



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2020 – 12:20 PM EDT

PDB ID : 6VWP
Title : Crystal structure of E. coli guanosine kinase in complex with ppGpp
Authors : Wang, B.; Grant, R.A.; Laub, M.T.
Deposited on : 2020-02-20
Resolution : 3.45 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

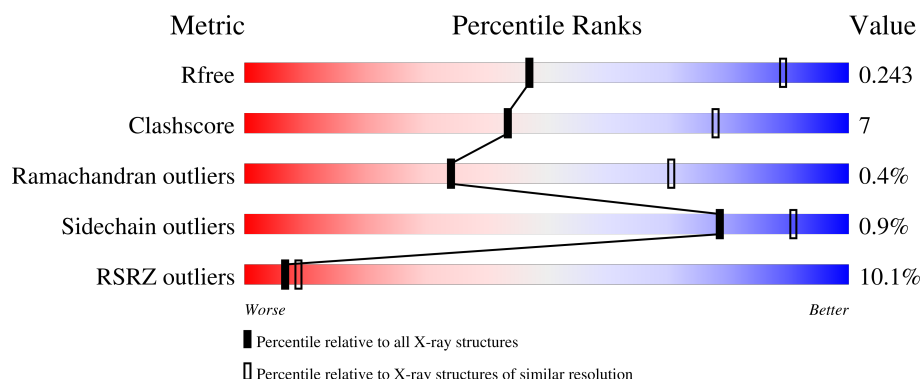
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 on 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	437	<div> <div>4%</div> <div>86%13%</div> </div>
1	B	437	<div> <div>5%</div> <div>82%15%</div> </div>
1	C	437	<div> <div>3%</div> <div>86%11%</div> </div>
1	D	437	<div> <div>7%</div> <div>83%16%</div> </div>
1	E	437	<div> <div>8%</div> <div>82%14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	437	
1	G	437	
1	H	437	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	K	C	505	-	-	-	X
4	K	G	504	-	-	-	X
5	MG	D	505	-	-	-	X
5	MG	E	506	-	-	-	X
5	MG	F	505	-	-	-	X
5	MG	H	506	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 51473 atoms, of which 24272 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 Inosine-guanosine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	H	N	O	S	0	0	0
			6389	2148	2984	588	653	16			
1	B	428	Total	C	H	N	O	S	0	0	0
			6368	2123	3006	579	643	17			
1	C	429	Total	C	H	N	O	S	0	0	0
			6365	2120	3009	580	640	16			
1	D	435	Total	C	H	N	O	S	0	0	0
			6415	2148	3010	588	653	16			
1	E	422	Total	C	H	N	O	S	0	0	0
			6316	2089	3006	571	634	16			
1	F	412	Total	C	H	N	O	S	0	0	0
			6248	2039	3022	555	616	16			
1	G	421	Total	C	H	N	O	S	0	0	0
			6321	2095	3005	573	632	16			
1	H	408	Total	C	H	N	O	S	0	0	0
			6128	2023	2934	547	608	16			

There are 24 discrepancies between the modelled and reference sequences:

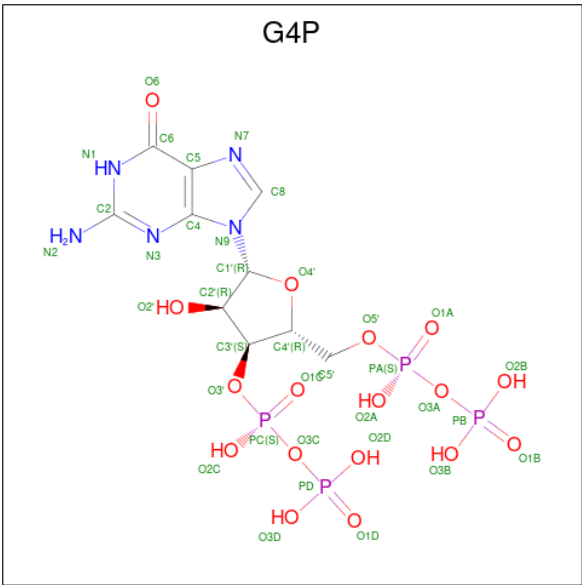
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P0AEW6
A	-1	SER	-	expression tag	UNP P0AEW6
A	0	HIS	-	expression tag	UNP P0AEW6
B	-2	GLY	-	expression tag	UNP P0AEW6
B	-1	SER	-	expression tag	UNP P0AEW6
B	0	HIS	-	expression tag	UNP P0AEW6
C	-2	GLY	-	expression tag	UNP P0AEW6
C	-1	SER	-	expression tag	UNP P0AEW6
C	0	HIS	-	expression tag	UNP P0AEW6
D	-2	GLY	-	expression tag	UNP P0AEW6
D	-1	SER	-	expression tag	UNP P0AEW6
D	0	HIS	-	expression tag	UNP P0AEW6
E	-2	GLY	-	expression tag	UNP P0AEW6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP P0AEW6
E	0	HIS	-	expression tag	UNP P0AEW6
F	-2	GLY	-	expression tag	UNP P0AEW6
F	-1	SER	-	expression tag	UNP P0AEW6
F	0	HIS	-	expression tag	UNP P0AEW6
G	-2	GLY	-	expression tag	UNP P0AEW6
G	-1	SER	-	expression tag	UNP P0AEW6
G	0	HIS	-	expression tag	UNP P0AEW6
H	-2	GLY	-	expression tag	UNP P0AEW6
H	-1	SER	-	expression tag	UNP P0AEW6
H	0	HIS	-	expression tag	UNP P0AEW6

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄) (labeled as "Ligand of Interest" by author).



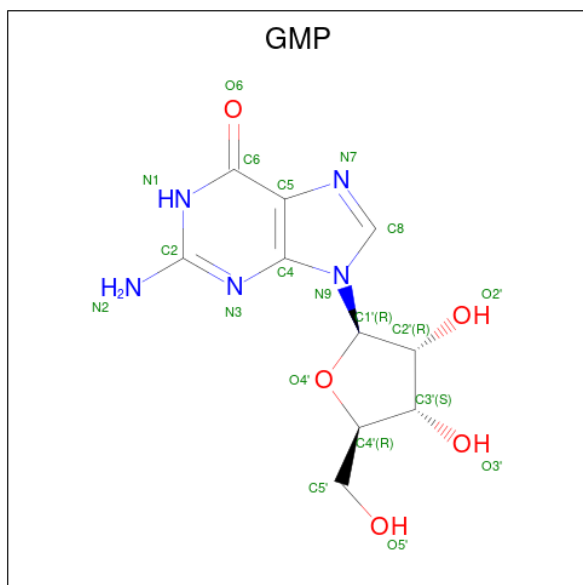
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			47	10	11	5	17	4		
2	B	1	Total	C	H	N	O	P	0	0
			47	10	11	5	17	4		
2	C	1	Total	C	H	N	O	P	0	0
			47	10	11	5	17	4		
2	D	1	Total	C	H	N	O	P	0	0
			47	10	11	5	17	4		
2	E	1	Total	C	H	N	O	P	0	0
			47	10	11	5	17	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	0	0
			47	10	11	5	17		
2	G	1	Total	C	H	N	O	0	0
			47	10	11	5	17		
2	H	1	Total	C	H	N	O	0	0
			47	10	11	5	17		

- Molecule 3 is GUANOSINE (three-letter code: GMP) (formula: C₁₀H₁₃N₅O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	A	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	B	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	B	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	C	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	C	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	D	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	D	1	Total	C	H	N	O	0	0
			33	10	13	5	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	E	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	F	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	F	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	G	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	G	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	H	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	H	1	Total	C	H	N	O	0	0
			33	10	13	5	5		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	2	Total	K	0	0
			2	2		
4	H	2	Total	K	0	0
			2	2		
4	B	2	Total	K	0	0
			2	2		
4	C	2	Total	K	0	0
			2	2		
4	A	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		

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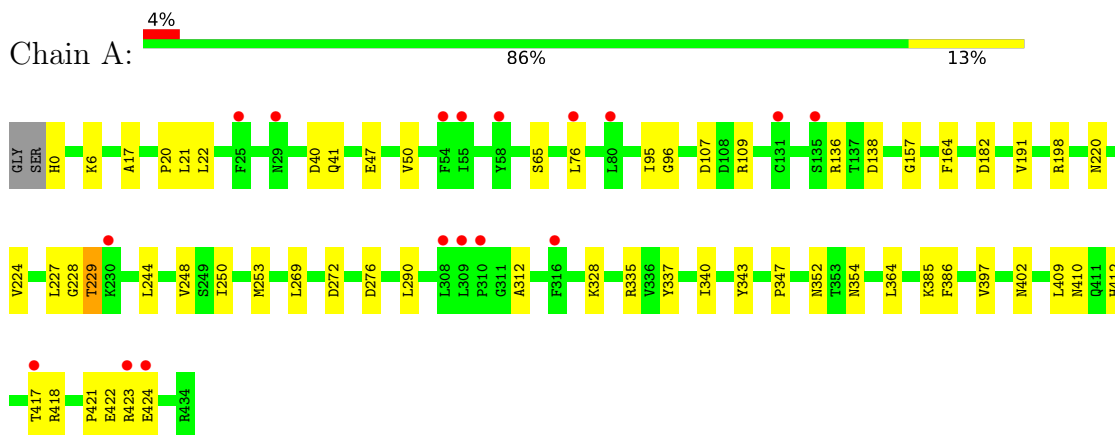
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0
5	H	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

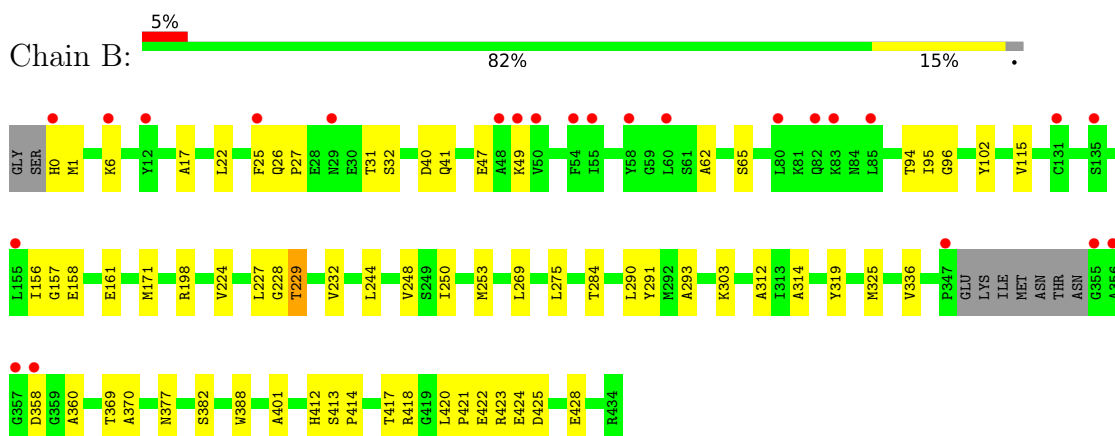
3 Residue-property plots [i](#)

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.

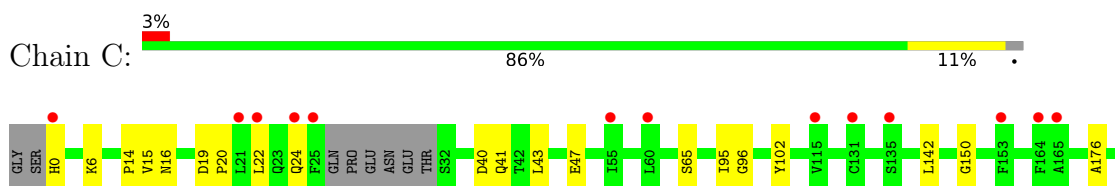
- Molecule 1: Inosine-guanosine kinase



- Molecule 1: Inosine-guanosine kinase

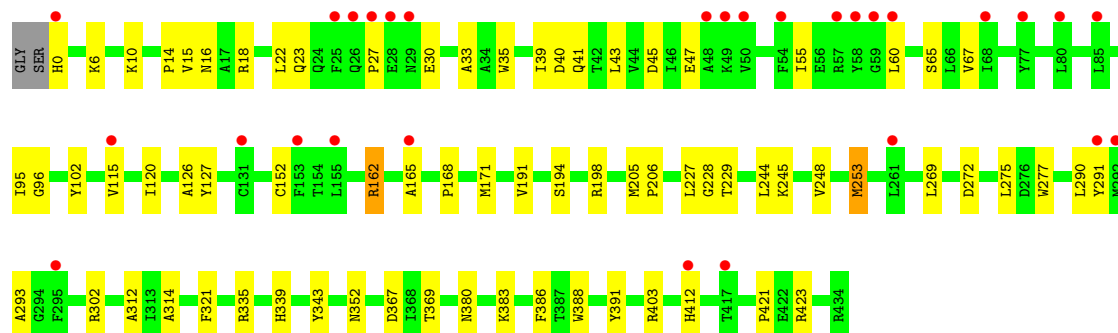
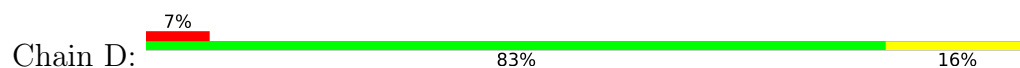


- Molecule 1: Inosine-guanosine kinase

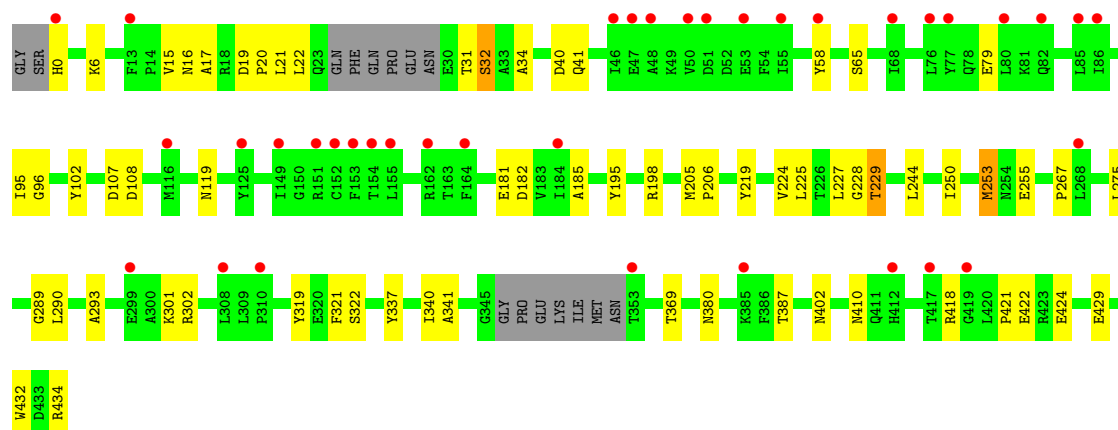
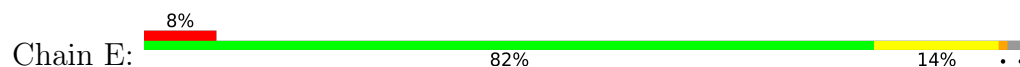




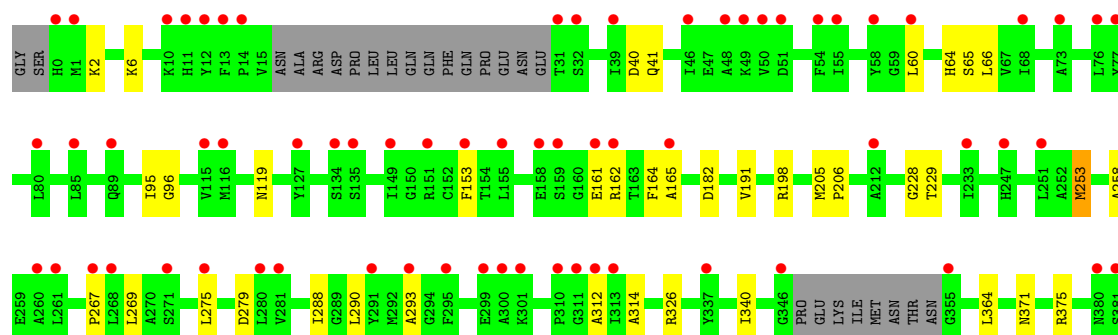
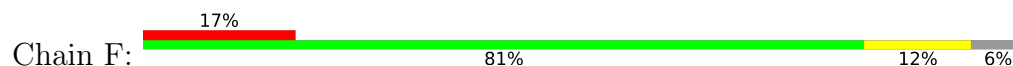
- Molecule 1: Inosine-guanosine kinase

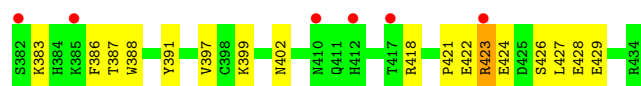


- Molecule 1: Inosine-guanosine kinase

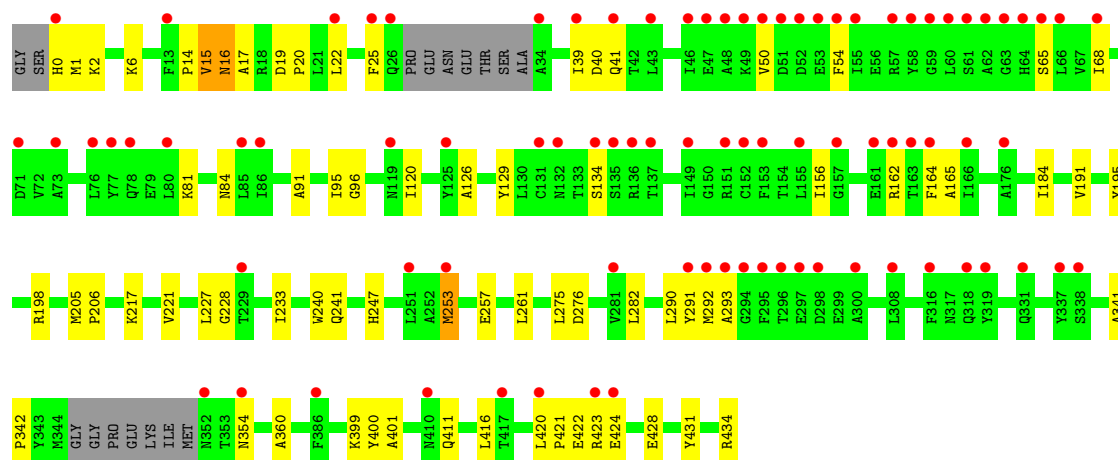
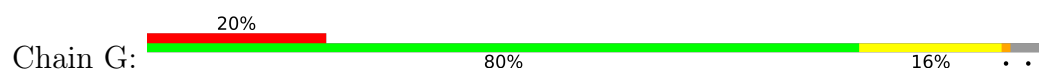


- Molecule 1: Inosine-guanosine kinase

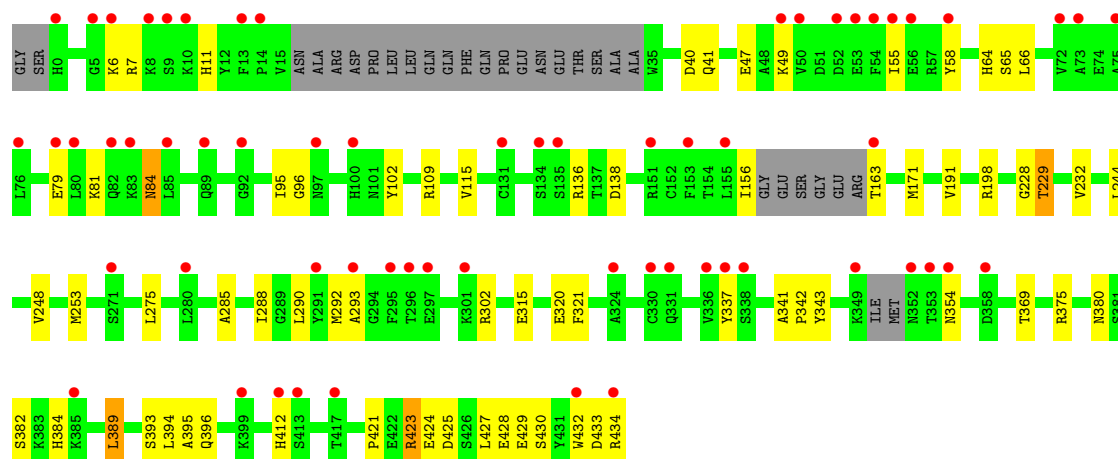
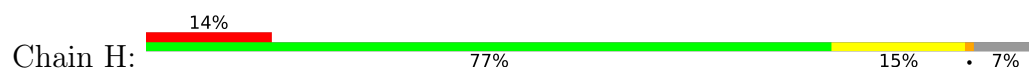




• Molecule 1: Inosine-guanosine kinase



• Molecule 1: Inosine-guanosine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.95Å 245.95Å 221.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.16 – 3.45 49.16 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.16-3.45) 94.0 (49.16-3.42)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.242 0.200 , 0.243	Depositor DCC
R_{free} test set	1991 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	133.5	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 108.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51473	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, K, GMP, MG

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	0.37	0/3485	0.53	0/4734
1	B	0.35	0/3441	0.52	0/4670
1	C	0.36	1/3434 (0.0%)	0.52	0/4662
1	D	0.32	0/3485	0.51	0/4734
1	E	0.31	0/3385	0.50	0/4593
1	F	0.28	0/3300	0.49	0/4476
1	G	0.29	0/3392	0.50	0/4602
1	H	0.32	0/3268	0.52	0/4436
All	All	0.33	1/27190 (0.0%)	0.51	0/36907

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419	GLY	C-N	-5.51	1.21	1.34

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	3405	2984	3303	48	0
1	B	3362	3006	3273	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3356	3009	3262	33	0
1	D	3405	3010	3303	49	0
1	E	3310	3006	3224	52	0
1	F	3226	3022	3143	45	0
1	G	3316	3005	3229	54	0
1	H	3194	2934	3103	66	0
2	A	36	11	11	0	0
2	B	36	11	11	0	0
2	C	36	11	11	0	0
2	D	36	11	11	3	0
2	E	36	11	11	1	0
2	F	36	11	11	1	0
2	G	36	11	11	0	0
2	H	36	11	11	0	0
3	A	40	26	26	0	0
3	B	40	26	26	0	0
3	C	40	26	26	0	0
3	D	40	26	26	0	0
3	E	40	26	26	2	0
3	F	40	26	26	1	0
3	G	40	26	26	1	0
3	H	40	26	26	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	27201	24272	26136	356	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 7.

The worst 5 of 356 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:424:GLU:OE2	1:D:423:ARG:HG3	1.60	1.01
1:A:421:PRO:HB3	1:B:422:GLU:HB3	1.47	0.96
1:A:109:ARG:NH2	1:A:138:ASP:OD2	2.12	0.82
1:B:228:GLY:O	1:B:229:THR:OG1	1.97	0.82
1:E:341:ALA:O	1:E:402:ASN:ND2	2.14	0.80

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	433/437 (99%)	411 (95%)	20 (5%)	2 (0%)	29	66
1	B	424/437 (97%)	406 (96%)	17 (4%)	1 (0%)	47	80
1	C	425/437 (97%)	408 (96%)	15 (4%)	2 (0%)	29	66
1	D	433/437 (99%)	410 (95%)	22 (5%)	1 (0%)	47	80
1	E	416/437 (95%)	399 (96%)	14 (3%)	3 (1%)	22	60
1	F	406/437 (93%)	390 (96%)	15 (4%)	1 (0%)	47	80
1	G	415/437 (95%)	400 (96%)	14 (3%)	1 (0%)	47	80
1	H	400/437 (92%)	385 (96%)	14 (4%)	1 (0%)	41	75
All	All	3352/3496 (96%)	3209 (96%)	131 (4%)	12 (0%)	34	70

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	229	THR
1	H	229	THR
1	A	229	THR
1	B	229	THR
1	E	15	VAL

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	364/369 (99%)	363 (100%)	1 (0%)	92	98
1	B	361/369 (98%)	358 (99%)	3 (1%)	81	92
1	C	358/369 (97%)	356 (99%)	2 (1%)	86	95
1	D	364/369 (99%)	360 (99%)	4 (1%)	73	88
1	E	355/369 (96%)	353 (99%)	2 (1%)	86	95
1	F	345/369 (94%)	343 (99%)	2 (1%)	86	95
1	G	356/369 (96%)	350 (98%)	6 (2%)	60	82
1	H	342/369 (93%)	337 (98%)	5 (2%)	65	84
All	All	2845/2952 (96%)	2820 (99%)	25 (1%)	78	91

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	387	THR
1	F	423	ARG
1	H	389	LEU
1	F	253	MET
1	G	16	ASN

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

Mol	Chain	Res	Type
1	A	64	HIS
1	C	384	HIS
1	E	327	HIS
1	G	354	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 19 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GMP	C	502	-	18,22,22	1.13	1 (5%)	20,33,33	2.60	4 (20%)
3	GMP	H	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.63	4 (20%)
3	GMP	G	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.61	4 (20%)
3	GMP	C	503	-	18,22,22	1.16	1 (5%)	20,33,33	2.56	4 (20%)
3	GMP	H	503	-	18,22,22	1.20	1 (5%)	20,33,33	2.60	4 (20%)
2	G4P	F	501	-	30,38,38	1.12	2 (6%)	43,61,61	1.78	9 (20%)
2	G4P	D	501	-	30,38,38	1.12	2 (6%)	43,61,61	1.90	10 (23%)
2	G4P	G	501	-	30,38,38	1.12	2 (6%)	43,61,61	2.10	11 (25%)
3	GMP	B	502	-	18,22,22	1.13	1 (5%)	20,33,33	2.60	4 (20%)
3	GMP	B	503	-	18,22,22	1.20	1 (5%)	20,33,33	2.59	4 (20%)
2	G4P	A	501	-	30,38,38	1.10	2 (6%)	43,61,61	2.12	12 (27%)
3	GMP	D	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.59	4 (20%)
3	GMP	E	502	-	18,22,22	1.15	1 (5%)	20,33,33	2.60	4 (20%)
2	G4P	H	501	-	30,38,38	1.06	2 (6%)	43,61,61	1.82	10 (23%)
3	GMP	F	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.62	4 (20%)
2	G4P	B	501	-	30,38,38	1.16	3 (10%)	43,61,61	2.10	12 (27%)
3	GMP	D	503	-	18,22,22	1.18	1 (5%)	20,33,33	2.58	4 (20%)
2	G4P	E	501	-	30,38,38	1.14	2 (6%)	43,61,61	1.95	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G4P	C	501	-	30,38,38	1.09	3 (10%)	43,61,61	1.92	11 (25%)
3	GMP	A	502	-	18,22,22	1.13	1 (5%)	20,33,33	2.61	4 (20%)
3	GMP	E	503	-	18,22,22	1.18	1 (5%)	20,33,33	2.61	4 (20%)
3	GMP	A	503	-	18,22,22	1.14	1 (5%)	20,33,33	2.59	4 (20%)
3	GMP	G	503	-	18,22,22	1.18	1 (5%)	20,33,33	2.59	4 (20%)
3	GMP	F	503	-	18,22,22	1.19	1 (5%)	20,33,33	2.60	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GMP	C	502	-	-	0/2/22/22	0/3/3/3
3	GMP	H	502	-	-	0/2/22/22	0/3/3/3
3	GMP	G	502	-	-	0/2/22/22	0/3/3/3
3	GMP	C	503	-	-	2/2/22/22	0/3/3/3
3	GMP	H	503	-	-	0/2/22/22	0/3/3/3
2	G4P	F	501	-	-	4/23/43/43	0/3/3/3
2	G4P	D	501	-	-	1/23/43/43	0/3/3/3
2	G4P	G	501	-	-	4/23/43/43	0/3/3/3
3	GMP	B	502	-	-	0/2/22/22	0/3/3/3
3	GMP	B	503	-	-	2/2/22/22	0/3/3/3
2	G4P	A	501	-	-	3/23/43/43	0/3/3/3
3	GMP	D	502	-	-	0/2/22/22	0/3/3/3
3	GMP	E	502	-	-	0/2/22/22	0/3/3/3
2	G4P	H	501	-	-	4/23/43/43	0/3/3/3
3	GMP	F	502	-	-	0/2/22/22	0/3/3/3
2	G4P	B	501	-	-	0/23/43/43	0/3/3/3
3	GMP	D	503	-	-	2/2/22/22	0/3/3/3
2	G4P	E	501	-	-	3/23/43/43	0/3/3/3
2	G4P	C	501	-	-	5/23/43/43	0/3/3/3
3	GMP	A	502	-	-	0/2/22/22	0/3/3/3
3	GMP	E	503	-	-	0/2/22/22	0/3/3/3
3	GMP	A	503	-	-	2/2/22/22	0/3/3/3
3	GMP	G	503	-	-	2/2/22/22	0/3/3/3
3	GMP	F	503	-	-	2/2/22/22	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	G4P	C6-C5	4.71	1.49	1.41
2	B	501	G4P	C6-C5	4.56	1.49	1.41
2	F	501	G4P	C6-C5	4.54	1.49	1.41
2	G	501	G4P	C6-C5	4.42	1.49	1.41
2	D	501	G4P	C6-C5	4.38	1.48	1.41

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	GMP	C5-C6-N1	-8.85	111.33	123.43
3	F	503	GMP	C5-C6-N1	-8.84	111.34	123.43
3	A	503	GMP	C5-C6-N1	-8.82	111.37	123.43
3	H	502	GMP	C5-C6-N1	-8.82	111.37	123.43
3	G	503	GMP	C5-C6-N1	-8.81	111.38	123.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	G4P	PA-O3A-PB-O2B
2	F	501	G4P	PA-O3A-PB-O3B
2	G	501	G4P	PA-O3A-PB-O2B
2	G	501	G4P	PA-O3A-PB-O3B
3	B	503	GMP	O4'-C4'-C5'-O5'

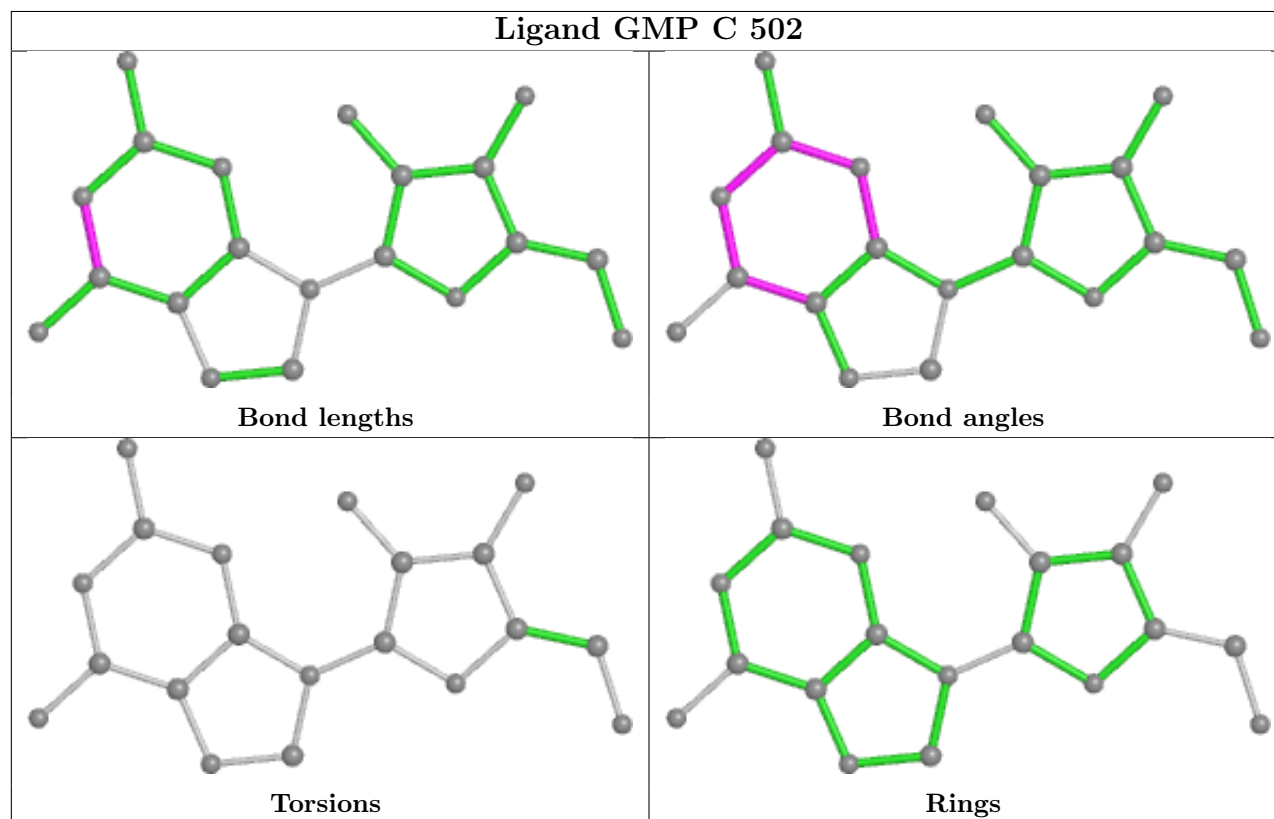
There are no ring outliers.

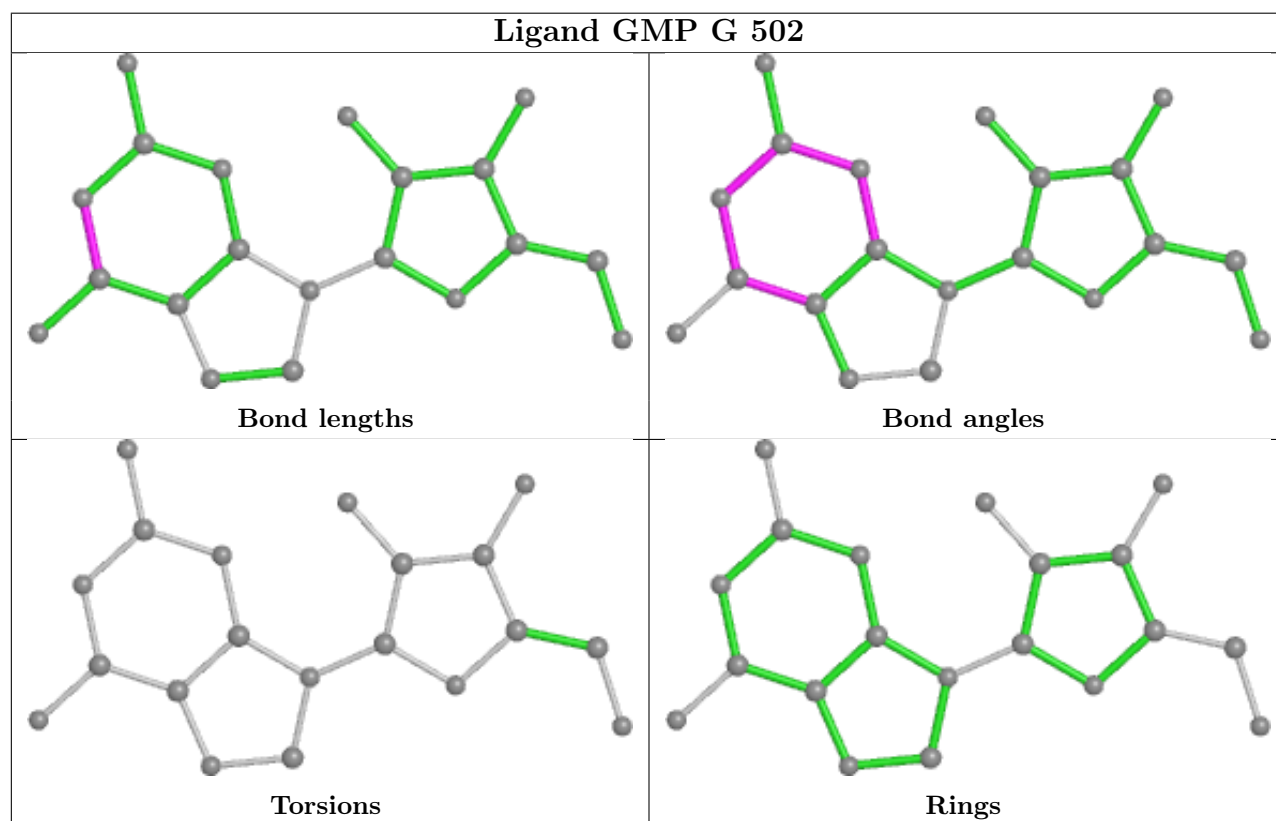
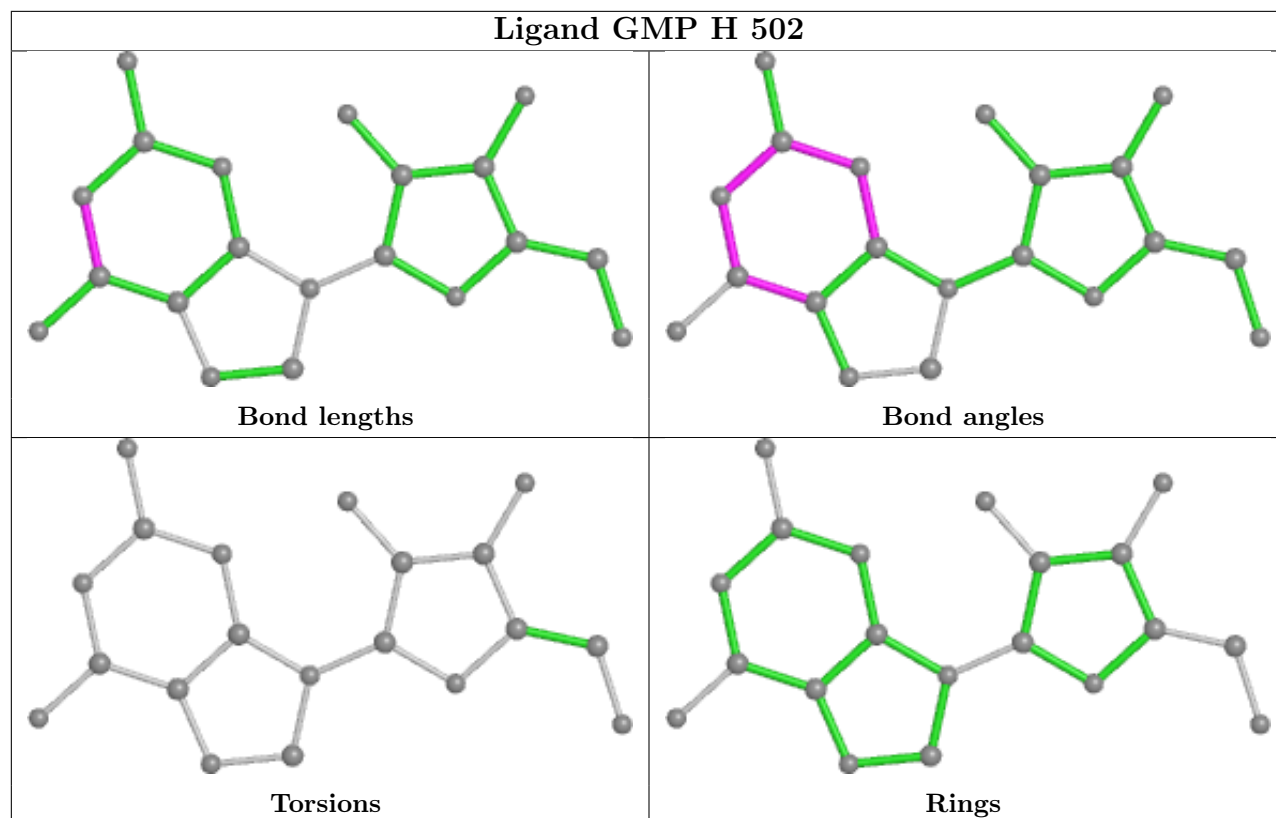
6 monomers are involved in 9 short contacts:

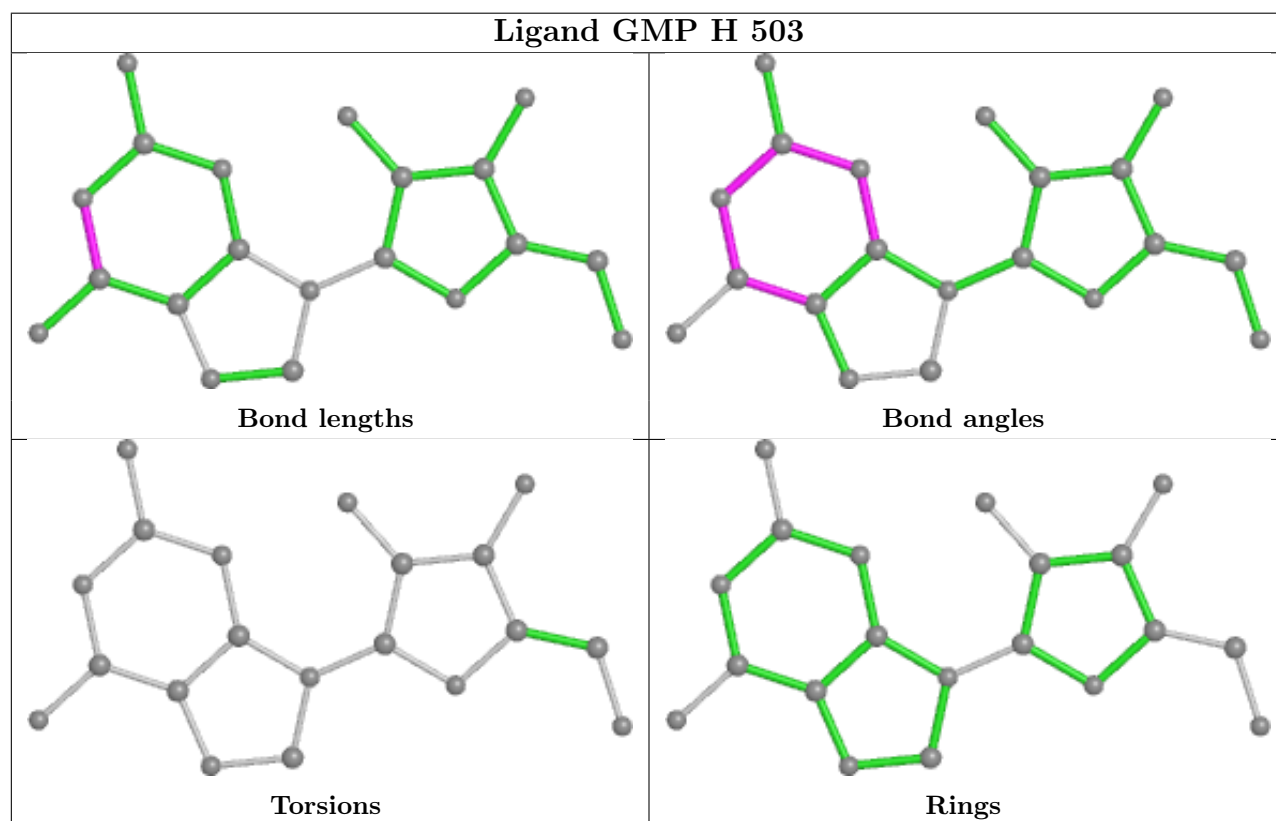
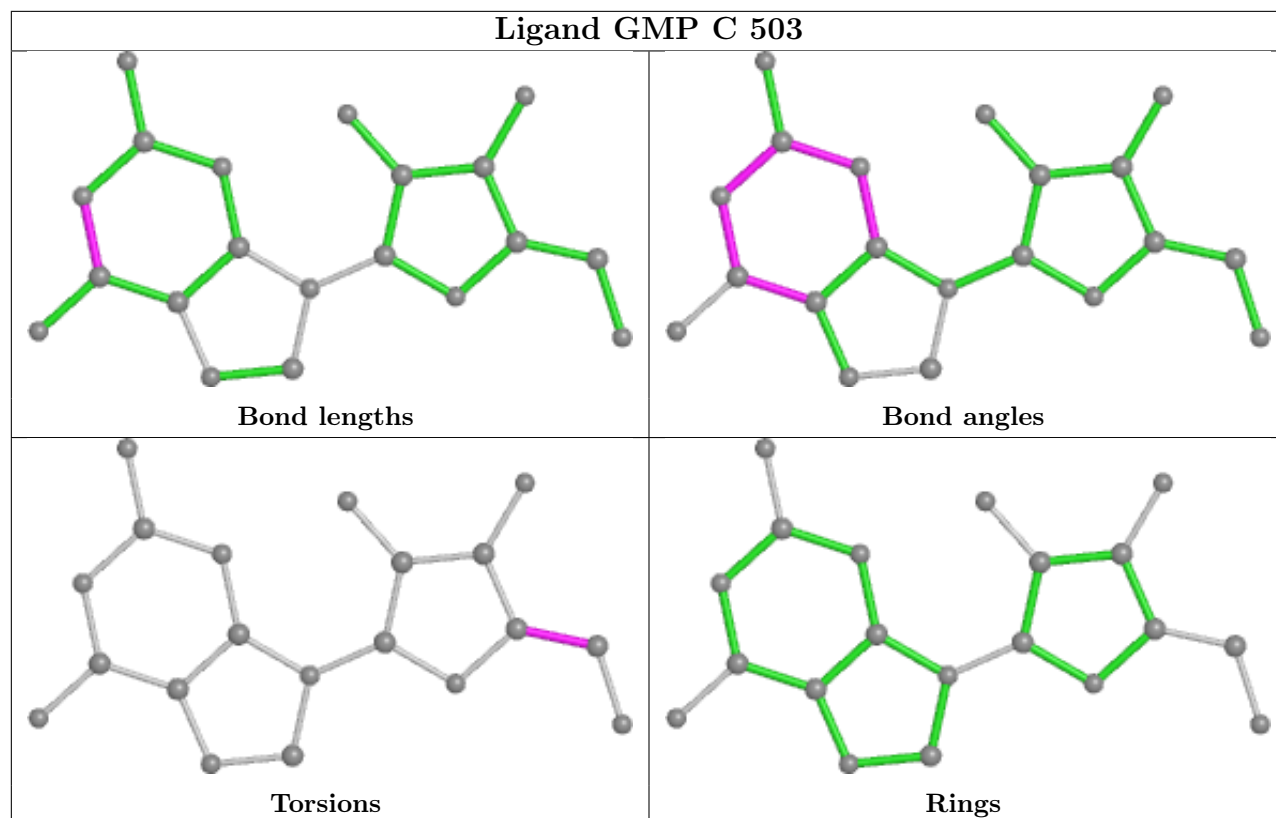
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	502	GMP	1	0
2	F	501	G4P	1	0
2	D	501	G4P	3	0
3	E	502	GMP	2	0
3	F	502	GMP	1	0
2	E	501	G4P	1	0

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.

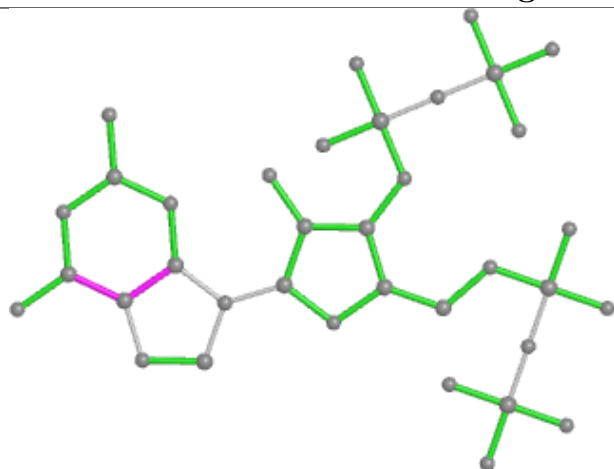
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



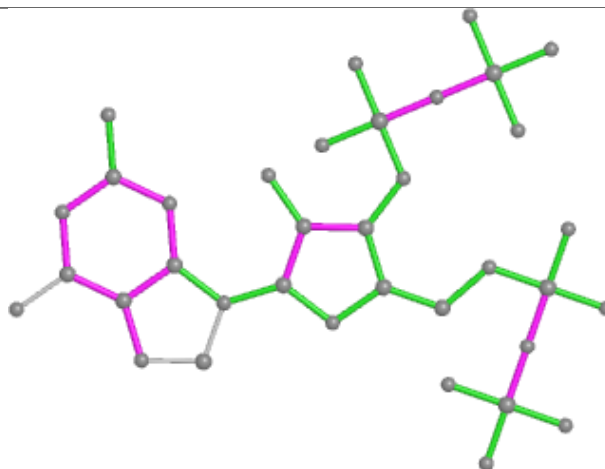




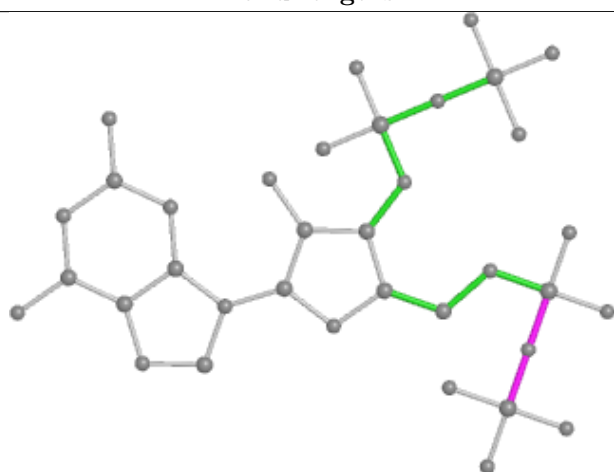
Ligand G4P F 501



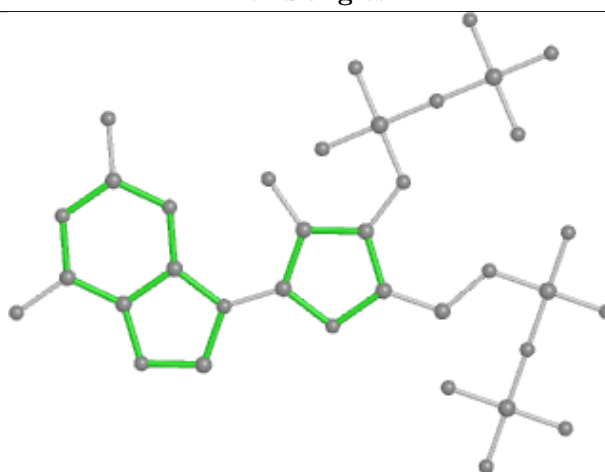
Bond lengths



Bond angles

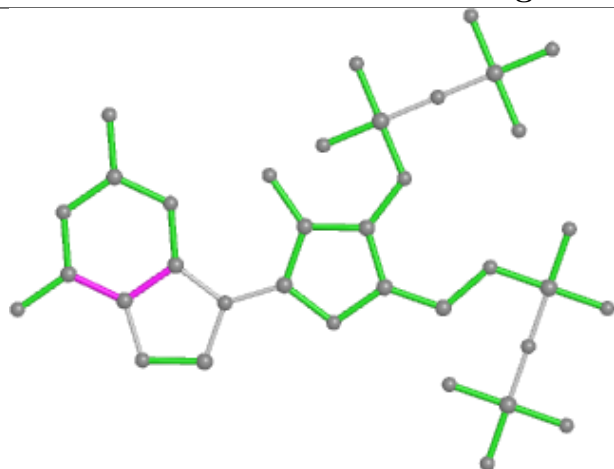


Torsions

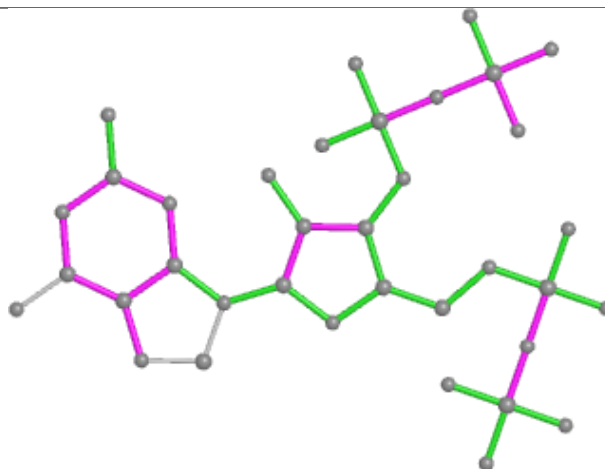


Rings

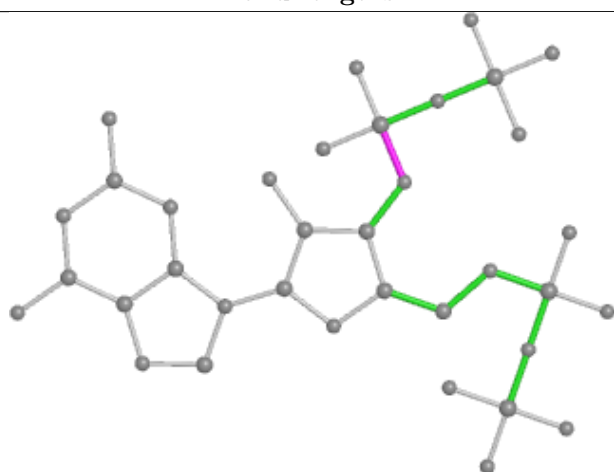
Ligand G4P D 501



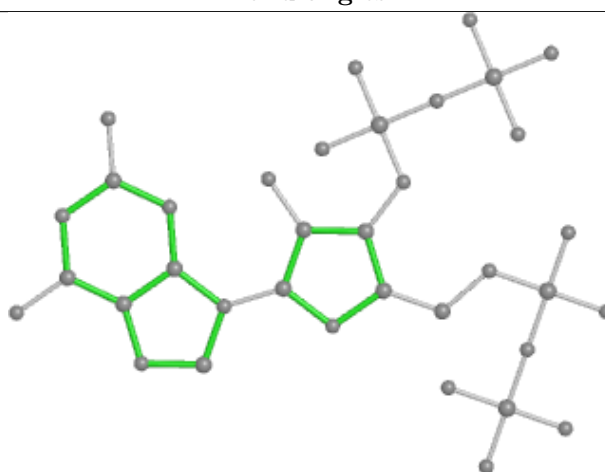
Bond lengths



Bond angles

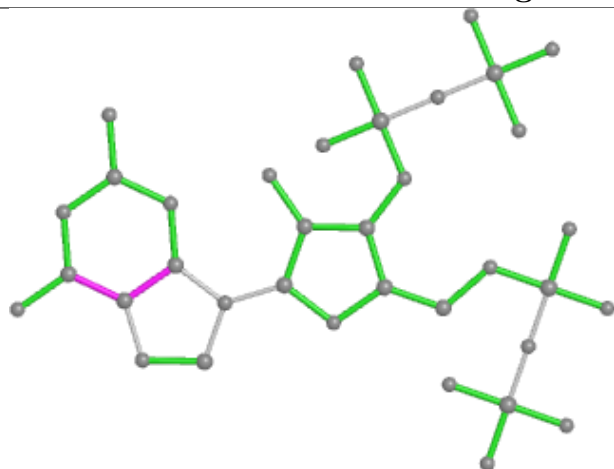


Torsions

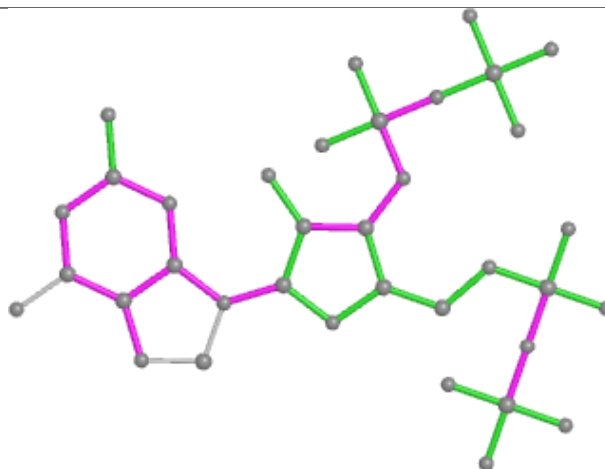


Rings

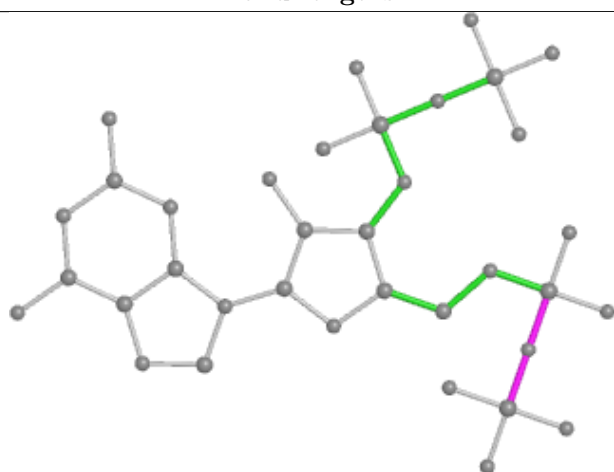
Ligand G4P G 501



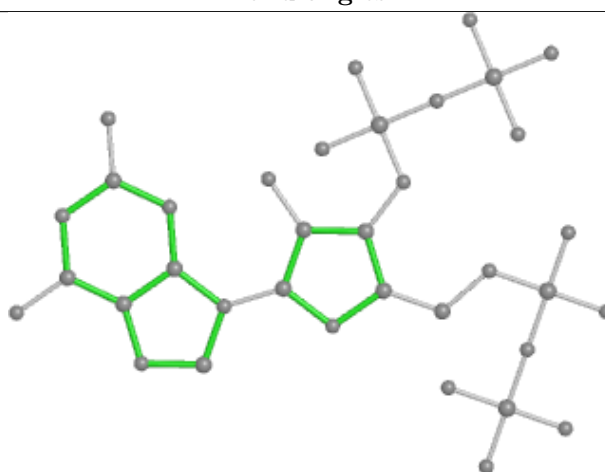
Bond lengths



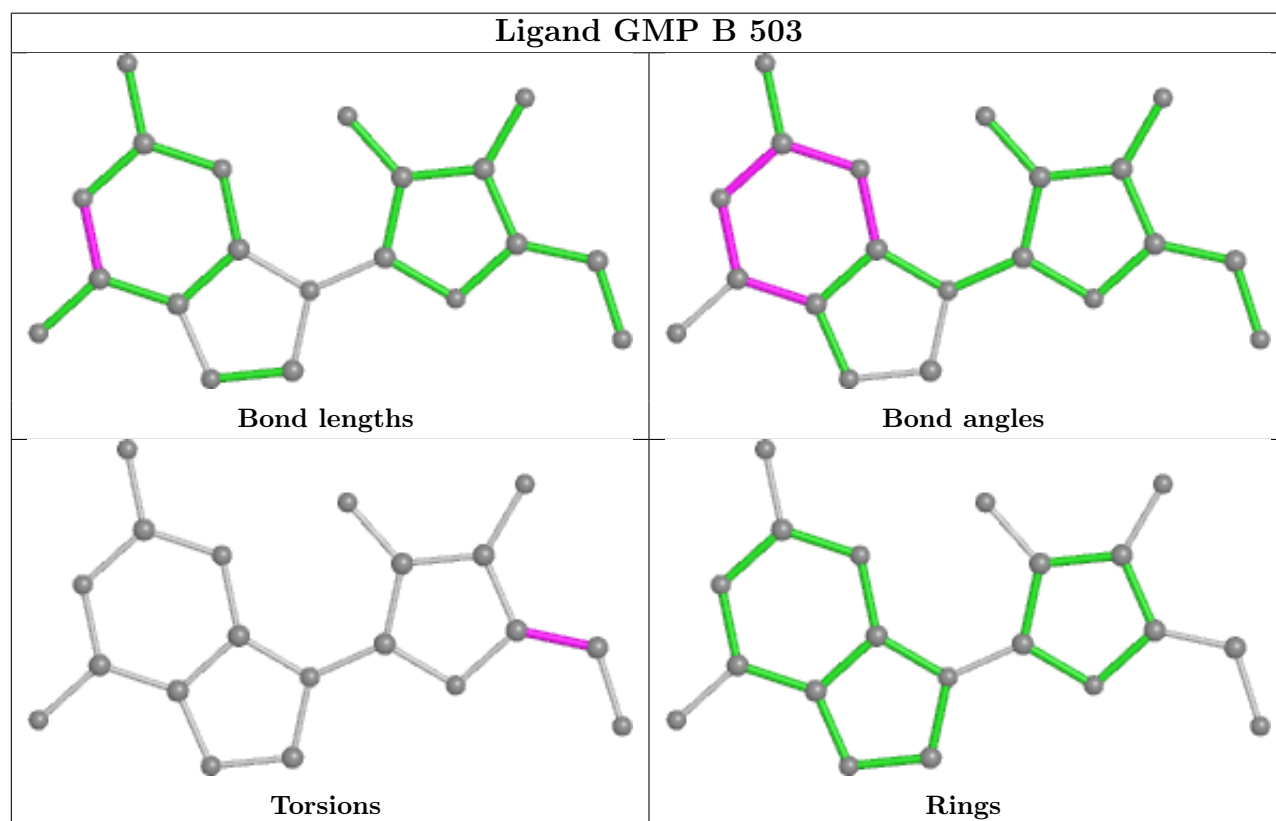
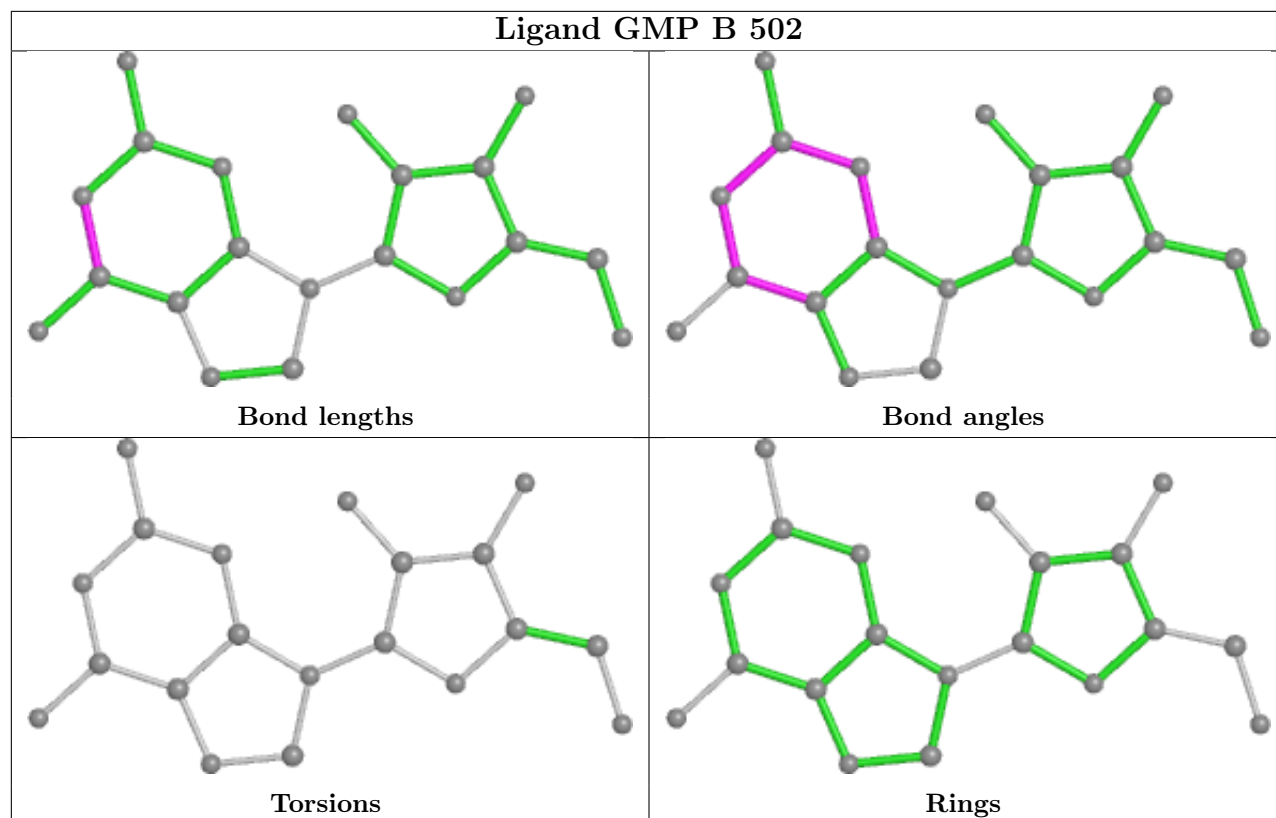
Bond angles



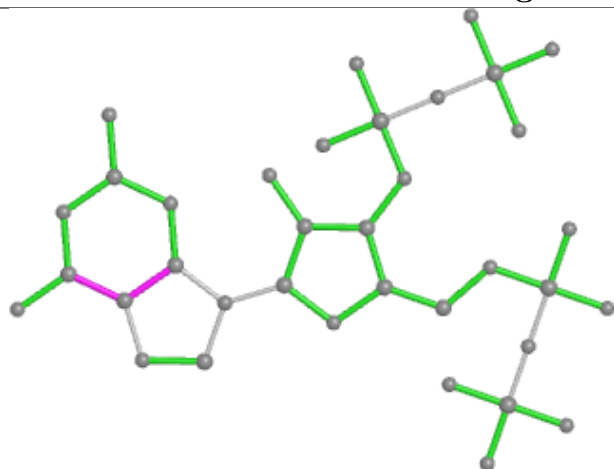
Torsions



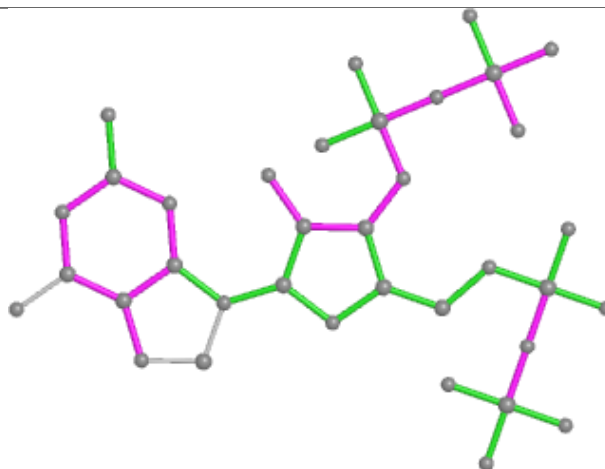
Rings



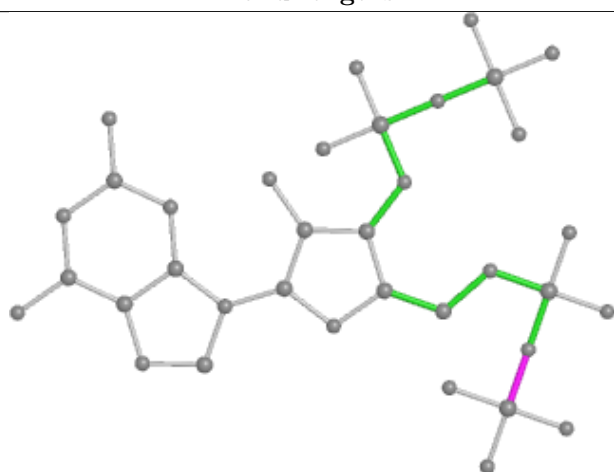
Ligand G4P A 501



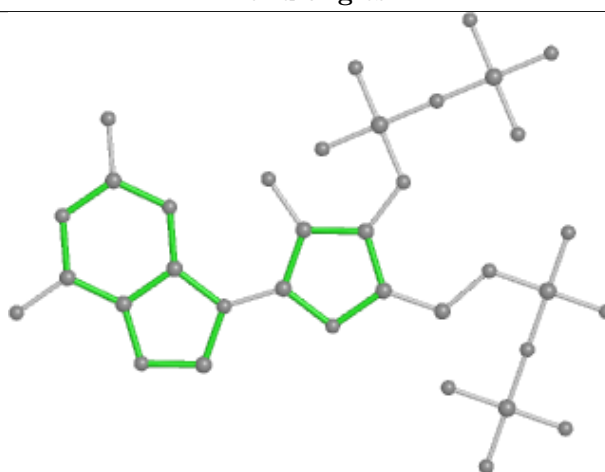
Bond lengths



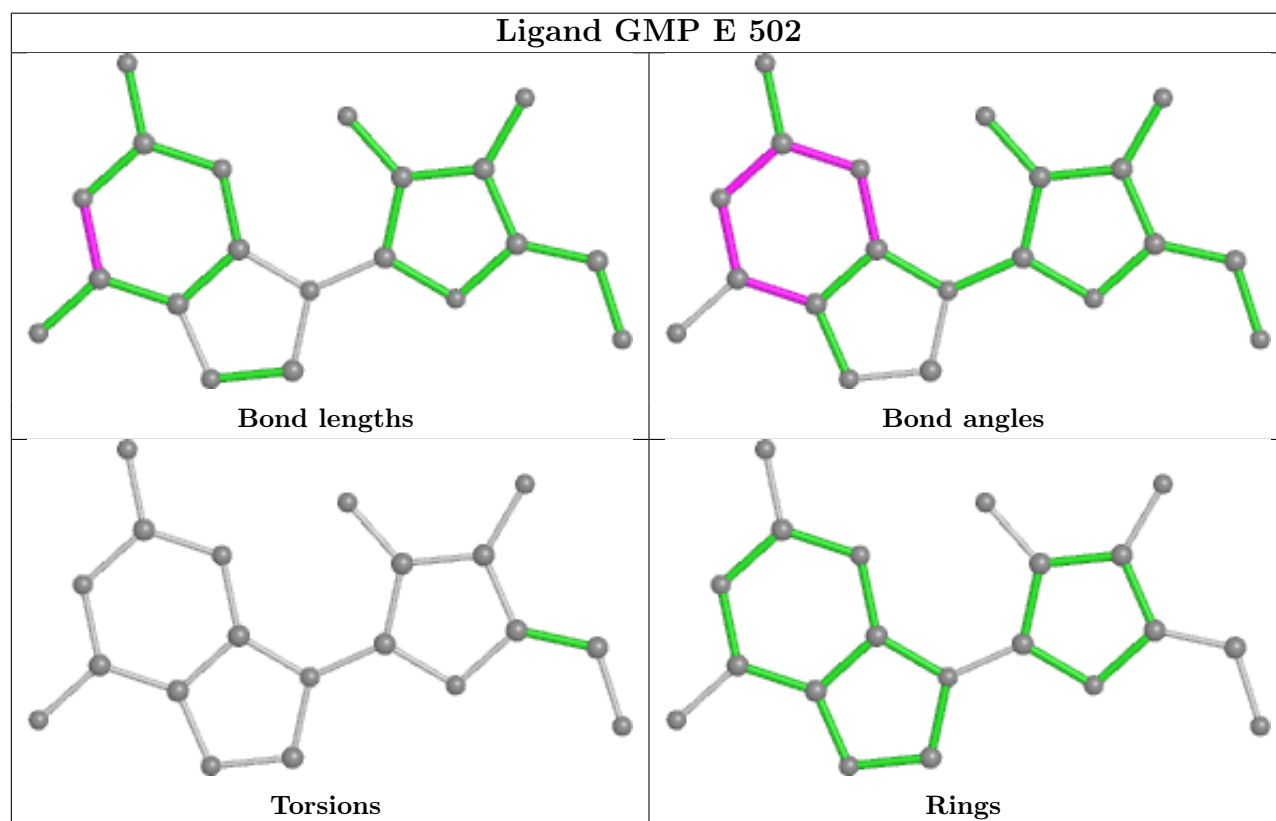
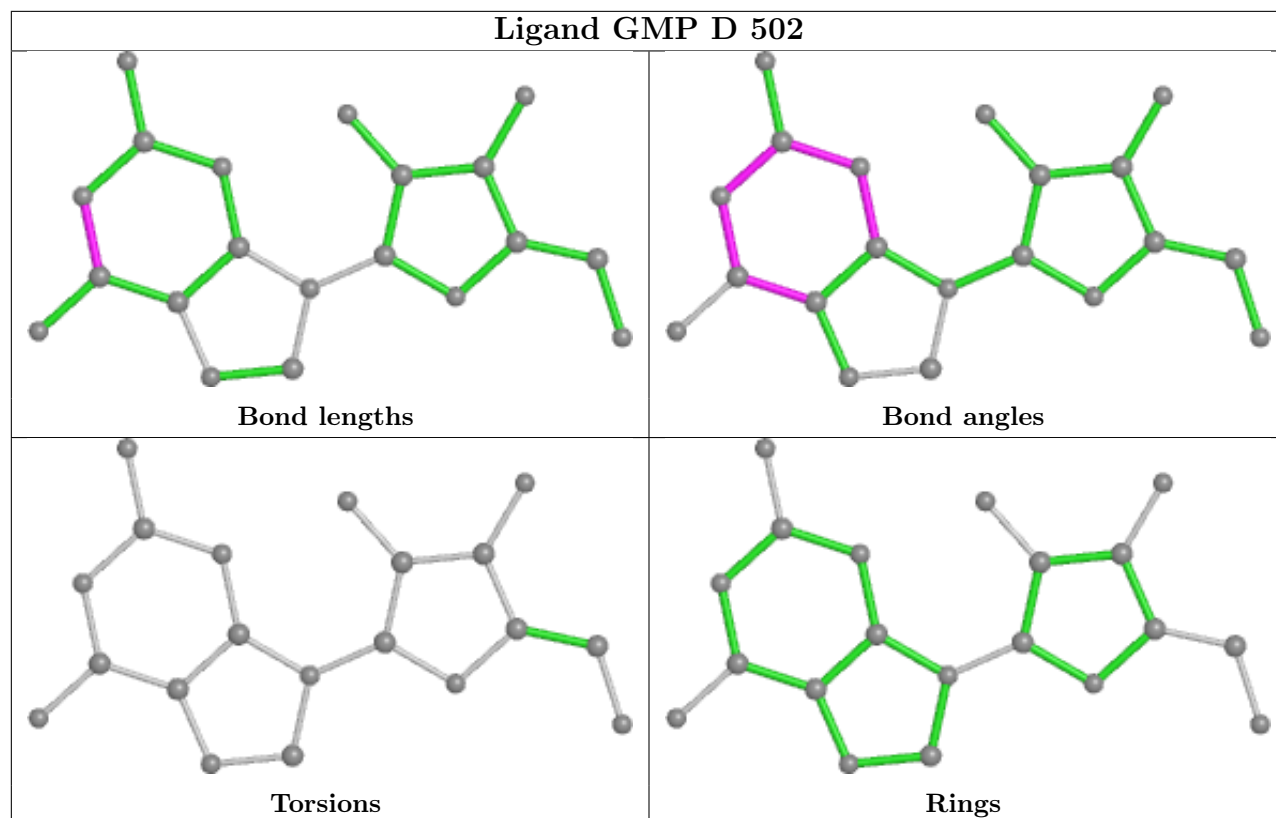
Bond angles



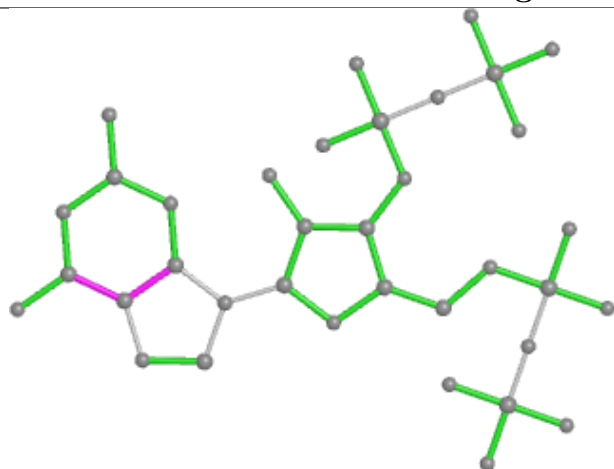
Torsions



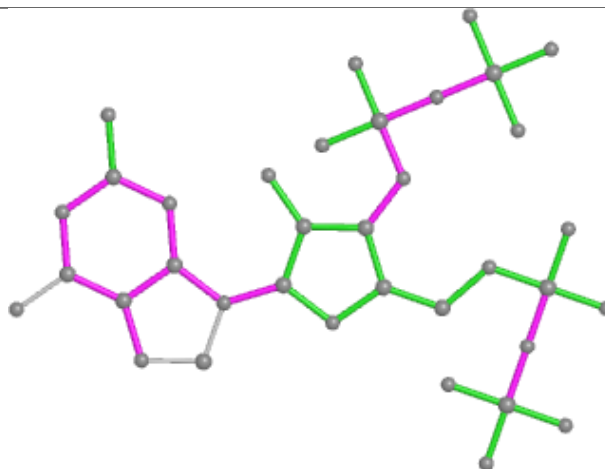
Rings



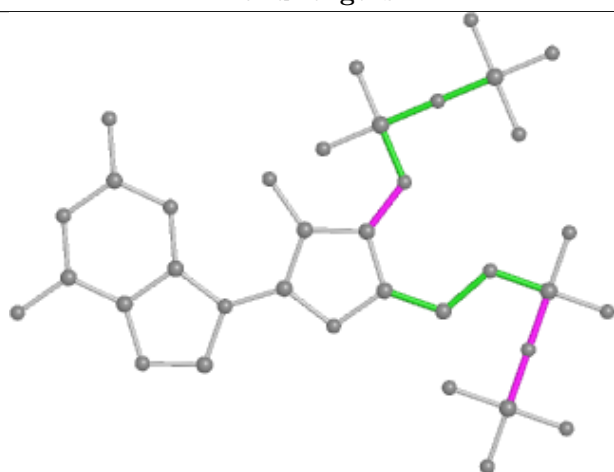
Ligand G4P H 501



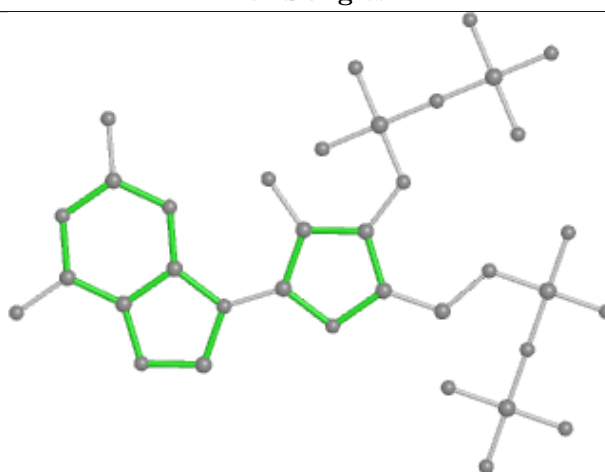
Bond lengths



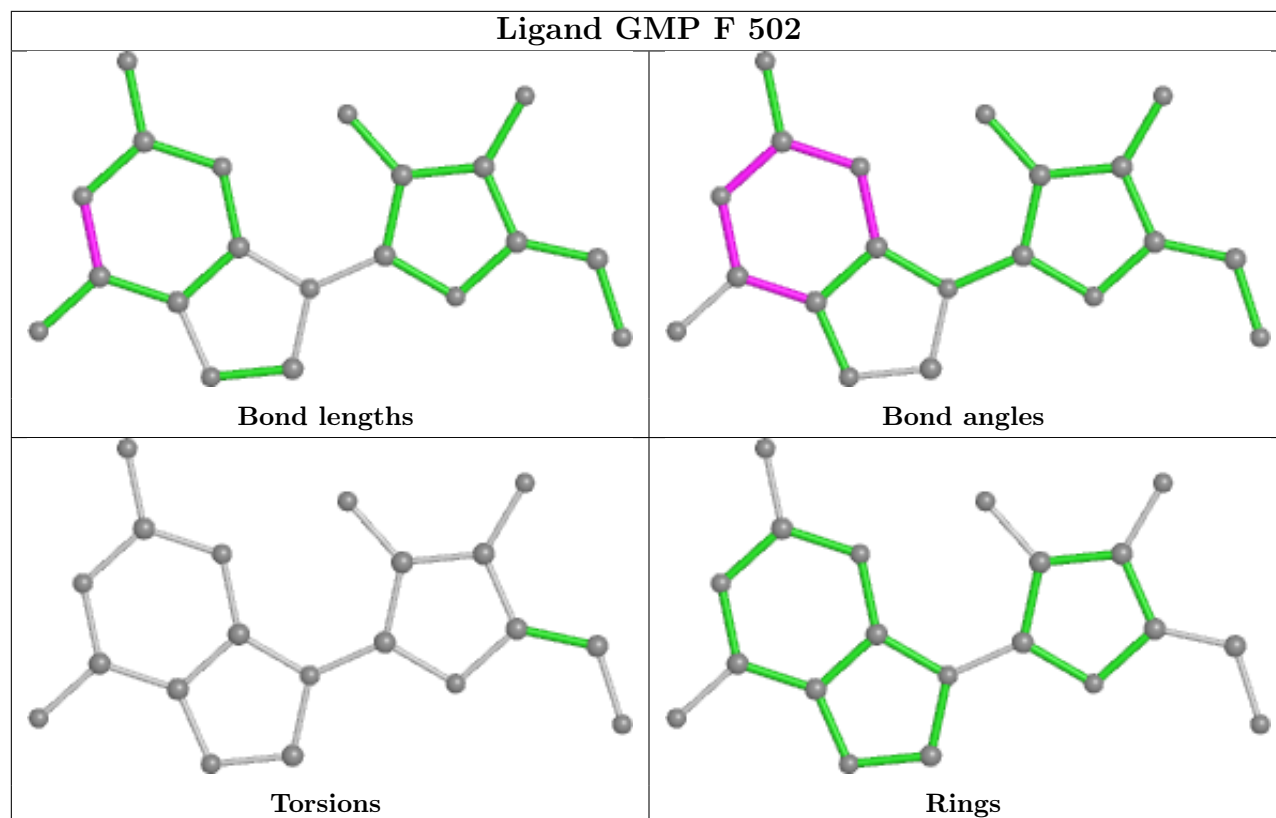
Bond angles



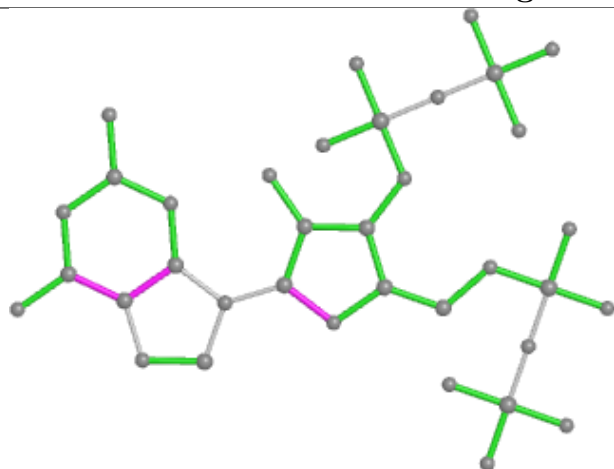
Torsions



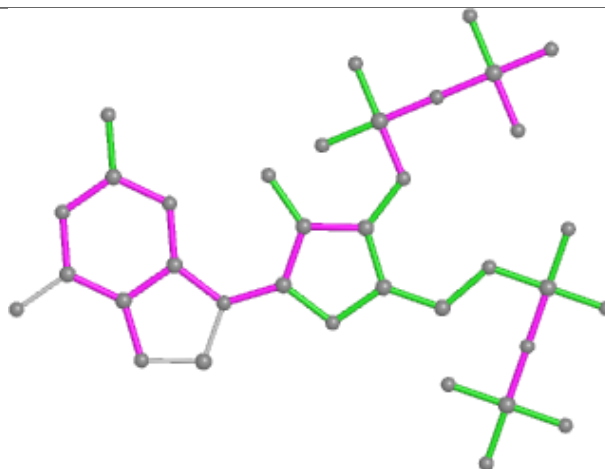
Rings



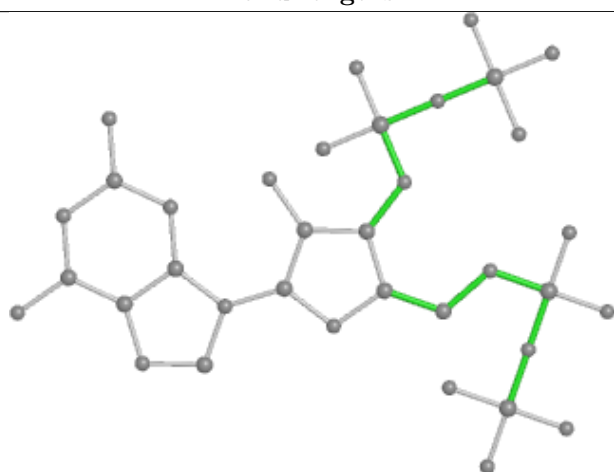
Ligand G4P B 501



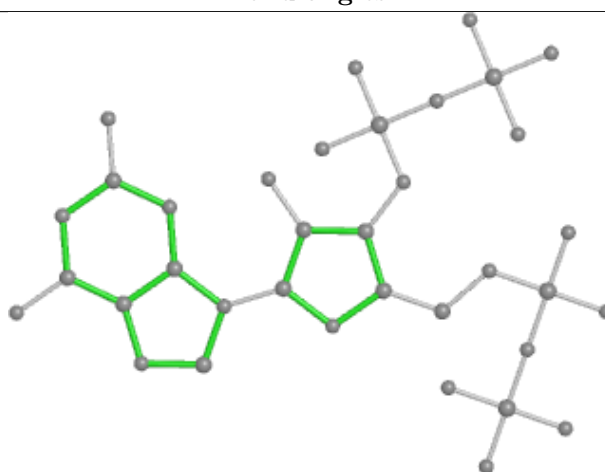
Bond lengths



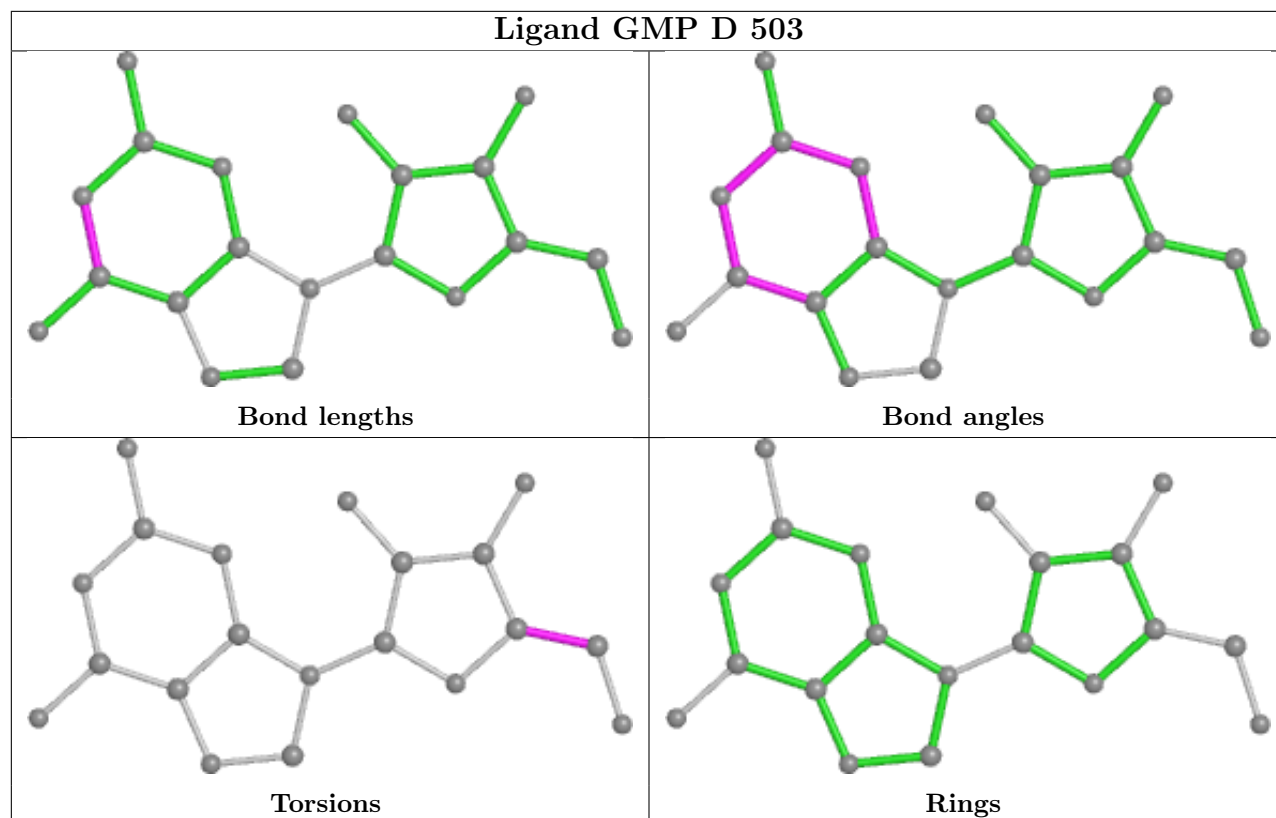
Bond angles



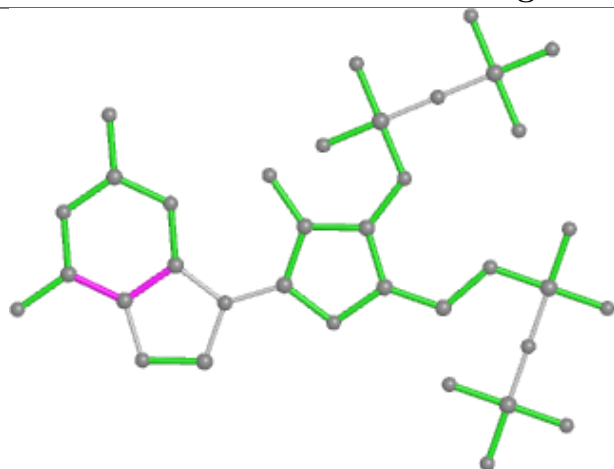
Torsions



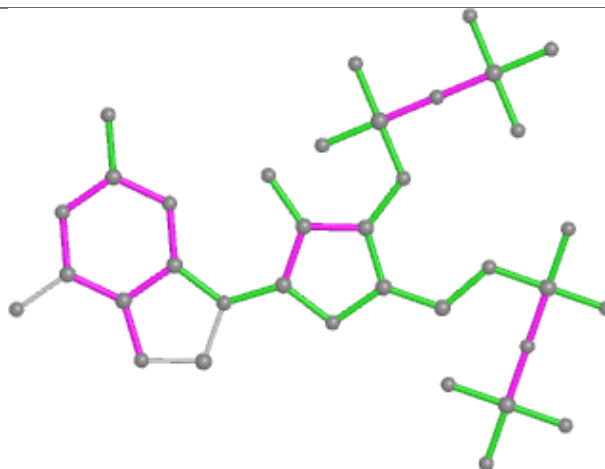
Rings



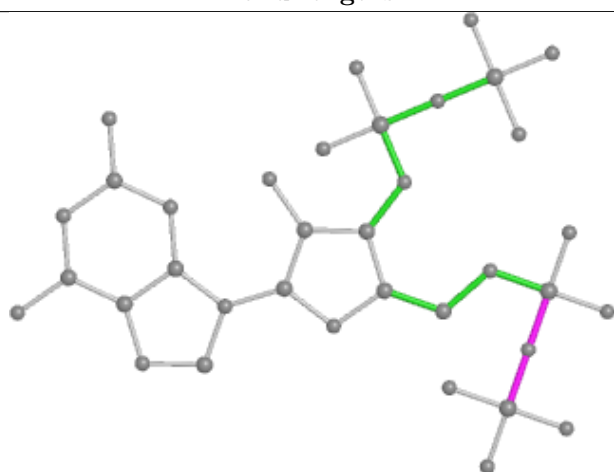
Ligand G4P E 501



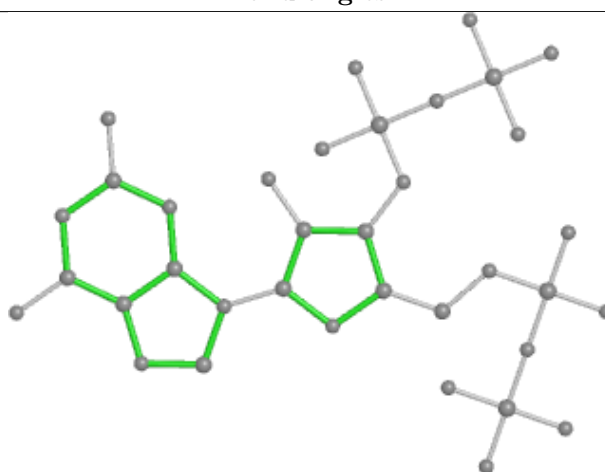
Bond lengths



Bond angles

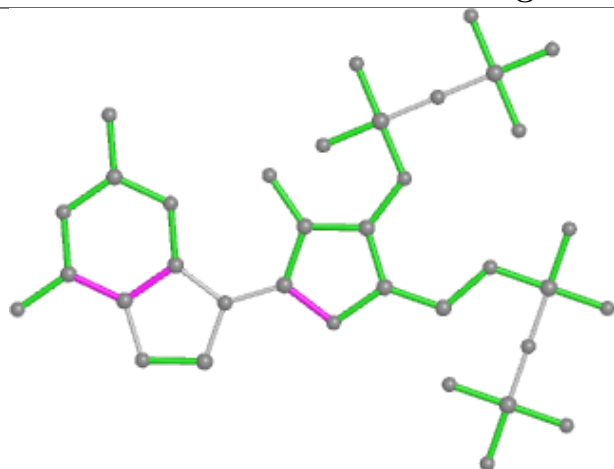


Torsions

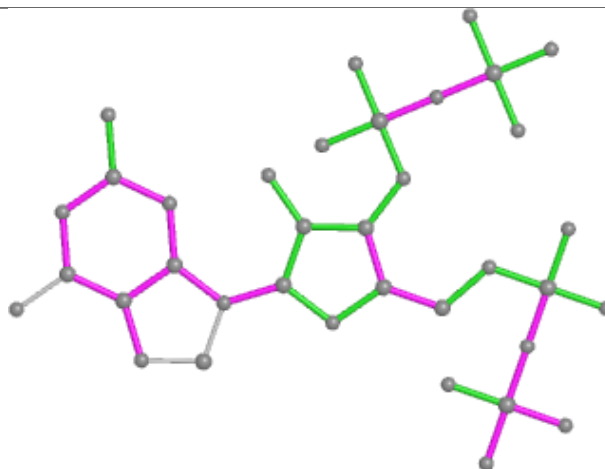


Rings

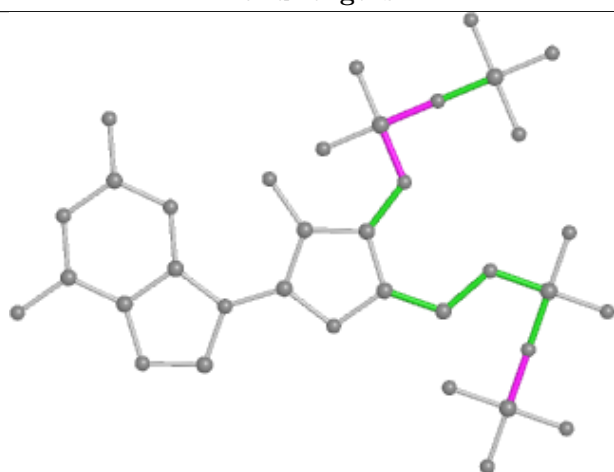
Ligand G4P C 501



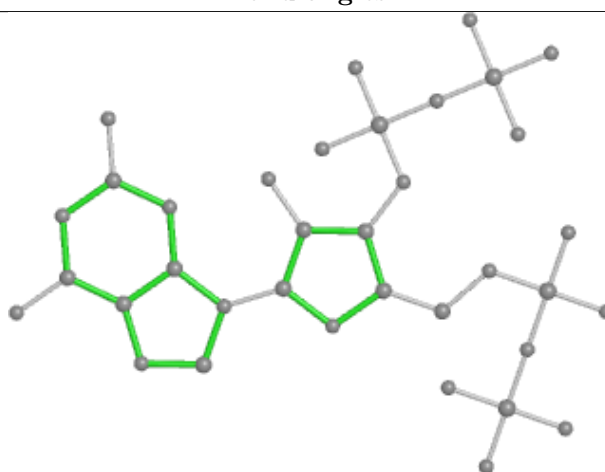
Bond lengths



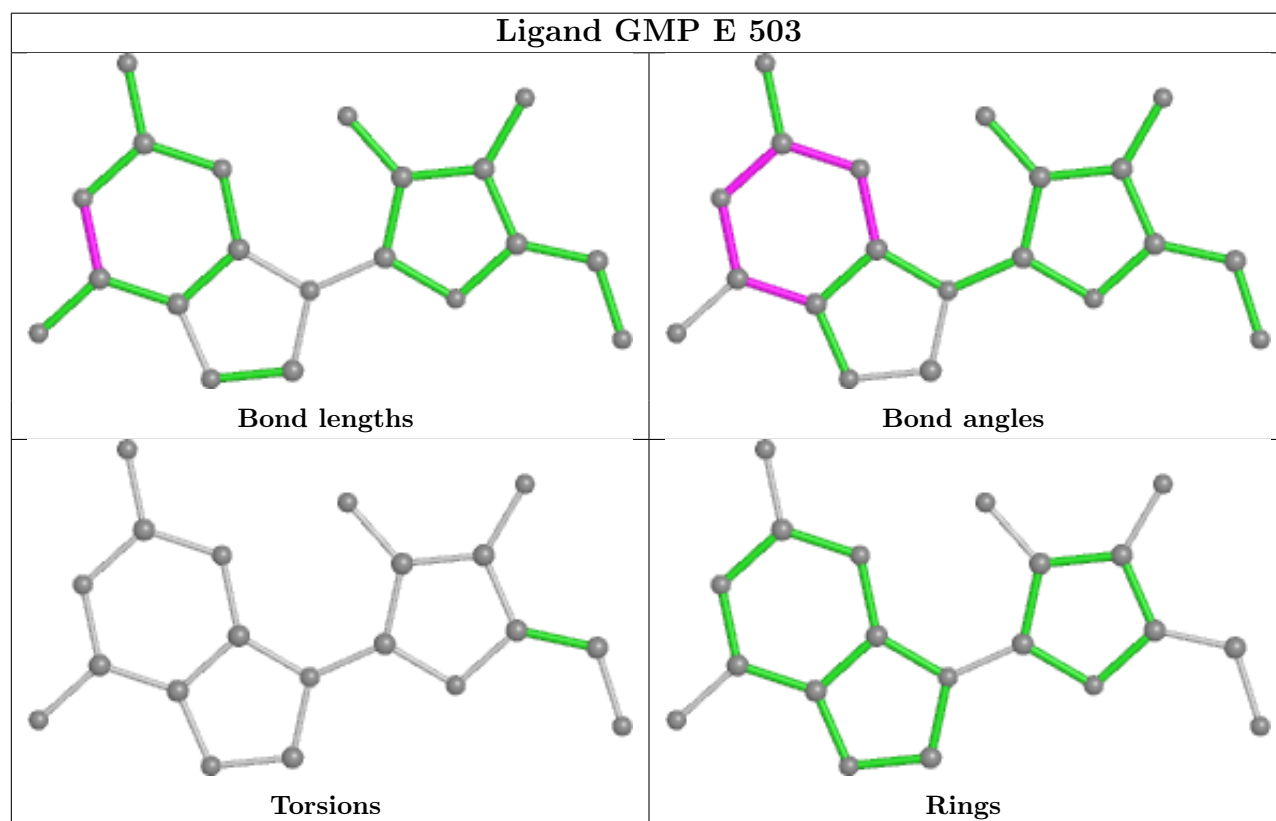
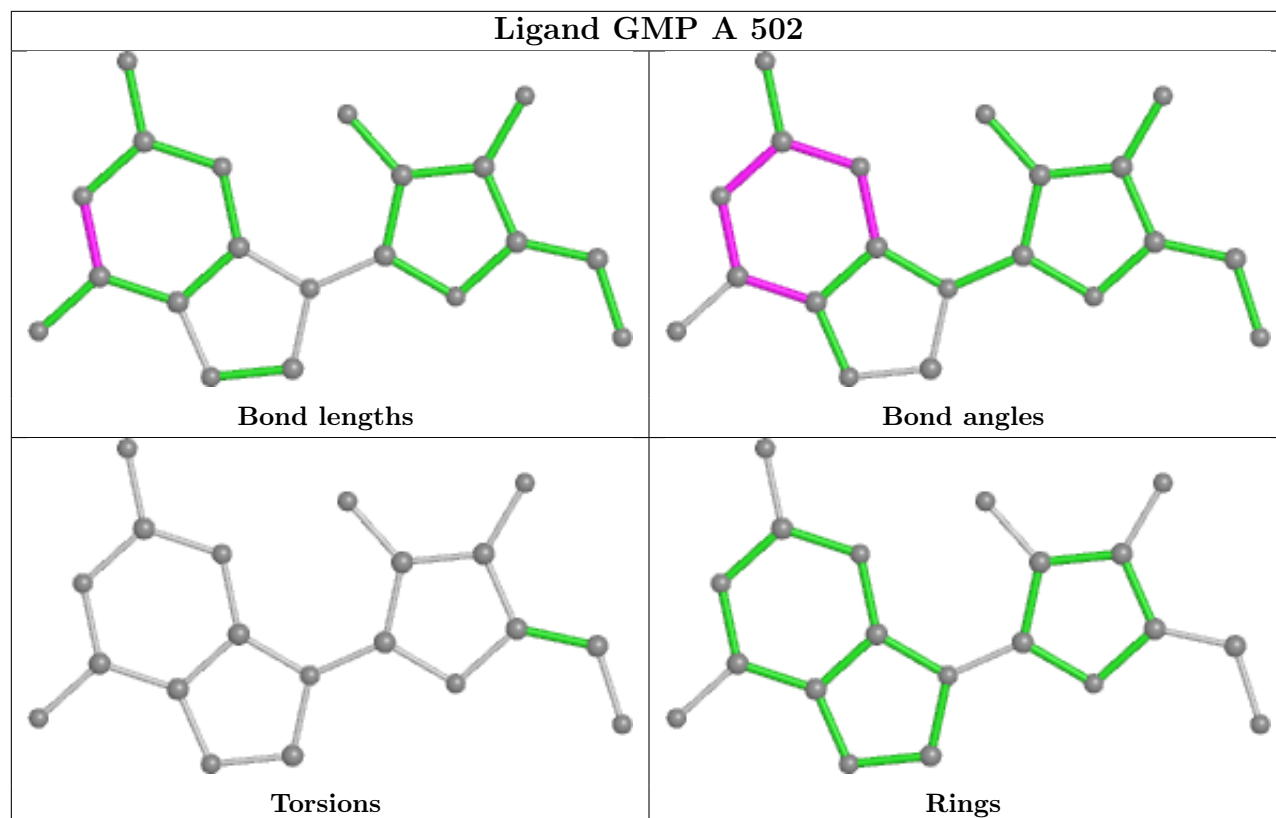
Bond angles

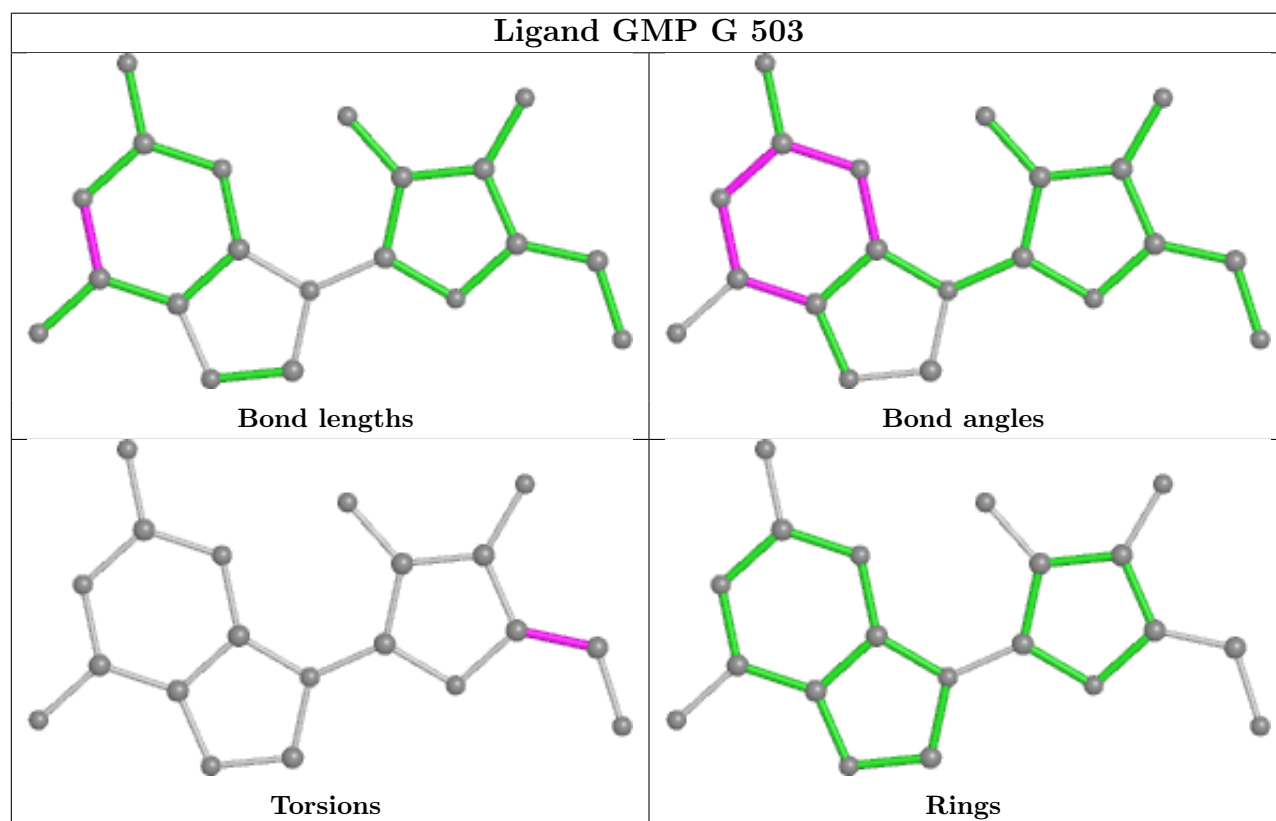
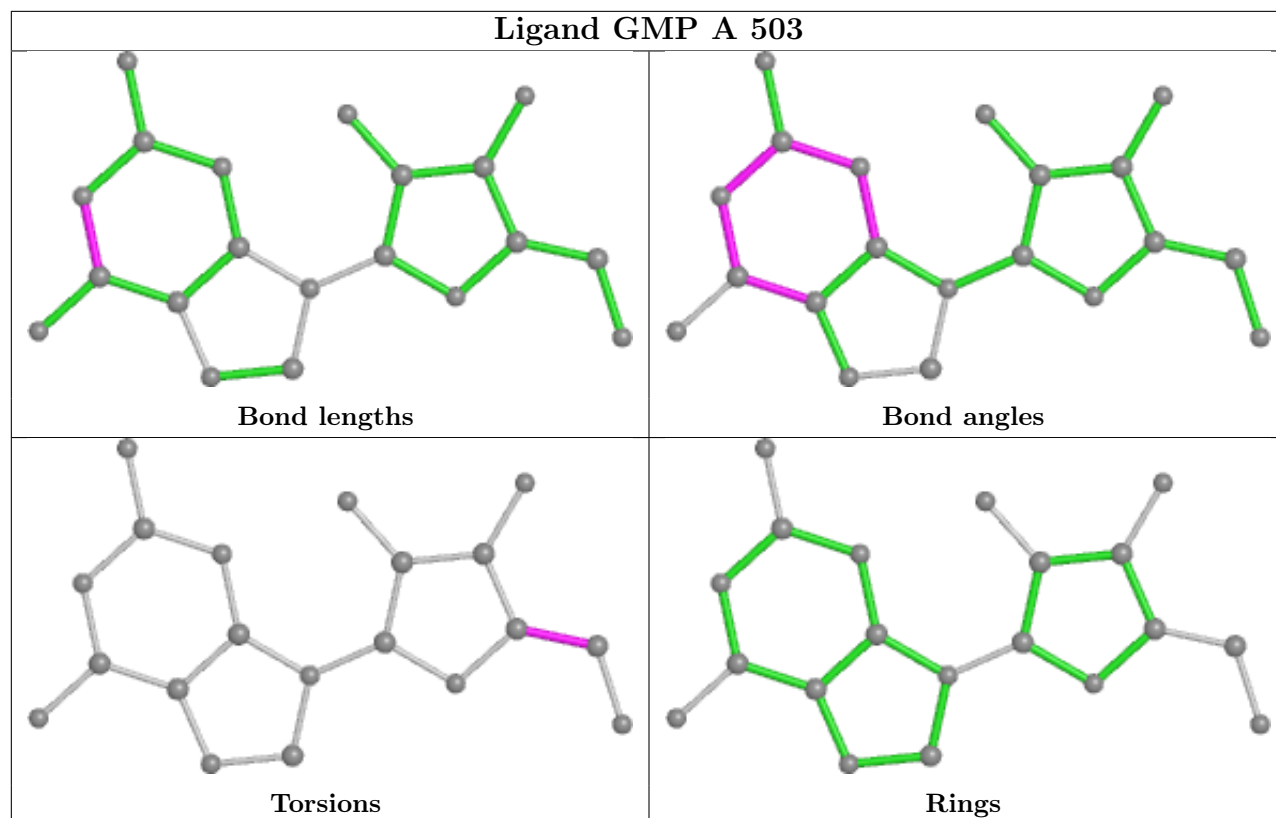


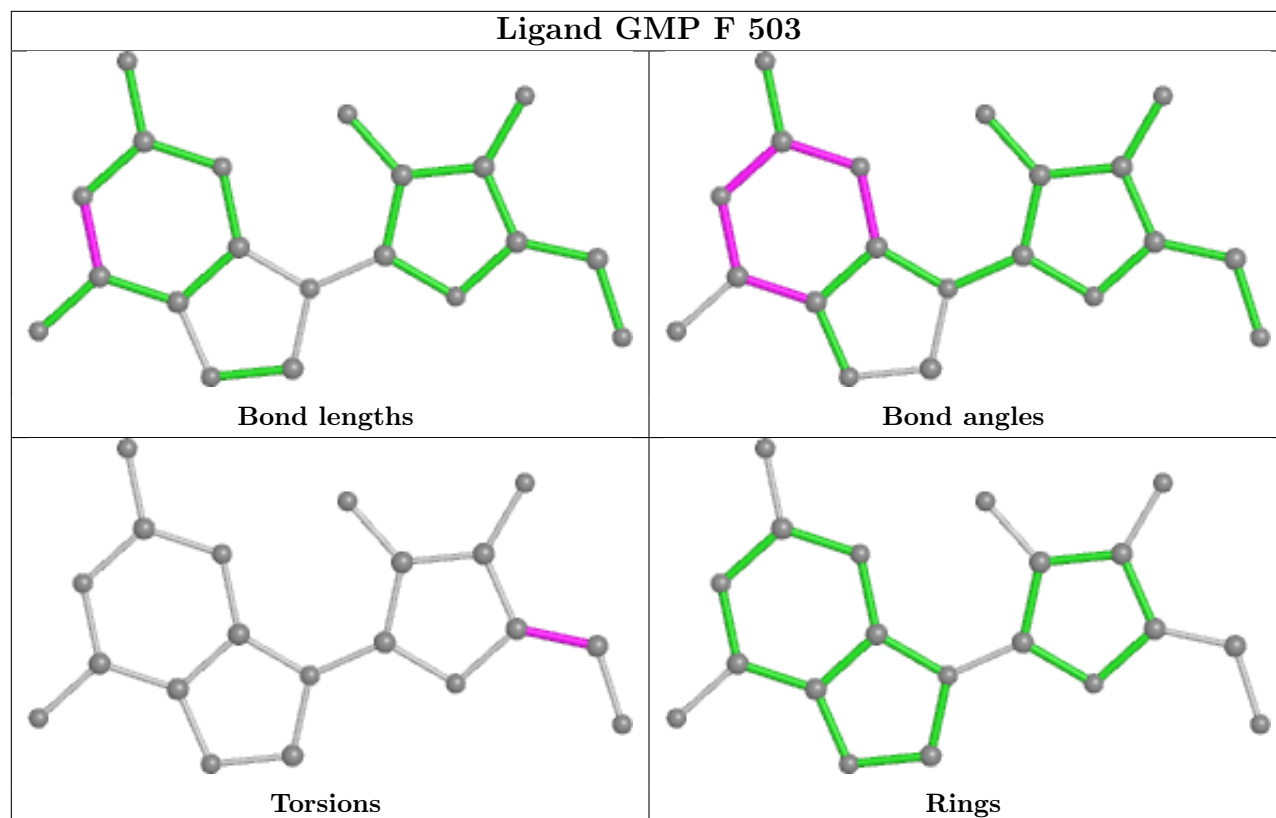
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	435/437 (99%)	0.46	17 (3%) 39 38	96, 118, 169, 209	0
1	B	428/437 (97%)	0.62	24 (5%) 24 24	95, 121, 170, 219	0
1	C	429/437 (98%)	0.44	14 (3%) 46 44	95, 120, 169, 202	0
1	D	435/437 (99%)	0.63	29 (6%) 17 19	95, 137, 196, 218	0
1	E	422/437 (96%)	0.64	37 (8%) 10 12	105, 144, 190, 220	0
1	F	412/437 (94%)	0.95	73 (17%) 1 2	116, 169, 207, 223	0
1	G	421/437 (96%)	1.11	86 (20%) 1 1	131, 182, 212, 228	0
1	H	408/437 (93%)	0.89	62 (15%) 2 3	106, 141, 201, 227	0
All	All	3390/3496 (96%)	0.71	342 (10%) 7 9	95, 141, 201, 228	0

The worst 5 of 342 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	50	VAL	8.8
1	G	60	LEU	7.1
1	B	355	GLY	6.7
1	F	50	VAL	6.5
1	C	25	PHE	6.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

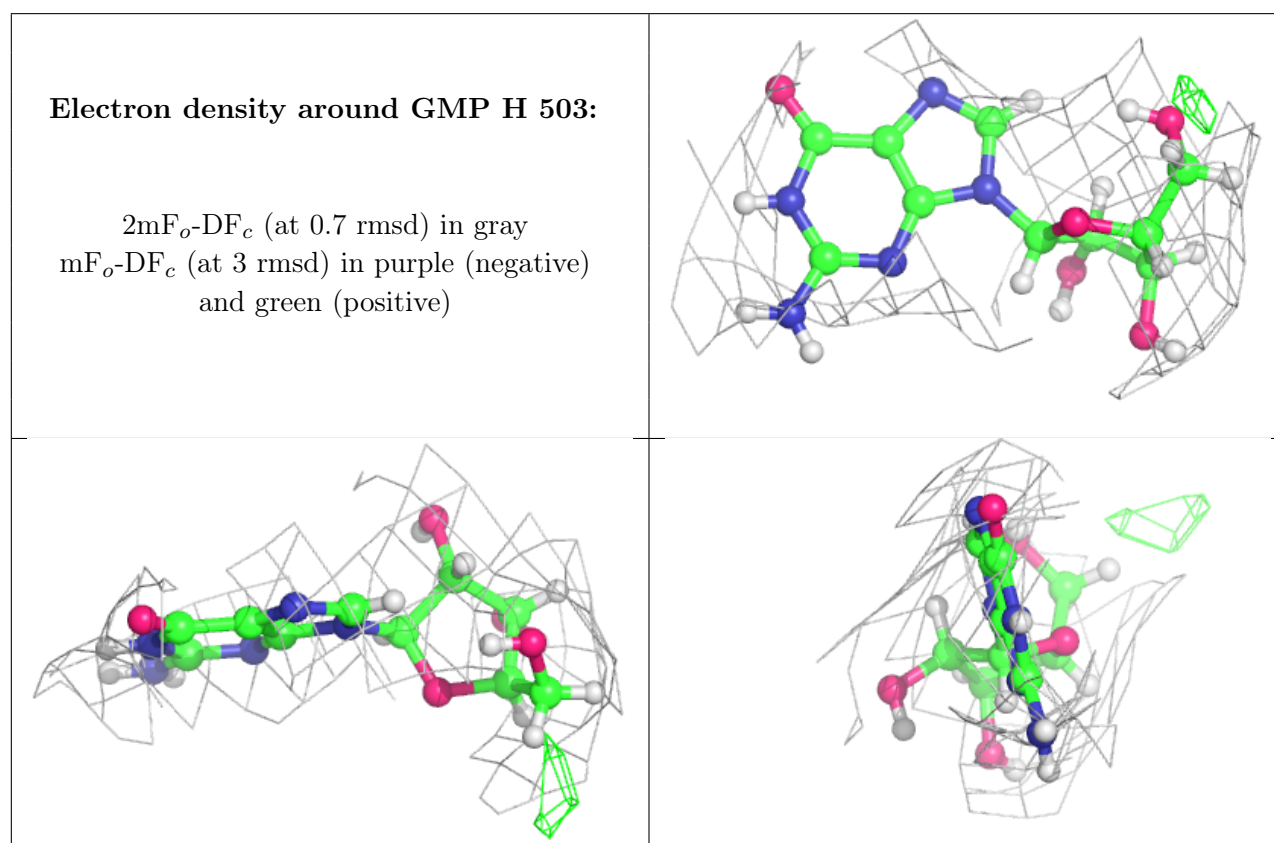
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	F	504	1/1	0.50	0.29	392,392,392,392	0
5	MG	E	506	1/1	0.56	2.37	146,146,146,146	0
4	K	C	505	1/1	0.65	0.43	198,198,198,198	0
5	MG	H	506	1/1	0.73	1.50	133,133,133,133	0
4	K	G	504	1/1	0.74	0.73	210,210,210,210	0
5	MG	D	505	1/1	0.77	0.78	143,143,143,143	0
3	GMP	H	503	20/20	0.77	0.24	119,168,224,228	0
3	GMP	C	503	20/20	0.79	0.34	105,147,201,221	0
3	GMP	F	503	20/20	0.79	0.26	174,215,279,282	0
5	MG	F	505	1/1	0.80	0.84	148,148,148,148	0
3	GMP	G	503	20/20	0.82	0.21	184,212,266,273	0
4	K	B	505	1/1	0.82	0.66	294,294,294,294	0
5	MG	G	505	1/1	0.83	0.78	177,177,177,177	0
5	MG	C	506	1/1	0.84	0.78	131,131,131,131	0
4	K	D	504	1/1	0.84	0.16	202,202,202,202	0
4	K	E	505	1/1	0.85	0.43	128,128,128,128	0
3	GMP	G	502	20/20	0.85	0.25	175,201,249,250	0
3	GMP	B	503	20/20	0.85	0.27	135,167,227,238	0
3	GMP	D	503	20/20	0.86	0.28	148,189,241,253	0
3	GMP	A	503	20/20	0.86	0.21	115,149,214,223	0
2	G4P	F	501	36/36	0.86	0.23	135,183,249,272	0
3	GMP	E	503	20/20	0.87	0.18	116,182,240,247	0
2	G4P	H	501	36/36	0.87	0.22	136,171,232,249	0
2	G4P	G	501	36/36	0.88	0.13	137,178,227,239	0
4	K	H	505	1/1	0.89	0.34	183,183,183,183	0
3	GMP	F	502	20/20	0.89	0.20	163,182,220,240	0
5	MG	A	505	1/1	0.89	0.78	139,139,139,139	0
2	G4P	A	501	36/36	0.90	0.19	94,133,192,226	0
2	G4P	E	501	36/36	0.90	0.19	117,151,220,257	0
3	GMP	E	502	20/20	0.91	0.28	137,161,197,213	0
4	K	H	504	1/1	0.92	0.65	160,160,160,160	0
2	G4P	D	501	36/36	0.93	0.18	94,123,187,212	0
2	G4P	C	501	36/36	0.93	0.17	94,121,198,233	0
3	GMP	D	502	20/20	0.94	0.24	125,152,194,229	0
2	G4P	B	501	36/36	0.94	0.15	97,135,196,219	0
4	K	E	504	1/1	0.94	0.30	135,135,135,135	0
3	GMP	A	502	20/20	0.94	0.27	95,116,164,203	0

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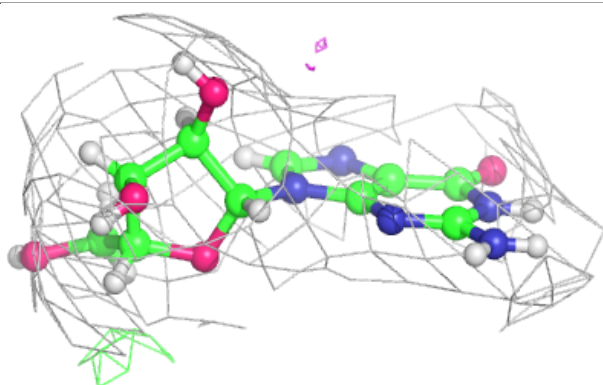
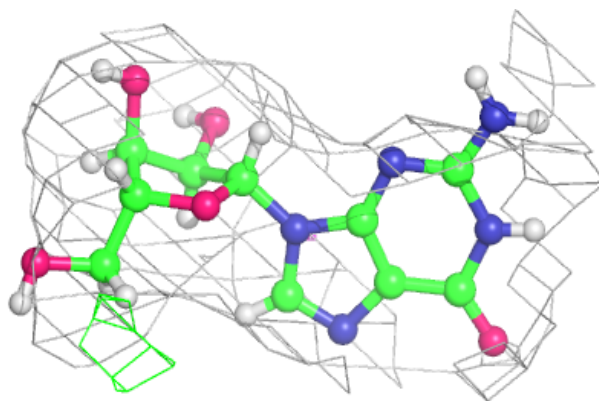
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GMP	B	502	20/20	0.94	0.27	94,108,131,187	0
3	GMP	C	502	20/20	0.95	0.29	94,124,169,215	0
3	GMP	H	502	20/20	0.96	0.35	108,137,192,196	0
4	K	B	504	1/1	0.97	0.41	113,113,113,113	0
4	K	C	504	1/1	0.97	0.32	94,94,94,94	0
4	K	A	504	1/1	0.97	0.52	145,145,145,145	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.

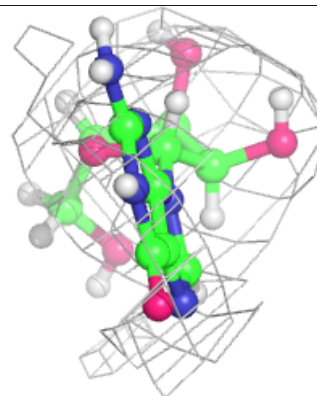
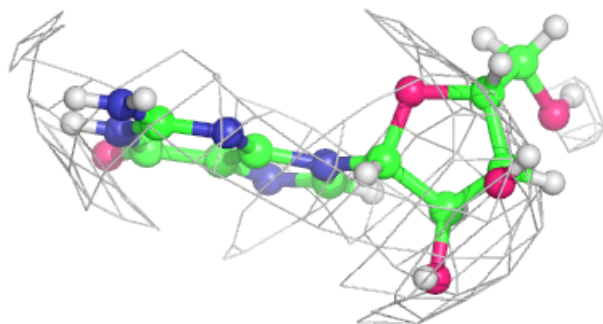
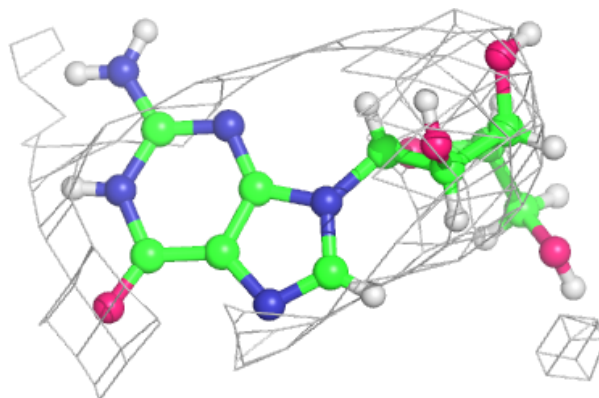


Electron density around GMP C 503:

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

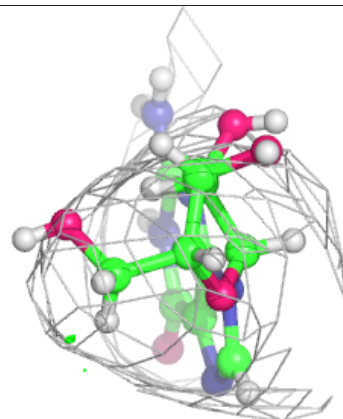
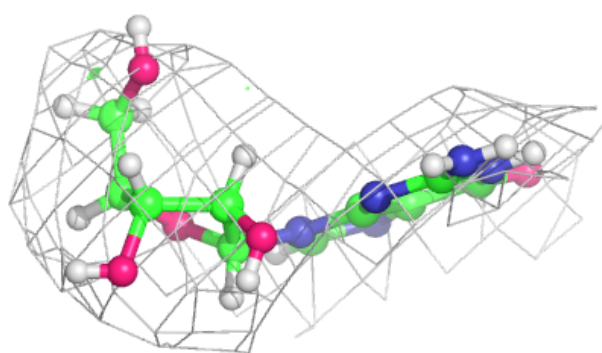
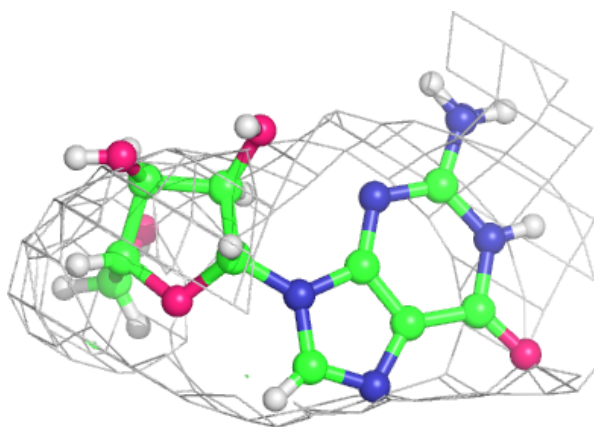
**Electron density around GMP F 503:**

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

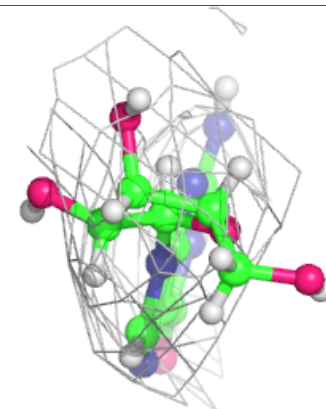
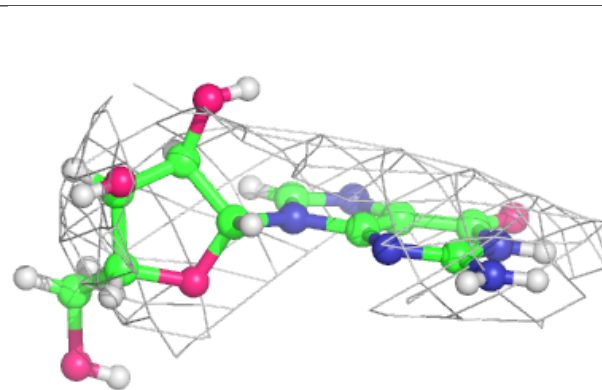
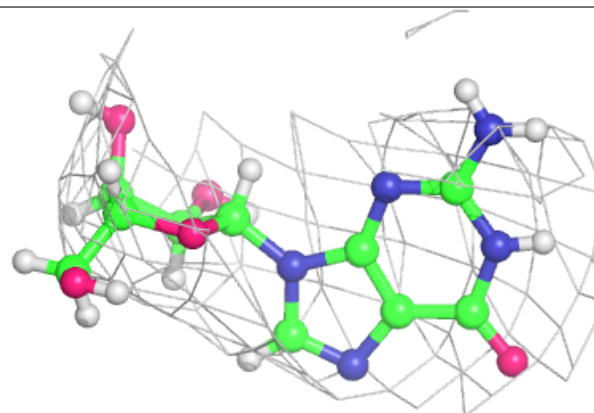


Electron density around GMP G 503:

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and green (positive)

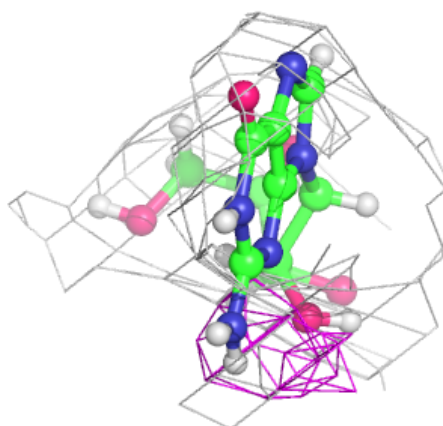
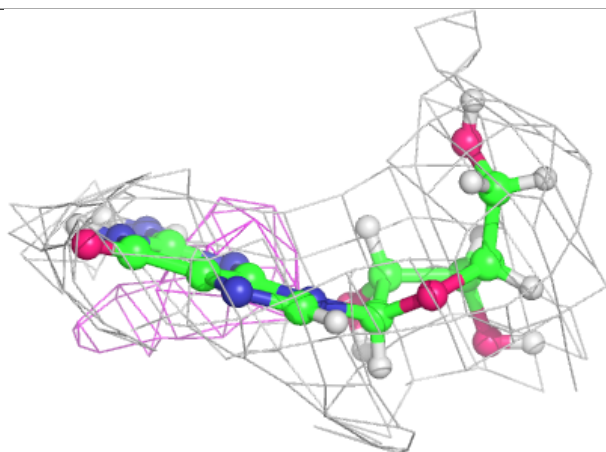
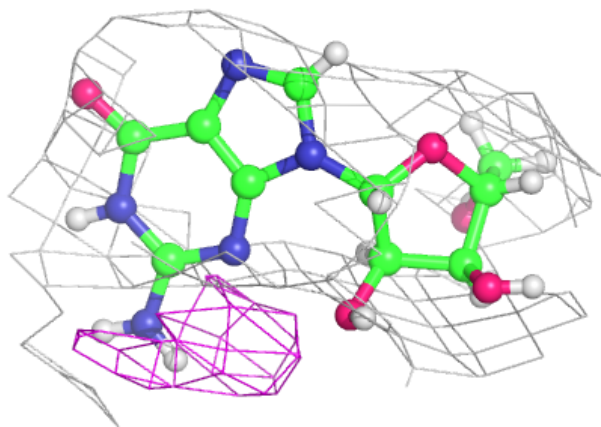
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and green (positive)



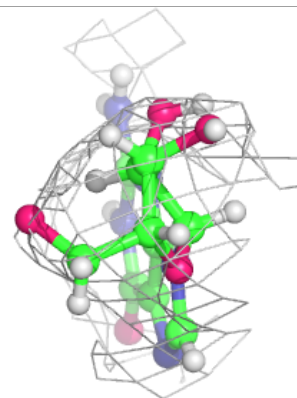
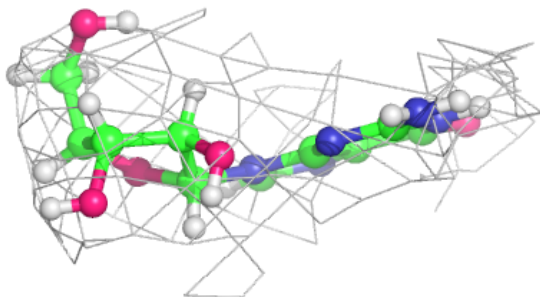
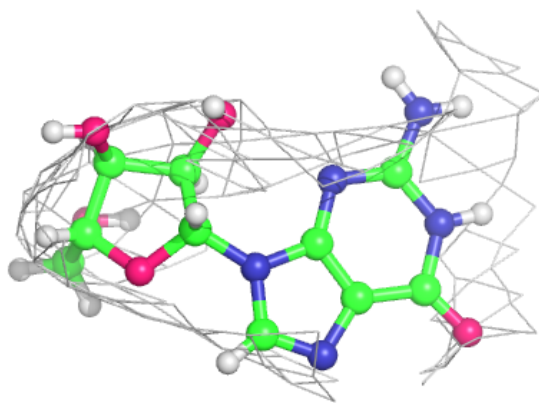
Electron density around GMP B 503:

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

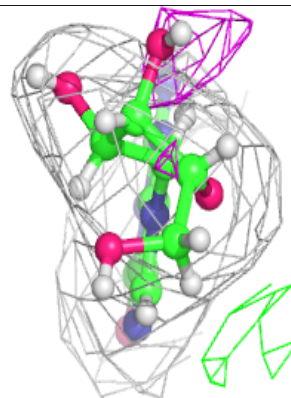
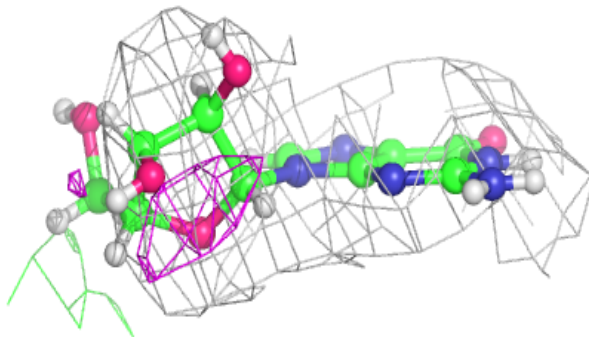
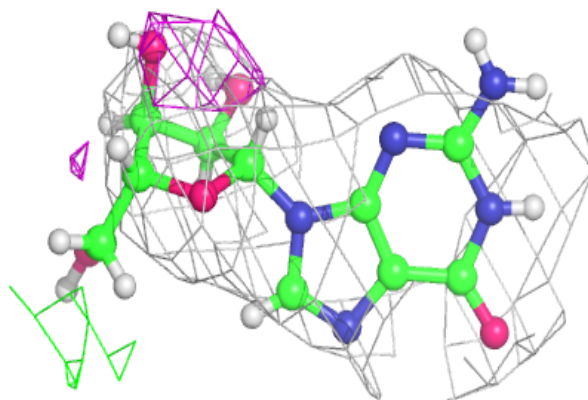


Electron density around GMP D 503:

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

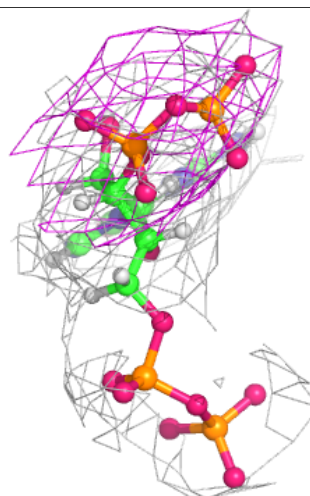
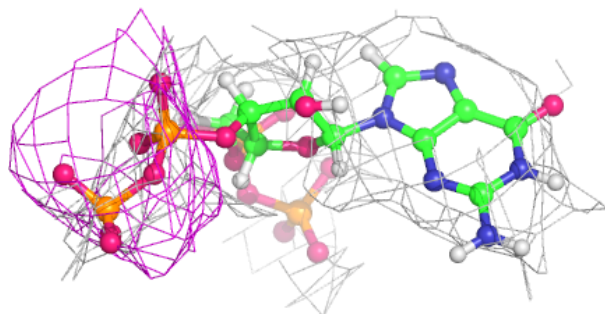
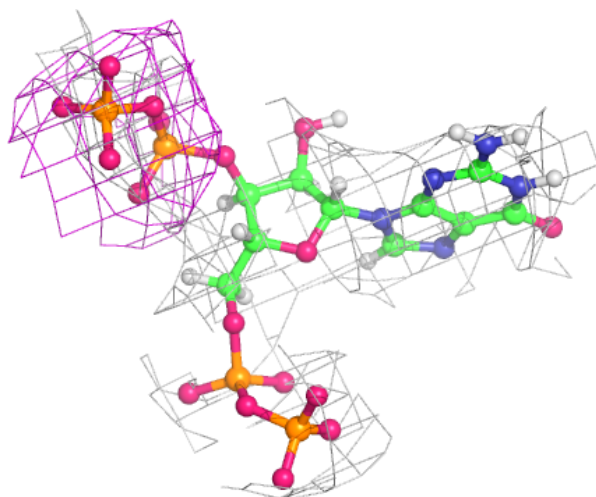
**Electron density around GMP A 503:**

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



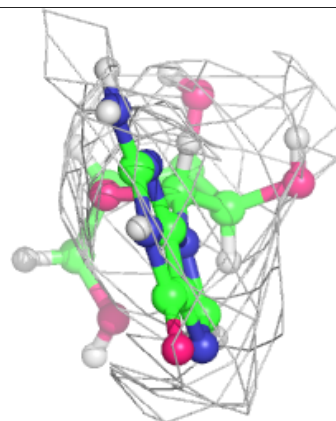
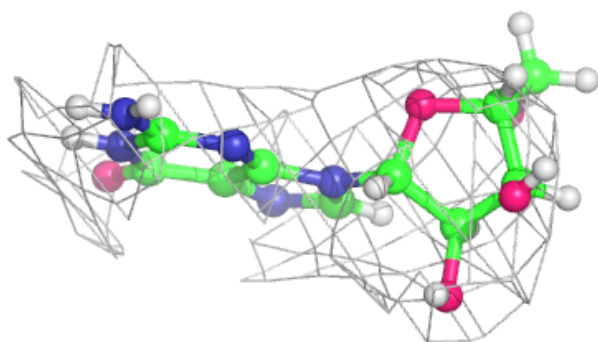
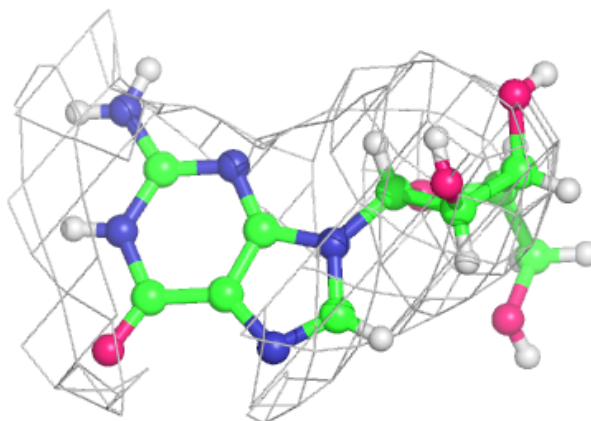
Electron density around G4P F 501:

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



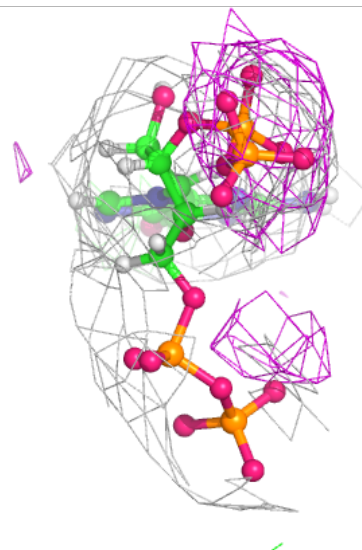
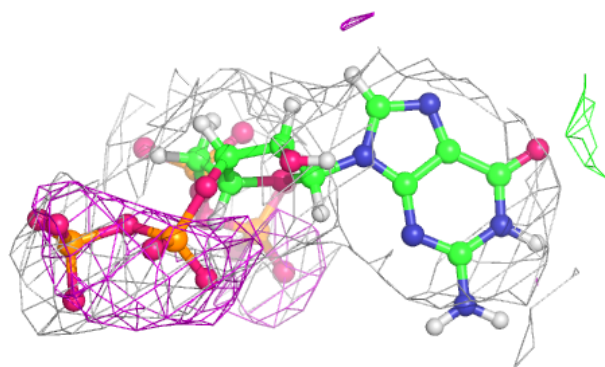
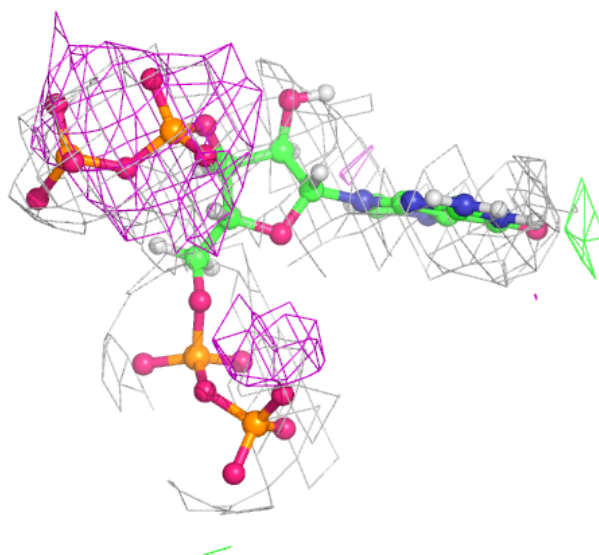
Electron density around GMP E 503:

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and green (positive)



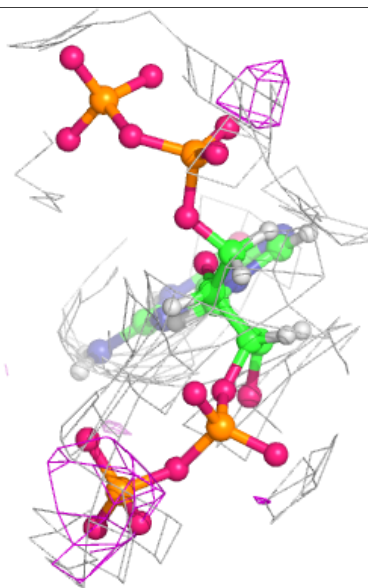
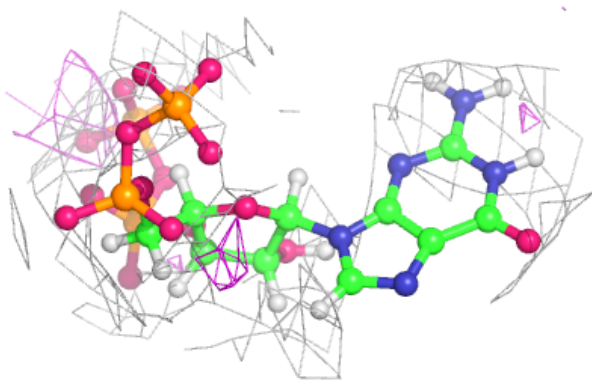
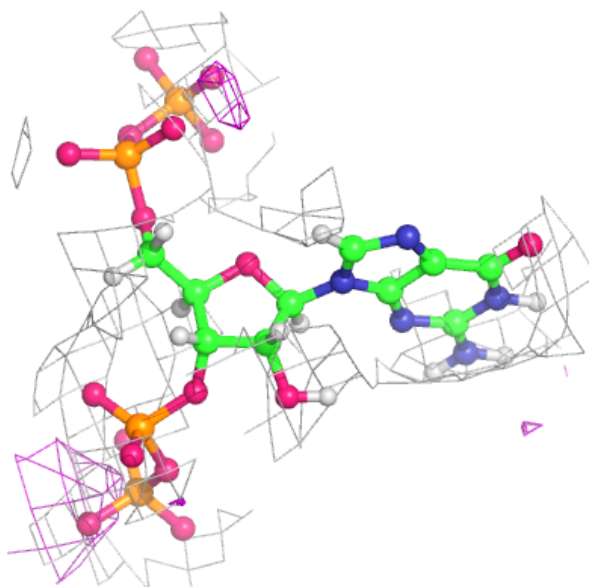
Electron density around G4P H 501:

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and green (positive)



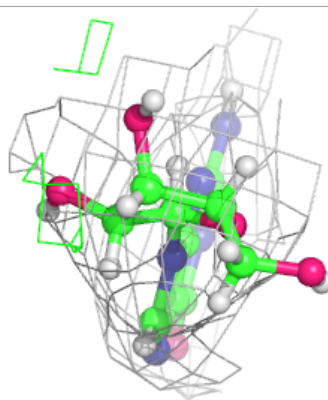
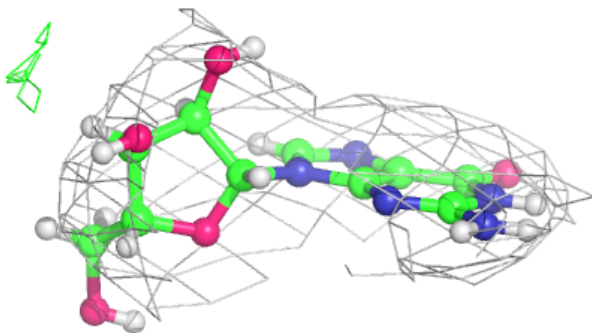
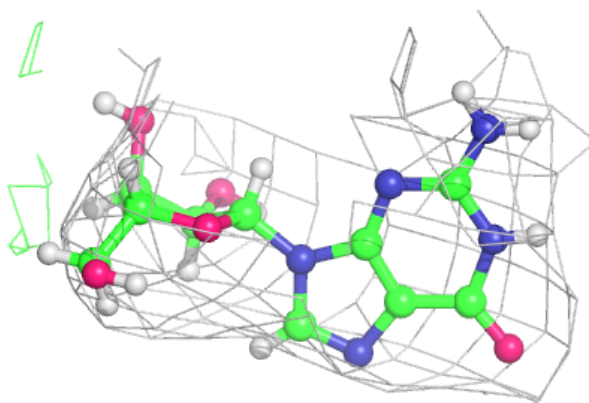
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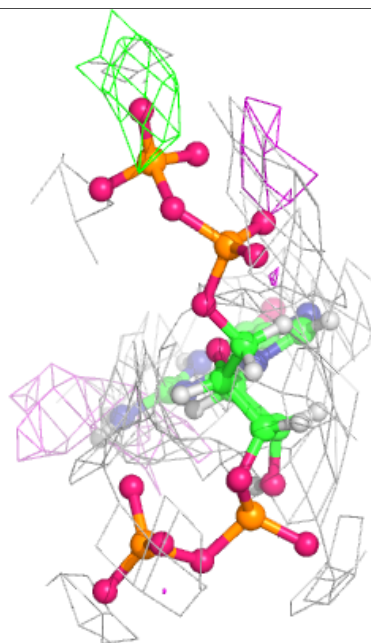
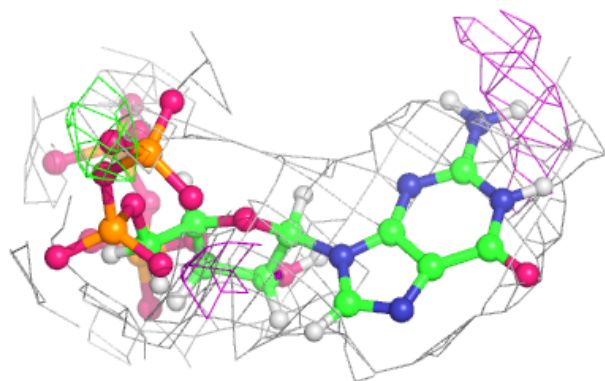
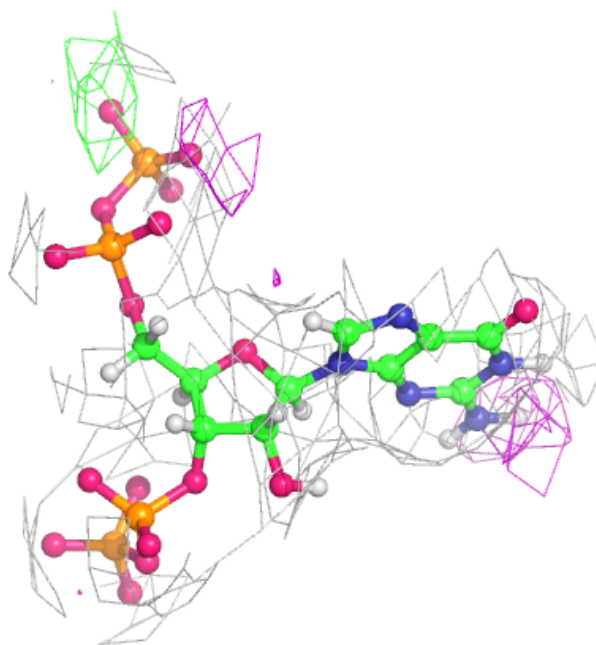
Electron density around GMP F 502:

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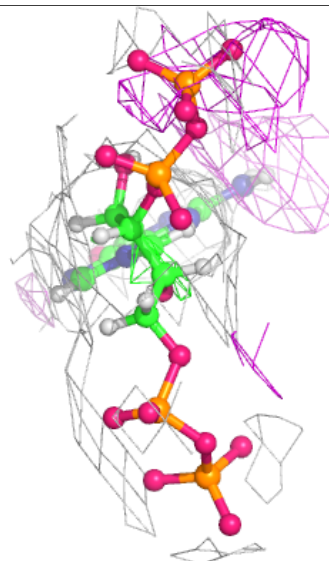
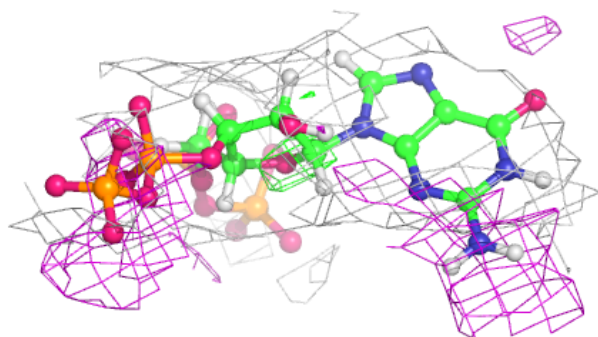
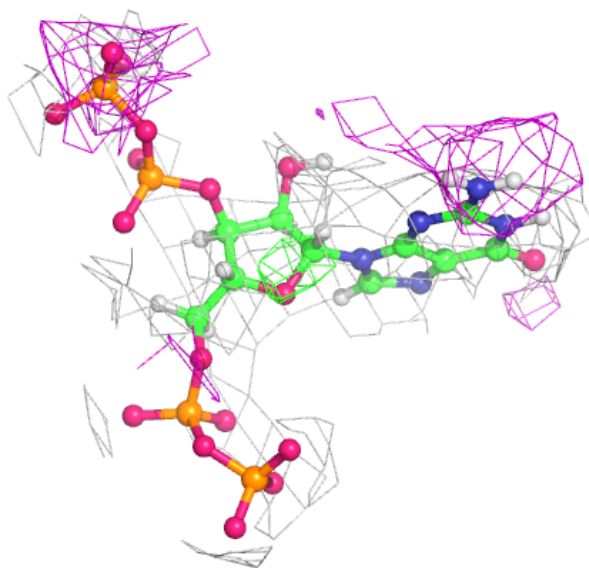
Electron density around G4P A 501:

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



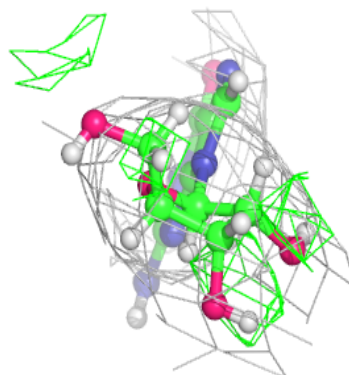
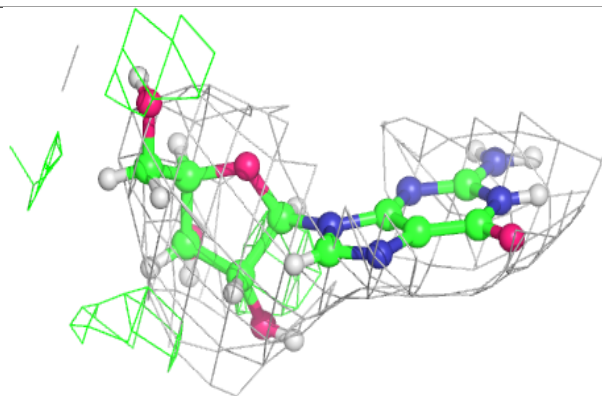
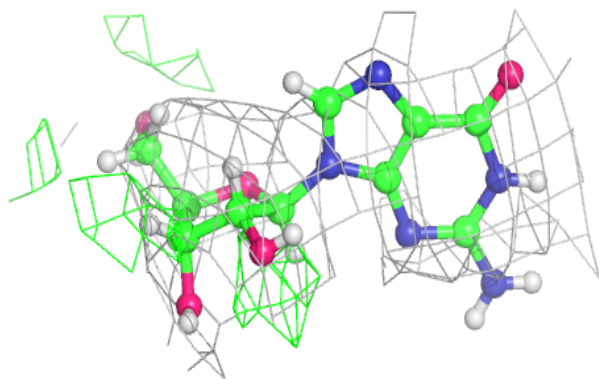
Electron density around G4P E 501:

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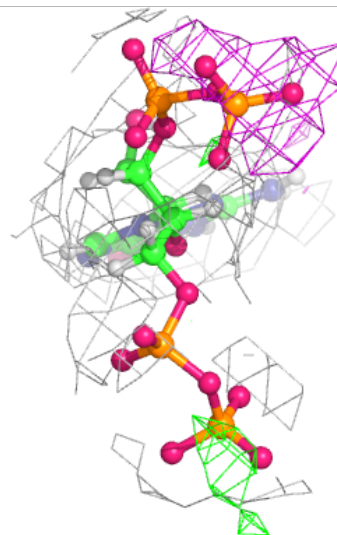
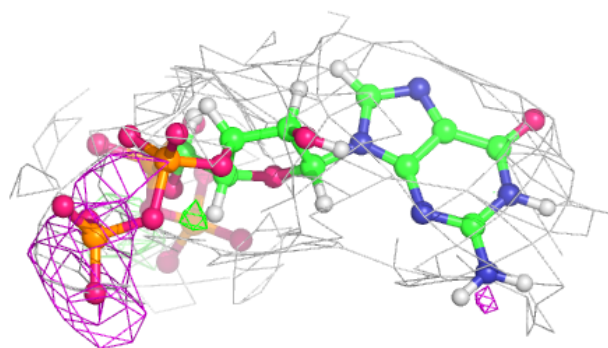
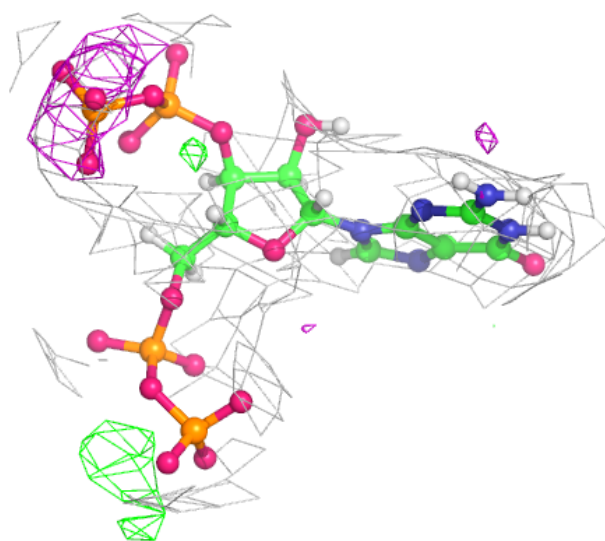
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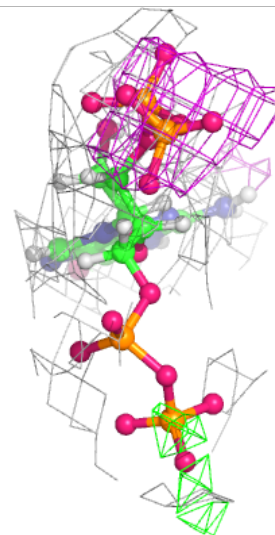
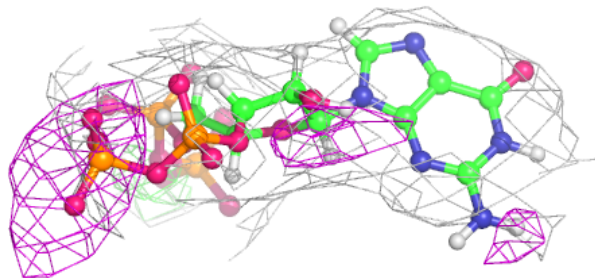
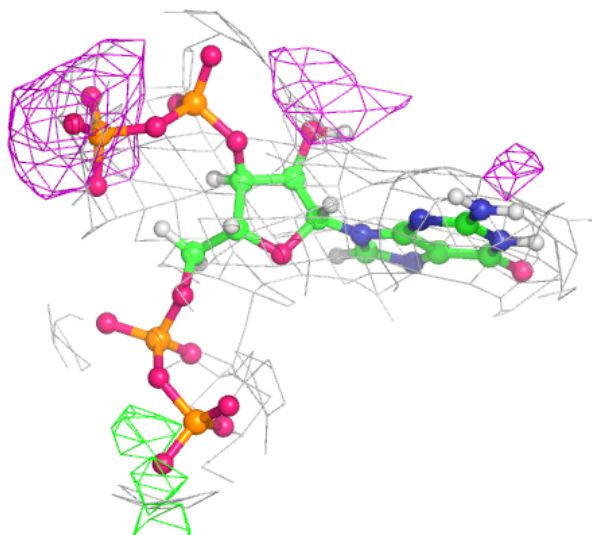
Electron density around G4P D 501:

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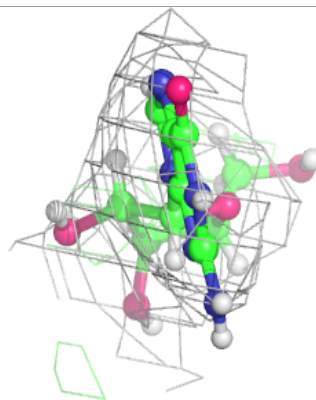
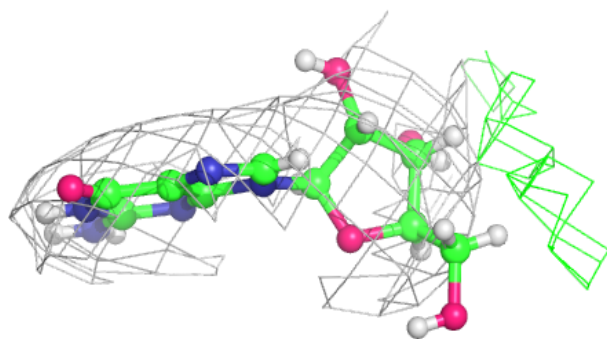
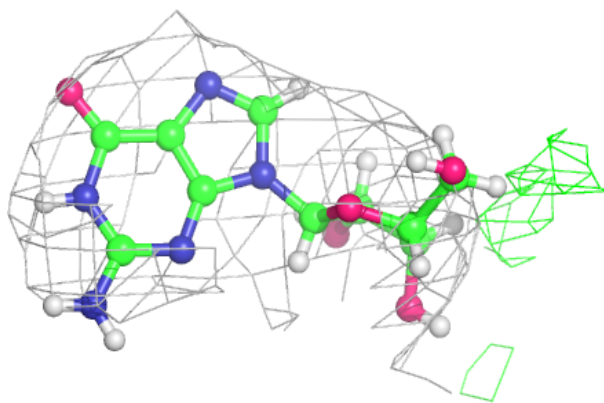
Electron density around G4P C 501:

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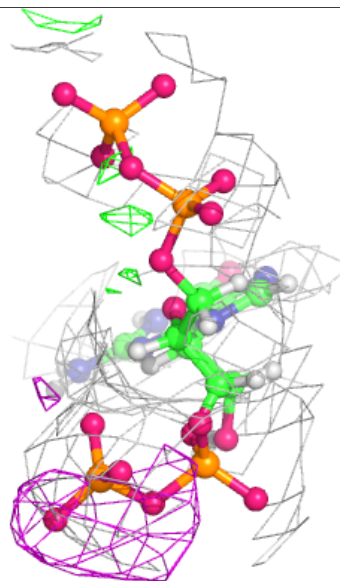
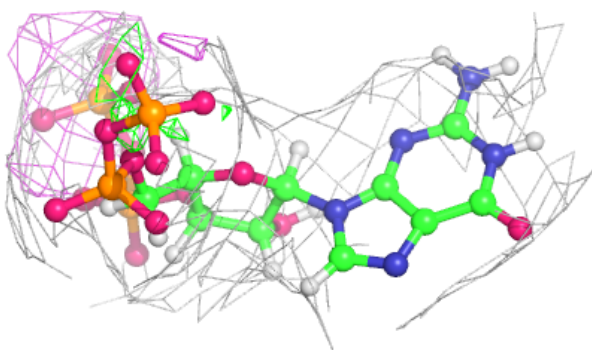
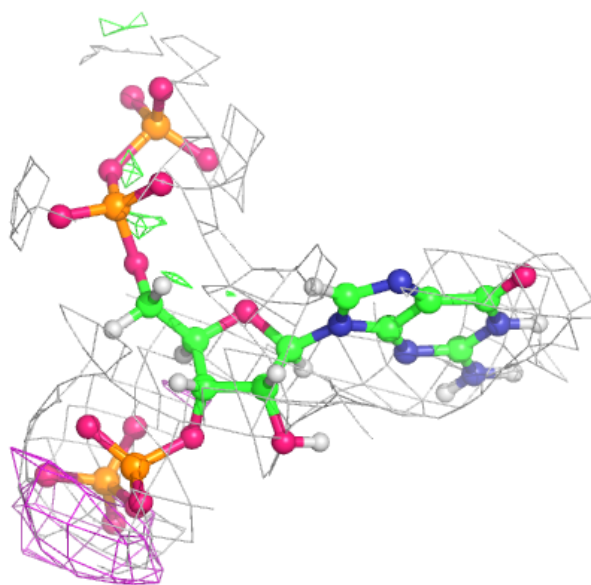
Electron density around GMP D 502:

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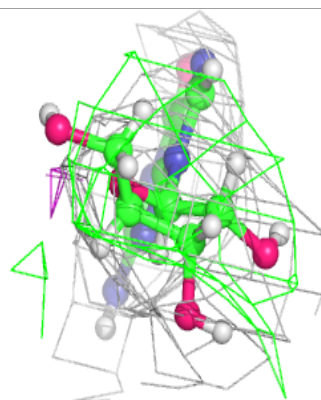
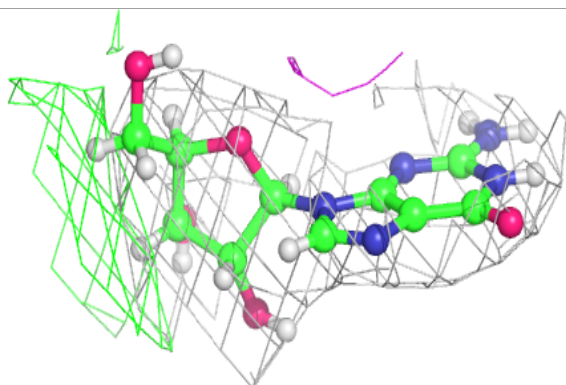
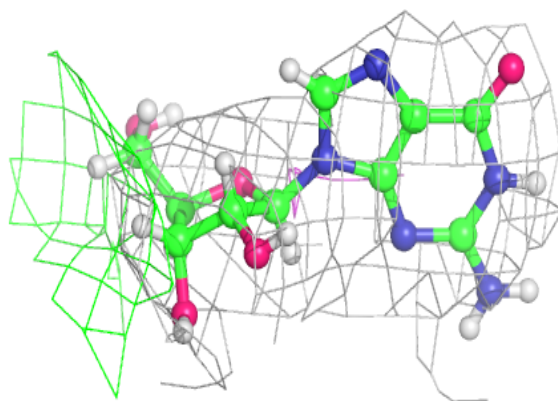
Electron density around G4P B 501:

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and green (positive)

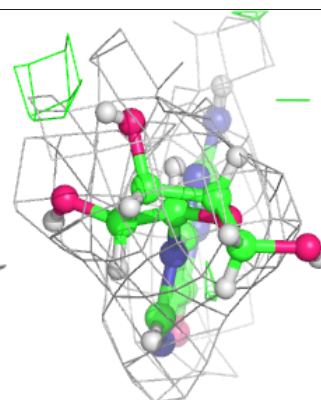
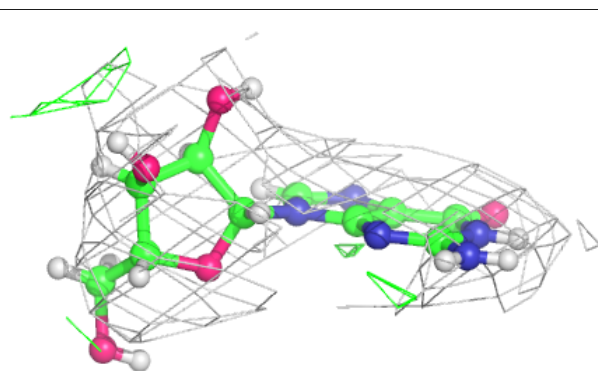
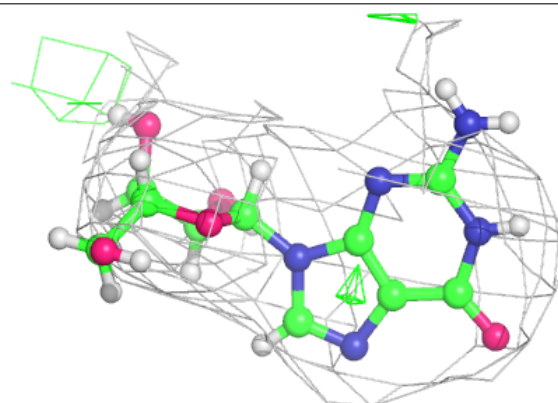


Electron density around GMP A 502:

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

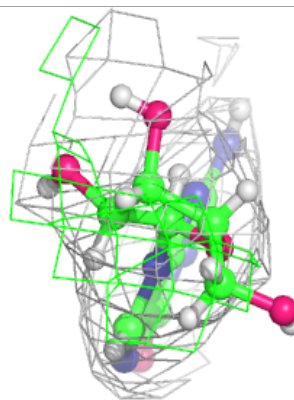
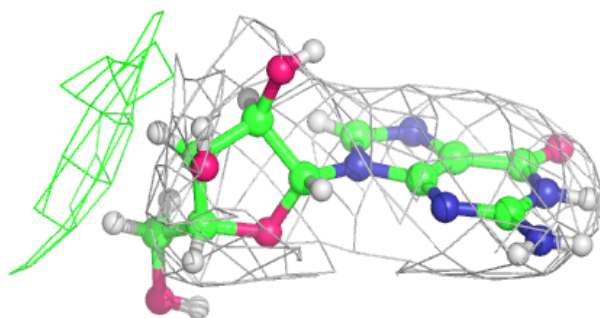
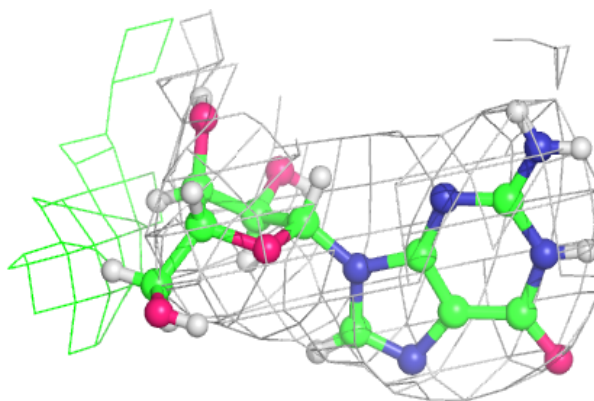
**Electron density around GMP B 502:**

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

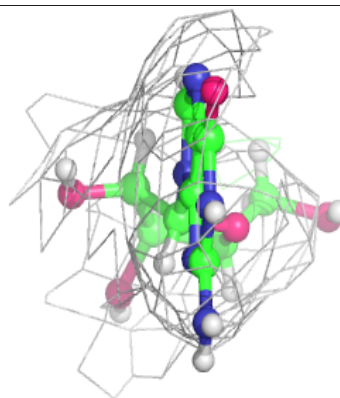
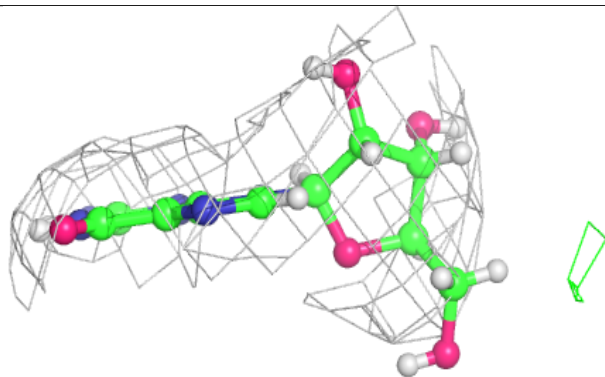
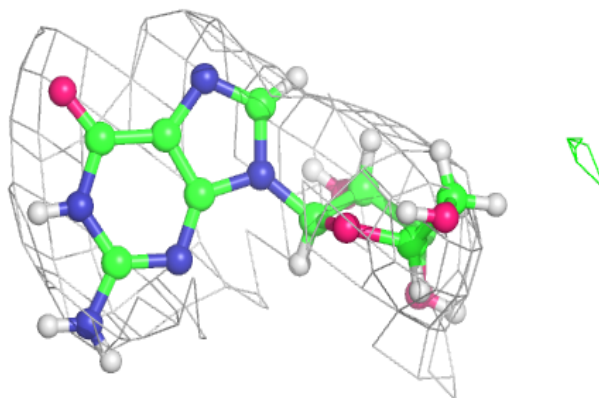


Electron density around GMP C 502:

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

**Electron density around GMP H 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.