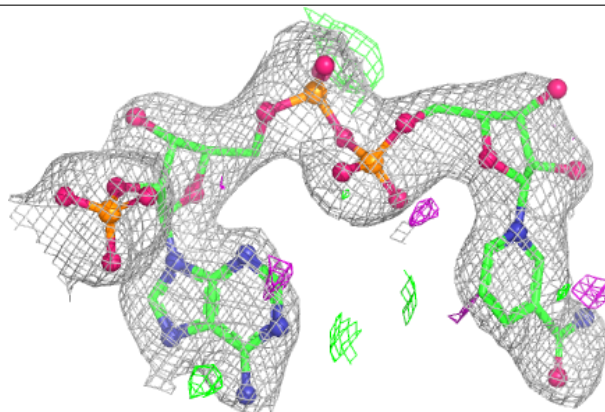


Electron density around NAP A 502:

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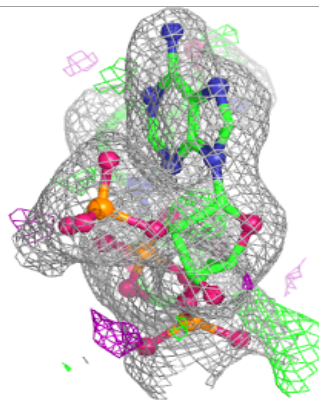
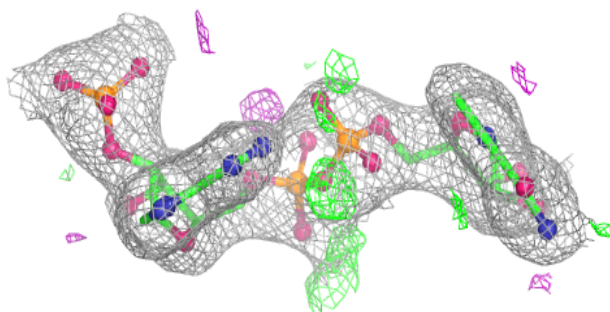
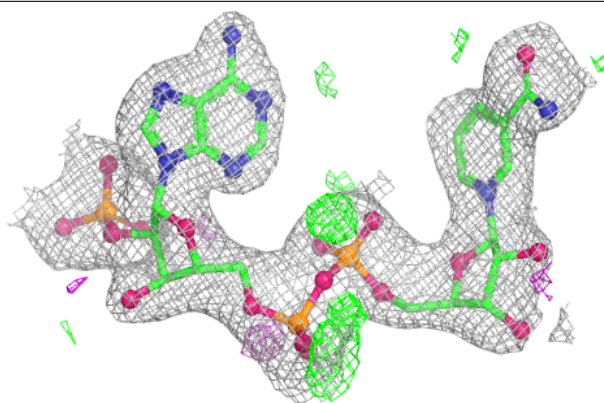
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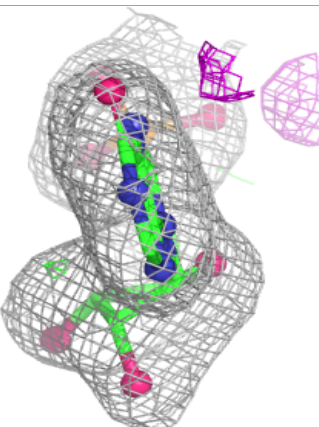
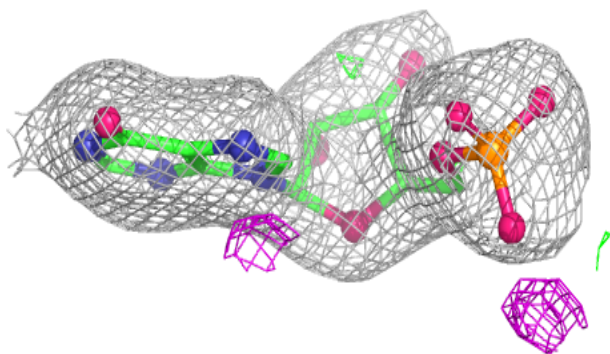
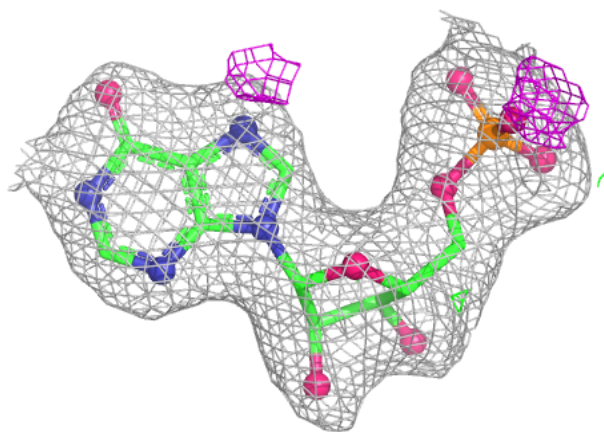


Electron density around NAP F 502:

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and green (positive)

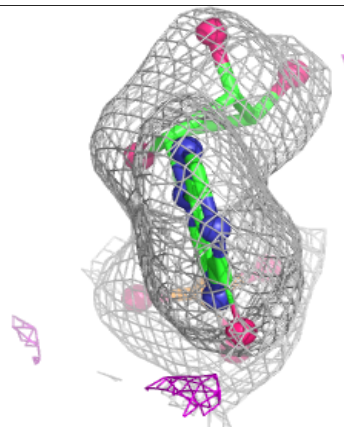
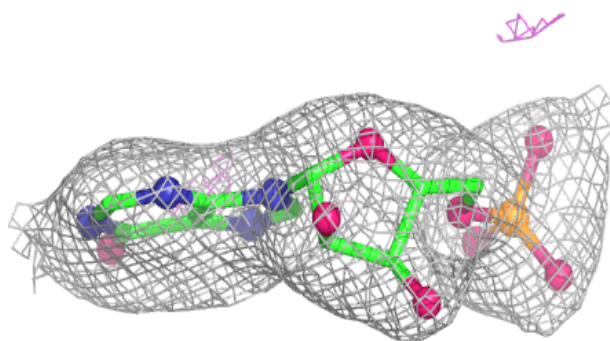
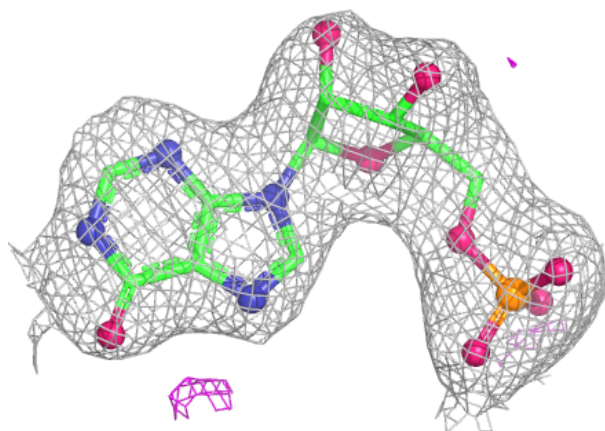
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and green (positive)



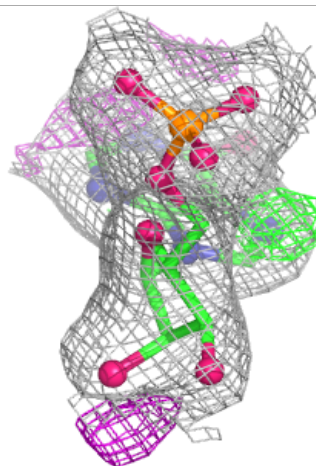
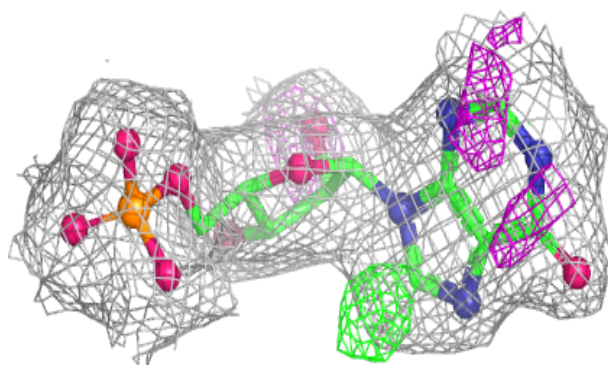
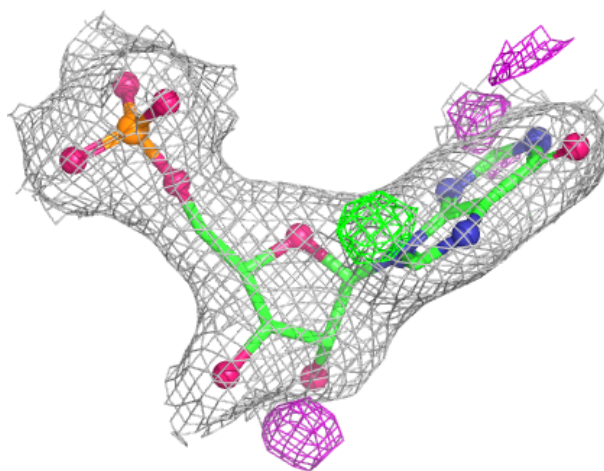
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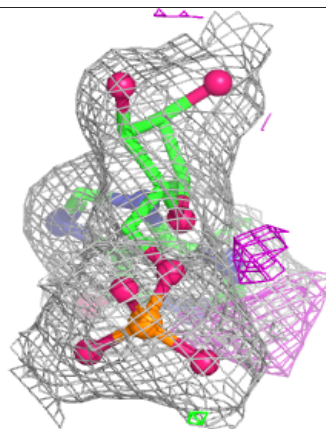
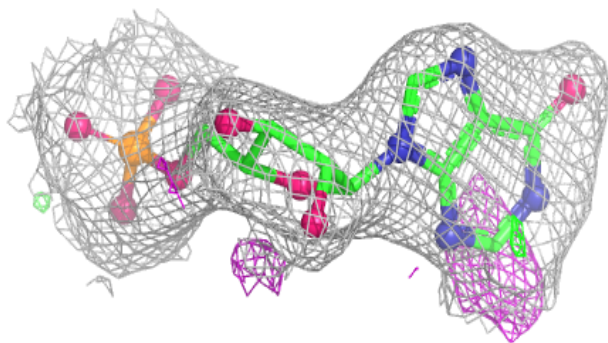
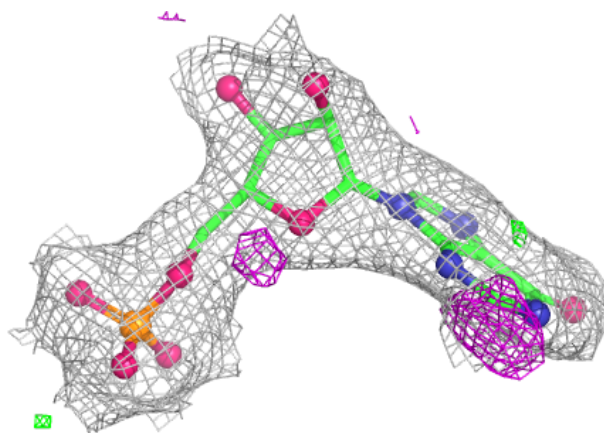
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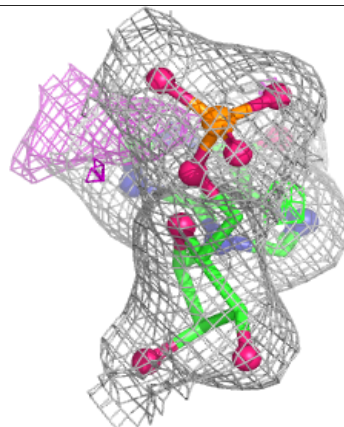
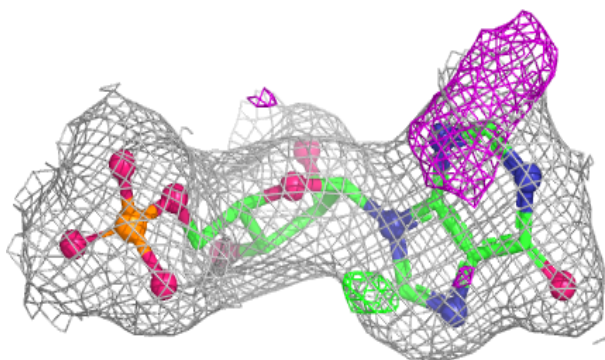
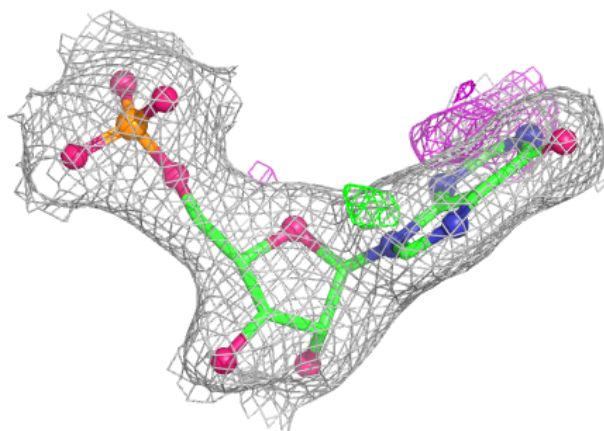
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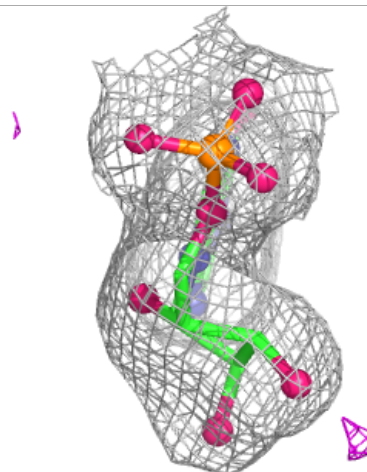
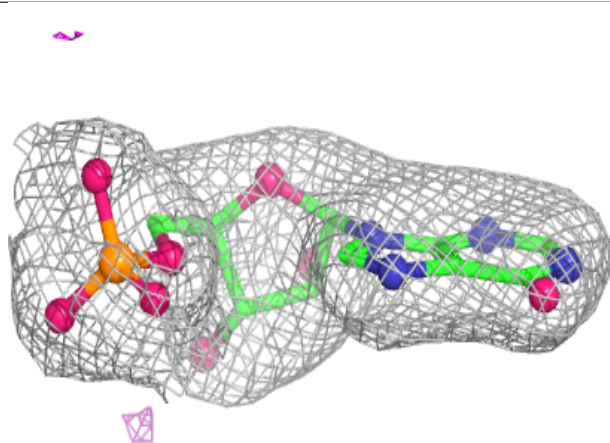
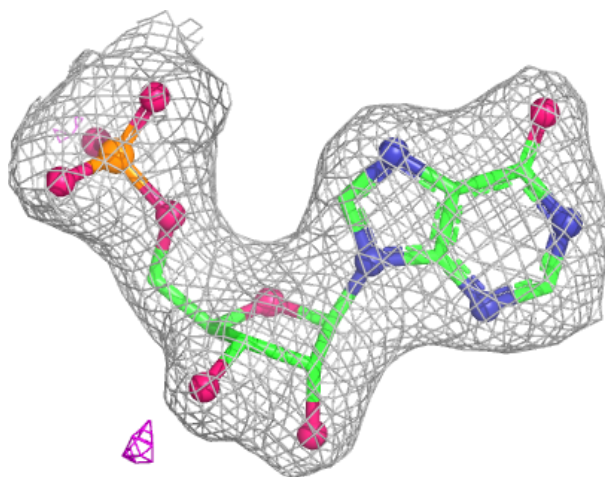
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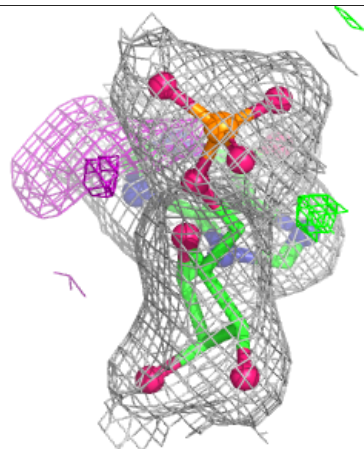
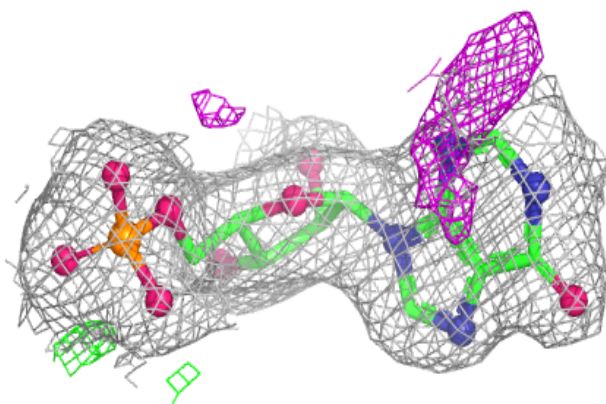
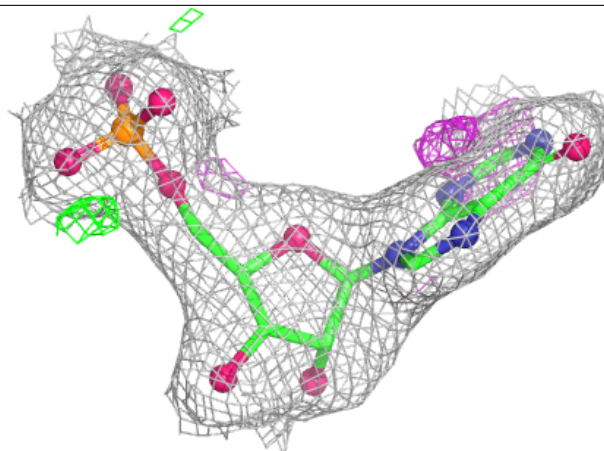
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and green (positive)



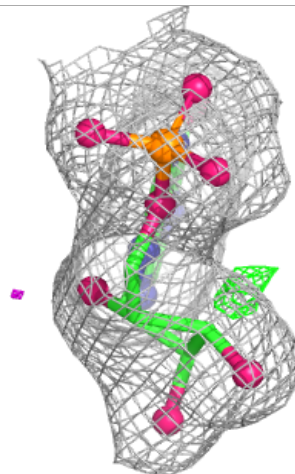
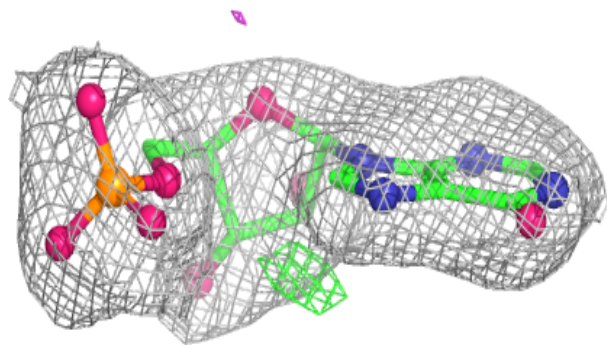
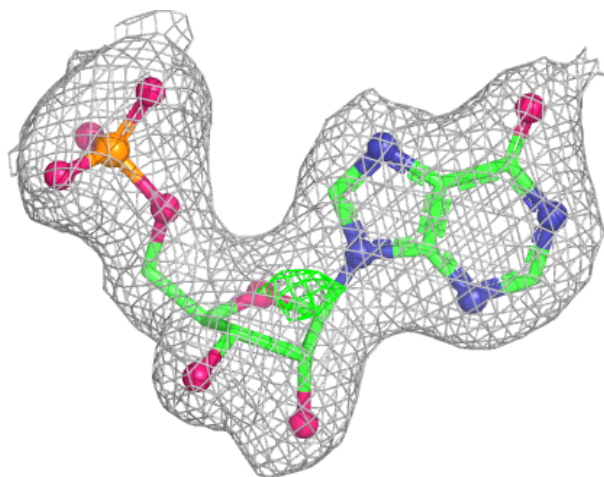
Electron density around IMP G 501:

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



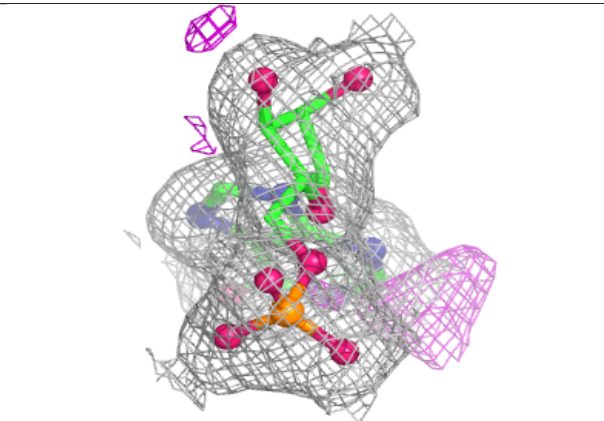
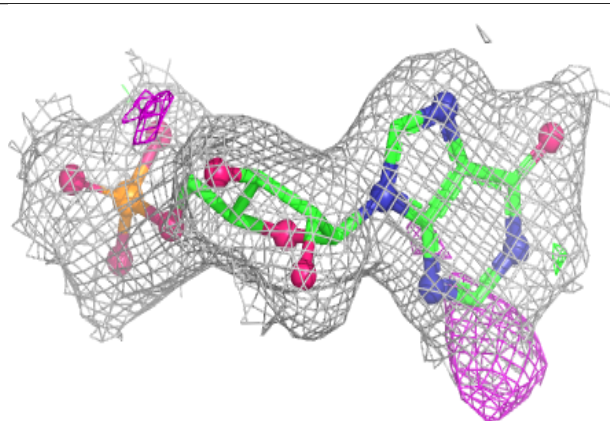
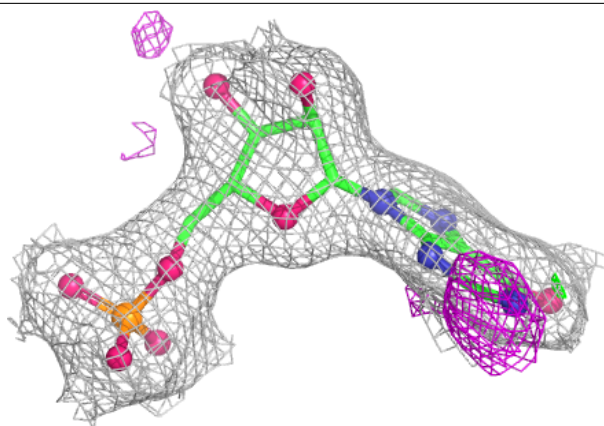
Electron density around IMP D 503:

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



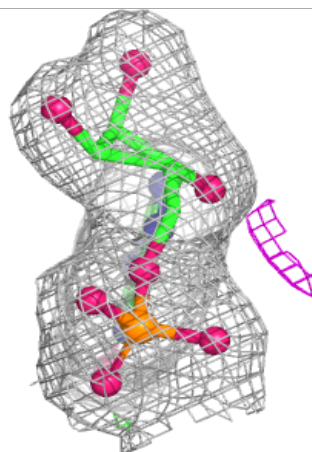
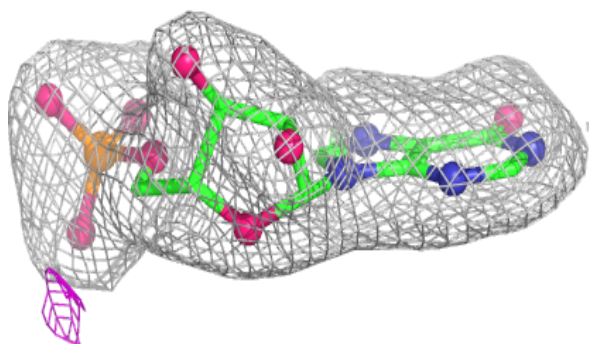
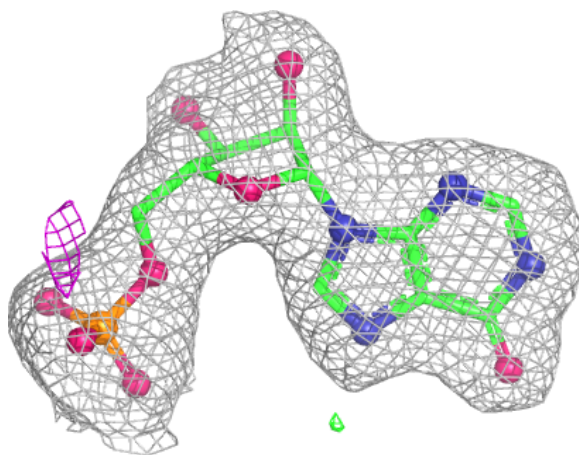
Electron density around IMP D 501:

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



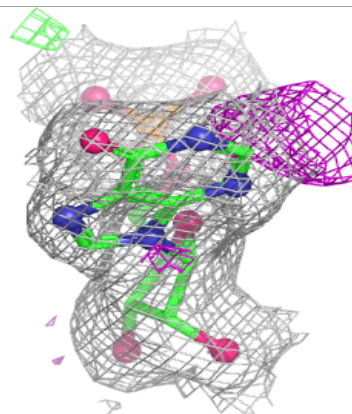
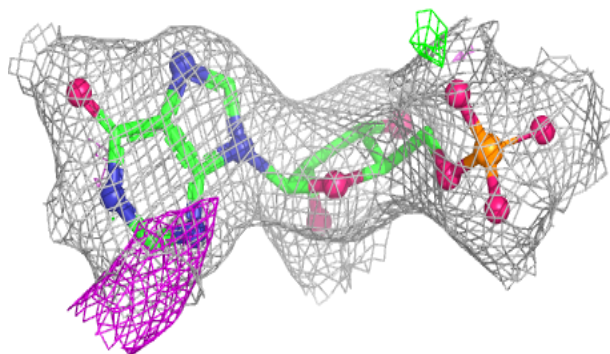
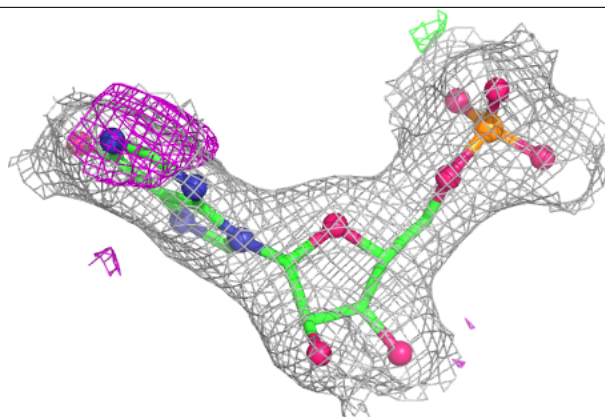
Electron density around IMP A 503:

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

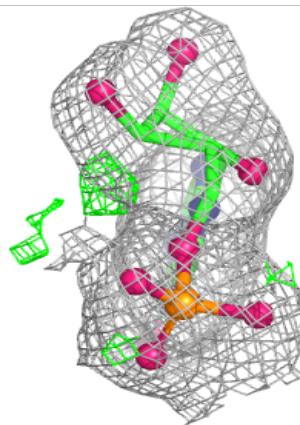
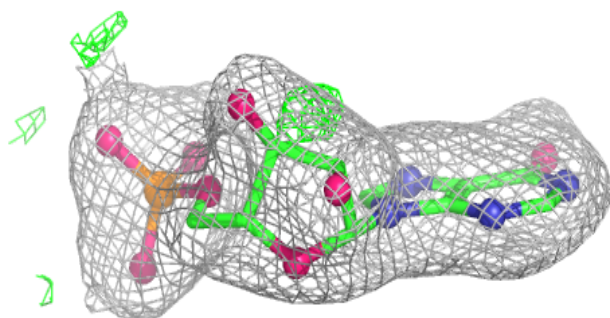
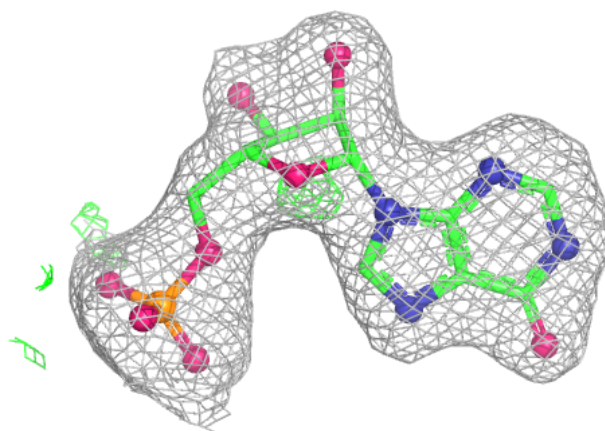


Electron density around IMP B 501:

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

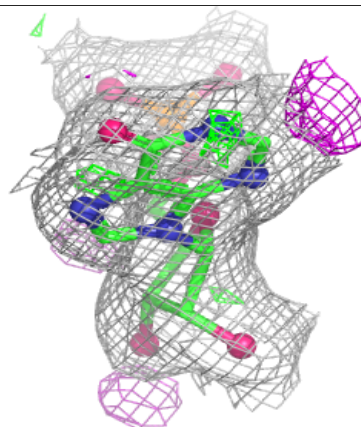
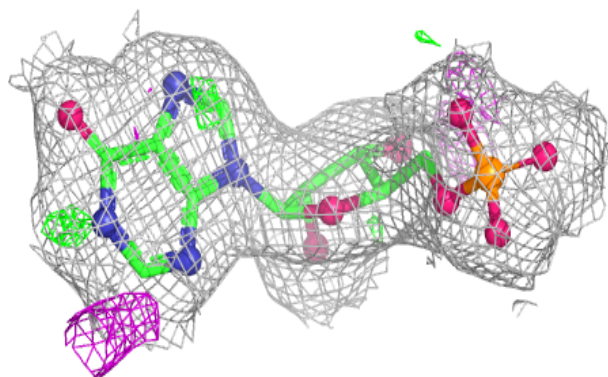
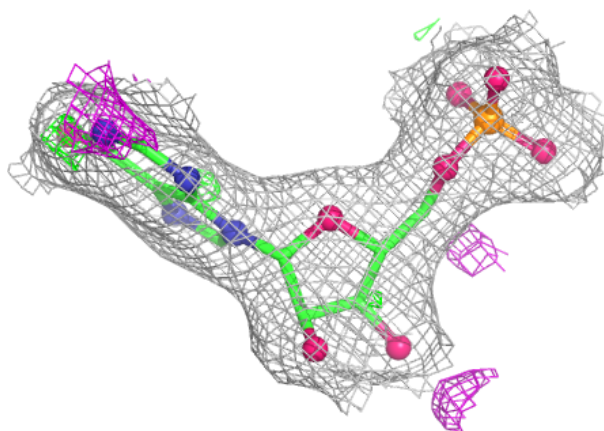
**Electron density around IMP B 503:**

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

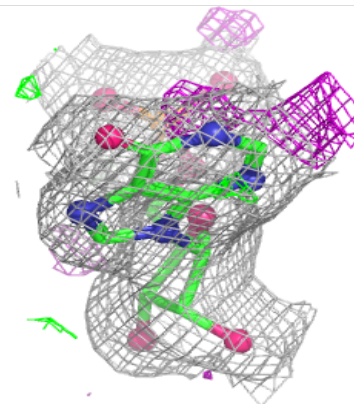
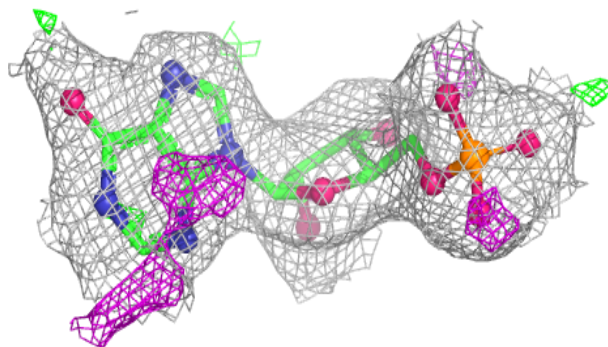
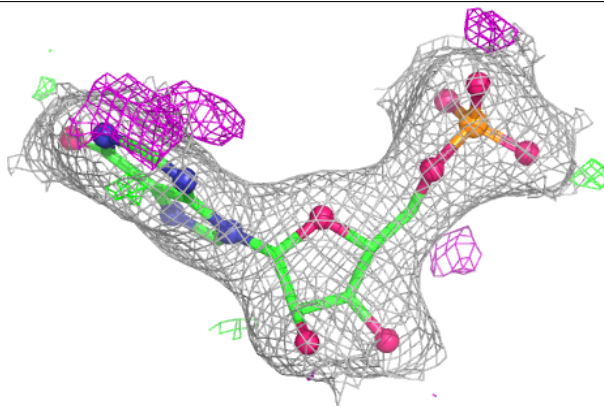


Electron density around IMP C 501:

$2mF_o-DF_c$ (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.