



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:42 AM UTC

PDB ID : 3WC0 / pdb_00003wc0
Title : Crystal structure of *C. albicans* tRNA(His) guanylyltransferase (Thg1) with GTP
Authors : Nakamura, A.; Nemoto, T.; Sonoda, T.; Yamashita, K.; Tanaka, I.; Yao, M.
Deposited on : 2013-05-24
Resolution : 3.03 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

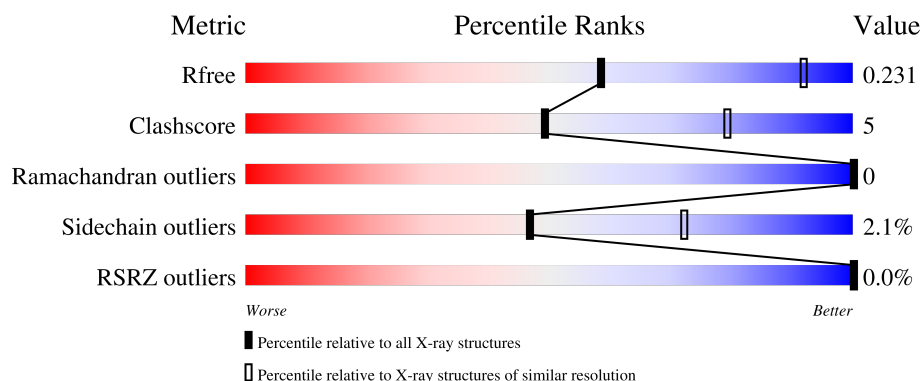
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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.



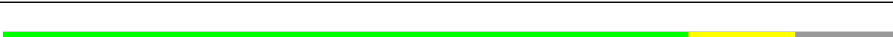
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	271	 80% 17% ..
1	B	271	 84% 14% .
1	C	271	 82% 15% ..
1	D	271	 85% 12% ..
1	E	271	 72% 16% • 11%

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Mol	Chain	Length	Quality of chain
1	F	271	 74%15%11%
1	G	271	 84%13%..
1	H	271	 78%19%..
1	I	271	 73%15%11%
1	J	271	 86%11%..
1	K	271	 80%16%..
1	L	271	 75%14%.11%
1	M	271	 79%18%..
1	N	271	 82%16%.
1	O	271	 82%14%..
1	P	271	 77%12%11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36341 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 Likely histidyl tRNA-specific guanylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	B	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	C	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	D	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	E	241	Total	C	N	O	S	0	0	0
			2057	1337	335	373	12			
1	F	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			
1	G	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	H	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	I	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			
1	J	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	K	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	L	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			
1	M	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	N	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	O	265	Total	C	N	O	S	0	0	0
			2267	1464	375	416	12			
1	P	242	Total	C	N	O	S	0	0	0
			2065	1341	336	376	12			

There are 48 discrepancies between the modelled and reference sequences:

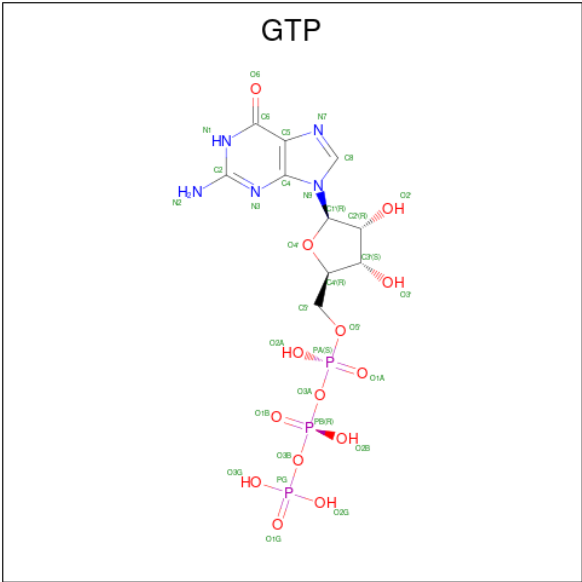
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5AFK5
A	-1	GLY	-	expression tag	UNP Q5AFK5
A	0	SER	-	expression tag	UNP Q5AFK5
B	-2	GLY	-	expression tag	UNP Q5AFK5
B	-1	GLY	-	expression tag	UNP Q5AFK5
B	0	SER	-	expression tag	UNP Q5AFK5
C	-2	GLY	-	expression tag	UNP Q5AFK5
C	-1	GLY	-	expression tag	UNP Q5AFK5
C	0	SER	-	expression tag	UNP Q5AFK5
D	-2	GLY	-	expression tag	UNP Q5AFK5
D	-1	GLY	-	expression tag	UNP Q5AFK5
D	0	SER	-	expression tag	UNP Q5AFK5
E	-2	GLY	-	expression tag	UNP Q5AFK5
E	-1	GLY	-	expression tag	UNP Q5AFK5
E	0	SER	-	expression tag	UNP Q5AFK5
F	-2	GLY	-	expression tag	UNP Q5AFK5
F	-1	GLY	-	expression tag	UNP Q5AFK5
F	0	SER	-	expression tag	UNP Q5AFK5
G	-2	GLY	-	expression tag	UNP Q5AFK5
G	-1	GLY	-	expression tag	UNP Q5AFK5
G	0	SER	-	expression tag	UNP Q5AFK5
H	-2	GLY	-	expression tag	UNP Q5AFK5
H	-1	GLY	-	expression tag	UNP Q5AFK5
H	0	SER	-	expression tag	UNP Q5AFK5
I	-2	GLY	-	expression tag	UNP Q5AFK5
I	-1	GLY	-	expression tag	UNP Q5AFK5
I	0	SER	-	expression tag	UNP Q5AFK5
J	-2	GLY	-	expression tag	UNP Q5AFK5
J	-1	GLY	-	expression tag	UNP Q5AFK5
J	0	SER	-	expression tag	UNP Q5AFK5
K	-2	GLY	-	expression tag	UNP Q5AFK5
K	-1	GLY	-	expression tag	UNP Q5AFK5
K	0	SER	-	expression tag	UNP Q5AFK5
L	-2	GLY	-	expression tag	UNP Q5AFK5
L	-1	GLY	-	expression tag	UNP Q5AFK5
L	0	SER	-	expression tag	UNP Q5AFK5
M	-2	GLY	-	expression tag	UNP Q5AFK5
M	-1	GLY	-	expression tag	UNP Q5AFK5
M	0	SER	-	expression tag	UNP Q5AFK5
N	-2	GLY	-	expression tag	UNP Q5AFK5
N	-1	GLY	-	expression tag	UNP Q5AFK5
N	0	SER	-	expression tag	UNP Q5AFK5

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP Q5AFK5
O	-1	GLY	-	expression tag	UNP Q5AFK5
O	0	SER	-	expression tag	UNP Q5AFK5
P	-2	GLY	-	expression tag	UNP Q5AFK5
P	-1	GLY	-	expression tag	UNP Q5AFK5
P	0	SER	-	expression tag	UNP Q5AFK5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	F	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	F	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	G	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	G	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	H	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	H	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	I	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	I	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	J	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	J	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	K	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	L	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	L	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	L	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	M	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	M	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	N	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	N	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	O	1	Total 32	C 10	N 5	O 14	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	P	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	E	2	Total	Mg	0	0
			2	2		
3	F	4	Total	Mg	0	0
			4	4		
3	G	3	Total	Mg	0	0
			3	3		
3	H	3	Total	Mg	0	0
			3	3		
3	I	3	Total	Mg	0	0
			3	3		
3	J	3	Total	Mg	0	0
			3	3		
3	K	2	Total	Mg	0	0
			2	2		
3	L	4	Total	Mg	0	0
			4	4		
3	M	3	Total	Mg	0	0
			3	3		
3	N	3	Total	Mg	0	0
			3	3		
3	O	3	Total	Mg	0	0
			3	3		
3	P	3	Total	Mg	0	0
			3	3		

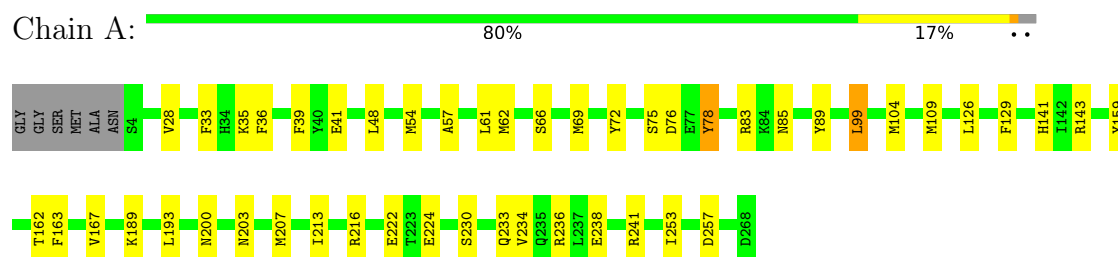
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	O 2	0	0
4	G	1	Total 1	O 1	0	0
4	H	2	Total 2	O 2	0	0
4	I	1	Total 1	O 1	0	0
4	K	1	Total 1	O 1	0	0
4	M	2	Total 2	O 2	0	0
4	N	3	Total 3	O 3	0	0
4	O	3	Total 3	O 3	0	0

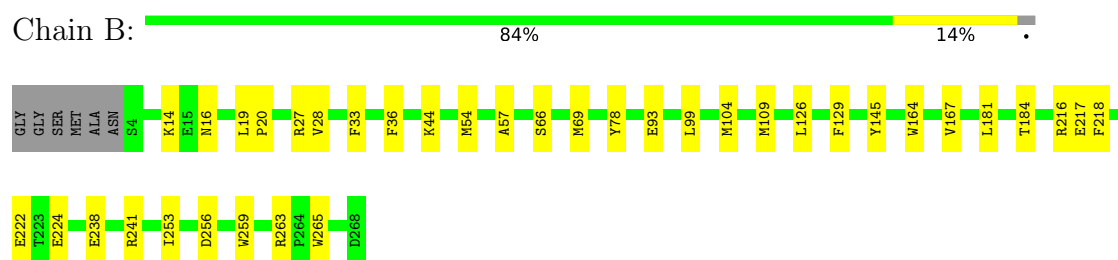
3 Residue-property plots

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

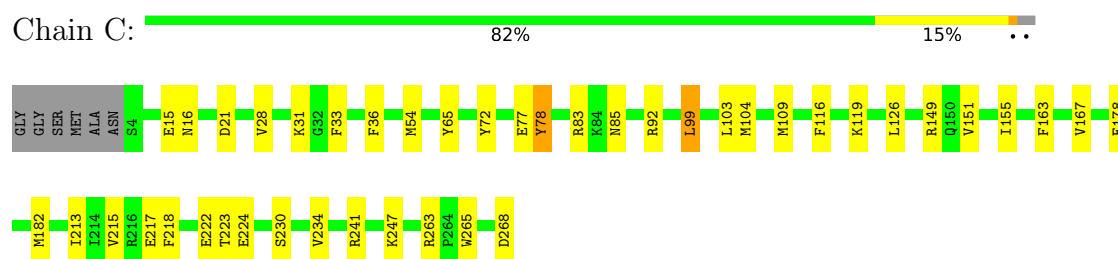
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase



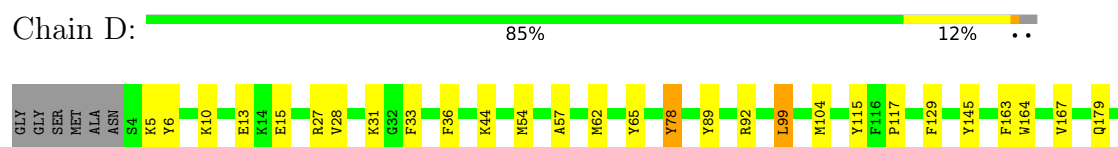
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

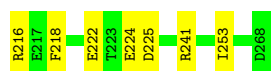


- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase



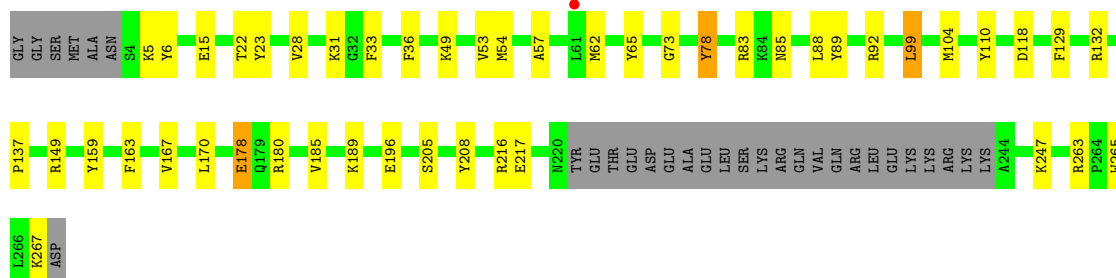
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase





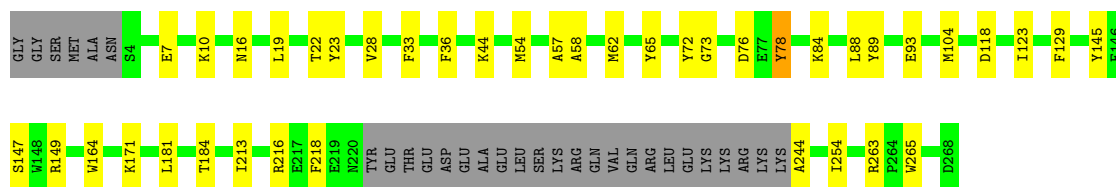
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain E: 72% 16% 11%



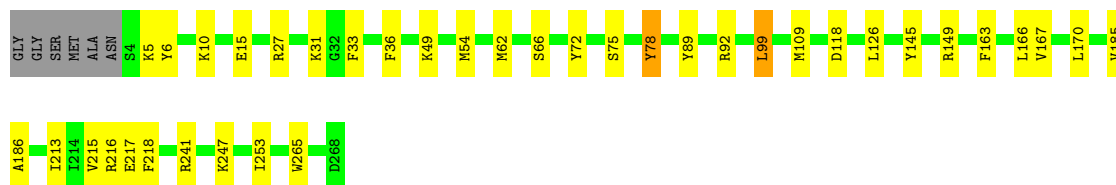
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain F: 74% 15% 11%



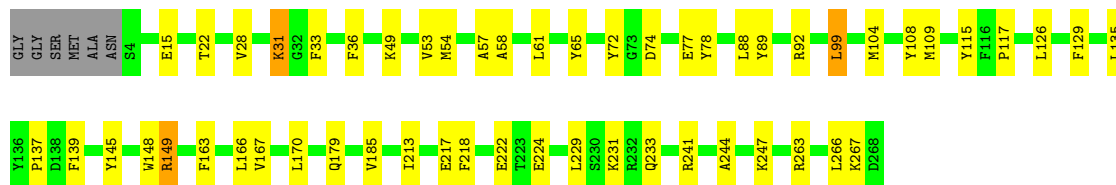
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain G: 84% 13% 3%



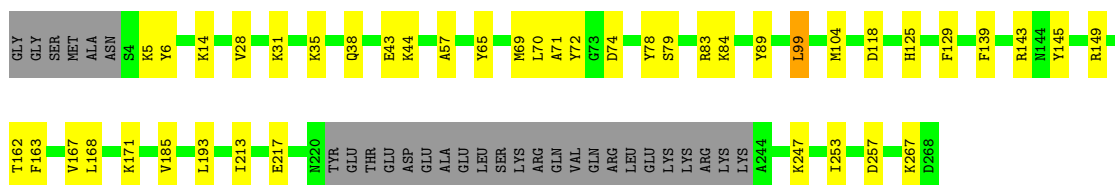
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain H: 78% 19% 3%



- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain I: 73% 15% 11%



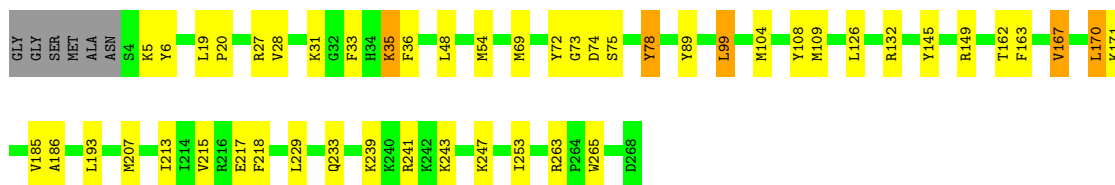
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain J: 86% 11% ..



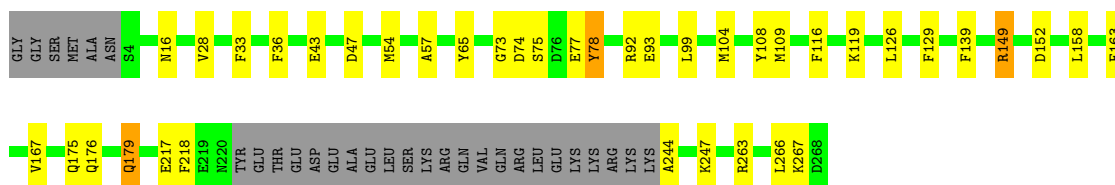
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain K: 80% 16% ..



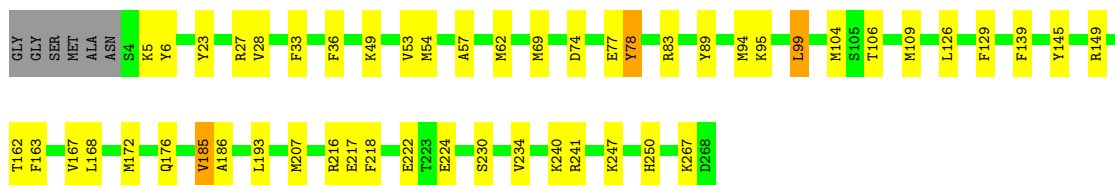
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain L: 75% 14% 11%



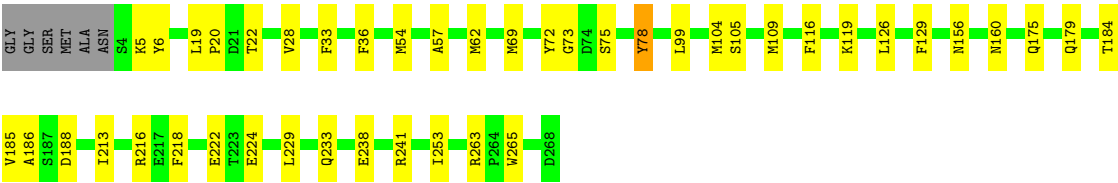
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain M: 79% 18% ..

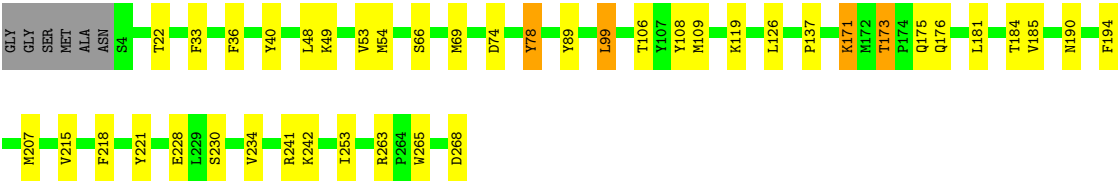
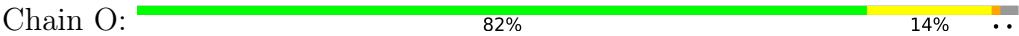


- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

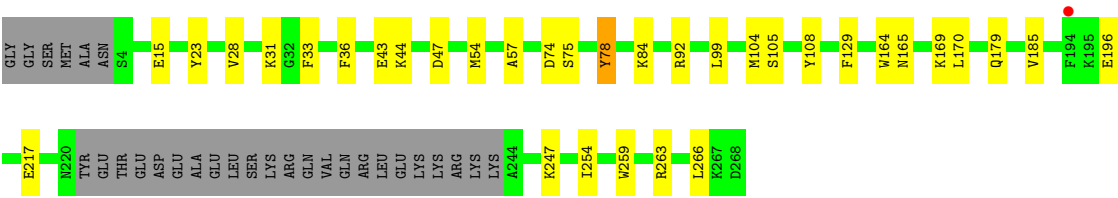
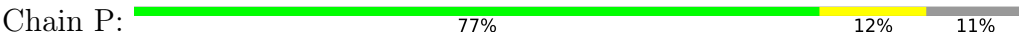
Chain N: 82% 16% .



• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase



• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.43Å 217.56Å 140.91Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	44.58 – 3.03 44.58 – 3.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.58-3.03) 98.9 (44.58-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.198 , 0.239 0.199 , 0.231	Depositor DCC
R_{free} test set	7040 reflections (7.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36341	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	0.33	0/2327	0.76	0/3135
1	B	0.35	0/2327	0.78	0/3135
1	C	0.35	0/2327	0.77	0/3135
1	D	0.37	0/2327	0.77	1/3135 (0.0%)
1	E	0.36	0/2115	0.79	0/2854
1	F	0.38	0/2123	0.76	0/2865
1	G	0.37	0/2327	0.81	2/3135 (0.1%)
1	H	0.37	0/2327	0.79	0/3135
1	I	0.37	0/2123	0.75	0/2865
1	J	0.36	0/2327	0.78	1/3135 (0.0%)
1	K	0.37	0/2327	0.79	3/3135 (0.1%)
1	L	0.36	0/2123	0.78	1/2865 (0.0%)
1	M	0.39	0/2327	0.77	0/3135
1	N	0.40	0/2327	0.78	1/3135 (0.0%)
1	O	0.40	0/2327	0.81	0/3135
1	P	0.37	0/2123	0.78	2/2865 (0.1%)
All	All	0.37	0/36204	0.78	11/48799 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	ASP	N-CA-C	5.97	118.37	109.59
1	P	254	ILE	N-CA-C	5.89	116.07	110.53
1	K	186	ALA	N-CA-C	5.64	117.42	111.28
1	J	75	SER	CB-CA-C	-5.51	110.21	116.54
1	G	186	ALA	N-CA-C	5.47	117.25	111.28
1	K	167	VAL	N-CA-C	5.23	115.89	110.82
1	P	75	SER	CB-CA-C	-5.17	110.60	116.54
1	G	75	SER	CB-CA-C	-5.10	110.68	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	75	SER	CB-CA-C	-5.07	110.71	116.54
1	K	75	SER	CB-CA-C	-5.05	110.73	116.54
1	L	75	SER	CB-CA-C	-5.02	110.77	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2267	0	2213	30	0
1	B	2267	0	2213	23	0
1	C	2267	0	2213	23	0
1	D	2267	0	2213	23	0
1	E	2057	0	1997	30	0
1	F	2065	0	2001	25	0
1	G	2267	0	2213	25	0
1	H	2267	0	2213	36	0
1	I	2065	0	2001	24	0
1	J	2267	0	2213	20	0
1	K	2267	0	2213	27	0
1	L	2065	0	2001	23	0
1	M	2267	0	2213	30	0
1	N	2267	0	2213	23	0
1	O	2267	0	2213	26	0
1	P	2065	0	2001	18	0
2	A	64	0	24	0	0
2	B	64	0	24	0	0
2	C	64	0	24	0	0
2	D	64	0	24	0	0
2	E	64	0	24	1	0
2	F	64	0	24	4	0
2	G	64	0	24	1	0
2	H	64	0	24	1	0
2	I	64	0	24	0	0
2	J	64	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	32	0	12	0	0
2	L	96	0	36	2	0
2	M	64	0	24	0	0
2	N	64	0	24	0	0
2	O	96	0	36	1	0
2	P	32	0	12	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	4	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	2	0	0	0	0
3	L	4	0	0	0	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	2	0	0	0	0
4	N	3	0	0	0	0
4	O	3	0	0	0	0
All	All	36341	0	34728	381	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 5.

All (381) 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:A:41:GLU:HG2	1:L:175:GLN:HE21	1.34	0.91
1:H:77:GLU:OE1	1:H:149:ARG:NH1	2.14	0.79
1:C:31:LYS:NZ	1:D:65:TYR:OH	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:263:ARG:HB3	1:P:266:LEU:HD13	1.70	0.73
1:L:92:ARG:NH1	2:L:301:GTP:O2G	2.25	0.70
1:K:31:LYS:NZ	1:L:65:TYR:OH	2.23	0.70
1:K:218:PHE:HZ	1:K:241:ARG:HG3	1.57	0.69
1:H:217:GLU:HG3	1:H:247:LYS:HD2	1.75	0.68
1:D:179:GLN:HG3	1:I:38:GLN:HE21	1.59	0.68
1:L:77:GLU:OE1	1:L:149:ARG:NH1	2.27	0.68
1:H:218:PHE:HZ	1:H:241:ARG:HG3	1.60	0.67
1:N:229:LEU:HD13	1:N:233:GLN:HE21	1.60	0.67
1:P:28:VAL:HG13	1:P:129:PHE:HB3	1.78	0.66
2:O:402:GTP:O1G	1:P:92:ARG:NH2	2.28	0.65
1:J:28:VAL:HG13	1:J:129:PHE:HB3	1.77	0.65
1:F:10:LYS:HE2	2:F:301:GTP:C8	2.32	0.65
1:L:28:VAL:HG13	1:L:129:PHE:HB3	1.79	0.64
1:I:217:GLU:HG3	1:I:247:LYS:HD2	1.80	0.64
1:A:62:MET:O	1:A:216:ARG:NH2	2.31	0.63
1:A:159:TYR:HD1	1:A:189:LYS:HE2	1.63	0.63
1:J:217:GLU:OE2	1:J:263:ARG:NH1	2.31	0.63
1:M:69:MET:HE3	1:M:83:ARG:HD3	1.81	0.63
1:K:28:VAL:HG21	1:K:104:MET:HG3	1.83	0.61
1:L:217:GLU:HG3	1:L:247:LYS:HD2	1.82	0.61
1:G:62:MET:O	1:G:216:ARG:NH2	2.33	0.60
1:C:217:GLU:HG3	1:C:247:LYS:HD2	1.83	0.60
1:J:89:TYR:HE2	1:J:99:LEU:HD22	1.67	0.60
1:K:218:PHE:CZ	1:K:241:ARG:HG3	2.37	0.60
1:M:109:MET:HE3	1:M:126:LEU:HD22	1.83	0.60
1:O:54:MET:HG2	1:O:108:TYR:HE1	1.67	0.60
1:F:28:VAL:HG13	1:F:129:PHE:HB3	1.84	0.59
1:G:99:LEU:HD13	1:H:31:LYS:HE2	1.85	0.59
1:B:28:VAL:HG13	1:B:129:PHE:HB3	1.85	0.59
1:B:217:GLU:OE2	1:B:263:ARG:NH1	2.36	0.59
1:M:217:GLU:HG3	1:M:247:LYS:HD2	1.83	0.59
1:P:33:PHE:HA	1:P:36:PHE:HB3	1.86	0.58
1:H:229:LEU:HB3	1:H:233:GLN:HG3	1.86	0.58
1:K:54:MET:HG2	1:K:108:TYR:HE1	1.69	0.58
1:C:218:PHE:HZ	1:C:241:ARG:HG3	1.68	0.57
1:I:143:ARG:NH2	1:I:257:ASP:OD1	2.38	0.57
1:B:218:PHE:HZ	1:B:241:ARG:HG3	1.69	0.57
1:A:41:GLU:HG2	1:L:175:GLN:NE2	2.11	0.57
1:E:217:GLU:HG3	1:E:247:LYS:HD2	1.87	0.57
1:N:156:ASN:O	1:N:160:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:VAL:HG13	1:E:129:PHE:HB3	1.87	0.56
1:G:109:MET:HE3	1:G:126:LEU:HD22	1.86	0.56
1:A:33:PHE:HA	1:A:36:PHE:HB3	1.87	0.56
1:A:89:TYR:HE2	1:A:99:LEU:HD22	1.70	0.56
1:D:163:PHE:O	1:D:167:VAL:HG23	2.04	0.56
1:A:28:VAL:HG13	1:A:129:PHE:HB3	1.88	0.56
1:F:16:ASN:ND2	1:F:93:GLU:OE1	2.34	0.56
1:O:221:TYR:OH	1:O:268:ASP:OD2	2.23	0.56
1:A:75:SER:OG	1:A:76:ASP:N	2.38	0.56
1:M:218:PHE:HZ	1:M:241:ARG:HG3	1.71	0.56
1:I:35:LYS:HE2	1:I:125:HIS:NE2	2.21	0.55
1:A:109:MET:HE3	1:A:126:LEU:HD22	1.88	0.55
1:J:54:MET:HG2	1:J:108:TYR:HE1	1.71	0.55
1:M:163:PHE:O	1:M:167:VAL:HG23	2.07	0.55
1:L:263:ARG:HB3	1:L:266:LEU:HD13	1.89	0.55
1:K:170:LEU:HD23	1:K:171:LYS:H	1.71	0.55
1:O:89:TYR:HE2	1:O:99:LEU:HD22	1.72	0.55
1:H:263:ARG:HB3	1:H:266:LEU:HD13	1.89	0.55
1:M:28:VAL:HG13	1:M:129:PHE:HB3	1.88	0.55
1:E:163:PHE:O	1:E:167:VAL:HG23	2.07	0.54
1:E:263:ARG:HG2	1:E:265:TRP:CZ2	2.41	0.54
1:P:54:MET:HG2	1:P:108:TYR:HE1	1.73	0.54
1:L:163:PHE:O	1:L:167:VAL:HG23	2.07	0.54
1:O:109:MET:HE3	1:O:126:LEU:HD22	1.88	0.54
1:P:44:LYS:HD3	1:P:164:TRP:CZ3	2.43	0.54
1:J:58:ALA:HA	1:J:104:MET:HE1	1.89	0.54
1:M:57:ALA:C	1:M:104:MET:HE1	2.33	0.54
1:N:62:MET:O	1:N:216:ARG:NH2	2.41	0.54
1:G:33:PHE:HA	1:G:36:PHE:HB3	1.88	0.54
1:O:230:SER:HA	1:O:234:VAL:HG23	1.90	0.54
1:F:7:GLU:OE2	2:F:301:GTP:N2	2.41	0.54
1:K:229:LEU:HD22	1:K:233:GLN:HE21	1.73	0.54
1:G:54:MET:HE3	1:G:78:TYR:HD2	1.72	0.54
1:C:77:GLU:OE1	1:C:149:ARG:NH2	2.42	0.53
1:D:179:GLN:HG3	1:I:38:GLN:NE2	2.21	0.53
1:D:222:GLU:O	1:D:224:GLU:N	2.38	0.53
1:M:54:MET:HE3	1:M:78:TYR:HD2	1.73	0.53
1:M:230:SER:HA	1:M:234:VAL:HG23	1.91	0.53
1:O:173:THR:HG22	1:O:176:GLN:HG3	1.88	0.53
1:A:163:PHE:O	1:A:167:VAL:HG23	2.08	0.53
1:A:143:ARG:NH2	1:A:257:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:89:TYR:HE2	1:K:99:LEU:HD22	1.73	0.53
1:A:39:PHE:O	1:L:176:GLN:HG2	2.09	0.53
1:D:54:MET:HE3	1:D:78:TYR:HD2	1.73	0.53
1:E:89:TYR:HE2	1:E:99:LEU:HD22	1.73	0.52
1:N:28:VAL:HG13	1:N:129:PHE:HB3	1.90	0.52
1:B:14:LYS:NZ	1:C:16:ASN:OD1	2.23	0.52
1:L:16:ASN:ND2	1:L:93:GLU:OE1	2.42	0.52
1:M:89:TYR:HE2	1:M:99:LEU:HD22	1.74	0.52
1:O:263:ARG:HG2	1:O:265:TRP:CZ2	2.43	0.52
1:A:233:GLN:OE1	1:A:236:ARG:NH2	2.42	0.52
1:J:230:SER:HA	1:J:234:VAL:HG23	1.91	0.52
1:M:185:VAL:HG12	1:M:186:ALA:H	1.75	0.52
1:I:89:TYR:CE2	1:I:99:LEU:HD22	2.45	0.52
1:B:27:ARG:HD3	1:B:145:TYR:OH	2.10	0.52
1:G:99:LEU:HB2	1:H:31:LYS:NZ	2.25	0.52
1:I:28:VAL:HG13	1:I:129:PHE:HB3	1.92	0.51
1:O:66:SER:HB3	1:O:242:LYS:HG2	1.92	0.51
1:I:72:TYR:HD1	1:I:213:ILE:HG13	1.75	0.51
1:L:116:PHE:CD1	1:L:119:LYS:HD2	2.45	0.51
1:N:185:VAL:HG22	1:N:186:ALA:H	1.75	0.51
1:H:54:MET:HG2	1:H:108:TYR:HE1	1.75	0.51
1:A:66:SER:HB2	1:A:241:ARG:HB3	1.92	0.51
1:J:15:GLU:CD	1:J:92:ARG:HH21	2.19	0.51
1:E:5:LYS:HE3	1:E:6:TYR:CZ	2.44	0.51
1:H:163:PHE:O	1:H:167:VAL:HG23	2.10	0.51
1:A:83:ARG:NH2	1:A:85:ASN:HB2	2.26	0.51
1:F:263:ARG:HG2	1:F:265:TRP:CZ2	2.46	0.51
1:J:77:GLU:OE2	1:J:149:ARG:NE	2.44	0.51
1:M:218:PHE:CZ	1:M:241:ARG:HG3	2.46	0.51
1:O:173:THR:HG23	1:O:175:GLN:H	1.75	0.51
1:H:28:VAL:HG13	1:H:129:PHE:HB3	1.93	0.50
1:E:65:TYR:CE2	1:E:99:LEU:HD21	2.45	0.50
1:F:62:MET:O	1:F:216:ARG:NH2	2.44	0.50
1:O:33:PHE:HA	1:O:36:PHE:HB3	1.92	0.50
1:A:230:SER:HA	1:A:234:VAL:HG23	1.94	0.50
1:N:57:ALA:C	1:N:104:MET:HE1	2.36	0.50
1:J:263:ARG:HG2	1:J:265:TRP:CZ2	2.46	0.50
1:K:163:PHE:O	1:K:167:VAL:HG23	2.12	0.50
1:C:222:GLU:O	1:C:224:GLU:N	2.41	0.50
1:H:109:MET:HE3	1:H:126:LEU:HD22	1.94	0.50
1:E:31:LYS:NZ	1:F:65:TYR:OH	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:172:MET:HG2	1:M:176:GLN:HB2	1.93	0.50
1:C:65:TYR:HE2	1:C:103:LEU:HD11	1.76	0.49
1:E:57:ALA:C	1:E:104:MET:HE1	2.37	0.49
1:A:141:HIS:NE2	1:C:21:ASP:OD2	2.27	0.49
1:H:65:TYR:CE2	1:H:99:LEU:HD21	2.47	0.49
1:K:109:MET:HE3	1:K:126:LEU:HD22	1.94	0.49
1:K:162:THR:HA	1:K:193:LEU:HD21	1.94	0.49
1:M:33:PHE:HA	1:M:36:PHE:HB3	1.93	0.49
1:M:62:MET:O	1:M:216:ARG:NH2	2.44	0.49
1:M:162:THR:HA	1:M:193:LEU:HD21	1.94	0.49
1:G:10:LYS:HD3	1:H:148:TRP:CH2	2.47	0.49
1:B:263:ARG:HG2	1:B:265:TRP:CZ2	2.48	0.49
1:I:89:TYR:HE2	1:I:99:LEU:HD22	1.77	0.49
1:B:109:MET:HE3	1:B:126:LEU:HD22	1.95	0.49
1:E:92:ARG:NH2	2:E:404:GTP:O1G	2.36	0.49
1:N:69:MET:HE1	1:N:218:PHE:HE1	1.78	0.49
1:C:263:ARG:HG2	1:C:265:TRP:CZ2	2.48	0.49
1:B:16:ASN:ND2	1:B:93:GLU:OE1	2.43	0.49
1:D:57:ALA:C	1:D:104:MET:HE1	2.38	0.49
1:H:72:TYR:HD1	1:H:213:ILE:HG13	1.78	0.49
1:P:259:TRP:O	1:P:263:ARG:NH1	2.42	0.49
1:H:57:ALA:C	1:H:104:MET:HE1	2.38	0.48
1:M:5:LYS:HE3	1:M:6:TYR:CZ	2.48	0.48
1:K:217:GLU:HG3	1:K:247:LYS:HD2	1.96	0.48
1:G:149:ARG:HH22	2:G:402:GTP:H4'	1.77	0.48
1:E:89:TYR:CE2	1:E:99:LEU:HD22	2.49	0.48
1:G:27:ARG:HD3	1:G:145:TYR:OH	2.13	0.48
1:P:23:TYR:CE1	1:P:84:LYS:HB2	2.48	0.48
1:O:171:LYS:N	1:O:171:LYS:HD2	2.29	0.48
1:E:5:LYS:HE3	1:E:6:TYR:OH	2.14	0.48
1:K:132:ARG:NH2	2:L:301:GTP:O3G	2.43	0.48
1:N:5:LYS:HE3	1:N:6:TYR:CZ	2.49	0.48
1:F:54:MET:HE3	1:F:78:TYR:HD2	1.77	0.48
1:J:89:TYR:CE2	1:J:99:LEU:HD22	2.48	0.48
1:I:163:PHE:O	1:I:167:VAL:HG23	2.14	0.48
1:N:263:ARG:HG2	1:N:265:TRP:CZ2	2.49	0.48
1:A:57:ALA:C	1:A:104:MET:HE1	2.39	0.47
1:N:54:MET:HE3	1:N:78:TYR:HD2	1.79	0.47
1:A:72:TYR:HD1	1:A:213:ILE:HG13	1.80	0.47
1:E:62:MET:O	1:E:216:ARG:NH2	2.47	0.47
1:F:88:LEU:HG	1:F:89:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:THR:HG23	1:C:268:ASP:OD2	2.15	0.47
1:D:44:LYS:HD3	1:D:164:TRP:CZ2	2.50	0.47
1:K:33:PHE:HA	1:K:36:PHE:HB3	1.95	0.47
1:P:57:ALA:C	1:P:104:MET:HE1	2.39	0.47
1:B:164:TRP:HA	1:B:167:VAL:HG12	1.97	0.47
1:E:23:TYR:OH	1:E:267:LYS:O	2.24	0.47
1:G:217:GLU:HG3	1:G:247:LYS:HD2	1.96	0.47
1:I:139:PHE:CD2	1:I:267:LYS:HG2	2.50	0.47
1:J:61:LEU:HD13	1:J:104:MET:HE3	1.95	0.47
1:K:69:MET:HE1	1:K:218:PHE:HE1	1.80	0.47
1:M:27:ARG:HD3	1:M:145:TYR:OH	2.15	0.47
1:M:207:MET:HE2	1:M:250:HIS:NE2	2.29	0.47
1:N:238:GLU:HG2	1:N:241:ARG:NH2	2.29	0.47
1:M:23:TYR:OH	1:M:267:LYS:O	2.28	0.47
1:C:109:MET:HE3	1:C:126:LEU:HD22	1.95	0.47
1:D:104:MET:HE2	1:D:104:MET:HA	1.97	0.47
1:E:22:THR:HG23	1:E:137:PRO:HA	1.96	0.47
1:E:33:PHE:HA	1:E:36:PHE:HB3	1.97	0.47
1:L:109:MET:HE3	1:L:126:LEU:HD22	1.96	0.47
1:O:40:TYR:O	1:O:119:LYS:NZ	2.41	0.47
1:G:89:TYR:HE2	1:G:99:LEU:HD22	1.80	0.47
1:O:218:PHE:CZ	1:O:241:ARG:HG3	2.50	0.47
1:H:89:TYR:CE2	1:H:99:LEU:HD22	2.49	0.46
1:P:217:GLU:HG3	1:P:247:LYS:HD2	1.95	0.46
1:E:132:ARG:NH2	2:F:301:GTP:O3G	2.46	0.46
1:K:5:LYS:HE3	1:K:6:TYR:CZ	2.51	0.46
1:D:62:MET:O	1:D:216:ARG:NH2	2.47	0.46
1:G:163:PHE:O	1:G:167:VAL:HG23	2.16	0.46
1:H:115:TYR:C	1:H:117:PRO:HD3	2.40	0.46
1:N:19:LEU:HD23	1:N:22:THR:HG21	1.97	0.46
1:O:218:PHE:HD1	1:O:265:TRP:CG	2.34	0.46
1:I:69:MET:HE3	1:I:83:ARG:HD3	1.96	0.46
1:N:184:THR:OG1	1:N:188:ASP:HB2	2.16	0.46
1:C:163:PHE:O	1:C:167:VAL:HG23	2.16	0.46
1:N:116:PHE:HB3	1:N:119:LYS:HB2	1.97	0.46
1:D:28:VAL:HG13	1:D:129:PHE:HB3	1.96	0.46
1:K:89:TYR:CE2	1:K:99:LEU:HD22	2.51	0.46
1:A:162:THR:HA	1:A:193:LEU:HD21	1.97	0.46
1:O:218:PHE:HZ	1:O:241:ARG:HG3	1.81	0.45
1:F:44:LYS:HD3	1:F:164:TRP:CH2	2.50	0.45
1:M:77:GLU:OE2	1:M:149:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:LEU:HG	1:H:89:TYR:CD2	2.51	0.45
1:J:62:MET:O	1:J:216:ARG:NH2	2.49	0.45
1:C:99:LEU:HB2	1:D:31:LYS:NZ	2.32	0.45
1:C:151:VAL:O	1:C:155:ILE:HG12	2.16	0.45
1:C:178:GLU:O	1:C:182:MET:HG2	2.17	0.45
1:D:218:PHE:HZ	1:D:241:ARG:HG3	1.82	0.45
1:K:48:LEU:HD12	1:K:207:MET:HE1	1.98	0.45
1:B:54:MET:HE3	1:B:78:TYR:HD2	1.81	0.45
1:B:238:GLU:HG2	1:B:241:ARG:NH2	2.31	0.45
1:D:89:TYR:HE2	1:D:99:LEU:HD22	1.80	0.45
1:D:33:PHE:HA	1:D:36:PHE:HB3	1.98	0.45
1:G:216:ARG:O	1:G:265:TRP:NE1	2.49	0.45
1:J:49:LYS:O	1:J:53:VAL:HG23	2.17	0.45
1:L:116:PHE:HB3	1:L:119:LYS:HB2	1.99	0.45
1:D:5:LYS:HE3	1:D:6:TYR:CZ	2.52	0.45
1:J:205:SER:HB3	1:J:208:TYR:CD2	2.52	0.45
1:K:73:GLY:HA3	1:K:78:TYR:CE2	2.51	0.45
1:C:54:MET:HE3	1:C:78:TYR:HD2	1.82	0.45
1:O:106:THR:HG23	1:P:105:SER:HB3	1.98	0.45
1:I:65:TYR:OH	1:J:31:LYS:NZ	2.49	0.45
1:J:139:PHE:CG	1:J:267:LYS:HG2	2.51	0.45
1:A:69:MET:HE3	1:A:83:ARG:HD3	1.97	0.44
1:D:115:TYR:C	1:D:117:PRO:HD3	2.42	0.44
1:G:92:ARG:HH22	2:H:402:GTP:PG	2.39	0.44
1:C:28:VAL:HG21	1:C:104:MET:HG3	1.99	0.44
1:F:145:TYR:O	1:F:149:ARG:HG2	2.18	0.44
1:L:33:PHE:HA	1:L:36:PHE:HB3	1.98	0.44
1:P:165:ASN:O	1:P:169:LYS:HB2	2.17	0.44
1:A:200:ASN:HD22	1:A:203:ASN:ND2	2.16	0.44
1:B:181:LEU:O	1:B:184:THR:HG22	2.17	0.44
1:B:222:GLU:O	1:B:224:GLU:N	2.44	0.44
1:H:104:MET:HE2	1:H:104:MET:HA	2.00	0.44
1:F:73:GLY:HA3	1:F:78:TYR:CE2	2.53	0.44
1:I:162:THR:HA	1:I:193:LEU:HD21	1.99	0.44
1:H:89:TYR:HE2	1:H:99:LEU:HD22	1.83	0.44
1:O:54:MET:HE3	1:O:78:TYR:HD2	1.82	0.44
1:A:54:MET:HE3	1:A:78:TYR:HD2	1.83	0.44
1:G:49:LYS:HB2	1:G:49:LYS:HE2	1.78	0.44
1:G:72:TYR:HD1	1:G:213:ILE:HG13	1.83	0.44
1:K:54:MET:HE3	1:K:78:TYR:HD2	1.81	0.44
1:M:69:MET:CE	1:M:83:ARG:HD3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:THR:HG23	1:O:137:PRO:HA	2.00	0.44
1:M:49:LYS:O	1:M:53:VAL:HG23	2.17	0.44
1:M:222:GLU:O	1:M:224:GLU:N	2.43	0.44
1:N:33:PHE:HA	1:N:36:PHE:HB3	2.00	0.44
1:E:159:TYR:HD1	1:E:189:LYS:HE2	1.83	0.44
1:I:70:LEU:HD11	1:I:213:ILE:HG23	2.00	0.44
1:O:99:LEU:HB2	1:P:31:LYS:NZ	2.33	0.44
1:O:190:ASN:O	1:O:194:PHE:HD1	2.00	0.44
1:O:268:ASP:OD1	1:O:268:ASP:N	2.49	0.44
1:F:57:ALA:C	1:F:104:MET:HE1	2.42	0.43
1:M:94:MET:HE1	1:M:95:LYS:HE2	2.00	0.43
1:A:61:LEU:HD13	1:A:104:MET:HE3	2.00	0.43
1:C:72:TYR:HD1	1:C:213:ILE:HG13	1.83	0.43
1:F:181:LEU:O	1:F:184:THR:HG22	2.18	0.43
1:H:49:LYS:O	1:H:53:VAL:HG23	2.17	0.43
1:F:33:PHE:HA	1:F:36:PHE:HB3	1.99	0.43
1:L:43:GLU:HB2	1:L:47:ASP:HA	2.00	0.43
1:O:69:MET:HE1	1:O:218:PHE:HE1	1.82	0.43
1:E:205:SER:HB3	1:E:208:TYR:CD2	2.53	0.43
1:N:73:GLY:HA3	1:N:78:TYR:CE2	2.53	0.43
1:D:27:ARG:HD3	1:D:145:TYR:OH	2.18	0.43
1:D:31:LYS:HE3	1:D:31:LYS:HB2	1.79	0.43
1:G:166:LEU:O	1:G:170:LEU:HB3	2.18	0.43
1:H:222:GLU:O	1:H:224:GLU:N	2.44	0.43
1:E:15:GLU:OE1	1:E:92:ARG:HD2	2.18	0.43
1:E:54:MET:HE3	1:E:78:TYR:HD2	1.82	0.43
1:I:31:LYS:NZ	1:J:65:TYR:OH	2.52	0.43
1:N:20:PRO:O	1:N:22:THR:HG23	2.19	0.43
1:C:33:PHE:HA	1:C:36:PHE:HB3	2.01	0.43
1:G:5:LYS:HE3	1:G:6:TYR:OH	2.18	0.43
1:H:61:LEU:HD13	1:H:104:MET:HE3	2.00	0.43
1:H:139:PHE:CG	1:H:267:LYS:HG2	2.54	0.43
1:I:43:GLU:HG3	1:I:44:LYS:N	2.33	0.43
1:J:76:ASP:OD1	2:J:401:GTP:O1A	2.37	0.43
1:P:54:MET:HE3	1:P:78:TYR:HD2	1.84	0.43
1:A:39:PHE:HD1	1:L:179:GLN:HB3	1.84	0.43
1:B:164:TRP:CE3	1:B:167:VAL:HG11	2.53	0.43
1:E:73:GLY:HA3	1:E:78:TYR:CE2	2.53	0.43
1:L:218:PHE:CE2	1:L:244:ALA:HB2	2.53	0.43
1:P:170:LEU:HD11	1:P:196:GLU:O	2.18	0.43
1:F:23:TYR:CD1	1:F:84:LYS:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:THR:CG2	1:N:105:SER:HB3	2.48	0.43
1:N:72:TYR:HD1	1:N:213:ILE:HG13	1.84	0.43
1:N:109:MET:HE3	1:N:126:LEU:HD22	2.01	0.43
1:P:54:MET:HE3	1:P:54:MET:HB3	1.94	0.43
1:G:89:TYR:CE2	1:G:99:LEU:HD22	2.54	0.42
1:D:89:TYR:CE2	1:D:99:LEU:HD22	2.54	0.42
1:G:31:LYS:HE2	1:H:65:TYR:OH	2.19	0.42
1:H:170:LEU:HD23	1:H:170:LEU:HA	1.87	0.42
1:G:5:LYS:HE3	1:G:6:TYR:CZ	2.54	0.42
1:H:218:PHE:CZ	1:H:241:ARG:HG3	2.47	0.42
1:D:44:LYS:HD3	1:D:164:TRP:CH2	2.55	0.42
1:E:83:ARG:NH2	1:E:85:ASN:HB2	2.34	0.42
1:B:216:ARG:O	1:B:265:TRP:NE1	2.52	0.42
1:F:72:TYR:HD1	1:F:213:ILE:HG13	1.85	0.42
1:H:15:GLU:OE1	1:H:92:ARG:HD2	2.20	0.42
1:D:10:LYS:HD2	1:D:13:GLU:OE2	2.20	0.42
1:L:73:GLY:HA3	1:L:78:TYR:CE2	2.54	0.42
1:C:230:SER:HA	1:C:234:VAL:HG23	2.01	0.42
1:F:218:PHE:CE2	1:F:244:ALA:HB2	2.55	0.42
1:L:139:PHE:CD2	1:L:267:LYS:HG2	2.55	0.42
1:F:147:SER:HA	1:F:254:ILE:HG12	2.01	0.42
1:H:15:GLU:CD	1:H:92:ARG:HH11	2.28	0.42
1:K:35:LYS:HE3	1:K:35:LYS:HA	2.01	0.42
1:E:49:LYS:O	1:E:53:VAL:HG23	2.20	0.42
1:G:15:GLU:OE1	1:G:92:ARG:HD2	2.20	0.42
1:H:58:ALA:HA	1:H:104:MET:HE1	2.02	0.42
1:H:218:PHE:CE2	1:H:244:ALA:HB2	2.55	0.42
1:F:19:LEU:HD23	1:F:22:THR:HG21	2.01	0.41
1:B:33:PHE:HA	1:B:36:PHE:HB3	2.01	0.41
1:B:57:ALA:C	1:B:104:MET:HE1	2.44	0.41
1:C:83:ARG:NH1	1:C:85:ASN:HB2	2.35	0.41
1:E:180:ARG:NH2	1:E:196:GLU:OE1	2.54	0.41
1:H:33:PHE:HA	1:H:36:PHE:HB3	2.02	0.41
1:K:72:TYR:HD1	1:K:213:ILE:HG13	1.85	0.41
1:M:89:TYR:CE2	1:M:99:LEU:HD22	2.54	0.41
1:O:181:LEU:O	1:O:184:THR:HG22	2.20	0.41
1:B:69:MET:HE1	1:B:218:PHE:HE1	1.84	0.41
1:F:76:ASP:OD1	2:F:303:GTP:O1A	2.38	0.41
1:G:66:SER:HB2	1:G:241:ARG:HB3	2.03	0.41
1:K:239:LYS:HE2	1:K:243:LYS:NZ	2.35	0.41
1:L:57:ALA:C	1:L:104:MET:HE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:GLU:C	1:N:224:GLU:H	2.27	0.41
1:E:88:LEU:HG	1:E:89:TYR:CD2	2.55	0.41
1:O:173:THR:HG23	1:O:175:GLN:N	2.36	0.41
1:B:256:ASP:OD2	1:B:259:TRP:HB2	2.21	0.41
1:F:58:ALA:HA	1:F:104:MET:HE1	2.02	0.41
1:I:57:ALA:C	1:I:104:MET:HE1	2.46	0.41
1:I:217:GLU:HG3	1:I:247:LYS:CD	2.48	0.41
1:I:84:LYS:HE3	1:I:84:LYS:HB3	1.84	0.41
1:I:145:TYR:O	1:I:149:ARG:HG2	2.20	0.41
1:C:15:GLU:OE1	1:C:92:ARG:HD2	2.21	0.41
1:E:178:GLU:HG2	1:N:175:GLN:CD	2.46	0.41
1:J:76:ASP:CG	2:J:401:GTP:O1A	2.62	0.41
1:M:104:MET:HE2	1:M:104:MET:HA	2.02	0.41
1:A:35:LYS:HG3	1:L:179:GLN:HG3	2.02	0.41
1:K:145:TYR:O	1:K:149:ARG:HG2	2.21	0.41
1:M:139:PHE:CD2	1:M:267:LYS:HG2	2.56	0.41
1:N:99:LEU:HD23	1:N:99:LEU:HA	1.79	0.41
1:O:48:LEU:HD12	1:O:207:MET:HE1	2.02	0.41
1:E:110:TYR:CZ	1:F:123:ILE:HB	2.55	0.41
1:G:218:PHE:HZ	1:G:241:ARG:HG3	1.85	0.41
1:I:5:LYS:HE3	1:I:6:TYR:CZ	2.55	0.41
1:K:19:LEU:HA	1:K:20:PRO:HD3	1.93	0.41
1:K:27:ARG:HD3	1:K:145:TYR:OH	2.20	0.41
1:P:43:GLU:HB2	1:P:47:ASP:HA	2.02	0.41
1:B:19:LEU:HA	1:B:20:PRO:HD3	1.89	0.41
1:A:48:LEU:HD12	1:A:207:MET:HE1	2.03	0.40
1:H:145:TYR:O	1:H:148:TRP:HB3	2.21	0.40
1:B:66:SER:HB2	1:B:241:ARG:HB3	2.03	0.40
1:A:222:GLU:O	1:A:224:GLU:N	2.47	0.40
1:I:71:ALA:HA	1:I:79:SER:O	2.21	0.40
1:I:118:ASP:OD1	1:I:118:ASP:N	2.51	0.40
1:A:54:MET:HE3	1:A:54:MET:HB3	1.98	0.40
1:A:234:VAL:O	1:A:238:GLU:HG3	2.21	0.40
1:C:116:PHE:HB3	1:C:119:LYS:HB2	2.02	0.40
1:F:22:THR:HG22	1:H:137:PRO:HB3	2.02	0.40
1:F:118:ASP:OD1	1:F:118:ASP:N	2.53	0.40
1:G:118:ASP:OD1	1:G:118:ASP:N	2.53	0.40
1:H:22:THR:HG21	1:H:135:LEU:HB3	2.03	0.40
1:L:54:MET:HG2	1:L:108:TYR:HE1	1.87	0.40
1:O:49:LYS:O	1:O:53:VAL:HG23	2.21	0.40
1:P:15:GLU:OE1	1:P:92:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:HD3	1:B:164:TRP:CZ3	2.57	0.40
1:B:218:PHE:CZ	1:B:241:ARG:HG3	2.51	0.40
1:D:15:GLU:OE1	1:D:92:ARG:HD2	2.22	0.40
1:E:118:ASP:OD1	1:E:118:ASP:N	2.55	0.40
1:E:159:TYR:OH	1:E:178:GLU:OE2	2.38	0.40
1:H:166:LEU:HD23	1:H:170:LEU:HD12	2.03	0.40
1:J:54:MET:HE3	1:J:78:TYR:HD2	1.86	0.40
1:K:263:ARG:HG2	1:K:265:TRP:CZ2	2.56	0.40
1:M:28:VAL:HG11	1:M:104:MET:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	B	263/271 (97%)	254 (97%)	9 (3%)	0	100	100
1	C	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	D	263/271 (97%)	253 (96%)	10 (4%)	0	100	100
1	E	237/271 (88%)	233 (98%)	4 (2%)	0	100	100
1	F	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
1	G	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	H	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	I	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
1	J	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	K	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	L	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
1	M	263/271 (97%)	255 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	O	263/271 (97%)	255 (97%)	8 (3%)	0	100	100
1	P	238/271 (88%)	234 (98%)	4 (2%)	0	100	100
All	All	4082/4336 (94%)	3971 (97%)	111 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/252 (99%)	246 (99%)	3 (1%)	63	79
1	B	249/252 (99%)	247 (99%)	2 (1%)	73	83
1	C	249/252 (99%)	246 (99%)	3 (1%)	63	79
1	D	249/252 (99%)	246 (99%)	3 (1%)	63	79
1	E	226/252 (90%)	220 (97%)	6 (3%)	39	68
1	F	227/252 (90%)	225 (99%)	2 (1%)	70	82
1	G	249/252 (99%)	244 (98%)	5 (2%)	48	73
1	H	249/252 (99%)	241 (97%)	8 (3%)	34	64
1	I	227/252 (90%)	219 (96%)	8 (4%)	32	62
1	J	249/252 (99%)	245 (98%)	4 (2%)	55	76
1	K	249/252 (99%)	241 (97%)	8 (3%)	34	64
1	L	227/252 (90%)	220 (97%)	7 (3%)	35	65
1	M	249/252 (99%)	243 (98%)	6 (2%)	43	70
1	N	249/252 (99%)	246 (99%)	3 (1%)	63	79
1	O	249/252 (99%)	240 (96%)	9 (4%)	31	62
1	P	227/252 (90%)	222 (98%)	5 (2%)	45	71
All	All	3873/4032 (96%)	3791 (98%)	82 (2%)	47	72

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	99	LEU
1	A	253	ILE
1	B	99	LEU
1	B	253	ILE
1	C	78	TYR
1	C	99	LEU
1	C	215	VAL
1	D	78	TYR
1	D	99	LEU
1	D	253	ILE
1	E	78	TYR
1	E	99	LEU
1	E	149	ARG
1	E	170	LEU
1	E	178	GLU
1	E	185	VAL
1	F	78	TYR
1	F	171	LYS
1	G	78	TYR
1	G	99	LEU
1	G	185	VAL
1	G	215	VAL
1	G	253	ILE
1	H	31	LYS
1	H	74	ASP
1	H	78	TYR
1	H	99	LEU
1	H	149	ARG
1	H	179	GLN
1	H	185	VAL
1	H	231	LYS
1	I	14	LYS
1	I	74	ASP
1	I	78	TYR
1	I	99	LEU
1	I	168	LEU
1	I	171	LYS
1	I	185	VAL
1	I	253	ILE
1	J	78	TYR
1	J	99	LEU

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Mol	Chain	Res	Type
1	J	179	GLN
1	J	253	ILE
1	K	35	LYS
1	K	74	ASP
1	K	78	TYR
1	K	99	LEU
1	K	170	LEU
1	K	185	VAL
1	K	215	VAL
1	K	253	ILE
1	L	74	ASP
1	L	78	TYR
1	L	99	LEU
1	L	149	ARG
1	L	152	ASP
1	L	158	LEU
1	L	179	GLN
1	M	74	ASP
1	M	78	TYR
1	M	99	LEU
1	M	168	LEU
1	M	185	VAL
1	M	240	LYS
1	N	78	TYR
1	N	179	GLN
1	N	253	ILE
1	O	74	ASP
1	O	78	TYR
1	O	99	LEU
1	O	171	LYS
1	O	173	THR
1	O	185	VAL
1	O	215	VAL
1	O	228	GLU
1	O	253	ILE
1	P	74	ASP
1	P	78	TYR
1	P	99	LEU
1	P	179	GLN
1	P	185	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	154	HIS
1	A	157	ASN
1	A	160	ASN
1	A	200	ASN
1	B	34	HIS
1	C	190	ASN
1	D	165	ASN
1	E	46	ASN
1	E	114	GLN
1	E	165	ASN
1	F	179	GLN
1	G	85	ASN
1	H	46	ASN
1	H	114	GLN
1	H	157	ASN
1	H	179	GLN
1	H	200	ASN
1	H	203	ASN
1	I	38	GLN
1	I	179	GLN
1	I	250	HIS
1	J	46	ASN
1	J	114	GLN
1	J	156	ASN
1	J	157	ASN
1	J	179	GLN
1	J	202	ASN
1	K	55	ASN
1	K	128	ASN
1	K	154	HIS
1	L	85	ASN
1	L	114	GLN
1	L	175	GLN
1	M	38	GLN
1	M	52	GLN
1	M	200	ASN
1	M	202	ASN
1	M	203	ASN
1	N	46	ASN
1	N	85	ASN
1	N	157	ASN
1	N	200	ASN

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Mol	Chain	Res	Type
1	N	202	ASN
1	N	233	GLN
1	O	34	HIS
1	O	85	ASN
1	O	128	ASN
1	O	200	ASN
1	P	46	ASN
1	P	114	GLN
1	P	179	GLN
1	P	200	ASN
1	P	202	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 80 ligands modelled in this entry, 48 are monoatomic - leaving 32 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
2	GTP	G	402	3	33,34,34	1.07	4 (12%)	50,54,54	1.62	9 (18%)
2	GTP	I	402	3	33,34,34	0.95	2 (6%)	50,54,54	1.63	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTP	M	402	3	33,34,34	1.04	3 (9%)	50,54,54	1.58	9 (18%)
2	GTP	L	301	3	33,34,34	1.02	3 (9%)	50,54,54	1.64	9 (18%)
2	GTP	D	302	3	33,34,34	1.12	4 (12%)	50,54,54	1.59	9 (18%)
2	GTP	N	402	3	33,34,34	0.93	1 (3%)	50,54,54	1.64	8 (16%)
2	GTP	O	401	3	33,34,34	1.03	2 (6%)	50,54,54	1.67	12 (24%)
2	GTP	H	401	3	33,34,34	0.90	1 (3%)	50,54,54	1.59	12 (24%)
2	GTP	E	404	3	33,34,34	1.05	5 (15%)	50,54,54	1.65	10 (20%)
2	GTP	D	301	3	33,34,34	0.93	1 (3%)	50,54,54	1.63	9 (18%)
2	GTP	M	401	3	33,34,34	0.92	1 (3%)	50,54,54	1.53	10 (20%)
2	GTP	N	401	3	33,34,34	1.04	3 (9%)	50,54,54	1.63	12 (24%)
2	GTP	E	401	3	33,34,34	1.17	3 (9%)	50,54,54	1.66	9 (18%)
2	GTP	H	402	3	33,34,34	0.91	2 (6%)	50,54,54	1.62	8 (16%)
2	GTP	A	402	3	33,34,34	1.02	4 (12%)	50,54,54	1.62	8 (16%)
2	GTP	O	406	3	33,34,34	0.93	2 (6%)	50,54,54	1.63	8 (16%)
2	GTP	B	401	3	33,34,34	1.00	3 (9%)	50,54,54	1.60	9 (18%)
2	GTP	F	303	3	33,34,34	0.93	2 (6%)	50,54,54	1.59	9 (18%)
2	GTP	J	402	3	33,34,34	1.03	3 (9%)	50,54,54	1.64	10 (20%)
2	GTP	I	401	3	33,34,34	1.08	3 (9%)	50,54,54	1.63	8 (16%)
2	GTP	A	401	3	33,34,34	1.19	4 (12%)	50,54,54	1.58	9 (18%)
2	GTP	J	401	3	33,34,34	0.95	2 (6%)	50,54,54	1.60	9 (18%)
2	GTP	B	402	3	33,34,34	0.99	2 (6%)	50,54,54	1.61	8 (16%)
2	GTP	C	405	3	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
2	GTP	K	401	3	33,34,34	1.11	4 (12%)	50,54,54	1.62	9 (18%)
2	GTP	F	301	3	33,34,34	1.06	2 (6%)	50,54,54	1.58	9 (18%)
2	GTP	L	303	3	33,34,34	1.03	4 (12%)	50,54,54	1.62	11 (22%)
2	GTP	L	304	3	33,34,34	0.98	3 (9%)	50,54,54	1.63	9 (18%)
2	GTP	C	401	3	33,34,34	1.06	4 (12%)	50,54,54	1.57	9 (18%)
2	GTP	G	401	3	33,34,34	0.99	3 (9%)	50,54,54	1.65	11 (22%)
2	GTP	O	402	3	33,34,34	0.94	2 (6%)	50,54,54	1.64	9 (18%)
2	GTP	P	401	3	33,34,34	1.00	3 (9%)	50,54,54	1.52	8 (16%)

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	GTP	G	402	3	-	7/22/38/38	0/3/3/3
2	GTP	I	402	3	-	11/22/38/38	0/3/3/3
2	GTP	M	402	3	-	10/22/38/38	0/3/3/3
2	GTP	L	301	3	-	7/22/38/38	0/3/3/3
2	GTP	D	302	3	-	7/22/38/38	0/3/3/3
2	GTP	N	402	3	-	6/22/38/38	0/3/3/3
2	GTP	O	401	3	-	6/22/38/38	0/3/3/3
2	GTP	H	401	3	-	5/22/38/38	0/3/3/3
2	GTP	E	404	3	-	6/22/38/38	0/3/3/3
2	GTP	D	301	3	-	9/22/38/38	0/3/3/3
2	GTP	M	401	3	-	4/22/38/38	0/3/3/3
2	GTP	N	401	3	-	2/22/38/38	0/3/3/3
2	GTP	E	401	3	-	10/22/38/38	0/3/3/3
2	GTP	H	402	3	-	3/22/38/38	0/3/3/3
2	GTP	A	402	3	-	10/22/38/38	0/3/3/3
2	GTP	O	406	3	-	5/22/38/38	0/3/3/3
2	GTP	B	401	3	-	11/22/38/38	0/3/3/3
2	GTP	F	303	3	-	5/22/38/38	0/3/3/3
2	GTP	J	402	3	-	7/22/38/38	0/3/3/3
2	GTP	I	401	3	-	4/22/38/38	0/3/3/3
2	GTP	A	401	3	-	9/22/38/38	0/3/3/3
2	GTP	J	401	3	-	8/22/38/38	0/3/3/3
2	GTP	B	402	3	-	12/22/38/38	0/3/3/3
2	GTP	C	405	3	-	4/22/38/38	0/3/3/3
2	GTP	K	401	3	-	5/22/38/38	0/3/3/3
2	GTP	F	301	3	-	7/22/38/38	0/3/3/3
2	GTP	L	303	3	-	3/22/38/38	0/3/3/3
2	GTP	L	304	3	-	10/22/38/38	0/3/3/3
2	GTP	C	401	3	-	7/22/38/38	0/3/3/3
2	GTP	G	401	3	-	5/22/38/38	0/3/3/3
2	GTP	O	402	3	-	7/22/38/38	0/3/3/3
2	GTP	P	401	3	-	5/22/38/38	0/3/3/3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	GTP	PA-O3A	3.44	1.63	1.59
2	E	401	GTP	PB-O3A	3.39	1.63	1.59
2	I	401	GTP	PB-O3A	3.35	1.63	1.59
2	F	301	GTP	PA-O3A	3.20	1.63	1.59
2	G	402	GTP	PA-O3A	3.08	1.62	1.59
2	J	402	GTP	PA-O3A	3.03	1.62	1.59
2	A	401	GTP	PB-O3A	3.02	1.62	1.59
2	A	401	GTP	PA-O3A	3.01	1.62	1.59
2	A	401	GTP	PB-O3B	2.99	1.62	1.59
2	D	302	GTP	PB-O3A	2.85	1.62	1.59
2	A	402	GTP	PA-O3A	2.83	1.62	1.59
2	M	402	GTP	PA-O3A	2.82	1.62	1.59
2	K	401	GTP	PA-O3A	2.81	1.62	1.59
2	D	302	GTP	PA-O3A	2.71	1.62	1.59
2	N	401	GTP	PA-O3A	2.65	1.62	1.59
2	L	303	GTP	PA-O3A	2.60	1.62	1.59
2	O	401	GTP	PB-O3A	2.59	1.62	1.59
2	O	401	GTP	PA-O3A	2.55	1.62	1.59
2	K	401	GTP	PB-O3A	2.50	1.62	1.59
2	K	401	GTP	PB-O3B	2.48	1.62	1.59
2	C	401	GTP	PB-O3B	2.48	1.62	1.59
2	C	401	GTP	PA-O3A	2.45	1.62	1.59
2	I	402	GTP	C2-N3	2.45	1.39	1.33
2	O	402	GTP	C2-N3	2.45	1.39	1.33
2	P	401	GTP	PA-O3A	2.45	1.62	1.59
2	L	304	GTP	PB-O3A	2.45	1.62	1.59
2	N	401	GTP	PB-O3B	2.45	1.62	1.59
2	D	302	GTP	PB-O3B	2.42	1.62	1.59
2	L	304	GTP	C2-N3	2.41	1.39	1.33
2	B	402	GTP	C2-N3	2.41	1.39	1.33
2	L	301	GTP	C2-N3	2.41	1.39	1.33
2	L	303	GTP	PB-O3A	2.40	1.62	1.59
2	D	301	GTP	C2-N3	2.36	1.38	1.33
2	H	402	GTP	C2-N3	2.35	1.38	1.33
2	G	402	GTP	C2-N3	2.35	1.38	1.33
2	J	401	GTP	C2-N3	2.35	1.38	1.33
2	J	402	GTP	C2-N3	2.33	1.38	1.33
2	F	301	GTP	C2-N3	2.32	1.38	1.33
2	M	401	GTP	C2-N3	2.32	1.38	1.33
2	B	401	GTP	C2-N3	2.28	1.38	1.33
2	C	401	GTP	PB-O3A	2.28	1.62	1.59
2	I	401	GTP	C2-N3	2.27	1.38	1.33
2	L	301	GTP	PA-O3A	2.27	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	402	GTP	C2-N3	2.26	1.38	1.33
2	G	401	GTP	C2-N3	2.26	1.38	1.33
2	O	406	GTP	C2-N3	2.26	1.38	1.33
2	G	401	GTP	PA-O3A	2.25	1.61	1.59
2	E	404	GTP	PB-O3A	2.24	1.61	1.59
2	N	402	GTP	C2-N3	2.24	1.38	1.33
2	K	401	GTP	C2-N3	2.24	1.38	1.33
2	B	401	GTP	PA-O3A	2.24	1.61	1.59
2	C	401	GTP	C2-N3	2.23	1.38	1.33
2	M	402	GTP	PB-O3A	2.22	1.61	1.59
2	A	402	GTP	C2-N3	2.22	1.38	1.33
2	E	404	GTP	PB-O3B	2.22	1.61	1.59
2	E	404	GTP	C2-N3	2.22	1.38	1.33
2	B	401	GTP	PB-O3A	2.20	1.61	1.59
2	C	405	GTP	C2-N3	2.19	1.38	1.33
2	H	402	GTP	PB-O3B	2.19	1.61	1.59
2	E	401	GTP	C2-N3	2.18	1.38	1.33
2	P	401	GTP	PB-O3A	2.15	1.61	1.59
2	I	402	GTP	PB-O3B	2.15	1.61	1.59
2	G	402	GTP	PB-O3A	2.13	1.61	1.59
2	L	301	GTP	PB-O3A	2.13	1.61	1.59
2	A	402	GTP	PB-O3A	2.12	1.61	1.59
2	D	302	GTP	C2-N3	2.12	1.38	1.33
2	E	404	GTP	PA-O3A	2.12	1.61	1.59
2	G	401	GTP	PB-O3A	2.11	1.61	1.59
2	N	401	GTP	PB-O3A	2.11	1.61	1.59
2	P	401	GTP	C2-N3	2.10	1.38	1.33
2	G	402	GTP	C5-N7	-2.09	1.34	1.39
2	B	402	GTP	C5-N7	-2.08	1.34	1.39
2	J	402	GTP	C5-N7	-2.07	1.34	1.39
2	A	401	GTP	C2-N3	2.07	1.38	1.33
2	A	402	GTP	C5-N7	-2.07	1.34	1.39
2	J	401	GTP	PA-O3A	2.06	1.61	1.59
2	L	303	GTP	C2-N3	2.06	1.38	1.33
2	O	406	GTP	C5-N7	-2.06	1.34	1.39
2	F	303	GTP	PB-O3B	2.06	1.61	1.59
2	I	401	GTP	PA-O3A	2.03	1.61	1.59
2	O	402	GTP	PB-O3A	2.02	1.61	1.59
2	F	303	GTP	C2-N3	2.01	1.38	1.33
2	L	303	GTP	PB-O3B	2.01	1.61	1.59
2	H	401	GTP	C2-N3	2.00	1.38	1.33
2	L	304	GTP	C5-N7	-2.00	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	404	GTP	C5-N7	-2.00	1.35	1.39

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GTP	C5-C4-N3	-5.41	119.78	128.39
2	I	401	GTP	C5-C4-N3	-5.40	119.79	128.39
2	K	401	GTP	C5-C4-N3	-5.29	119.97	128.39
2	L	301	GTP	C5-C4-N3	-5.28	119.98	128.39
2	G	401	GTP	C5-C4-N3	-5.25	120.04	128.39
2	O	402	GTP	C5-C4-N3	-5.23	120.07	128.39
2	J	401	GTP	C5-C4-N3	-5.21	120.11	128.39
2	G	402	GTP	C5-C4-N3	-5.14	120.20	128.39
2	B	401	GTP	C5-C4-N3	-5.14	120.22	128.39
2	O	406	GTP	C5-C4-N3	-5.11	120.26	128.39
2	B	402	GTP	C5-C4-N3	-5.04	120.36	128.39
2	L	304	GTP	C5-C4-N3	-5.03	120.39	128.39
2	A	402	GTP	C5-C4-N3	-5.01	120.41	128.39
2	C	401	GTP	C5-C4-N3	-5.00	120.43	128.39
2	A	401	GTP	C5-C4-N3	-4.98	120.46	128.39
2	F	301	GTP	C5-C4-N3	-4.98	120.47	128.39
2	F	303	GTP	C5-C4-N3	-4.96	120.49	128.39
2	P	401	GTP	C5-C4-N3	-4.96	120.49	128.39
2	D	301	GTP	C5-C4-N3	-4.94	120.53	128.39
2	I	401	GTP	C2-N3-C4	4.92	120.77	112.30
2	D	302	GTP	C5-C4-N3	-4.91	120.57	128.39
2	I	402	GTP	C5-C4-N3	-4.90	120.59	128.39
2	L	303	GTP	C2-N3-C4	4.90	120.73	112.30
2	J	402	GTP	C5-C4-N3	-4.89	120.61	128.39
2	E	401	GTP	C2-N3-C4	4.88	120.71	112.30
2	N	402	GTP	C5-C4-N3	-4.88	120.62	128.39
2	L	301	GTP	C2-N3-C4	4.85	120.66	112.30
2	G	402	GTP	C2-N3-C4	4.84	120.63	112.30
2	H	401	GTP	C5-C4-N3	-4.84	120.69	128.39
2	H	402	GTP	C5-C4-N3	-4.83	120.71	128.39
2	O	406	GTP	C2-N3-C4	4.83	120.61	112.30
2	D	301	GTP	C2-N3-C4	4.83	120.61	112.30
2	K	401	GTP	C2-N3-C4	4.83	120.61	112.30
2	L	303	GTP	C5-C4-N3	-4.82	120.72	128.39
2	O	402	GTP	C2-N3-C4	4.79	120.55	112.30
2	C	405	GTP	C5-C4-N3	-4.79	120.77	128.39
2	N	402	GTP	C2-N3-C4	4.78	120.54	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	304	GTP	C2-N3-C4	4.78	120.53	112.30
2	A	402	GTP	C2-N3-C4	4.78	120.53	112.30
2	I	402	GTP	C2-N3-C4	4.77	120.51	112.30
2	M	402	GTP	C2-N3-C4	4.76	120.50	112.30
2	O	401	GTP	C2-N3-C4	4.76	120.50	112.30
2	F	303	GTP	C2-N3-C4	4.76	120.50	112.30
2	B	402	GTP	C2-N3-C4	4.76	120.49	112.30
2	A	401	GTP	C2-N3-C4	4.70	120.40	112.30
2	M	401	GTP	C5-C4-N3	-4.69	120.92	128.39
2	J	401	GTP	C2-N3-C4	4.69	120.38	112.30
2	H	402	GTP	C2-N3-C4	4.67	120.35	112.30
2	E	404	GTP	C5-C4-N3	-4.67	120.96	128.39
2	E	404	GTP	C2-N3-C4	4.65	120.31	112.30
2	D	302	GTP	C2-N3-C4	4.65	120.31	112.30
2	M	402	GTP	C5-C4-N3	-4.65	120.99	128.39
2	C	405	GTP	C2-N3-C4	4.65	120.30	112.30
2	B	401	GTP	C2-N3-C4	4.63	120.28	112.30
2	C	401	GTP	C2-N3-C4	4.62	120.25	112.30
2	J	402	GTP	C2-N3-C4	4.62	120.25	112.30
2	G	401	GTP	C2-N3-C4	4.60	120.22	112.30
2	F	301	GTP	C2-N3-C4	4.59	120.21	112.30
2	O	401	GTP	C5-C4-N3	-4.53	121.17	128.39
2	H	401	GTP	C2-N3-C4	4.52	120.08	112.30
2	N	401	GTP	C5-C4-N3	-4.47	121.28	128.39
2	P	401	GTP	C2-N3-C4	4.46	119.97	112.30
2	M	401	GTP	C2-N3-C4	4.42	119.92	112.30
2	N	401	GTP	C2-N3-C4	4.41	119.89	112.30
2	O	402	GTP	N9-C4-N3	3.79	133.54	125.95
2	G	402	GTP	N9-C4-N3	3.76	133.48	125.95
2	I	402	GTP	N9-C4-N3	3.66	133.28	125.95
2	L	301	GTP	N9-C4-N3	3.60	133.15	125.95
2	B	402	GTP	N9-C4-N3	3.60	133.15	125.95
2	L	304	GTP	N9-C4-N3	3.59	133.14	125.95
2	F	301	GTP	N9-C4-N3	3.59	133.12	125.95
2	O	406	GTP	N9-C4-N3	3.54	133.03	125.95
2	D	301	GTP	N9-C4-N3	3.53	133.01	125.95
2	J	402	GTP	N9-C4-N3	3.52	132.99	125.95
2	A	402	GTP	N9-C4-N3	3.48	132.91	125.95
2	E	401	GTP	N9-C4-N3	3.47	132.89	125.95
2	K	401	GTP	N9-C4-N3	3.45	132.85	125.95
2	N	402	GTP	N9-C4-N3	3.42	132.80	125.95
2	I	401	GTP	N9-C4-N3	3.42	132.79	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	GTP	N9-C4-N3	3.42	132.79	125.95
2	C	405	GTP	N9-C4-N3	3.38	132.72	125.95
2	J	401	GTP	N9-C4-N3	3.36	132.67	125.95
2	H	402	GTP	N9-C4-N3	3.35	132.66	125.95
2	B	401	GTP	N9-C4-N3	3.33	132.61	125.95
2	E	404	GTP	N9-C4-N3	3.28	132.51	125.95
2	M	402	GTP	N9-C4-N3	3.18	132.31	125.95
2	A	401	GTP	N9-C4-N3	3.15	132.24	125.95
2	G	401	GTP	C2-N1-C6	-3.13	119.44	125.11
2	D	302	GTP	N9-C4-N3	3.12	132.20	125.95
2	N	401	GTP	C2'-C1'-N9	-3.11	104.60	113.25
2	C	401	GTP	N9-C4-N3	3.09	132.13	125.95
2	F	303	GTP	N9-C4-N3	3.07	132.10	125.95
2	E	401	GTP	C2-N1-C6	-3.03	119.61	125.11
2	J	401	GTP	C2-N1-C6	-3.03	119.62	125.11
2	M	401	GTP	N9-C4-N3	3.02	132.00	125.95
2	P	401	GTP	N9-C4-N3	3.00	131.94	125.95
2	L	301	GTP	C2-N1-C6	-2.98	119.70	125.11
2	I	402	GTP	N9-C8-N7	-2.97	107.89	113.40
2	G	402	GTP	C2-N1-C6	-2.96	119.75	125.11
2	O	401	GTP	N9-C8-N7	-2.95	107.92	113.40
2	O	402	GTP	C2-N1-C6	-2.95	119.76	125.11
2	L	303	GTP	N9-C4-N3	2.95	131.85	125.95
2	B	401	GTP	C2-N1-C6	-2.94	119.78	125.11
2	I	401	GTP	C2-N1-C6	-2.93	119.79	125.11
2	H	401	GTP	C2-N1-C6	-2.92	119.81	125.11
2	J	402	GTP	O6-C6-C5	-2.91	118.85	126.53
2	O	406	GTP	O6-C6-C5	-2.91	118.85	126.53
2	B	402	GTP	O6-C6-C5	-2.91	118.86	126.53
2	B	402	GTP	C2-N1-C6	-2.90	119.84	125.11
2	K	401	GTP	C2-N1-C6	-2.89	119.87	125.11
2	G	402	GTP	O6-C6-C5	-2.88	118.92	126.53
2	D	301	GTP	O6-C6-C5	-2.88	118.93	126.53
2	N	402	GTP	C2-N1-C6	-2.88	119.90	125.11
2	J	402	GTP	C2-N1-C6	-2.87	119.90	125.11
2	A	402	GTP	C2-N1-C6	-2.87	119.91	125.11
2	E	404	GTP	O6-C6-C5	-2.87	118.96	126.53
2	O	406	GTP	C2-N1-C6	-2.86	119.92	125.11
2	N	402	GTP	O6-C6-C5	-2.85	119.00	126.53
2	D	302	GTP	C2-N1-C6	-2.85	119.94	125.11
2	H	402	GTP	C2-N1-C6	-2.85	119.94	125.11
2	H	401	GTP	N9-C4-N3	2.84	131.62	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	401	GTP	C2-N1-C6	-2.84	119.97	125.11
2	L	304	GTP	C2-N1-C6	-2.83	119.98	125.11
2	L	303	GTP	C2-N1-C6	-2.82	120.00	125.11
2	F	301	GTP	O6-C6-C5	-2.82	119.10	126.53
2	A	402	GTP	O6-C6-C5	-2.81	119.11	126.53
2	A	401	GTP	C2-N1-C6	-2.80	120.02	125.11
2	M	401	GTP	C2-N1-C6	-2.80	120.02	125.11
2	O	401	GTP	N9-C4-N3	2.80	131.56	125.95
2	D	301	GTP	C2-N1-C6	-2.79	120.05	125.11
2	M	402	GTP	C2-N1-C6	-2.77	120.09	125.11
2	O	401	GTP	C2'-C1'-N9	-2.77	105.55	113.25
2	L	304	GTP	O6-C6-C5	-2.76	119.23	126.53
2	F	301	GTP	C2-N1-C6	-2.76	120.10	125.11
2	E	404	GTP	C2-N1-C6	-2.76	120.11	125.11
2	N	402	GTP	N9-C8-N7	-2.76	108.29	113.40
2	M	402	GTP	O6-C6-C5	-2.74	119.29	126.53
2	C	401	GTP	C2-N1-C6	-2.74	120.14	125.11
2	M	402	GTP	N9-C8-N7	-2.73	108.33	113.40
2	O	401	GTP	C2-N1-C6	-2.73	120.17	125.11
2	H	402	GTP	O6-C6-C5	-2.72	119.34	126.53
2	C	405	GTP	C2-N1-C6	-2.72	120.17	125.11
2	O	402	GTP	O6-C6-C5	-2.72	119.36	126.53
2	M	402	GTP	C5-C6-N1	2.72	120.17	113.25
2	N	401	GTP	N9-C8-N7	-2.71	108.37	113.40
2	G	402	GTP	C5-C6-N1	2.71	120.16	113.25
2	I	402	GTP	O6-C6-C5	-2.71	119.38	126.53
2	I	402	GTP	C2-N1-C6	-2.71	120.19	125.11
2	H	402	GTP	N9-C8-N7	-2.69	108.41	113.40
2	E	404	GTP	N9-C8-N7	-2.69	108.42	113.40
2	N	401	GTP	O3B-PB-O1B	-2.69	102.62	110.70
2	L	301	GTP	O6-C6-C5	-2.68	119.46	126.53
2	B	402	GTP	C5-C6-N1	2.67	120.06	113.25
2	F	303	GTP	C2-N1-C6	-2.67	120.27	125.11
2	C	405	GTP	O6-C6-C5	-2.67	119.49	126.53
2	B	401	GTP	N9-C8-N7	-2.66	108.46	113.40
2	L	304	GTP	N9-C8-N7	-2.66	108.47	113.40
2	N	401	GTP	N9-C4-N3	2.65	131.25	125.95
2	C	405	GTP	N9-C8-N7	-2.65	108.49	113.40
2	D	301	GTP	N9-C8-N7	-2.64	108.50	113.40
2	E	401	GTP	C8-N7-C5	2.64	108.96	104.26
2	G	402	GTP	N9-C8-N7	-2.64	108.51	113.40
2	F	301	GTP	N9-C8-N7	-2.64	108.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	402	GTP	C5-C6-N1	2.64	119.96	113.25
2	H	401	GTP	N9-C8-N7	-2.64	108.51	113.40
2	B	401	GTP	C8-N7-C5	2.63	108.95	104.26
2	N	402	GTP	C5-C6-N1	2.63	119.95	113.25
2	N	401	GTP	C2-N1-C6	-2.62	120.35	125.11
2	D	301	GTP	C5-C6-N1	2.62	119.92	113.25
2	L	304	GTP	C5-C6-N1	2.62	119.92	113.25
2	L	301	GTP	C5-C6-N1	2.61	119.90	113.25
2	L	301	GTP	C8-N7-C5	2.61	108.91	104.26
2	I	402	GTP	C8-N7-C5	2.61	108.91	104.26
2	G	401	GTP	O6-C6-C5	-2.61	119.65	126.53
2	O	402	GTP	N9-C8-N7	-2.60	108.58	113.40
2	H	402	GTP	C5-C6-N1	2.60	119.86	113.25
2	A	402	GTP	C5-C6-N1	2.59	119.85	113.25
2	H	401	GTP	C8-N7-C5	2.59	108.88	104.26
2	O	406	GTP	C5-C6-N1	2.58	119.83	113.25
2	N	401	GTP	C8-N7-C5	2.58	108.85	104.26
2	J	402	GTP	C5-C6-N1	2.57	119.80	113.25
2	I	402	GTP	C5-C6-N1	2.57	119.80	113.25
2	E	404	GTP	C5-C6-N1	2.57	119.80	113.25
2	L	301	GTP	N9-C8-N7	-2.57	108.64	113.40
2	A	402	GTP	N9-C8-N7	-2.56	108.65	113.40
2	J	401	GTP	C5-C6-N1	2.55	119.75	113.25
2	D	302	GTP	C2'-C1'-N9	-2.55	106.15	113.25
2	L	303	GTP	C5-C6-N1	2.55	119.75	113.25
2	B	402	GTP	N9-C8-N7	-2.55	108.67	113.40
2	E	401	GTP	C5-C6-N1	2.54	119.73	113.25
2	E	401	GTP	N9-C8-N7	-2.54	108.68	113.40
2	O	401	GTP	C8-N7-C5	2.54	108.79	104.26
2	M	401	GTP	N9-C8-N7	-2.54	108.70	113.40
2	D	302	GTP	N9-C8-N7	-2.53	108.71	113.40
2	O	401	GTP	C5-C6-N1	2.52	119.68	113.25
2	J	401	GTP	N9-C8-N7	-2.52	108.72	113.40
2	J	402	GTP	N9-C8-N7	-2.52	108.72	113.40
2	K	401	GTP	C8-N7-C5	2.52	108.75	104.26
2	F	303	GTP	N9-C8-N7	-2.52	108.72	113.40
2	G	401	GTP	C5-C6-N1	2.52	119.67	113.25
2	N	402	GTP	C8-N7-C5	2.51	108.74	104.26
2	I	401	GTP	O6-C6-C5	-2.50	119.92	126.53
2	K	401	GTP	N9-C8-N7	-2.50	108.76	113.40
2	C	401	GTP	C8-N7-C5	2.50	108.71	104.26
2	F	301	GTP	C5-C6-N1	2.50	119.61	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	402	GTP	C8-N7-C5	2.49	108.70	104.26
2	C	401	GTP	N9-C8-N7	-2.49	108.78	113.40
2	F	303	GTP	C8-N7-C5	2.48	108.69	104.26
2	E	401	GTP	C3'-C2'-C1'	2.48	106.16	101.46
2	J	401	GTP	C8-N7-C5	2.48	108.68	104.26
2	I	401	GTP	C5-C6-N1	2.48	119.56	113.25
2	O	402	GTP	C8-N7-C5	2.47	108.67	104.26
2	O	406	GTP	N9-C8-N7	-2.47	108.82	113.40
2	K	401	GTP	C5-C6-N1	2.47	119.54	113.25
2	C	405	GTP	C5-C6-N1	2.47	119.54	113.25
2	L	303	GTP	C2'-C1'-N9	-2.47	106.38	113.25
2	L	303	GTP	O6-C6-C5	-2.47	120.02	126.53
2	L	303	GTP	N9-C8-N7	-2.46	108.83	113.40
2	L	304	GTP	C8-N7-C5	2.46	108.64	104.26
2	D	302	GTP	C5-C6-N1	2.46	119.51	113.25
2	G	401	GTP	N9-C8-N7	-2.45	108.85	113.40
2	M	401	GTP	O6-C6-C5	-2.45	120.06	126.53
2	G	402	GTP	C8-N7-C5	2.44	108.61	104.26
2	F	301	GTP	C8-N7-C5	2.44	108.60	104.26
2	I	401	GTP	C8-N7-C5	2.43	108.59	104.26
2	K	401	GTP	O6-C6-C5	-2.43	120.12	126.53
2	A	401	GTP	C5-C6-N1	2.43	119.43	113.25
2	B	401	GTP	C5-C6-N1	2.42	119.42	113.25
2	A	402	GTP	C8-N7-C5	2.42	108.57	104.26
2	C	405	GTP	C8-N7-C5	2.42	108.57	104.26
2	A	401	GTP	N9-C8-N7	-2.41	108.92	113.40
2	P	401	GTP	C8-N7-C5	2.40	108.53	104.26
2	D	302	GTP	O6-C6-C5	-2.40	120.20	126.53
2	E	404	GTP	C8-N7-C5	2.39	108.52	104.26
2	O	401	GTP	O6-C6-C5	-2.39	120.23	126.53
2	M	402	GTP	C8-N7-C5	2.39	108.51	104.26
2	O	401	GTP	O2B-PB-O3A	2.39	113.72	107.27
2	D	302	GTP	C8-N7-C5	2.38	108.51	104.26
2	O	406	GTP	C8-N7-C5	2.38	108.51	104.26
2	M	401	GTP	C5-C6-N1	2.38	119.32	113.25
2	D	301	GTP	C8-N7-C5	2.38	108.50	104.26
2	G	401	GTP	C8-N7-C5	2.38	108.50	104.26
2	N	401	GTP	O3G-PG-O3B	2.37	112.60	104.64
2	J	401	GTP	O6-C6-C5	-2.37	120.27	126.53
2	A	401	GTP	C8-N7-C5	2.35	108.45	104.26
2	C	401	GTP	C5-C6-N1	2.34	119.21	113.25
2	L	303	GTP	C8-N7-C5	2.34	108.43	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	GTP	C8-N7-C5	2.33	108.42	104.26
2	P	401	GTP	O6-C6-C5	-2.33	120.38	126.53
2	F	303	GTP	C5-C6-N1	2.33	119.19	113.25
2	P	401	GTP	N9-C8-N7	-2.33	109.09	113.40
2	B	401	GTP	C3'-C2'-C1'	2.31	105.82	101.46
2	A	401	GTP	O6-C6-C5	-2.30	120.46	126.53
2	M	401	GTP	O3G-PG-O3B	2.29	112.33	104.64
2	I	401	GTP	N9-C8-N7	-2.29	109.16	113.40
2	J	402	GTP	C8-N7-C5	2.27	108.31	104.26
2	J	402	GTP	O2A-PA-O3A	2.27	113.41	107.27
2	H	401	GTP	C5-C6-N1	2.27	119.03	113.25
2	P	401	GTP	C5-C6-N1	2.25	118.98	113.25
2	F	303	GTP	C3'-C2'-C1'	2.25	105.71	101.46
2	M	401	GTP	C8-N7-C5	2.24	108.26	104.26
2	B	401	GTP	O6-C6-C5	-2.24	120.62	126.53
2	K	401	GTP	C3'-C2'-C1'	2.24	105.70	101.46
2	E	401	GTP	O6-C6-C5	-2.23	120.65	126.53
2	J	401	GTP	C3'-C2'-C1'	2.22	105.66	101.46
2	L	301	GTP	C3'-C2'-C1'	2.21	105.65	101.46
2	L	303	GTP	C3'-C2'-C1'	2.21	105.65	101.46
2	F	303	GTP	O6-C6-C5	-2.20	120.71	126.53
2	N	401	GTP	C5-C6-N1	2.20	118.86	113.25
2	C	401	GTP	O6-C6-C5	-2.20	120.73	126.53
2	L	304	GTP	O2B-PB-O3A	2.19	113.20	107.27
2	E	404	GTP	O2B-PB-O3A	2.19	113.18	107.27
2	A	401	GTP	O3G-PG-O3B	2.16	111.89	104.64
2	J	402	GTP	C3'-C2'-C1'	2.16	105.55	101.46
2	G	401	GTP	C3'-C2'-C1'	2.15	105.53	101.46
2	L	303	GTP	N2-C2-N1	2.14	121.29	116.76
2	H	401	GTP	C3'-C2'-C1'	2.14	105.51	101.46
2	N	401	GTP	O6-C6-C5	-2.13	120.91	126.53
2	G	401	GTP	O2B-PB-O3A	2.10	112.94	107.27
2	O	401	GTP	N2-C2-N1	2.09	121.18	116.76
2	H	401	GTP	O6-C6-C5	-2.09	121.01	126.53
2	H	401	GTP	C4-C5-N7	-2.08	107.37	110.67
2	M	401	GTP	C3'-C2'-C1'	2.07	105.38	101.46
2	C	401	GTP	O3G-PG-O3B	2.07	111.59	104.64
2	G	401	GTP	C2'-C1'-N9	-2.07	107.49	113.25
2	G	402	GTP	C3'-C2'-C1'	2.06	105.36	101.46
2	M	402	GTP	N1-C2-N3	-2.05	119.57	123.32
2	H	401	GTP	O2B-PB-O3A	2.05	112.80	107.27
2	I	402	GTP	N1-C2-N3	-2.04	119.58	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	GTP	N1-C2-N3	-2.03	119.60	123.32
2	E	404	GTP	C3'-C2'-C1'	2.03	105.30	101.46
2	O	402	GTP	C3'-C2'-C1'	2.03	105.30	101.46
2	H	401	GTP	O3G-PG-O3B	2.03	111.44	104.64
2	F	301	GTP	C3'-C2'-C1'	2.02	105.28	101.46
2	N	401	GTP	C4-C5-N7	-2.02	107.47	110.67
2	O	401	GTP	O3G-PG-O3B	2.01	111.36	104.64
2	C	405	GTP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GTP	C5'-O5'-PA-O3A
2	A	401	GTP	C5'-O5'-PA-O1A
2	A	402	GTP	PB-O3B-PG-O3G
2	A	402	GTP	C5'-O5'-PA-O3A
2	A	402	GTP	C5'-O5'-PA-O1A
2	A	402	GTP	C5'-O5'-PA-O2A
2	B	401	GTP	PB-O3B-PG-O2G
2	B	401	GTP	C5'-O5'-PA-O3A
2	B	401	GTP	C5'-O5'-PA-O1A
2	B	402	GTP	PB-O3B-PG-O2G
2	B	402	GTP	PB-O3B-PG-O3G
2	B	402	GTP	C5'-O5'-PA-O3A
2	B	402	GTP	C5'-O5'-PA-O1A
2	B	402	GTP	C5'-O5'-PA-O2A
2	C	401	GTP	C5'-O5'-PA-O3A
2	C	401	GTP	C5'-O5'-PA-O1A
2	D	301	GTP	PB-O3B-PG-O3G
2	D	301	GTP	C5'-O5'-PA-O3A
2	D	301	GTP	C5'-O5'-PA-O1A
2	D	301	GTP	C5'-O5'-PA-O2A
2	D	302	GTP	C5'-O5'-PA-O3A
2	D	302	GTP	C5'-O5'-PA-O1A
2	E	401	GTP	C5'-O5'-PA-O3A
2	E	401	GTP	C5'-O5'-PA-O1A
2	E	404	GTP	PB-O3B-PG-O3G
2	F	301	GTP	C5'-O5'-PA-O3A
2	F	301	GTP	C5'-O5'-PA-O1A
2	F	301	GTP	C5'-O5'-PA-O2A
2	F	301	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	F	303	GTP	C5'-O5'-PA-O3A
2	F	303	GTP	C5'-O5'-PA-O1A
2	F	303	GTP	C5'-O5'-PA-O2A
2	G	401	GTP	C5'-O5'-PA-O1A
2	G	402	GTP	C5'-O5'-PA-O3A
2	G	402	GTP	C5'-O5'-PA-O1A
2	G	402	GTP	C5'-O5'-PA-O2A
2	H	401	GTP	C5'-O5'-PA-O3A
2	H	401	GTP	C5'-O5'-PA-O1A
2	I	402	GTP	PB-O3B-PG-O3G
2	J	401	GTP	C5'-O5'-PA-O3A
2	J	401	GTP	C5'-O5'-PA-O1A
2	J	401	GTP	C5'-O5'-PA-O2A
2	J	402	GTP	C5'-O5'-PA-O3A
2	J	402	GTP	C5'-O5'-PA-O2A
2	J	402	GTP	O4'-C4'-C5'-O5'
2	K	401	GTP	C5'-O5'-PA-O3A
2	K	401	GTP	C5'-O5'-PA-O1A
2	L	301	GTP	C5'-O5'-PA-O3A
2	L	301	GTP	C5'-O5'-PA-O1A
2	L	301	GTP	C5'-O5'-PA-O2A
2	L	303	GTP	PB-O3B-PG-O2G
2	L	304	GTP	PB-O3B-PG-O2G
2	L	304	GTP	PB-O3B-PG-O3G
2	L	304	GTP	O4'-C4'-C5'-O5'
2	M	401	GTP	PB-O3A-PA-O5'
2	M	401	GTP	C5'-O5'-PA-O3A
2	M	401	GTP	C5'-O5'-PA-O1A
2	M	402	GTP	PB-O3B-PG-O2G
2	M	402	GTP	PB-O3B-PG-O3G
2	M	402	GTP	C5'-O5'-PA-O3A
2	M	402	GTP	C5'-O5'-PA-O1A
2	M	402	GTP	C5'-O5'-PA-O2A
2	N	402	GTP	PB-O3B-PG-O3G
2	N	402	GTP	C5'-O5'-PA-O3A
2	N	402	GTP	C5'-O5'-PA-O2A
2	O	401	GTP	C5'-O5'-PA-O3A
2	O	401	GTP	C5'-O5'-PA-O1A
2	O	402	GTP	PB-O3B-PG-O3G
2	P	401	GTP	C5'-O5'-PA-O3A
2	P	401	GTP	C5'-O5'-PA-O1A
2	P	401	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	C	405	GTP	O4'-C4'-C5'-O5'
2	C	405	GTP	C3'-C4'-C5'-O5'
2	F	301	GTP	C3'-C4'-C5'-O5'
2	G	402	GTP	C3'-C4'-C5'-O5'
2	H	402	GTP	O4'-C4'-C5'-O5'
2	H	402	GTP	C3'-C4'-C5'-O5'
2	J	402	GTP	C3'-C4'-C5'-O5'
2	O	406	GTP	O4'-C4'-C5'-O5'
2	E	401	GTP	O4'-C4'-C5'-O5'
2	F	303	GTP	O4'-C4'-C5'-O5'
2	G	402	GTP	O4'-C4'-C5'-O5'
2	I	401	GTP	O4'-C4'-C5'-O5'
2	I	402	GTP	O4'-C4'-C5'-O5'
2	I	402	GTP	C3'-C4'-C5'-O5'
2	J	401	GTP	O4'-C4'-C5'-O5'
2	L	304	GTP	C3'-C4'-C5'-O5'
2	M	402	GTP	O4'-C4'-C5'-O5'
2	M	402	GTP	C3'-C4'-C5'-O5'
2	O	402	GTP	O4'-C4'-C5'-O5'
2	O	402	GTP	C3'-C4'-C5'-O5'
2	O	406	GTP	C3'-C4'-C5'-O5'
2	E	401	GTP	C3'-C4'-C5'-O5'
2	F	303	GTP	C3'-C4'-C5'-O5'
2	I	401	GTP	C3'-C4'-C5'-O5'
2	A	401	GTP	O4'-C4'-C5'-O5'
2	A	401	GTP	C3'-C4'-C5'-O5'
2	A	402	GTP	C3'-C4'-C5'-O5'
2	B	401	GTP	O4'-C4'-C5'-O5'
2	B	401	GTP	C3'-C4'-C5'-O5'
2	D	301	GTP	C3'-C4'-C5'-O5'
2	J	401	GTP	C3'-C4'-C5'-O5'
2	P	401	GTP	O4'-C4'-C5'-O5'
2	B	402	GTP	O4'-C4'-C5'-O5'
2	D	301	GTP	O4'-C4'-C5'-O5'
2	D	302	GTP	C3'-C4'-C5'-O5'
2	P	401	GTP	C3'-C4'-C5'-O5'
2	A	402	GTP	O4'-C4'-C5'-O5'
2	C	401	GTP	O4'-C4'-C5'-O5'
2	D	302	GTP	O4'-C4'-C5'-O5'
2	B	402	GTP	C3'-C4'-C5'-O5'
2	C	401	GTP	C3'-C4'-C5'-O5'
2	A	402	GTP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	B	402	GTP	PG-O3B-PB-O1B
2	E	401	GTP	PA-O3A-PB-O1B
2	L	304	GTP	PA-O3A-PB-O1B
2	O	402	GTP	PA-O3A-PB-O1B
2	E	401	GTP	C4'-C5'-O5'-PA
2	I	401	GTP	C4'-C5'-O5'-PA
2	H	401	GTP	PB-O3A-PA-O5'
2	J	401	GTP	PB-O3B-PG-O1G
2	A	401	GTP	PA-O3A-PB-O2B
2	B	401	GTP	PA-O3A-PB-O2B
2	B	401	GTP	PB-O3A-PA-O1A
2	B	402	GTP	PB-O3A-PA-O1A
2	E	401	GTP	PG-O3B-PB-O1B
2	E	404	GTP	PA-O3A-PB-O2B
2	I	401	GTP	PG-O3B-PB-O2B
2	I	402	GTP	PA-O3A-PB-O2B
2	L	303	GTP	PA-O3A-PB-O2B
2	L	304	GTP	PB-O3A-PA-O1A
2	A	401	GTP	C5'-O5'-PA-O2A
2	B	401	GTP	C5'-O5'-PA-O2A
2	C	401	GTP	C5'-O5'-PA-O2A
2	D	302	GTP	C5'-O5'-PA-O2A
2	E	401	GTP	C5'-O5'-PA-O2A
2	G	401	GTP	C5'-O5'-PA-O3A
2	G	401	GTP	C5'-O5'-PA-O2A
2	H	401	GTP	C5'-O5'-PA-O2A
2	I	402	GTP	C5'-O5'-PA-O3A
2	I	402	GTP	C5'-O5'-PA-O1A
2	I	402	GTP	C5'-O5'-PA-O2A
2	J	402	GTP	C5'-O5'-PA-O1A
2	K	401	GTP	C5'-O5'-PA-O2A
2	M	401	GTP	C5'-O5'-PA-O2A
2	N	402	GTP	C5'-O5'-PA-O1A
2	O	401	GTP	C5'-O5'-PA-O2A
2	K	401	GTP	O4'-C4'-C5'-O5'
2	D	301	GTP	PA-O3A-PB-O2B
2	F	301	GTP	PG-O3B-PB-O2B
2	G	402	GTP	PG-O3B-PB-O2B
2	H	402	GTP	PG-O3B-PB-O2B
2	L	301	GTP	PA-O3A-PB-O2B
2	L	304	GTP	PG-O3B-PB-O1B
2	M	402	GTP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	N	401	GTP	PA-O3A-PB-O2B
2	N	402	GTP	PA-O3A-PB-O2B
2	O	402	GTP	PA-O3A-PB-O2B
2	O	406	GTP	PG-O3B-PB-O2B
2	B	401	GTP	C4'-C5'-O5'-PA
2	E	404	GTP	O4'-C4'-C5'-O5'
2	L	303	GTP	O4'-C4'-C5'-O5'
2	A	401	GTP	C4'-C5'-O5'-PA
2	O	406	GTP	C4'-C5'-O5'-PA
2	B	402	GTP	PA-O3A-PB-O1B
2	E	401	GTP	PA-O3A-PB-O2B
2	L	301	GTP	PG-O3B-PB-O1B
2	M	402	GTP	PG-O3B-PB-O1B
2	K	401	GTP	C3'-C4'-C5'-O5'
2	D	301	GTP	PB-O3B-PG-O1G
2	I	402	GTP	PB-O3B-PG-O1G
2	L	304	GTP	PB-O3B-PG-O1G
2	M	402	GTP	PB-O3B-PG-O1G
2	A	401	GTP	PB-O3B-PG-O2G
2	D	301	GTP	PB-O3B-PG-O2G
2	E	401	GTP	PB-O3B-PG-O3G
2	E	404	GTP	PB-O3B-PG-O2G
2	I	402	GTP	PB-O3B-PG-O2G
2	J	401	GTP	PB-O3B-PG-O2G
2	J	401	GTP	PB-O3B-PG-O3G
2	O	402	GTP	PB-O3B-PG-O2G
2	A	402	GTP	PA-O3A-PB-O2B
2	B	401	GTP	PA-O3A-PB-O1B
2	B	402	GTP	PG-O3B-PB-O2B
2	C	401	GTP	PA-O3A-PB-O2B
2	C	405	GTP	PG-O3B-PB-O1B
2	C	405	GTP	PG-O3B-PB-O2B
2	D	302	GTP	PA-O3A-PB-O1B
2	D	302	GTP	PA-O3A-PB-O2B
2	E	404	GTP	PA-O3A-PB-O1B
2	G	401	GTP	PA-O3A-PB-O1B
2	G	401	GTP	PA-O3A-PB-O2B
2	G	402	GTP	PG-O3B-PB-O1B
2	I	402	GTP	PA-O3A-PB-O1B
2	J	402	GTP	PG-O3B-PB-O1B
2	J	402	GTP	PG-O3B-PB-O2B
2	L	301	GTP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	L	304	GTP	PA-O3A-PB-O2B
2	O	401	GTP	PA-O3A-PB-O1B
2	O	401	GTP	PA-O3A-PB-O2B
2	O	402	GTP	PB-O3A-PA-O2A
2	O	406	GTP	PG-O3B-PB-O1B
2	A	402	GTP	PB-O3B-PG-O1G
2	N	402	GTP	PB-O3B-PG-O1G
2	H	401	GTP	O4'-C4'-C5'-O5'
2	O	401	GTP	O4'-C4'-C5'-O5'
2	A	401	GTP	PB-O3A-PA-O2A
2	A	402	GTP	PB-O3A-PA-O2A
2	B	401	GTP	PB-O3A-PA-O2A
2	B	402	GTP	PB-O3A-PA-O2A
2	C	401	GTP	PA-O3A-PB-O1B
2	E	404	GTP	PB-O3A-PA-O2A
2	F	301	GTP	PG-O3B-PB-O1B
2	I	402	GTP	PB-O3A-PA-O2A
2	L	301	GTP	PA-O3A-PB-O1B
2	L	304	GTP	PB-O3A-PA-O2A
2	N	401	GTP	PA-O3A-PB-O1B

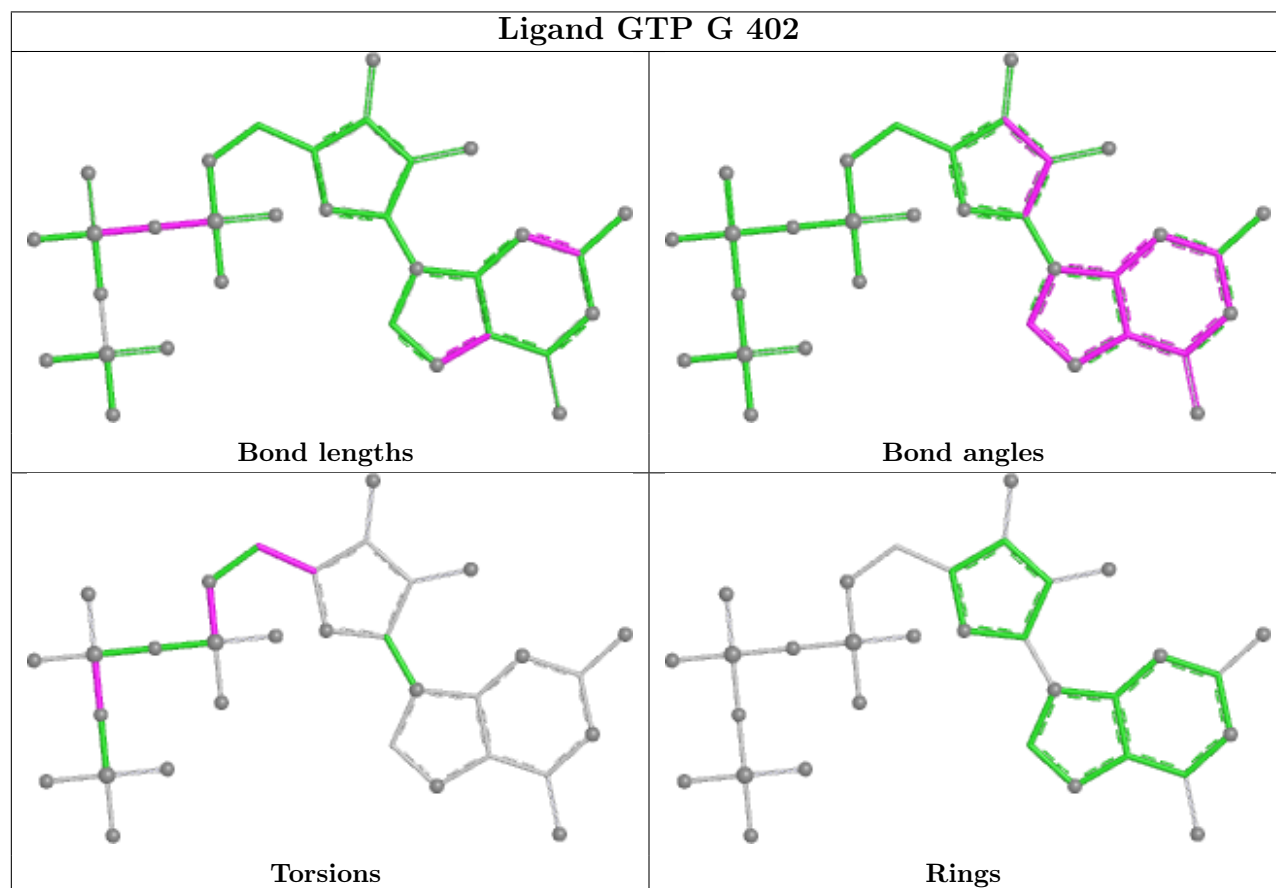
There are no ring outliers.

8 monomers are involved in 12 short contacts:

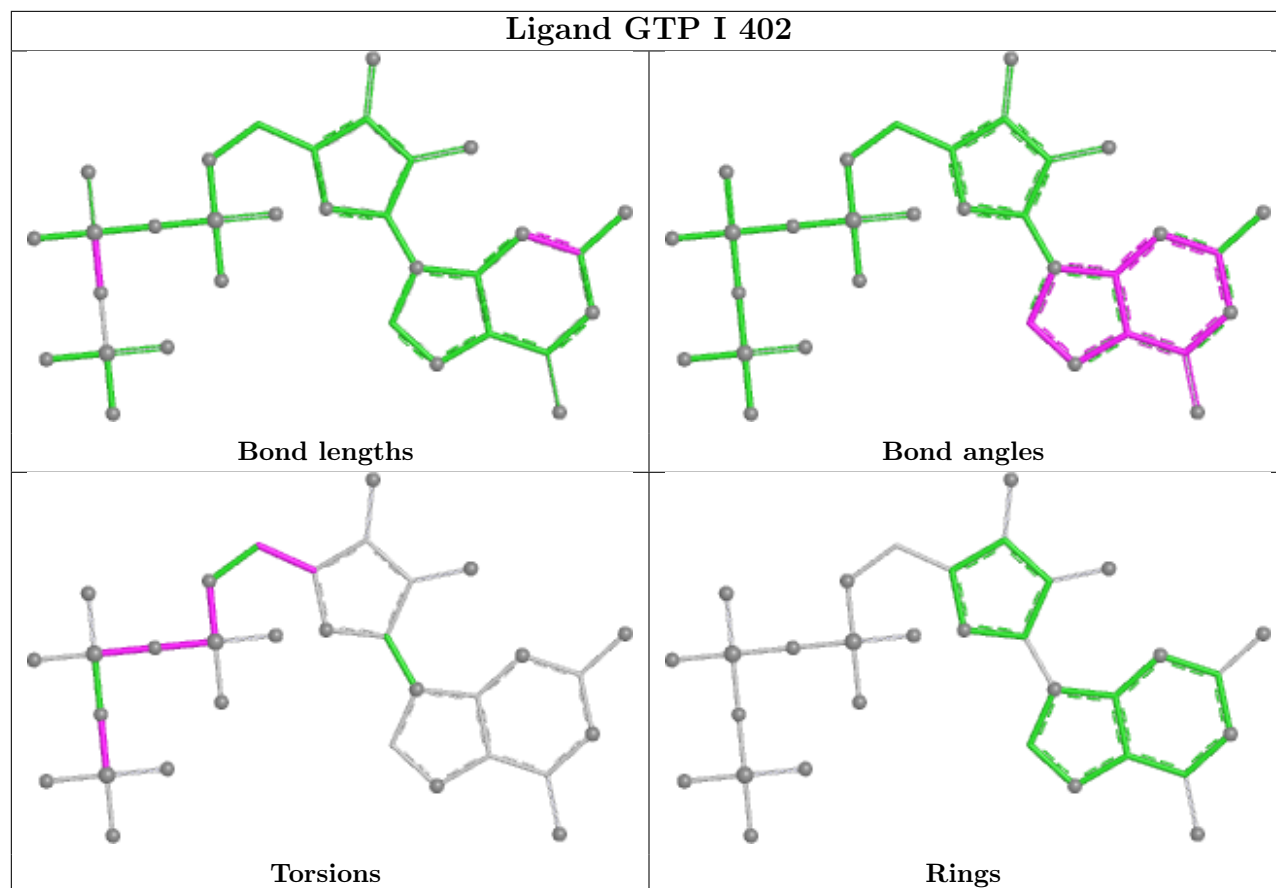
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	402	GTP	1	0
2	L	301	GTP	2	0
2	E	404	GTP	1	0
2	H	402	GTP	1	0
2	F	303	GTP	1	0
2	J	401	GTP	2	0
2	F	301	GTP	3	0
2	O	402	GTP	1	0

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

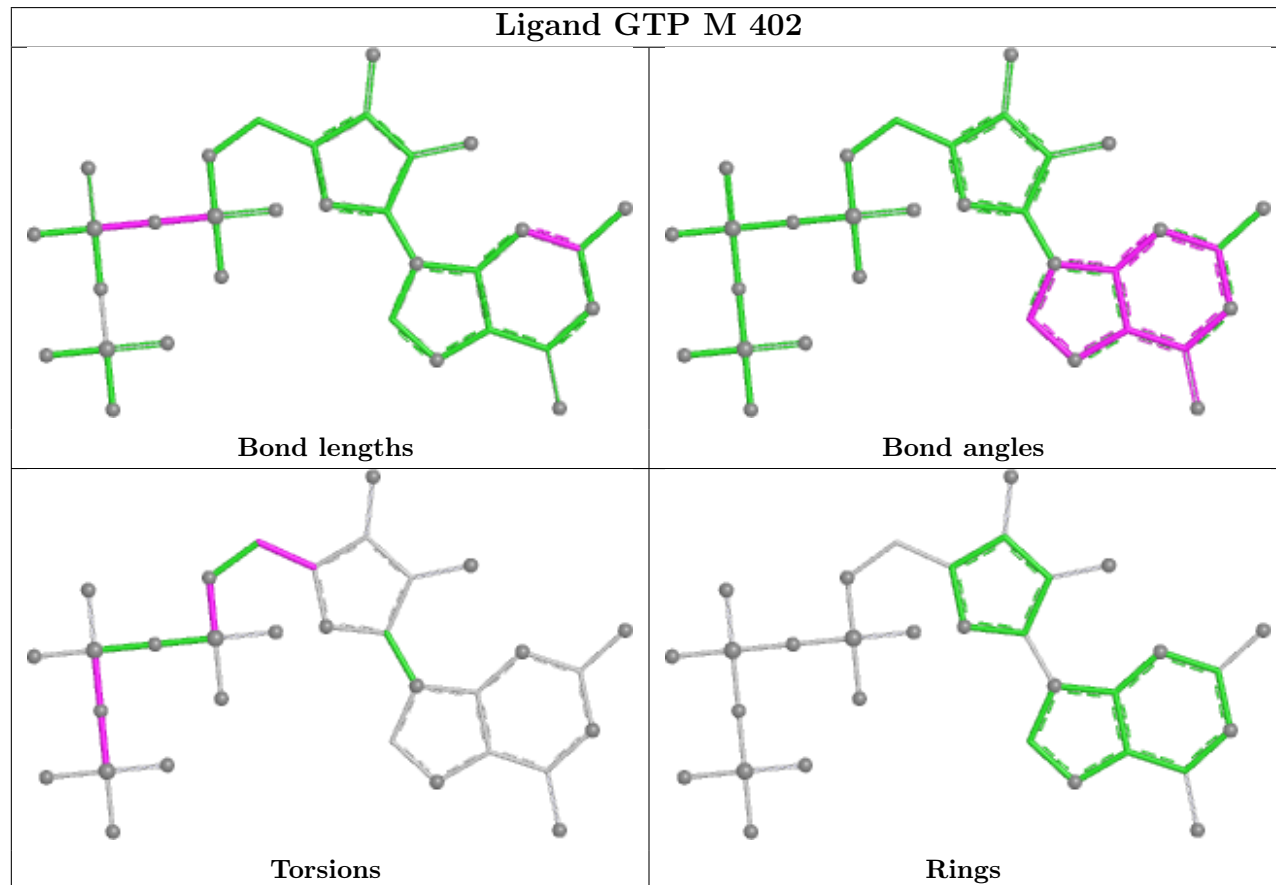
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



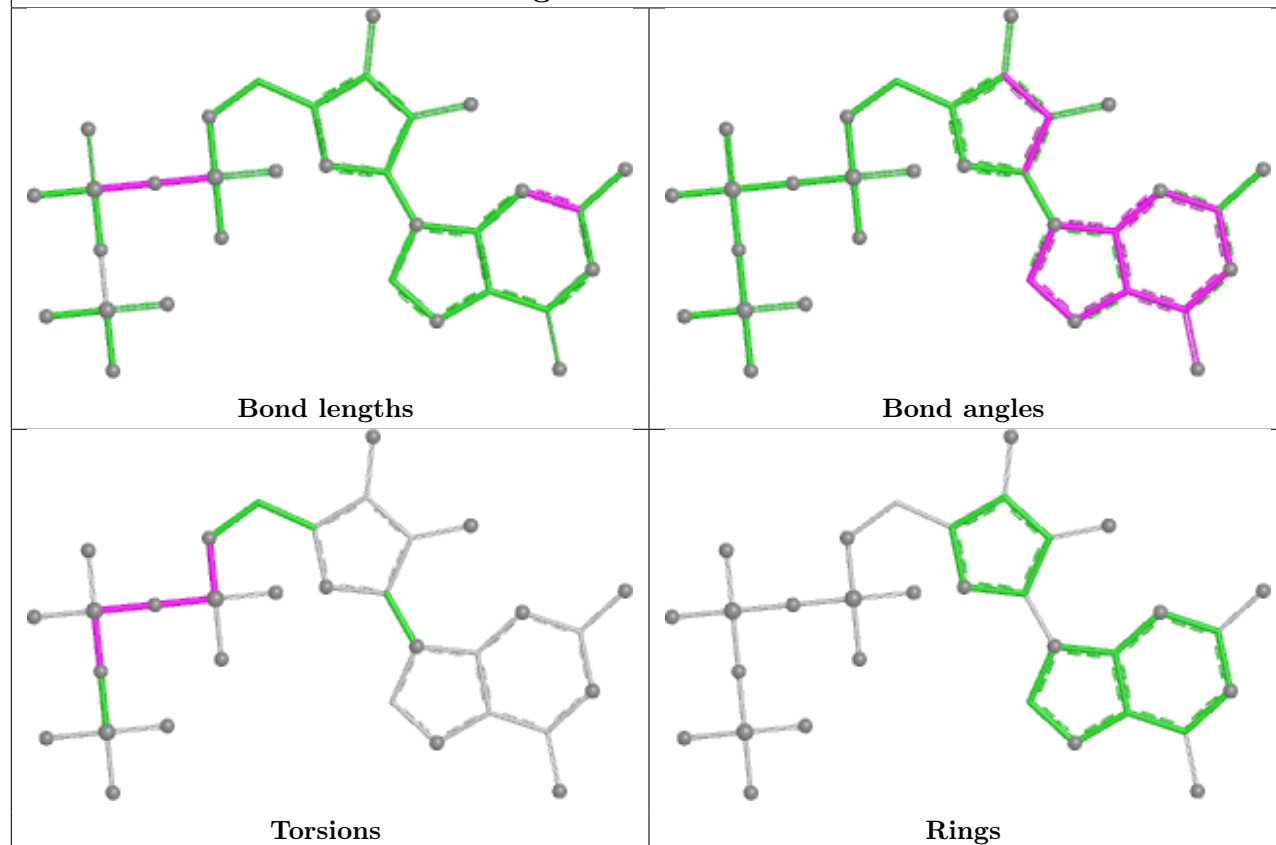
Ligand GTP I 402



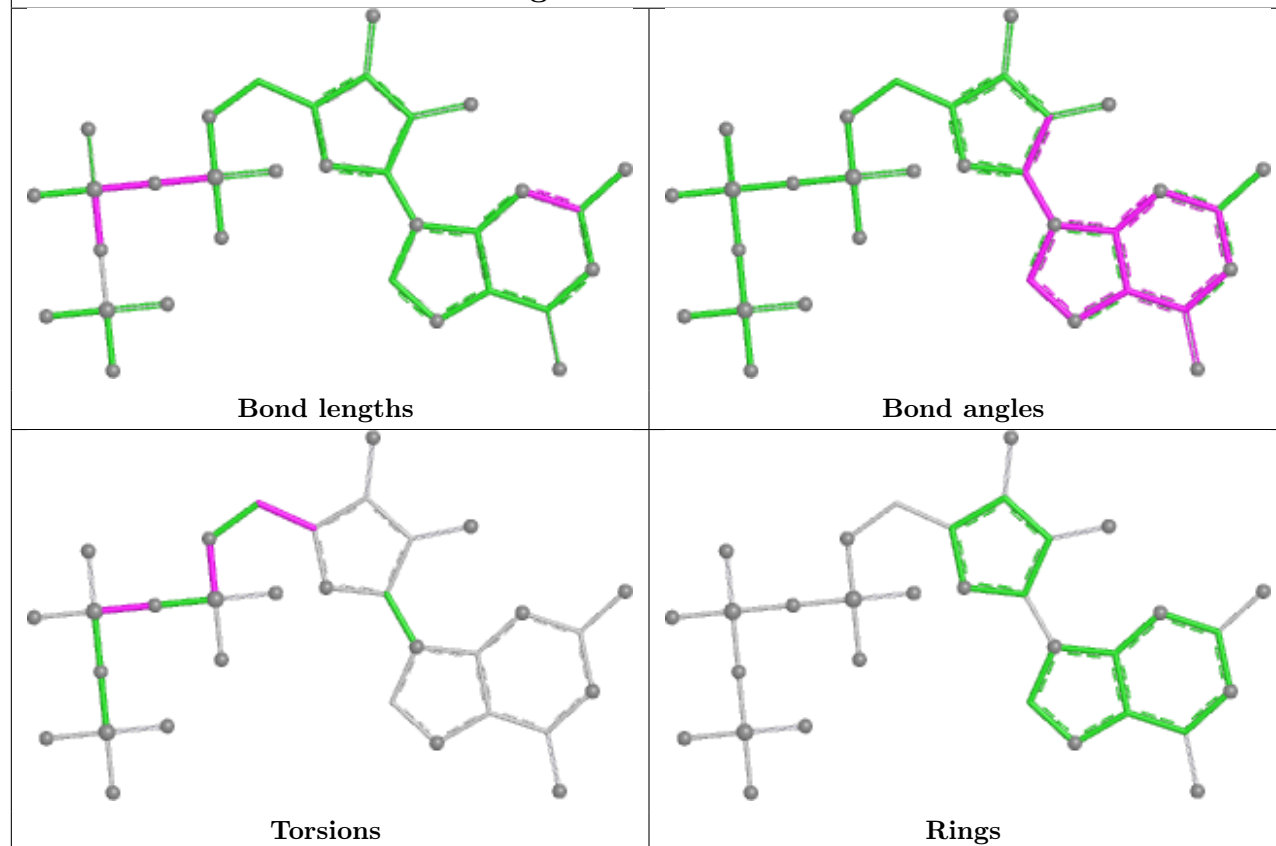
Ligand GTP M 402



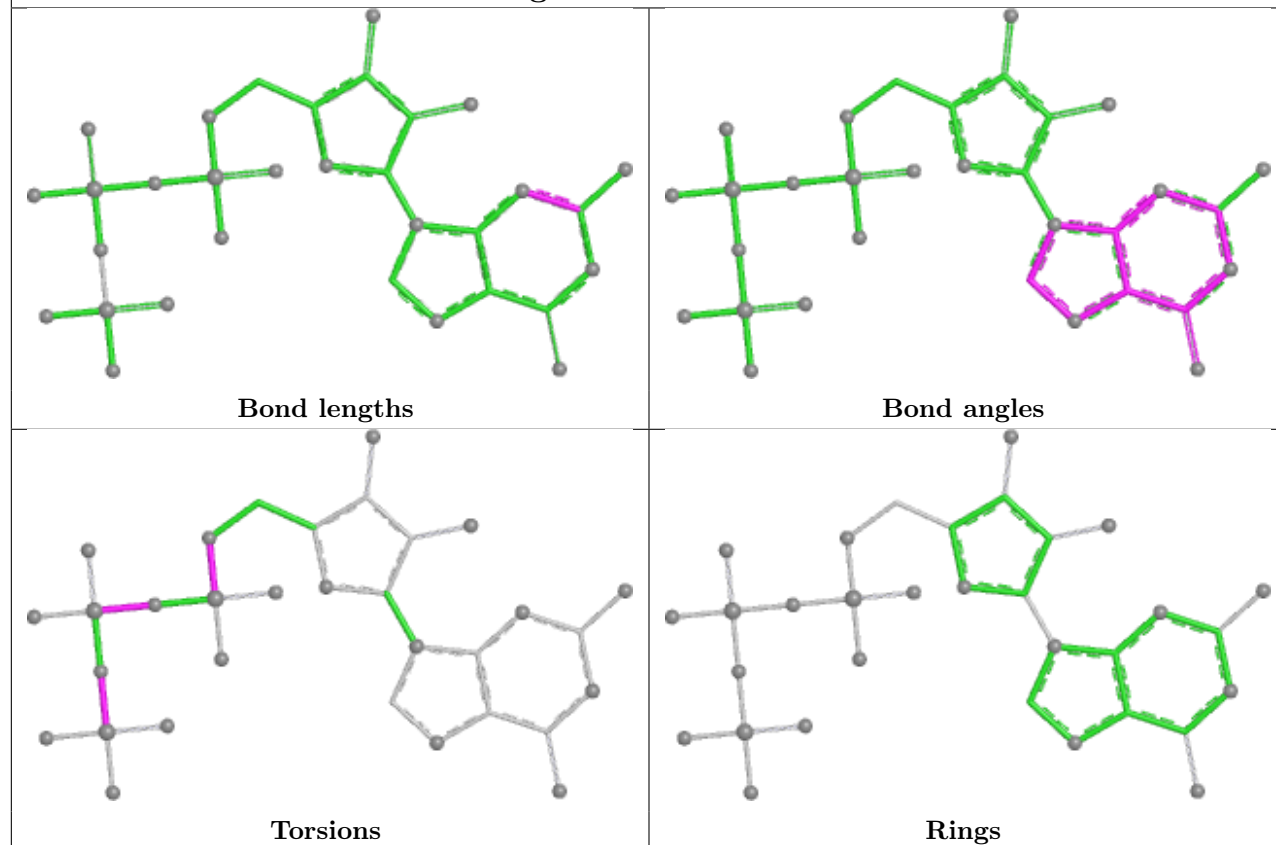
Ligand GTP L 301



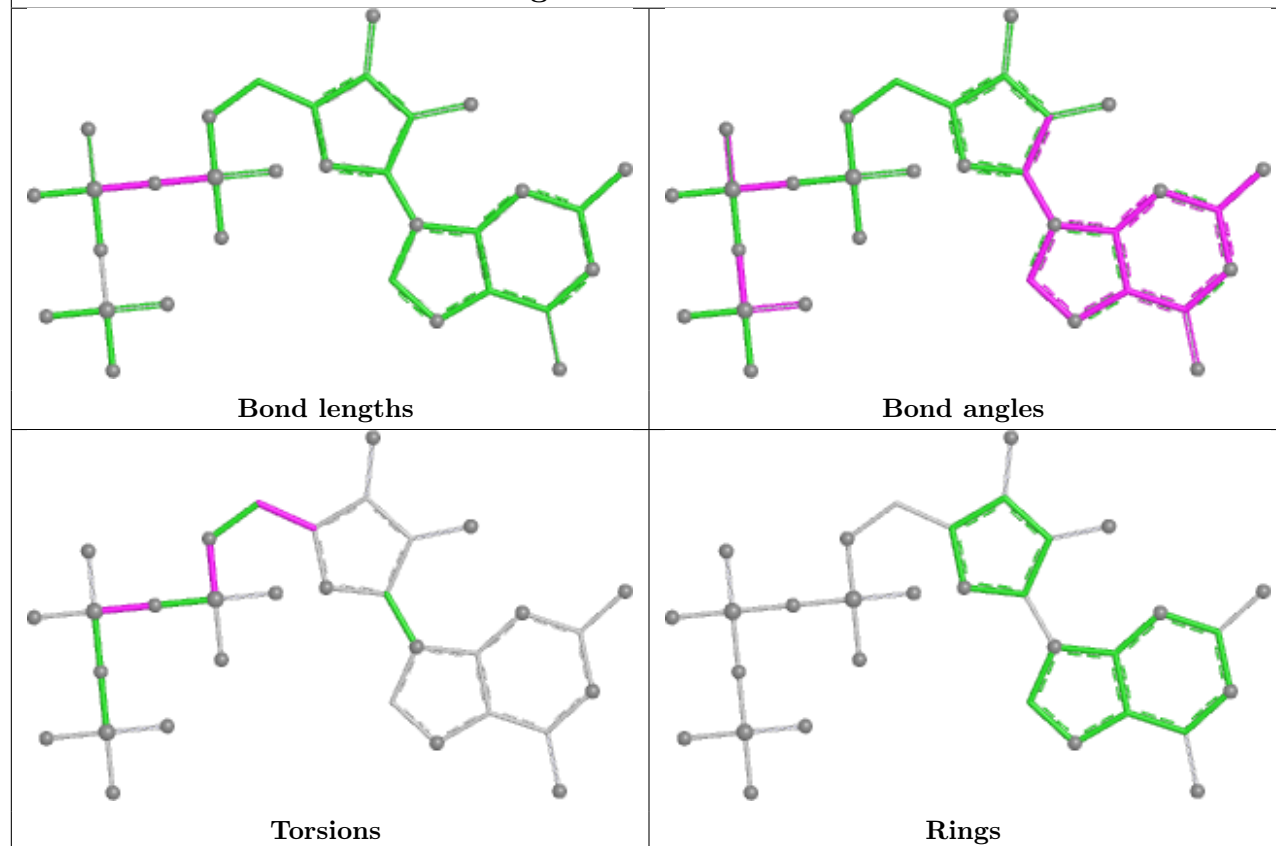
Ligand GTP D 302

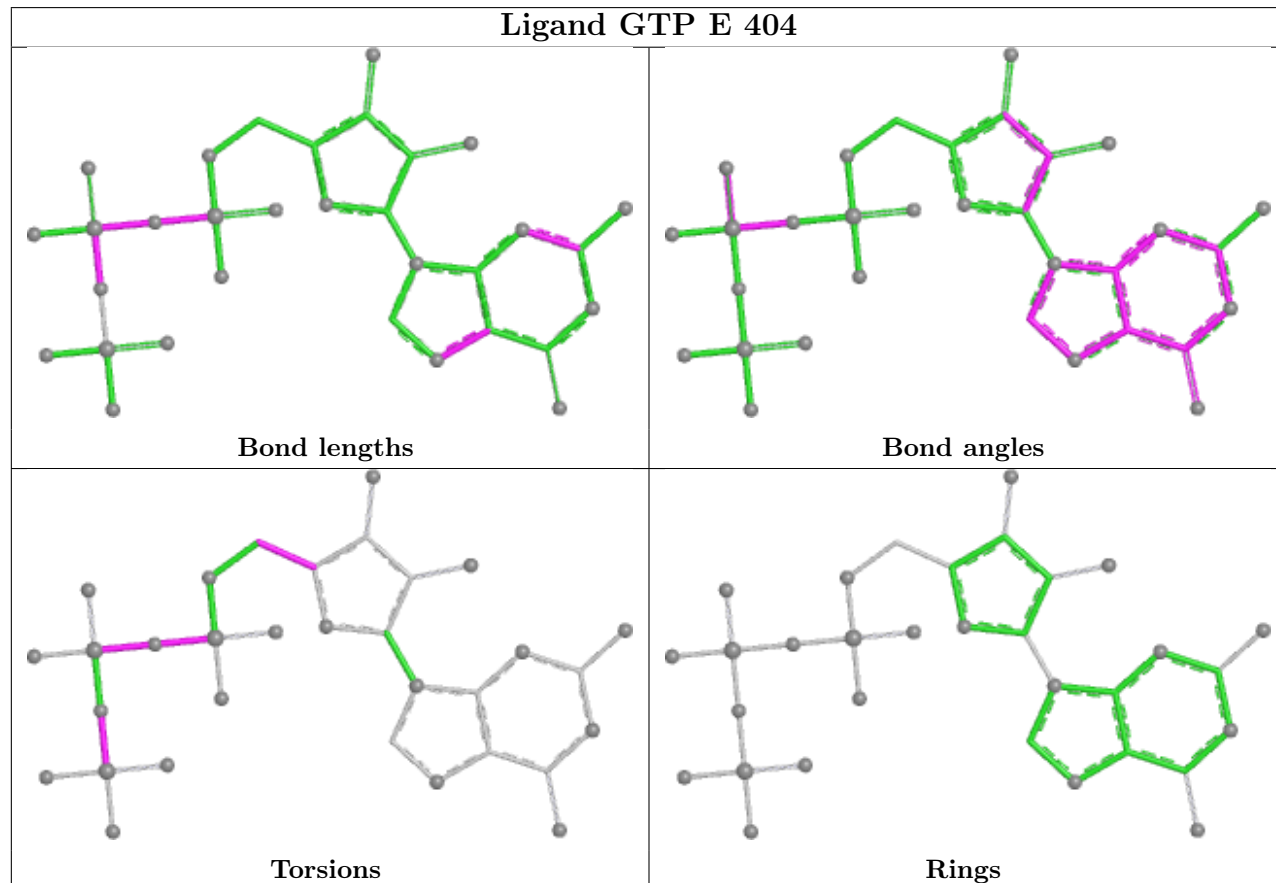
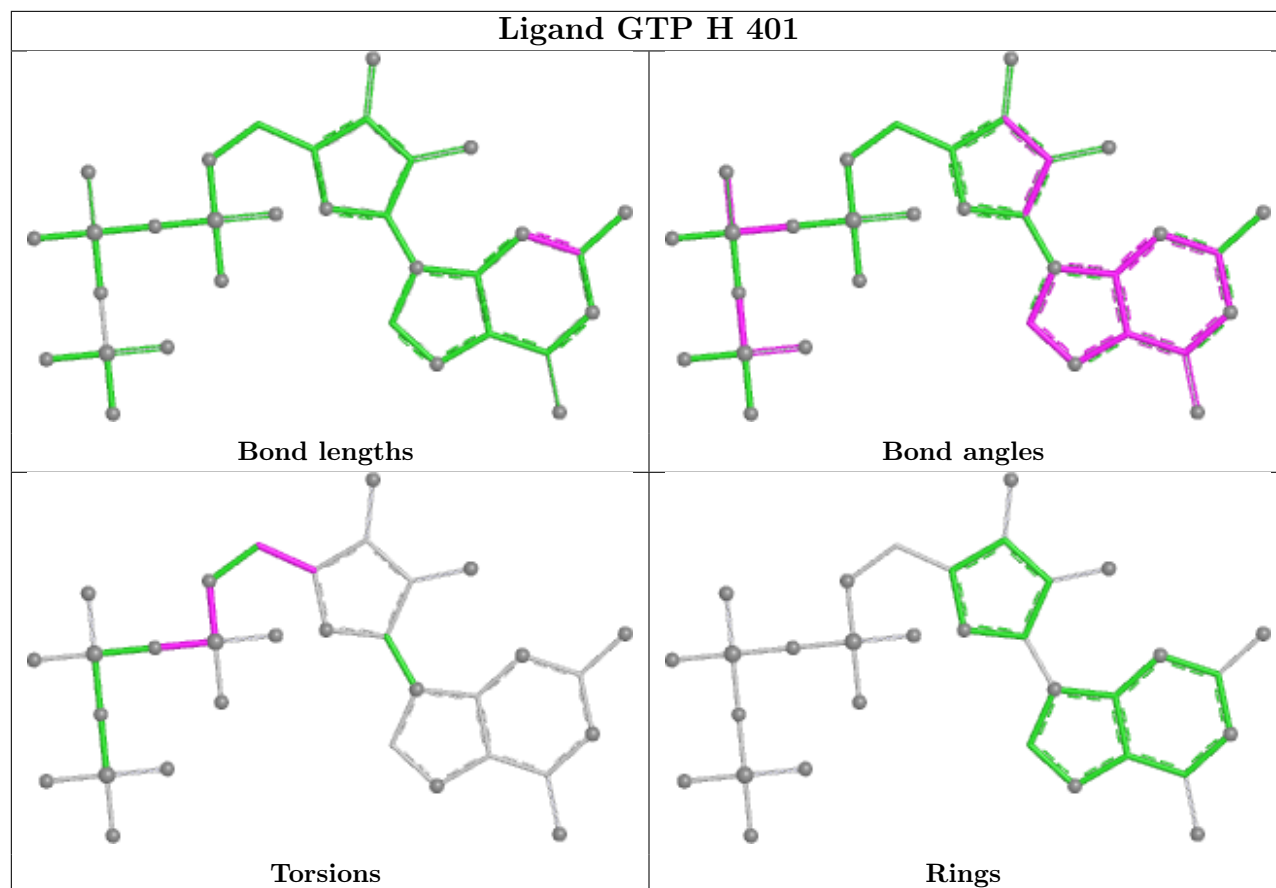


Ligand GTP N 402

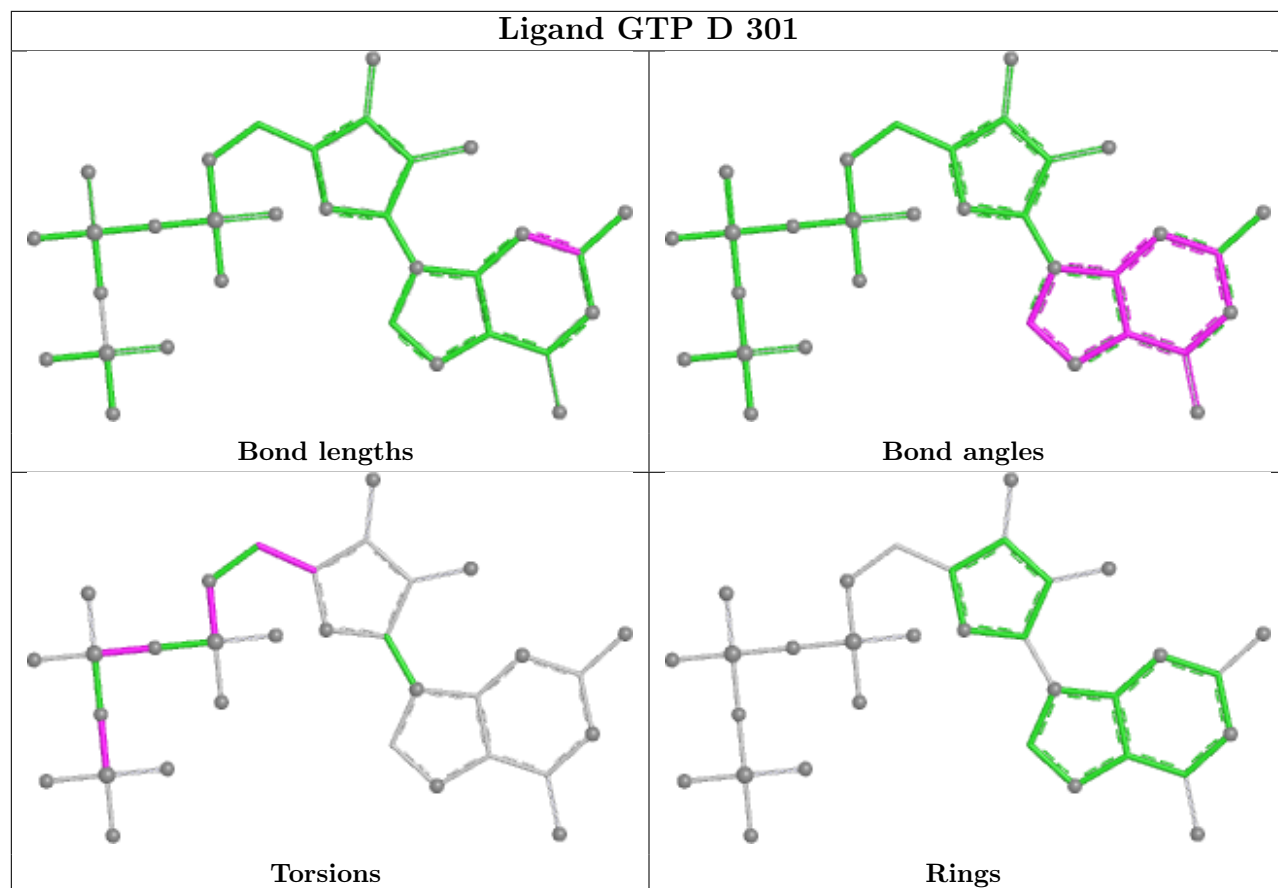


Ligand GTP O 401

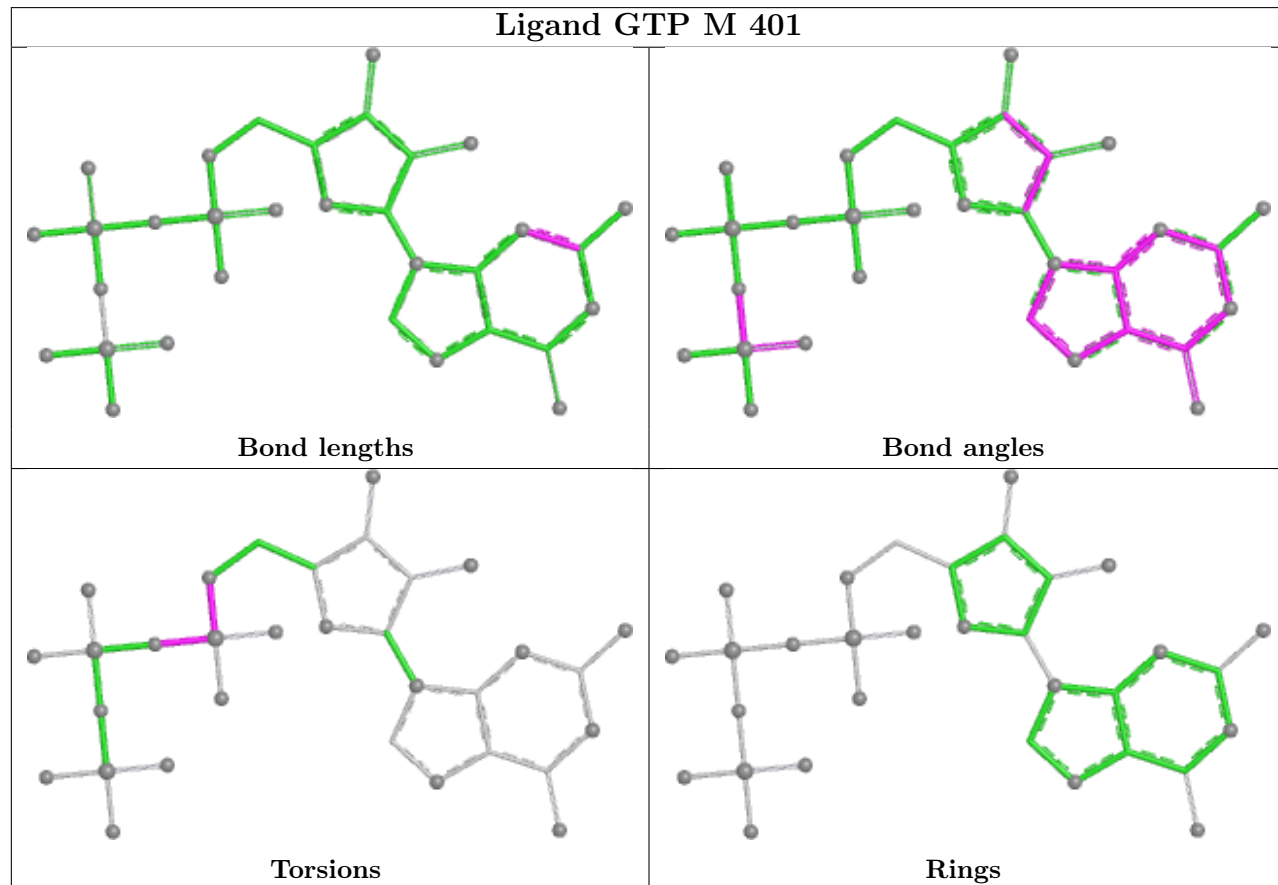




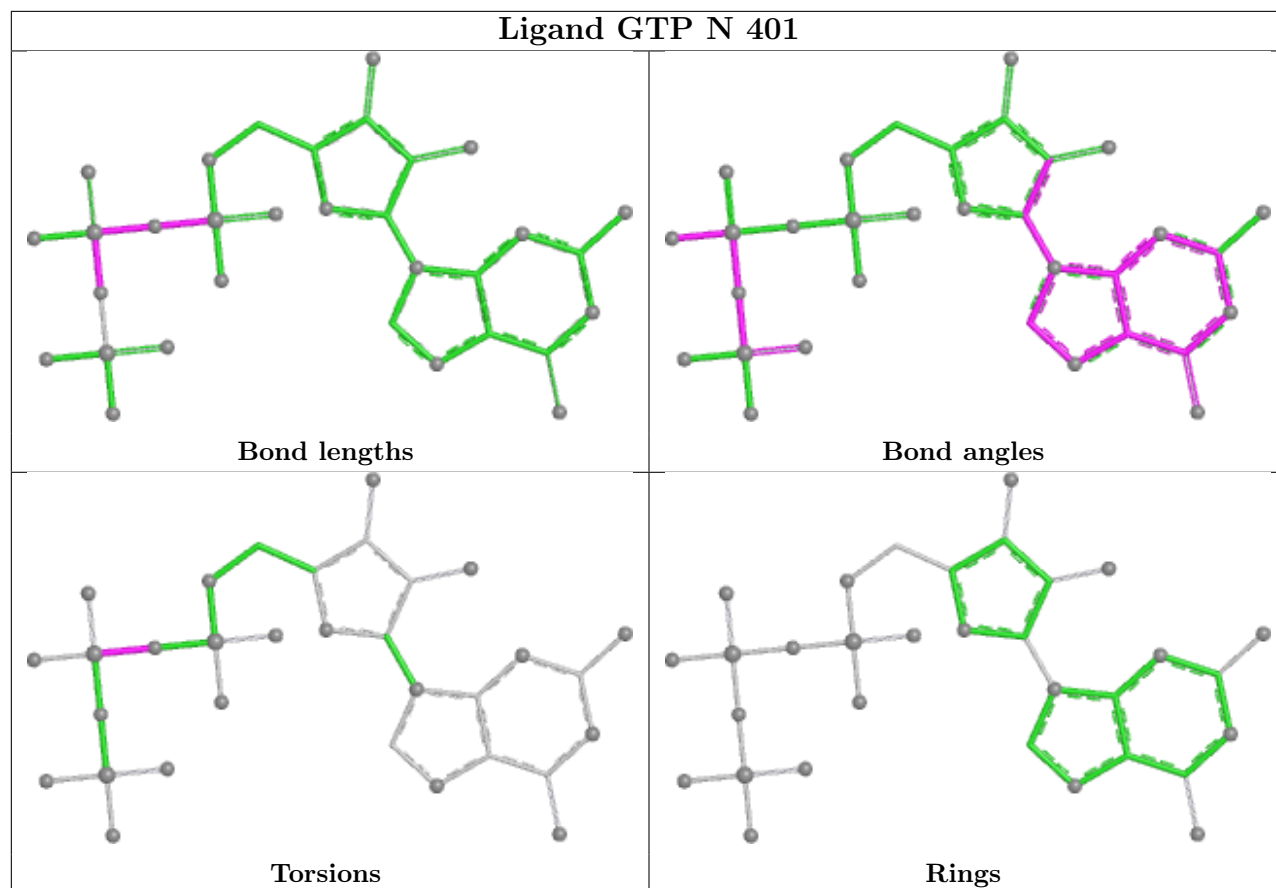
Ligand GTP D 301



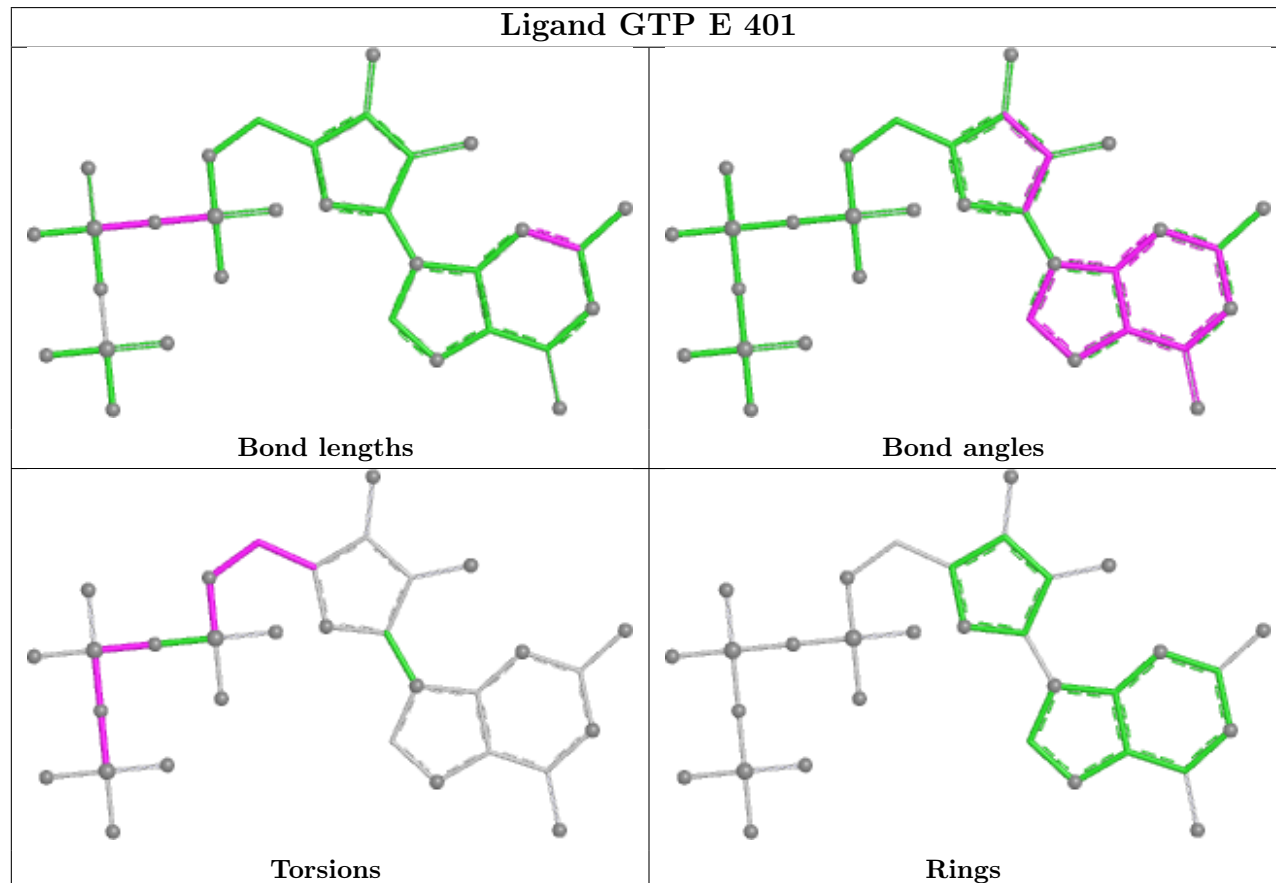
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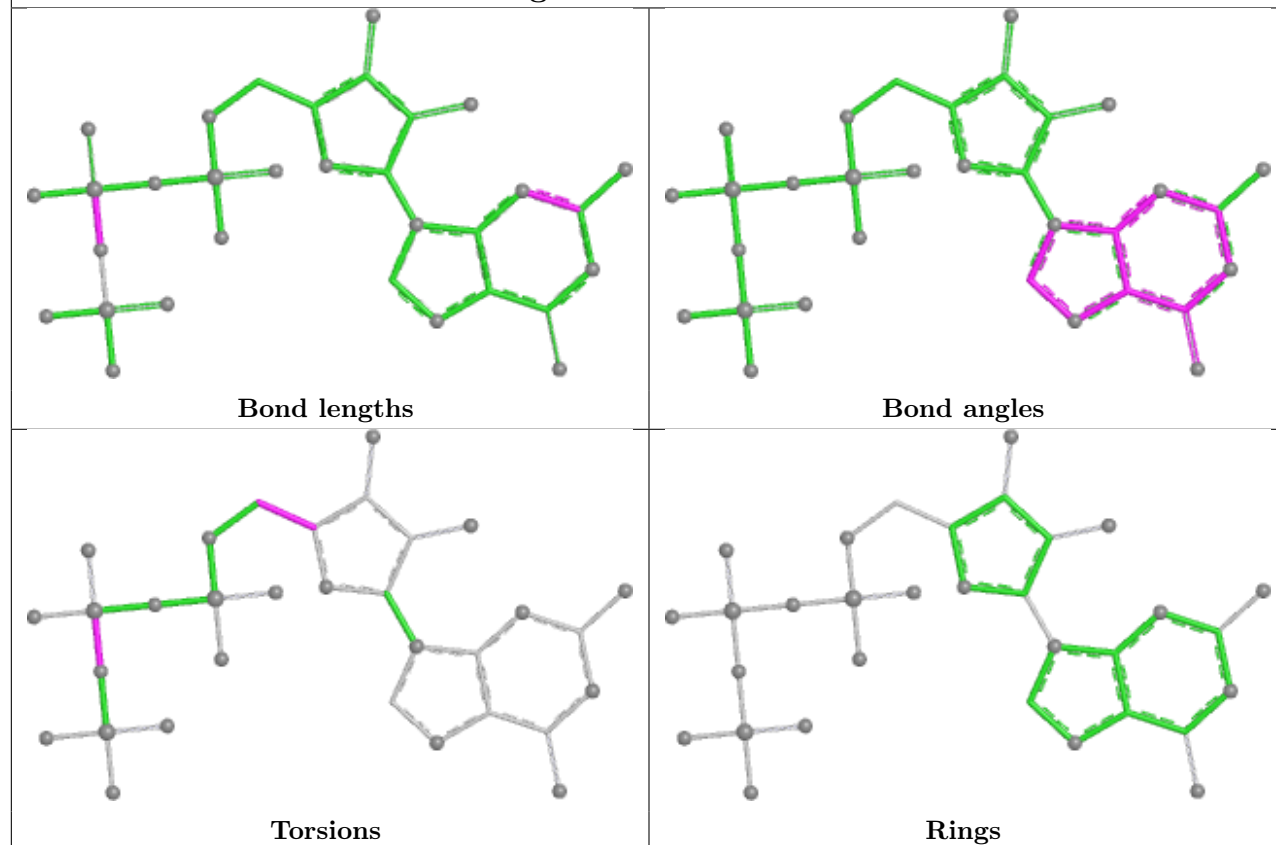
Ligand GTP N 401



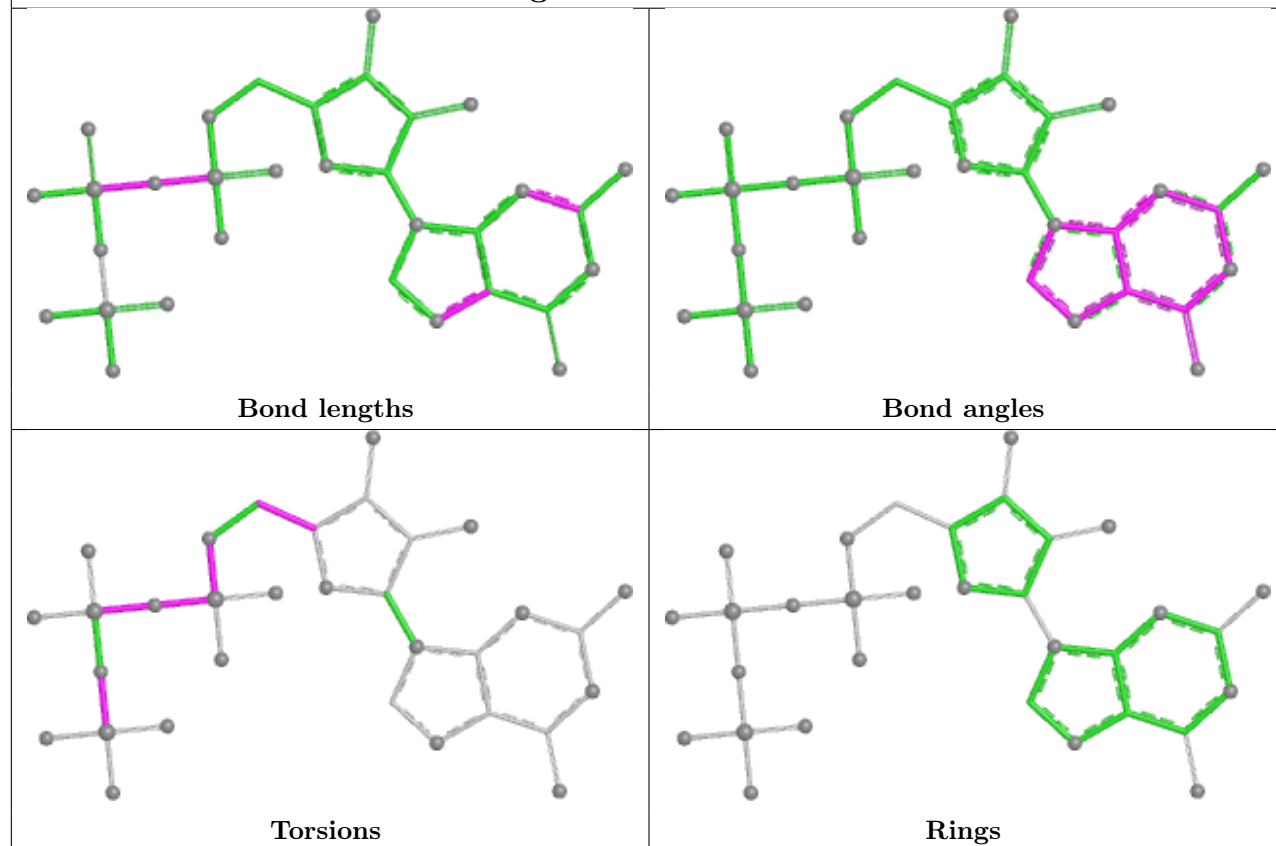
Ligand GTP E 401



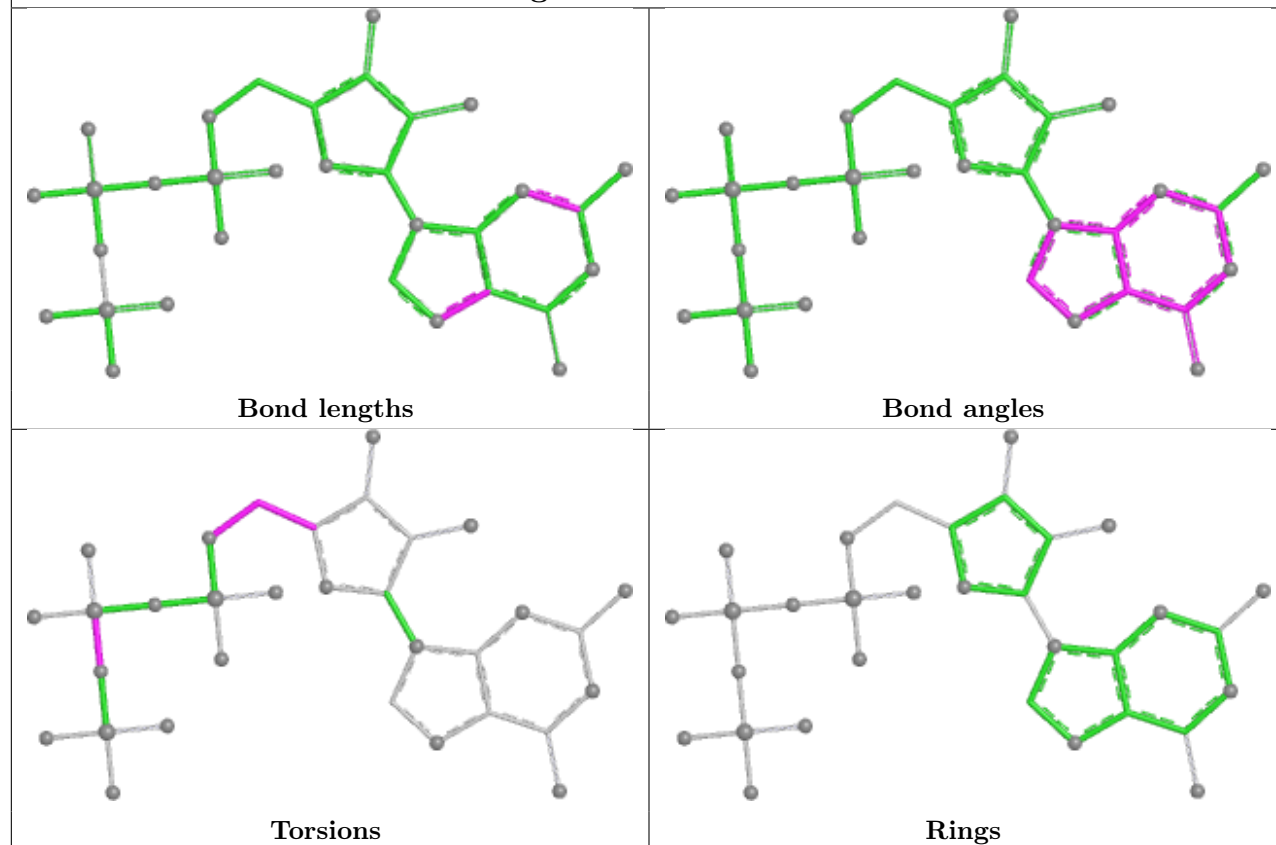
Ligand GTP H 402



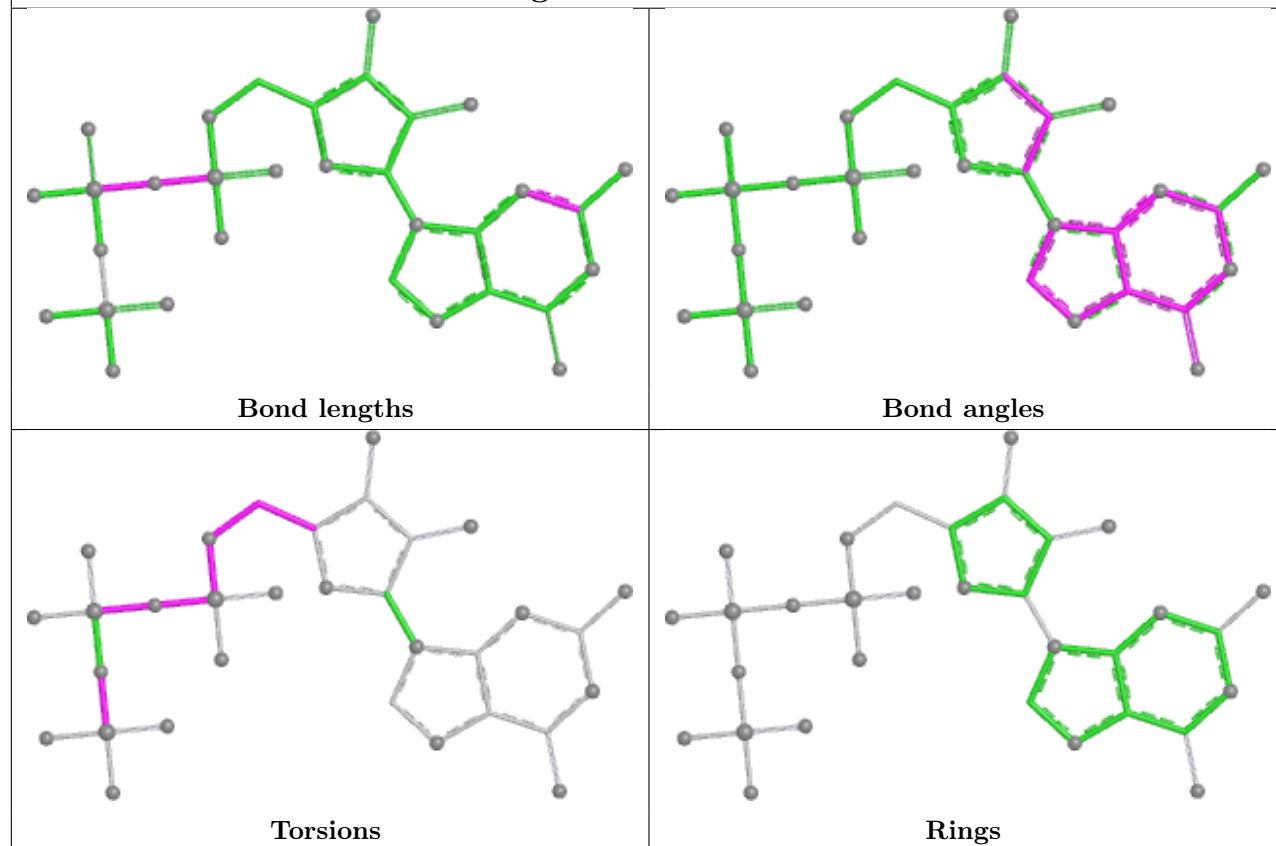
Ligand GTP A 402



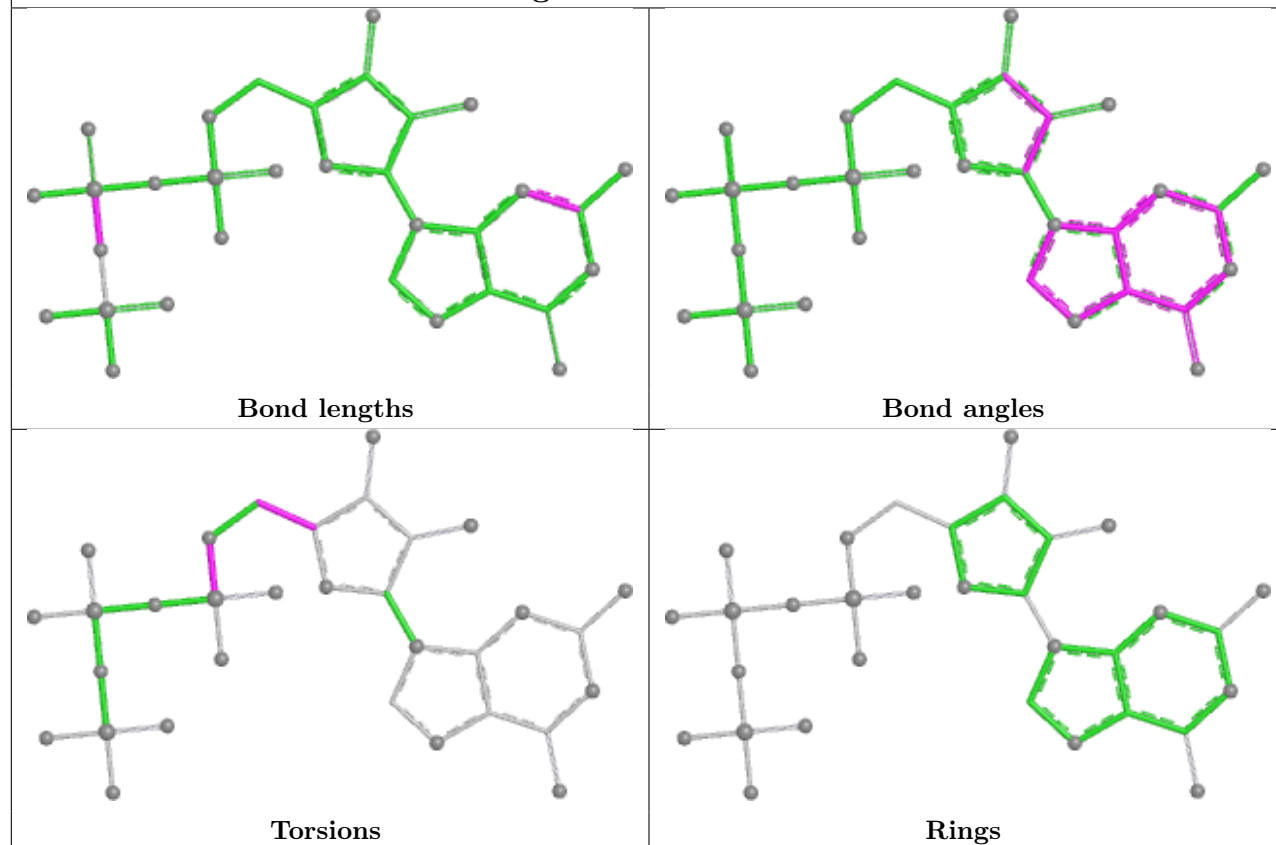
Ligand GTP O 406



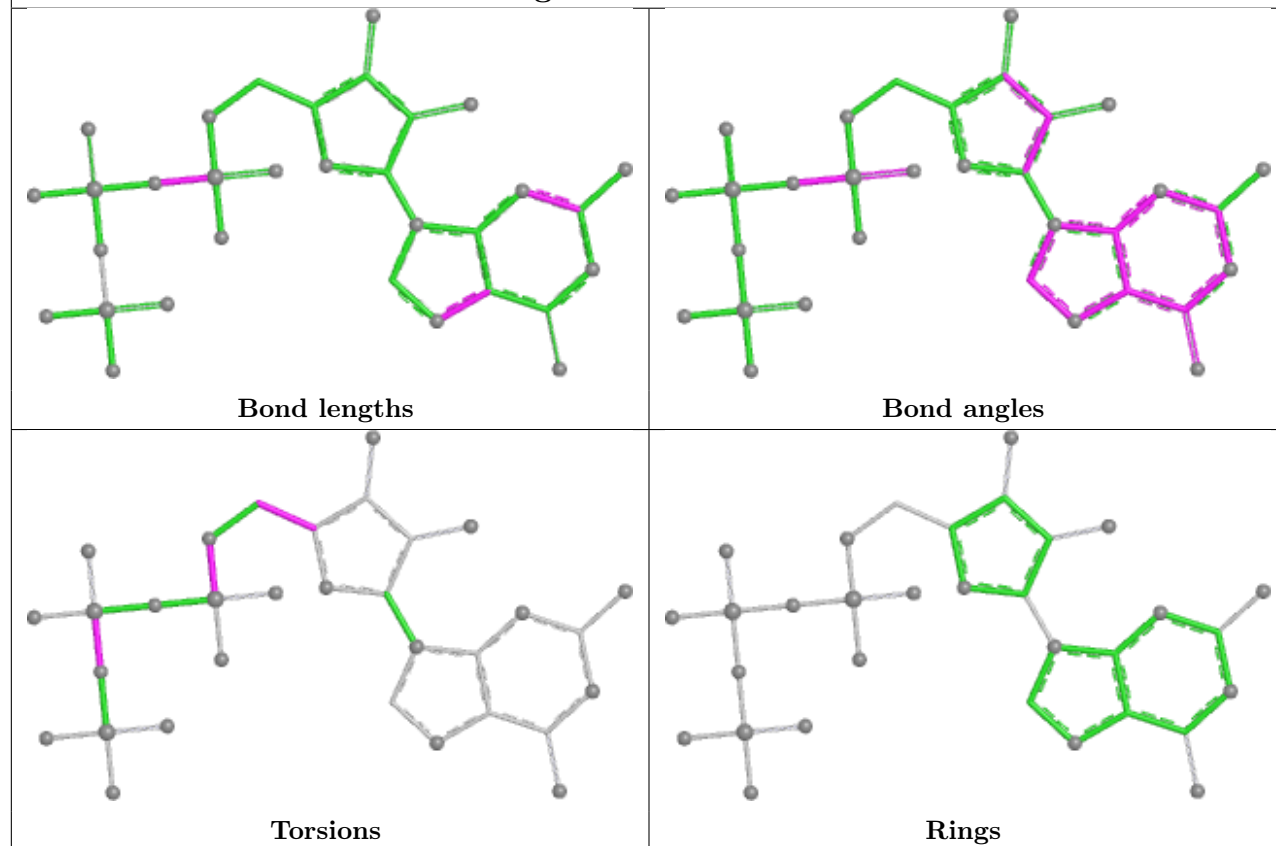
Ligand GTP B 401



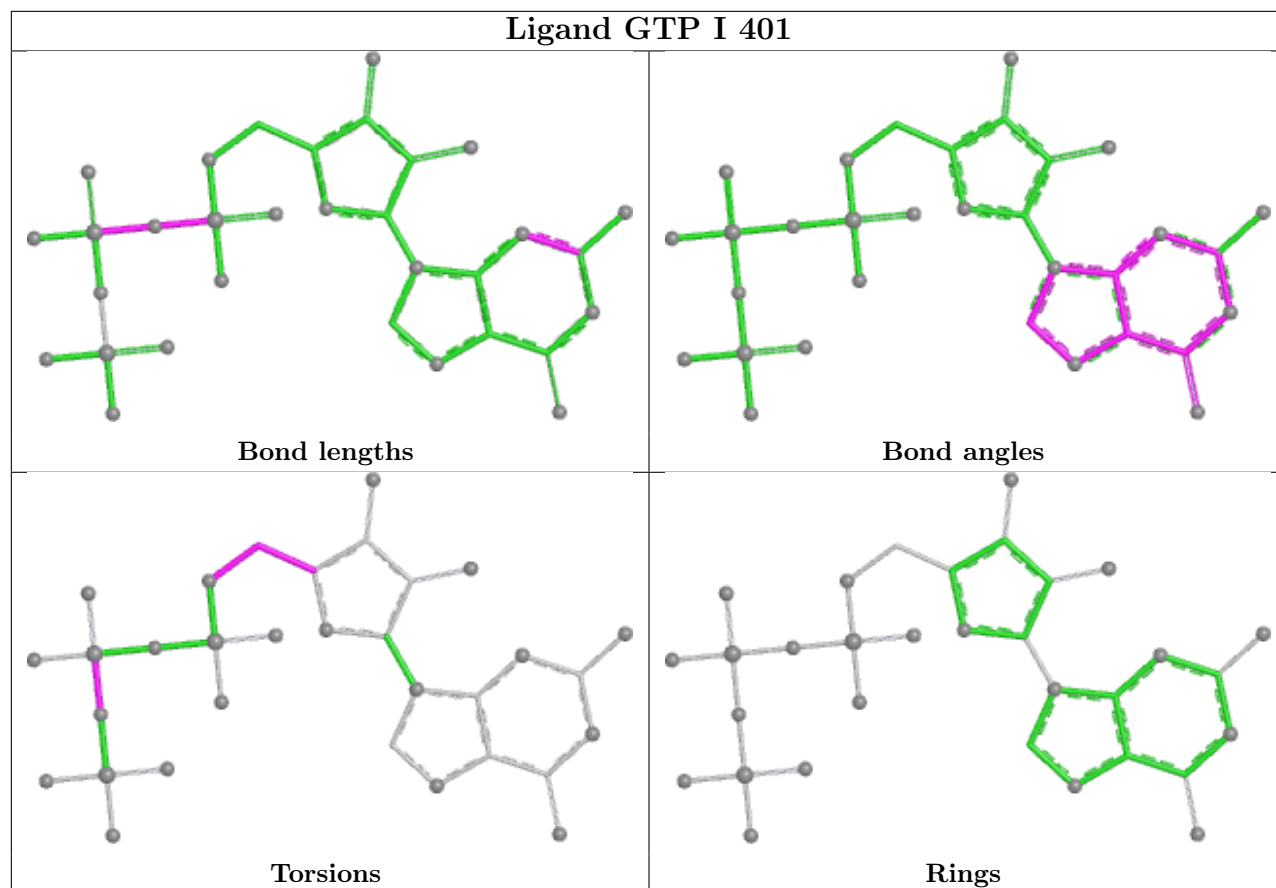
Ligand GTP F 303



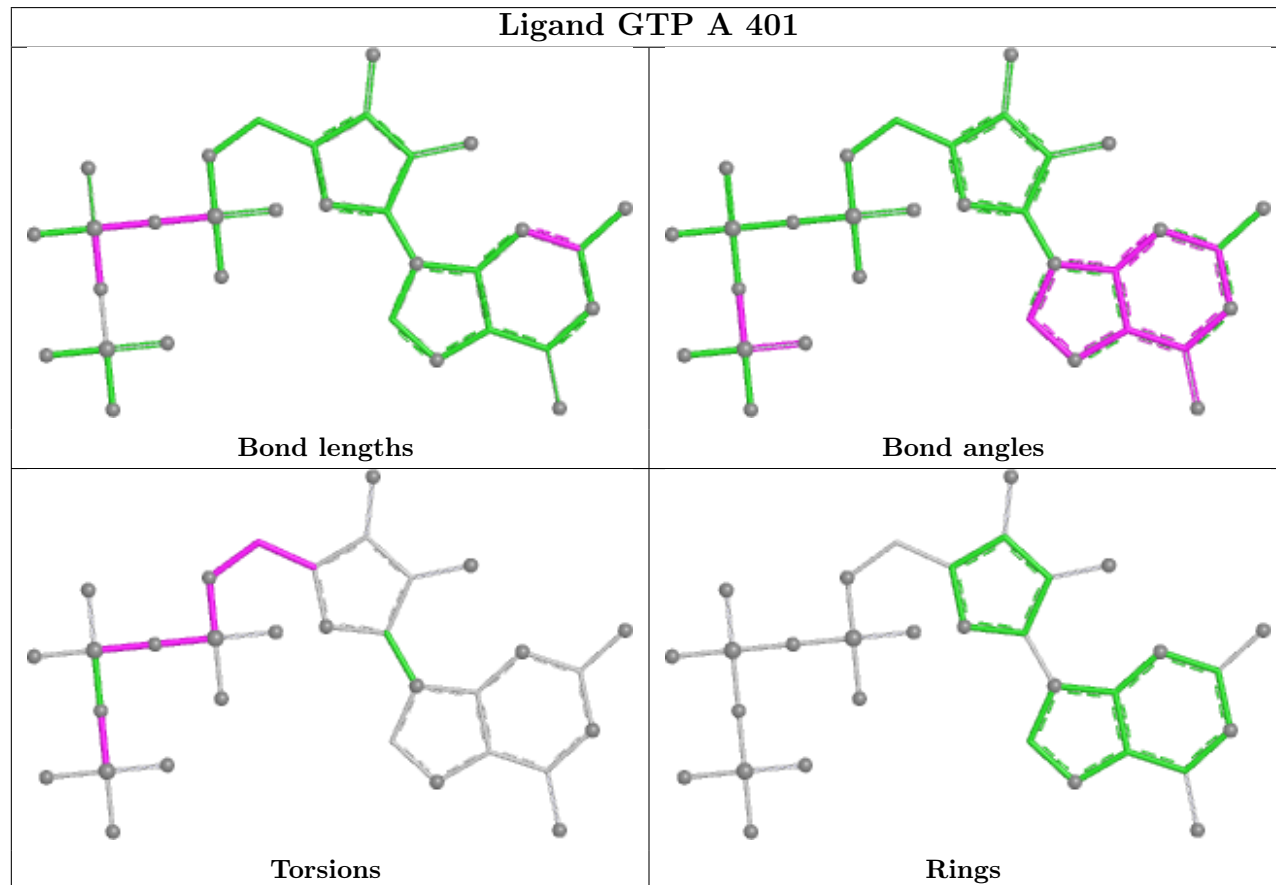
Ligand GTP J 402



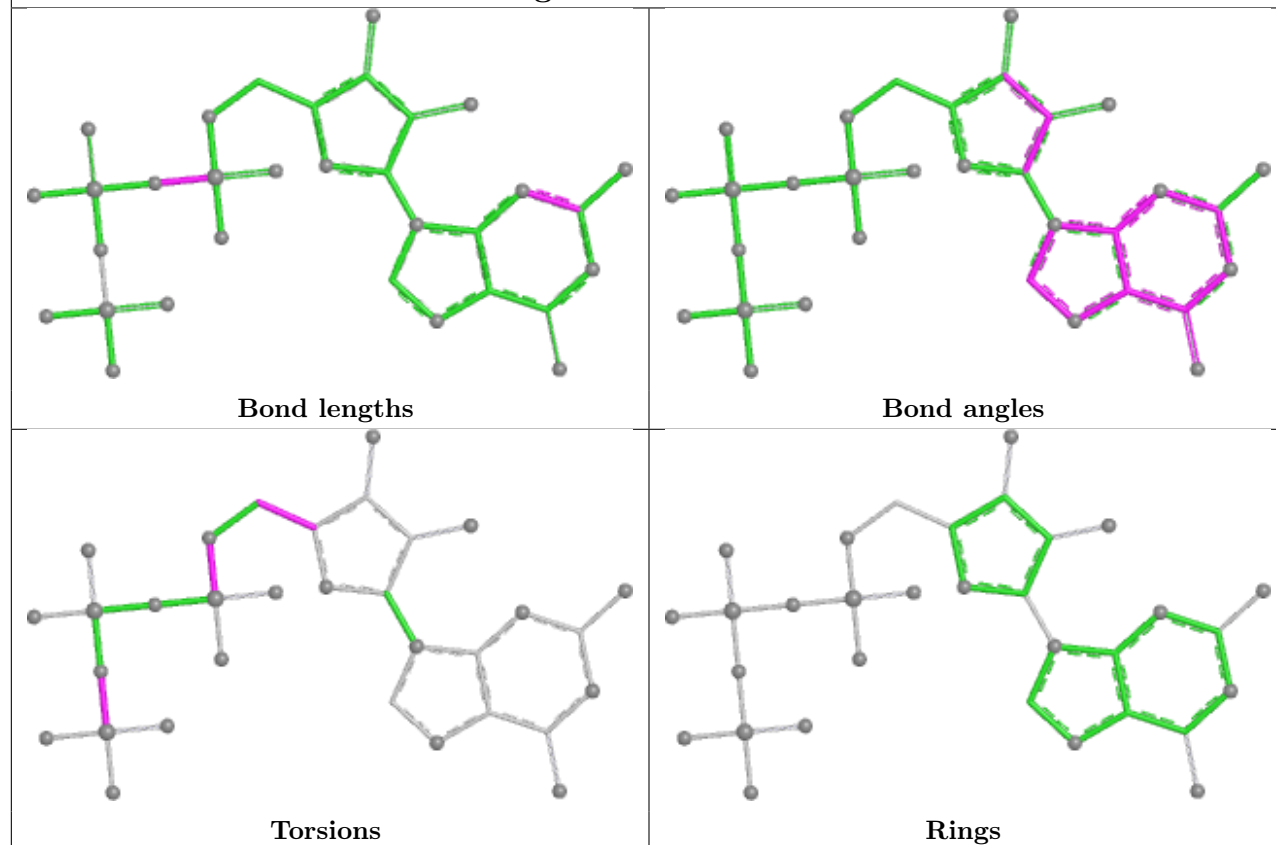
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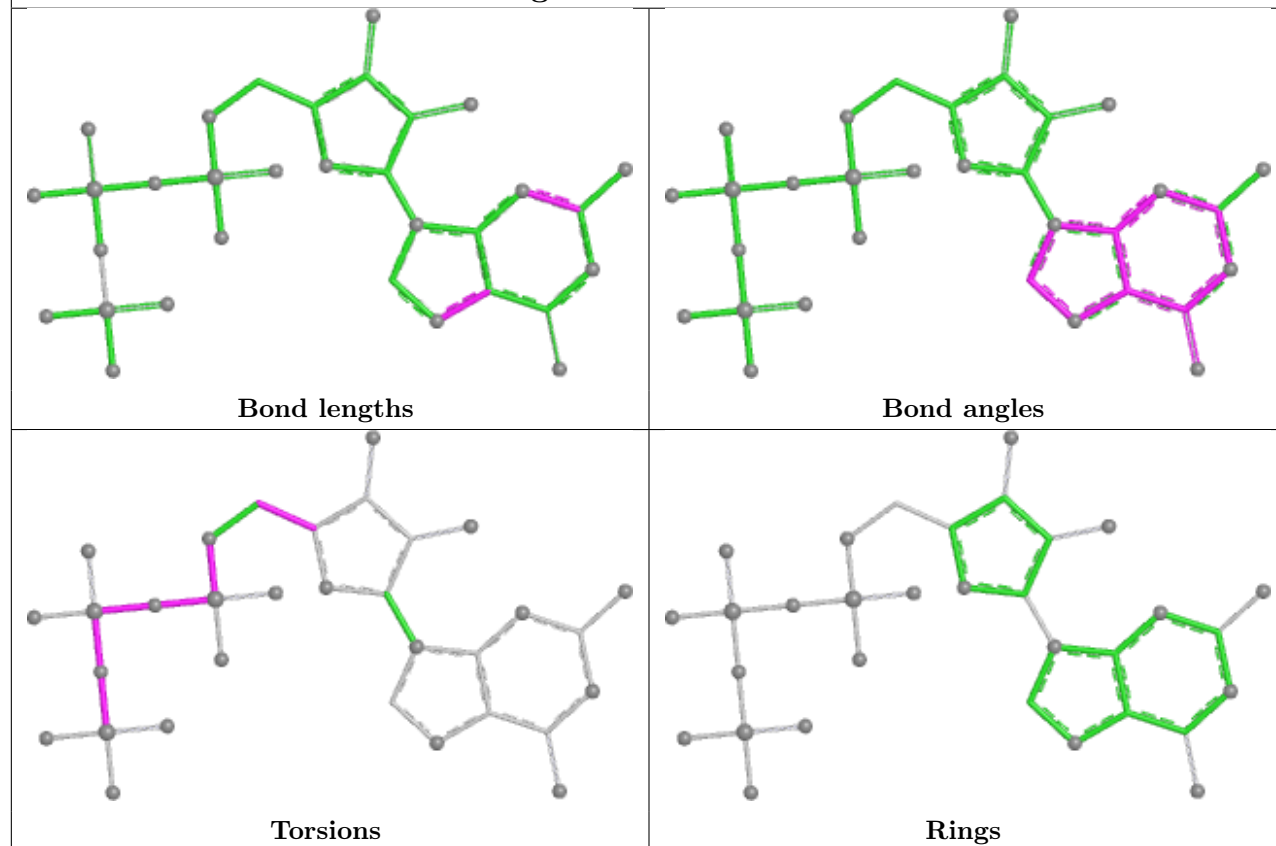
Ligand GTP A 401



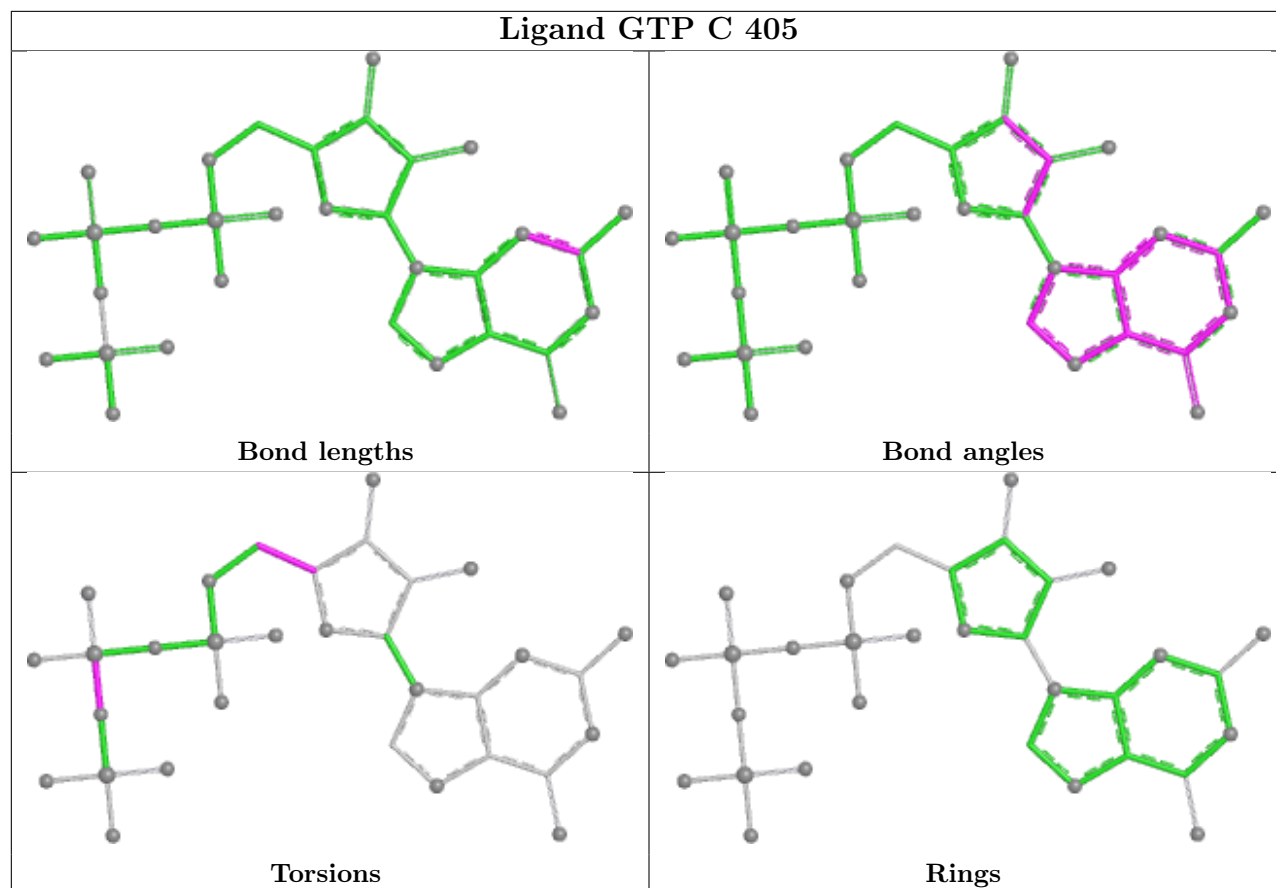
Ligand GTP J 401



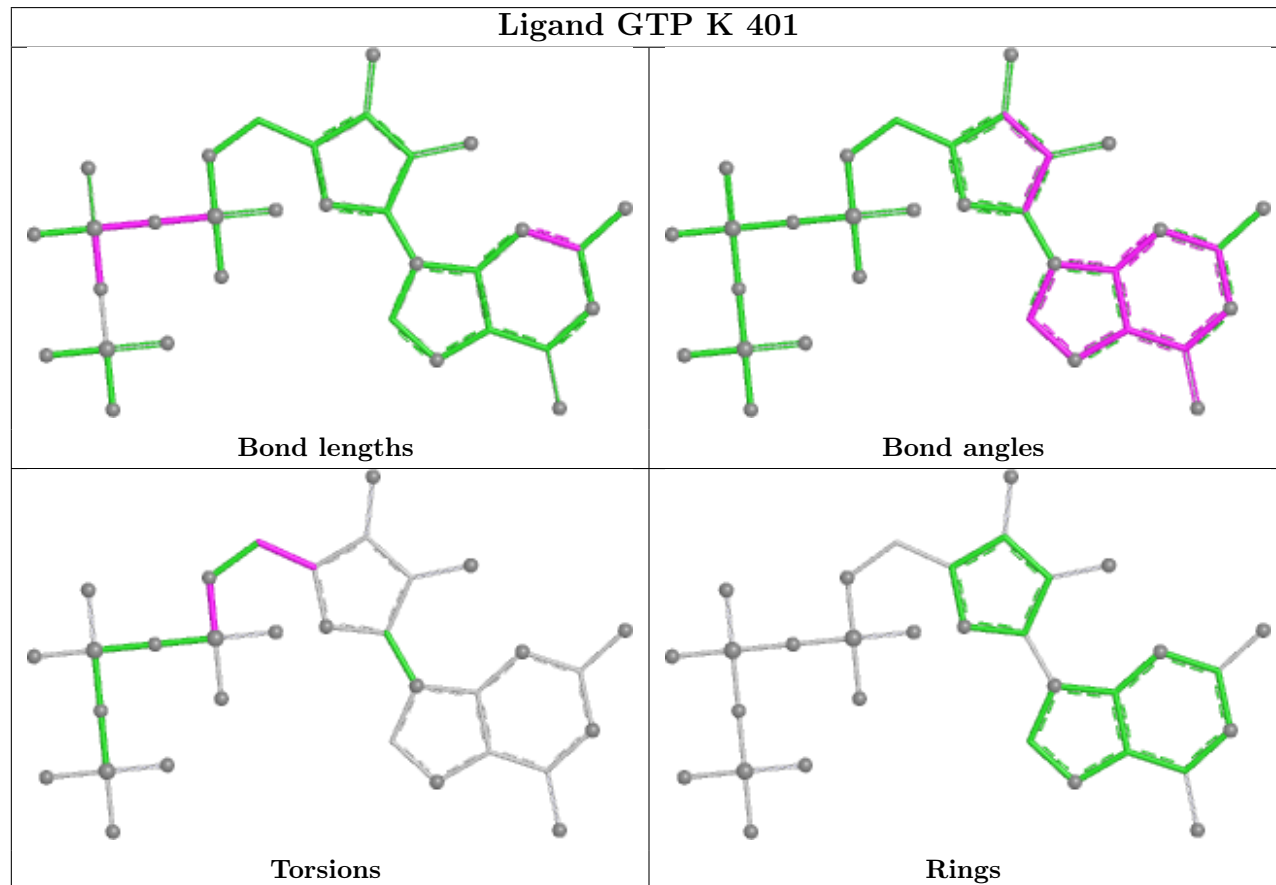
Ligand GTP B 402



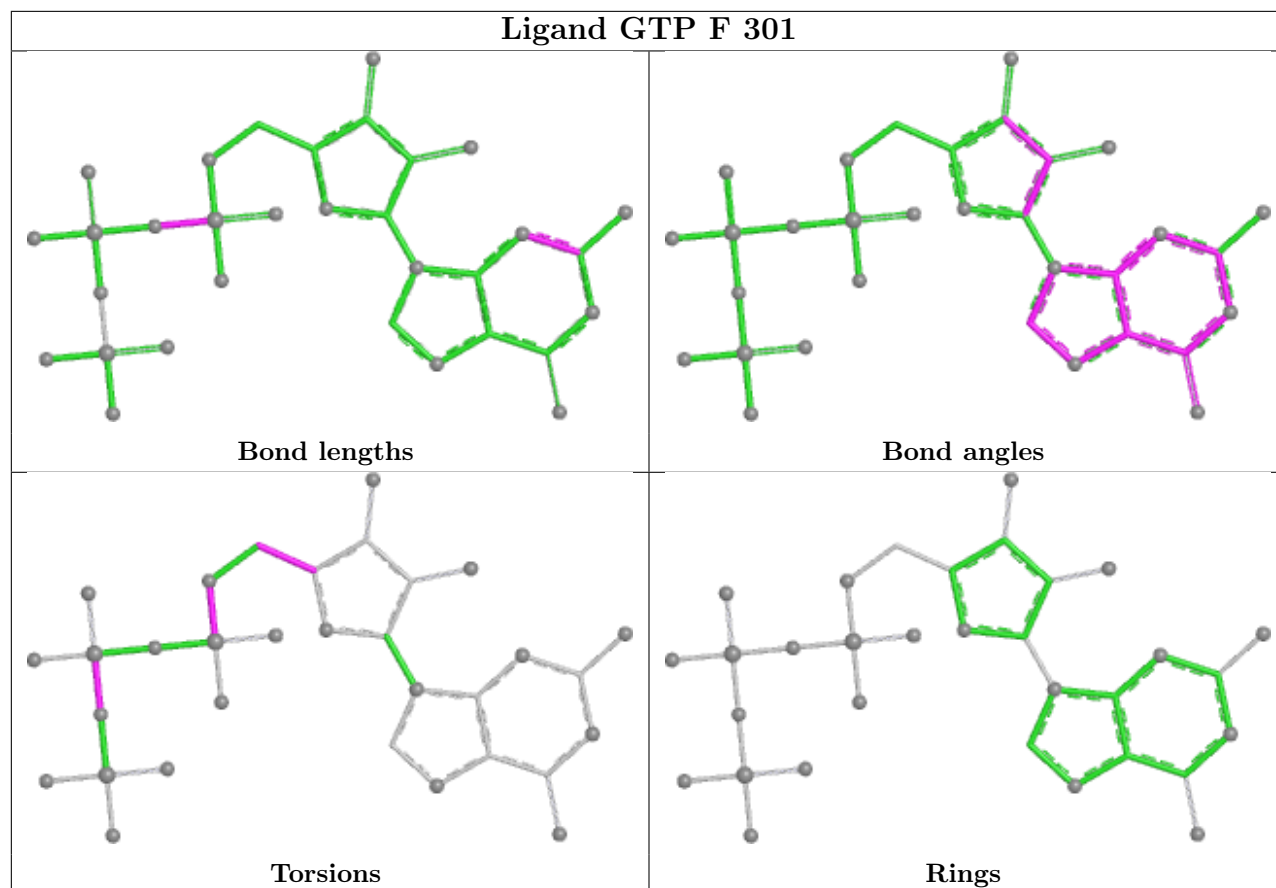
Ligand GTP C 405



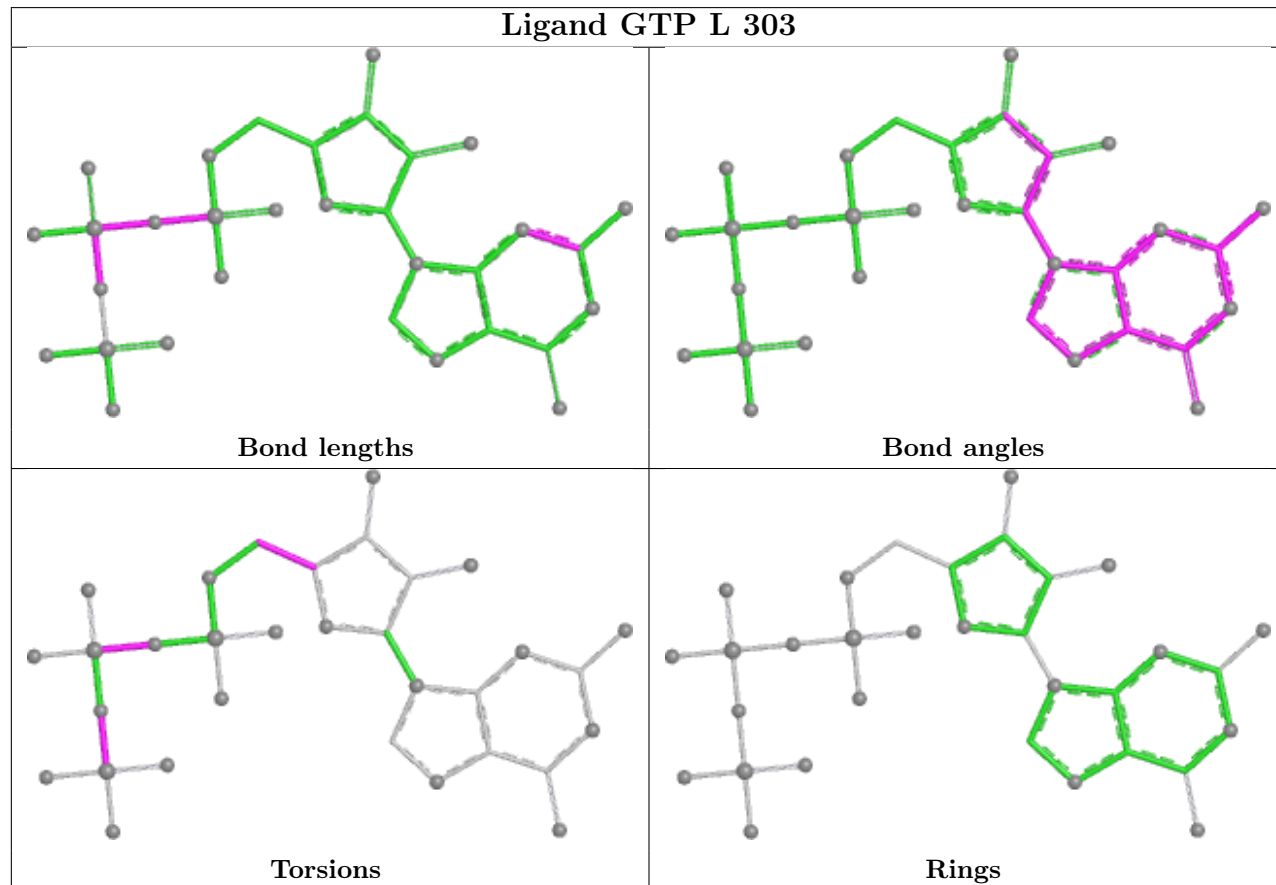
Ligand GTP K 401



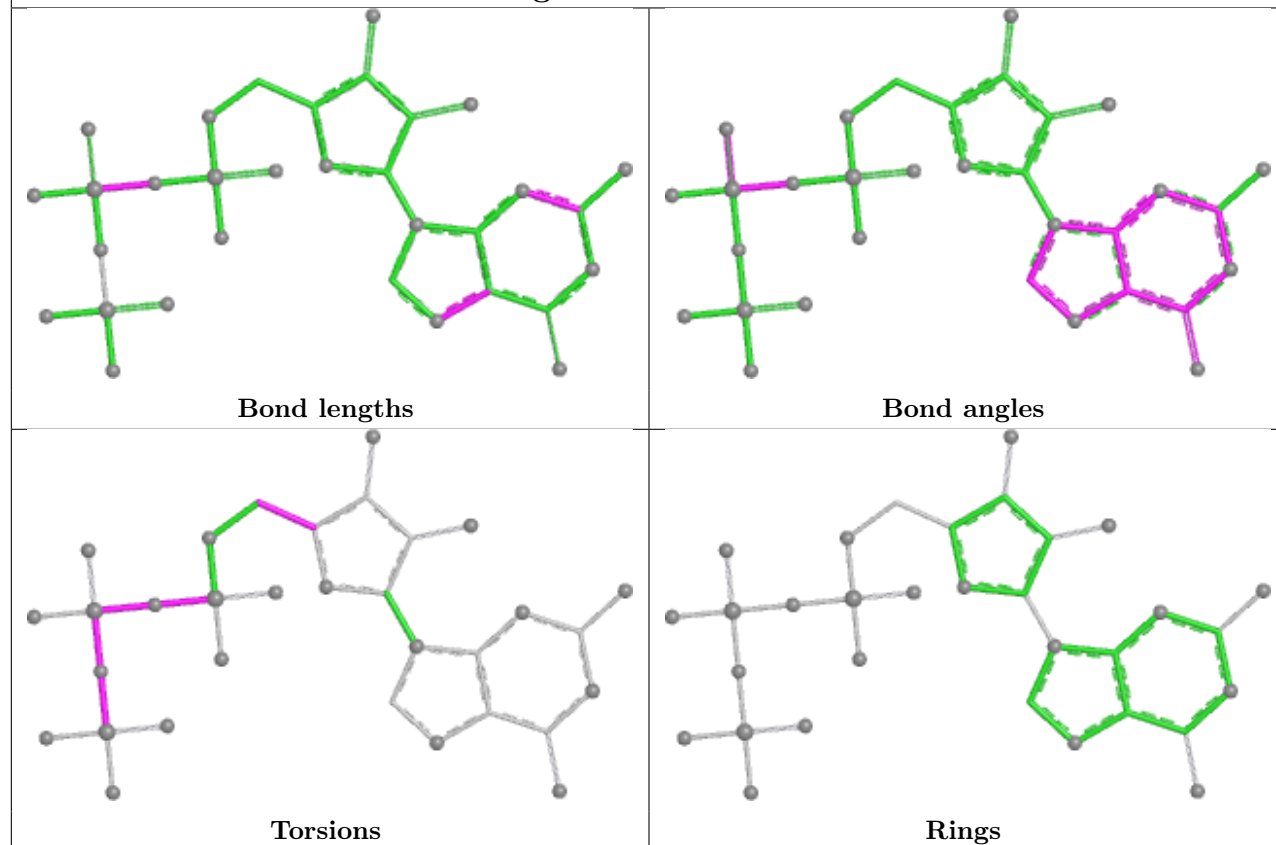
Ligand GTP F 301



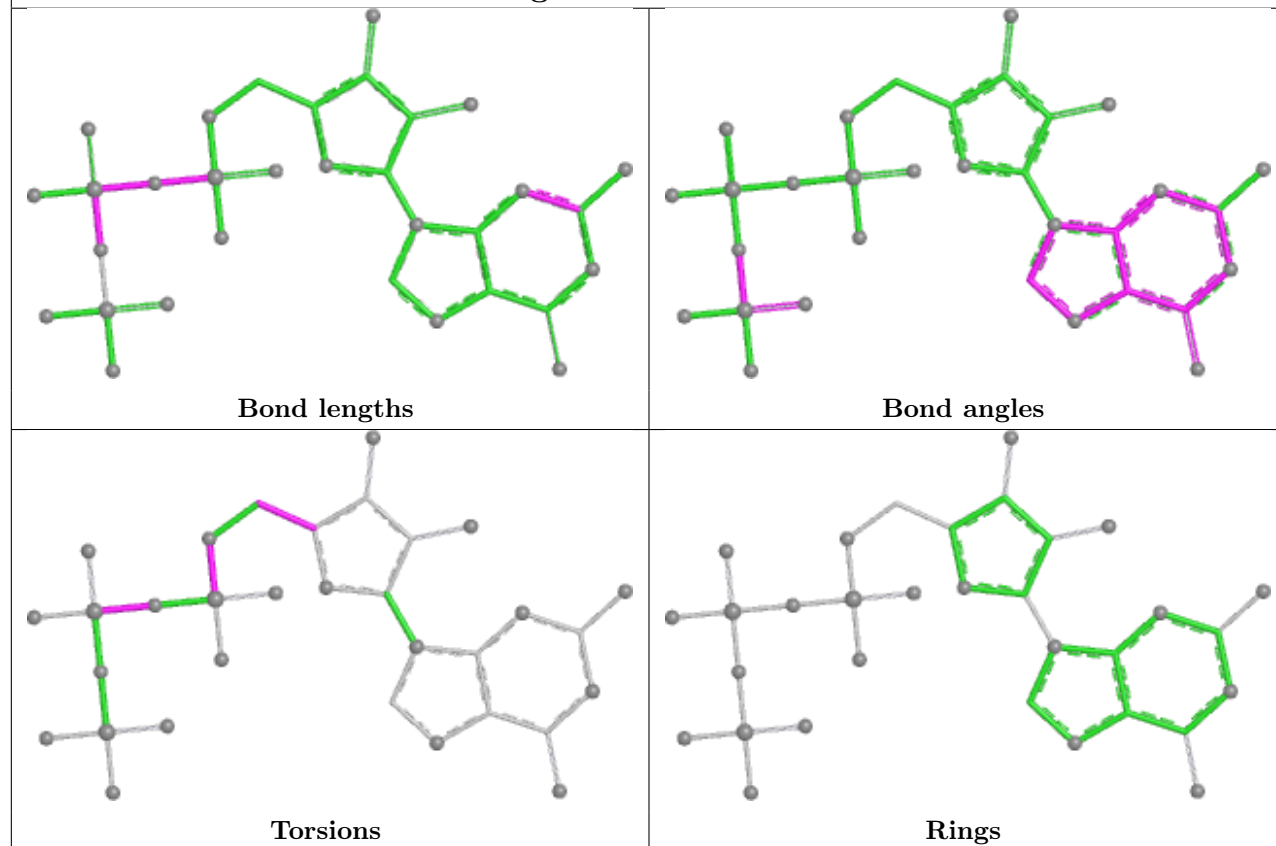
Ligand GTP L 303

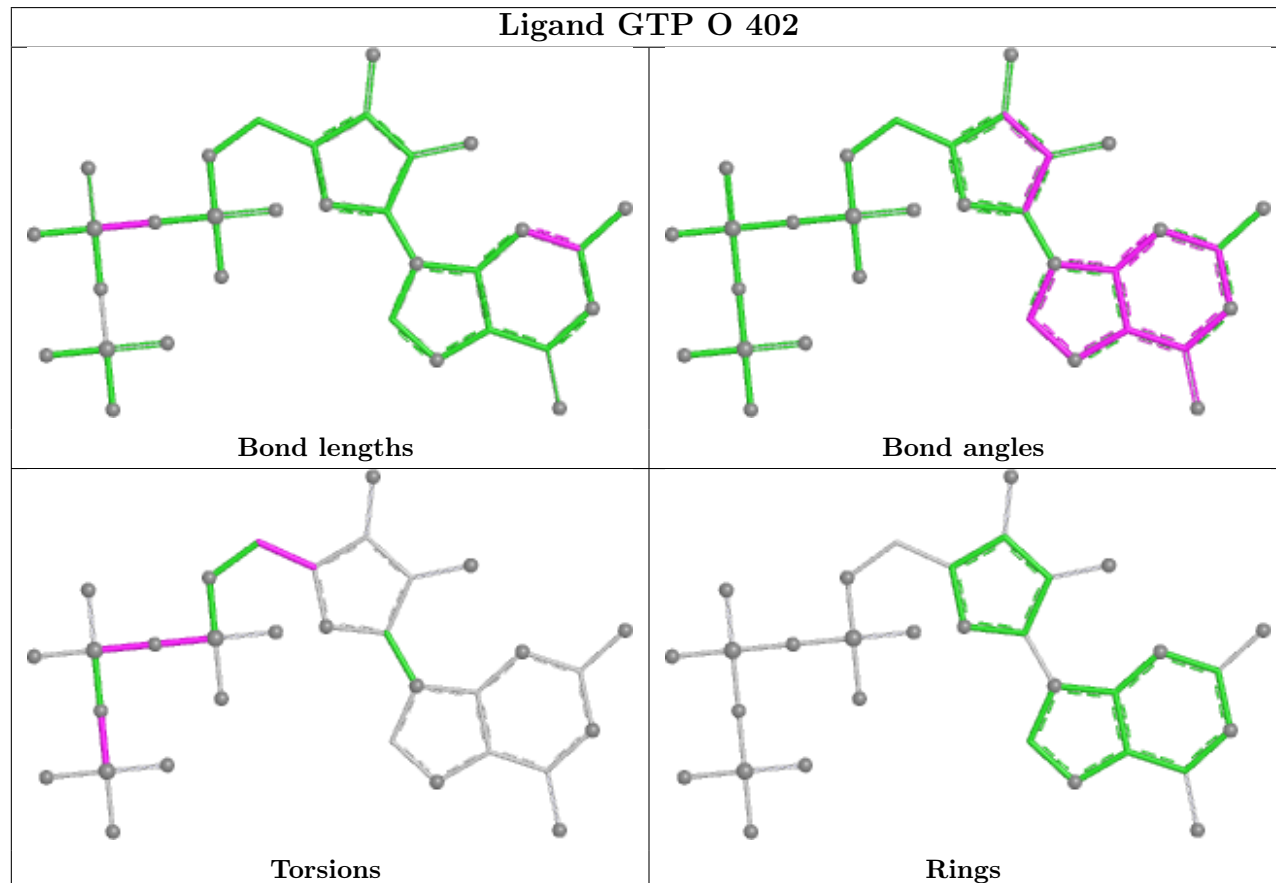
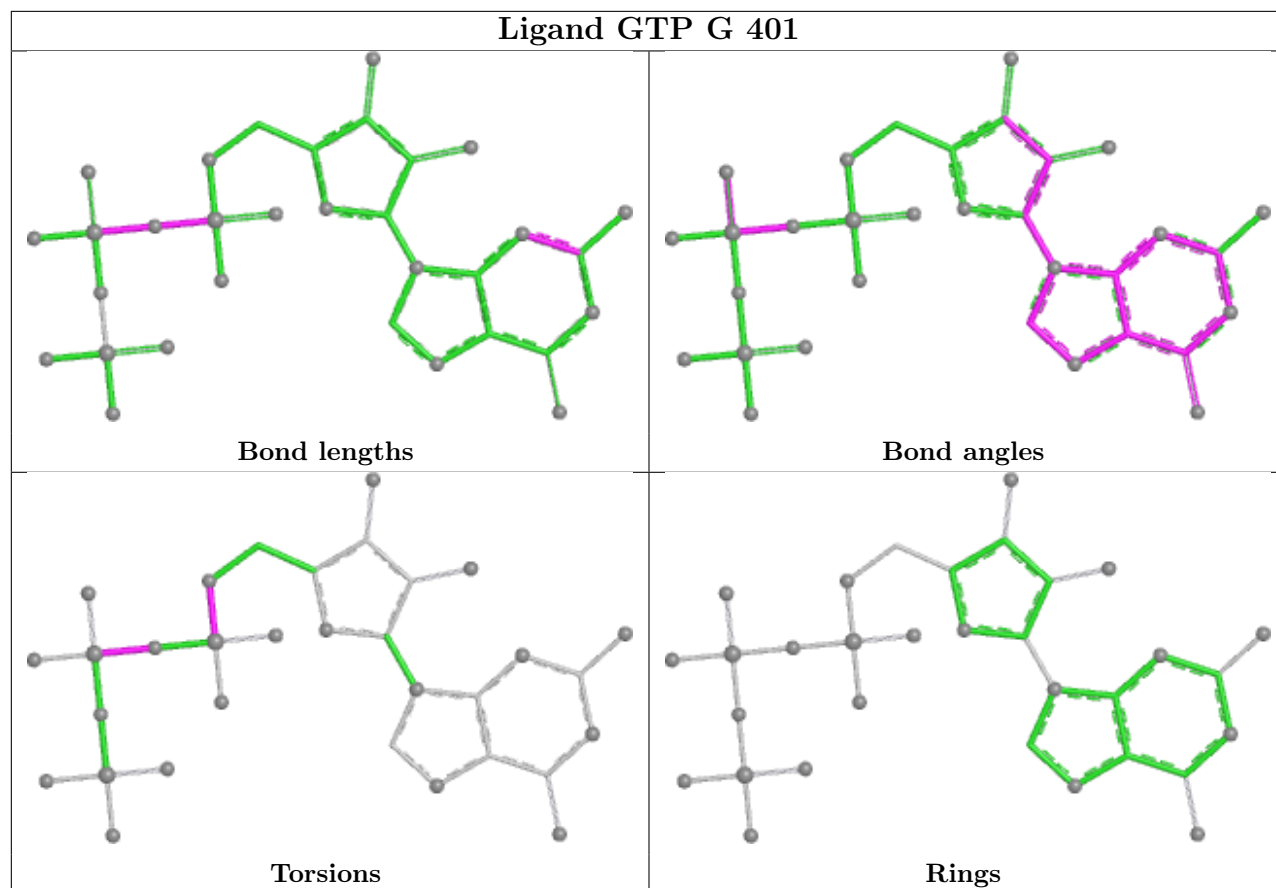


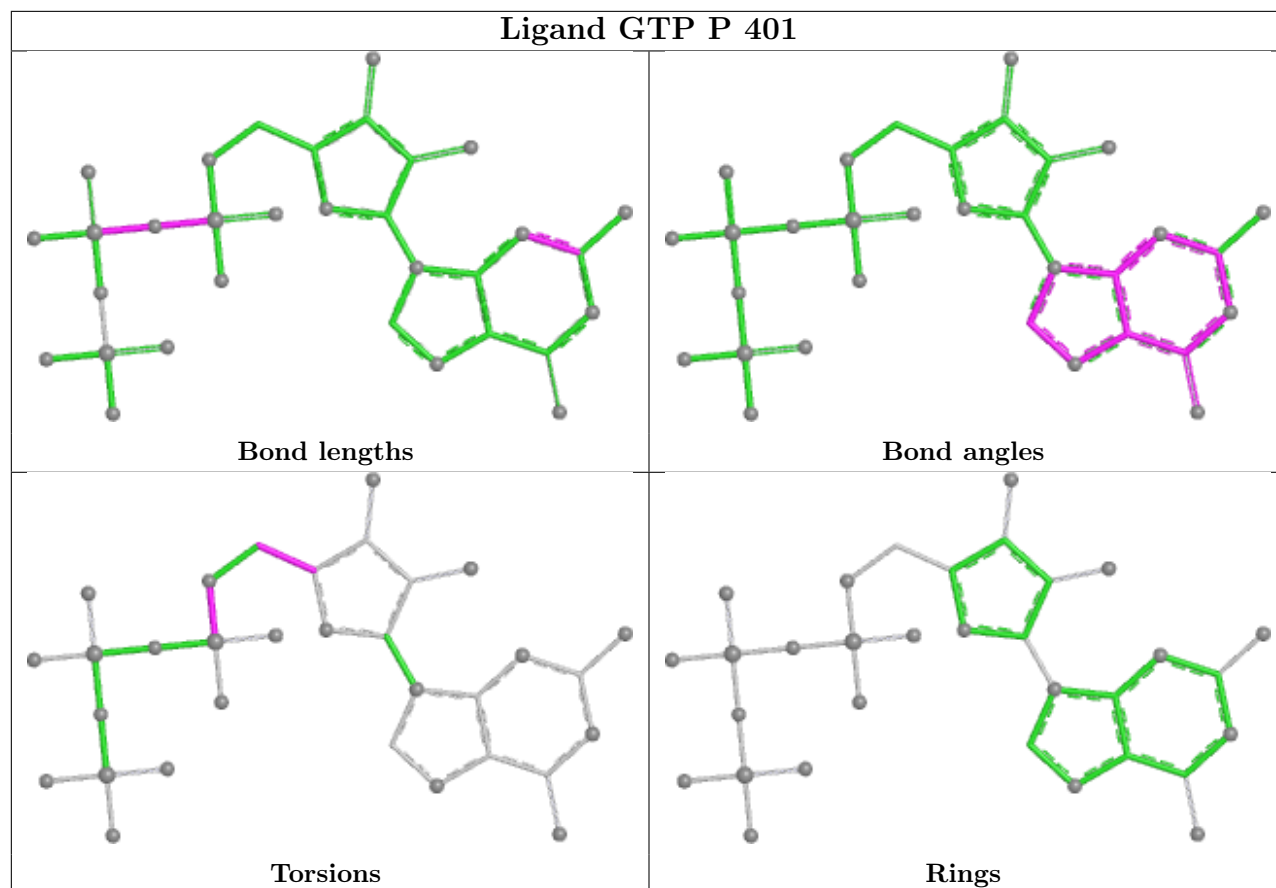
Ligand GTP L 304



Ligand GTP C 401







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	265/271 (97%)	-0.47	0 100 100	56, 90, 141, 156	0
1	B	265/271 (97%)	-0.54	0 100 100	50, 82, 139, 162	0
1	C	265/271 (97%)	-0.45	0 100 100	48, 92, 130, 138	0
1	D	265/271 (97%)	-0.66	0 100 100	45, 69, 108, 128	0
1	E	241/271 (88%)	-0.05	1 (0%) 88 76	44, 106, 147, 162	0
1	F	242/271 (89%)	-0.60	0 100 100	38, 67, 107, 126	0
1	G	265/271 (97%)	-0.46	0 100 100	38, 81, 139, 150	0
1	H	265/271 (97%)	-0.63	0 100 100	34, 65, 126, 146	0
1	I	242/271 (89%)	-0.57	0 100 100	40, 72, 119, 135	0
1	J	265/271 (97%)	-0.50	0 100 100	41, 82, 141, 162	0
1	K	265/271 (97%)	-0.45	0 100 100	36, 83, 142, 168	0
1	L	242/271 (89%)	-0.59	0 100 100	48, 78, 110, 135	0
1	M	265/271 (97%)	-0.68	0 100 100	31, 59, 122, 139	0
1	N	265/271 (97%)	-0.66	0 100 100	28, 58, 120, 144	0
1	O	265/271 (97%)	-0.70	0 100 100	40, 60, 118, 148	0
1	P	242/271 (89%)	-0.18	1 (0%) 88 76	40, 93, 179, 188	0
All	All	4124/4336 (95%)	-0.51	2 (0%) 100 100	28, 77, 137, 188	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	61	LEU	2.3
1	P	194	PHE	2.1

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 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	MG	G	403	1/1	0.62	0.13	69,69,69,69	0
3	MG	L	305	1/1	0.65	0.22	67,67,67,67	0
3	MG	C	404	1/1	0.68	0.17	54,54,54,54	0
3	MG	J	405	1/1	0.70	0.15	43,43,43,43	0
3	MG	C	402	1/1	0.70	0.14	82,82,82,82	0
3	MG	N	403	1/1	0.73	0.12	51,51,51,51	0
3	MG	K	402	1/1	0.75	0.11	100,100,100,100	0
3	MG	F	306	1/1	0.76	0.15	45,45,45,45	0
3	MG	O	403	1/1	0.76	0.14	48,48,48,48	0
3	MG	D	303	1/1	0.77	0.11	77,77,77,77	0
3	MG	F	304	1/1	0.78	0.12	60,60,60,60	0
3	MG	B	403	1/1	0.78	0.12	71,71,71,71	0
2	GTP	L	301	32/32	0.79	0.09	123,138,167,192	0
2	GTP	K	401	32/32	0.80	0.12	129,146,177,177	0
3	MG	D	305	1/1	0.80	0.18	53,53,53,53	0
3	MG	I	405	1/1	0.81	0.13	34,34,34,34	0
3	MG	A	403	1/1	0.81	0.13	73,73,73,73	0
3	MG	A	405	1/1	0.81	0.13	45,45,45,45	0
3	MG	H	403	1/1	0.82	0.13	67,67,67,67	0
3	MG	G	405	1/1	0.83	0.13	50,50,50,50	0
3	MG	F	302	1/1	0.84	0.14	61,61,61,61	0
3	MG	I	403	1/1	0.86	0.14	54,54,54,54	0
3	MG	H	405	1/1	0.87	0.20	31,31,31,31	0
3	MG	E	402	1/1	0.87	0.10	91,91,91,91	0
3	MG	L	307	1/1	0.88	0.09	27,27,27,27	0
2	GTP	E	401	32/32	0.89	0.09	62,102,120,156	0
3	MG	L	302	1/1	0.89	0.06	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	M	403	1/1	0.90	0.10	54,54,54,54	0
3	MG	B	405	1/1	0.91	0.13	56,56,56,56	0
2	GTP	A	401	32/32	0.92	0.07	60,81,91,96	0
2	GTP	P	401	32/32	0.92	0.08	58,101,113,116	0
2	GTP	F	301	32/32	0.92	0.08	64,129,135,137	0
3	MG	N	405	1/1	0.92	0.13	23,23,23,23	0
2	GTP	D	301	32/32	0.92	0.07	70,113,118,119	0
3	MG	O	405	1/1	0.92	0.10	25,25,25,25	0
3	MG	P	402	1/1	0.92	0.06	65,65,65,65	0
3	MG	K	403	1/1	0.93	0.07	220,220,220,220	0
3	MG	J	403	1/1	0.93	0.07	54,54,54,54	0
2	GTP	C	401	32/32	0.94	0.07	64,104,111,111	0
2	GTP	I	401	32/32	0.94	0.08	10,93,102,127	0
3	MG	P	404	1/1	0.94	0.09	42,42,42,42	0
2	GTP	O	406	32/32	0.95	0.06	39,129,133,134	0
3	MG	M	405	1/1	0.95	0.09	21,21,21,21	0
2	GTP	G	402	32/32	0.95	0.08	44,143,155,155	0
2	GTP	G	401	32/32	0.95	0.07	45,84,90,92	0
2	GTP	M	401	32/32	0.96	0.07	25,55,68,72	0
2	GTP	F	303	32/32	0.96	0.07	37,76,89,95	0
2	GTP	B	401	32/32	0.96	0.06	63,86,95,115	0
2	GTP	D	302	32/32	0.96	0.06	25,66,71,73	0
2	GTP	H	401	32/32	0.96	0.06	30,57,66,66	0
2	GTP	A	402	32/32	0.96	0.07	43,122,128,129	0
2	GTP	I	402	32/32	0.96	0.06	39,94,103,104	0
2	GTP	E	404	32/32	0.96	0.07	20,101,105,107	0
2	GTP	C	405	32/32	0.96	0.07	40,103,115,121	0
2	GTP	L	303	32/32	0.97	0.06	39,69,78,80	0
2	GTP	J	401	32/32	0.97	0.06	43,69,74,75	0
2	GTP	M	402	32/32	0.97	0.05	31,95,104,106	0
2	GTP	N	401	32/32	0.97	0.06	0,63,68,70	0
2	GTP	N	402	32/32	0.97	0.07	18,114,121,123	0
2	GTP	O	401	32/32	0.97	0.07	21,57,70,85	0
2	GTP	O	402	32/32	0.97	0.07	22,113,118,118	0
2	GTP	J	402	32/32	0.97	0.06	37,100,121,122	0
3	MG	E	403	1/1	0.97	0.04	68,68,68,68	0
2	GTP	B	402	32/32	0.97	0.05	59,123,126,126	0
2	GTP	H	402	32/32	0.97	0.07	26,92,99,101	0
3	MG	D	304	1/1	0.98	0.04	46,46,46,46	0
2	GTP	L	304	32/32	0.98	0.06	28,120,123,124	0
3	MG	G	404	1/1	0.98	0.03	39,39,39,39	0
3	MG	I	404	1/1	0.98	0.05	61,61,61,61	0

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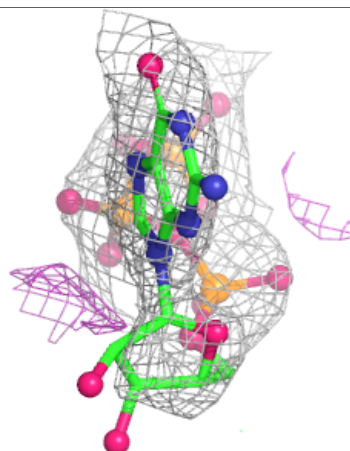
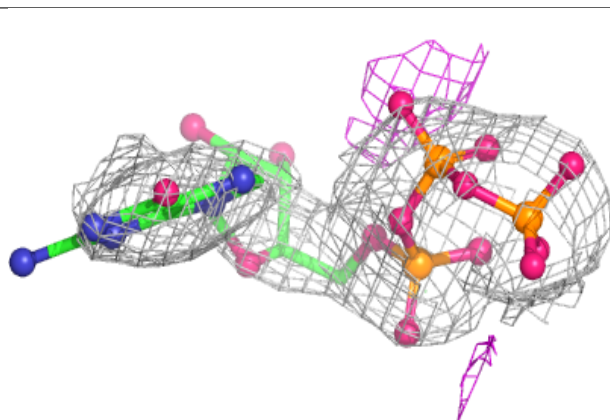
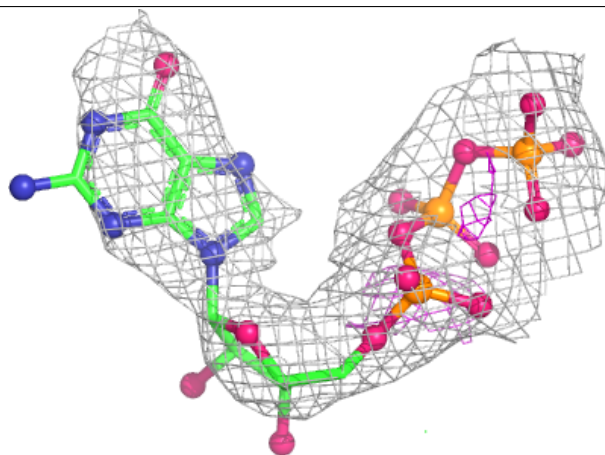
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	P	403	1/1	0.98	0.05	42,42,42,42	0
3	MG	F	305	1/1	0.98	0.04	46,46,46,46	0
3	MG	L	306	1/1	0.99	0.05	59,59,59,59	0
3	MG	B	404	1/1	0.99	0.02	42,42,42,42	0
3	MG	O	404	1/1	0.99	0.04	27,27,27,27	0
3	MG	H	404	1/1	0.99	0.03	29,29,29,29	0
3	MG	M	404	1/1	0.99	0.02	16,16,16,16	0
3	MG	C	403	1/1	0.99	0.02	53,53,53,53	0
3	MG	A	404	1/1	0.99	0.03	39,39,39,39	0
3	MG	N	404	1/1	1.00	0.02	38,38,38,38	0
3	MG	J	404	1/1	1.00	0.02	47,47,47,47	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.

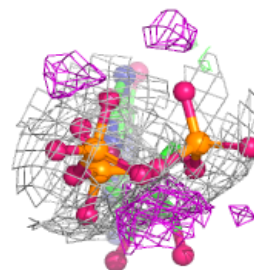
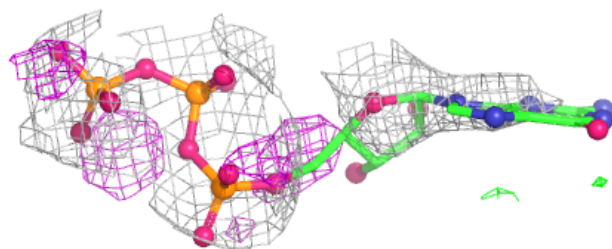
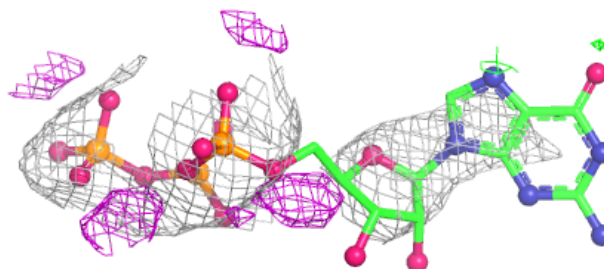
Electron density around GTP L 301:

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

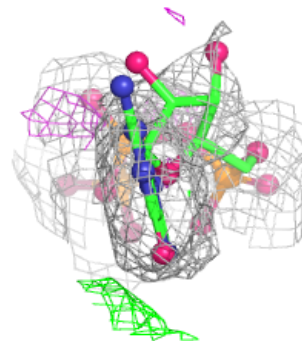
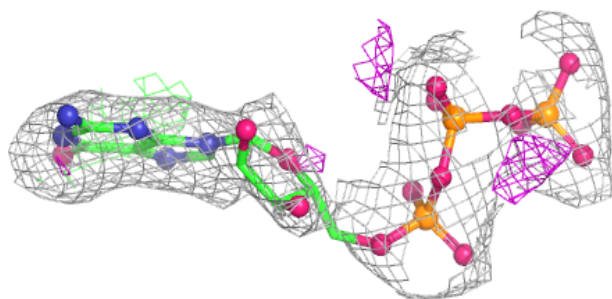
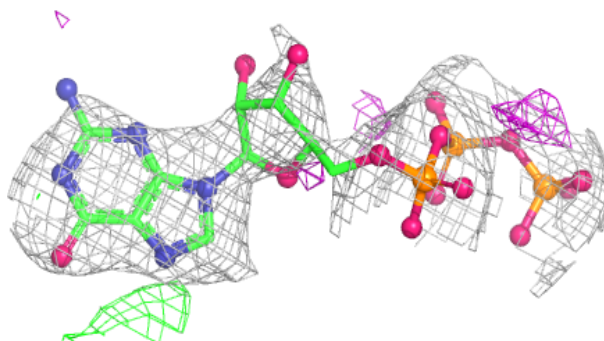


Electron density around GTP K 401:

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

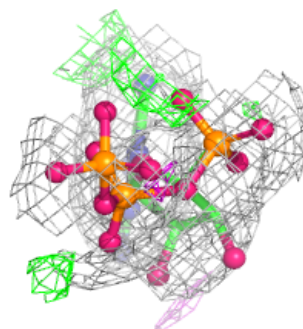
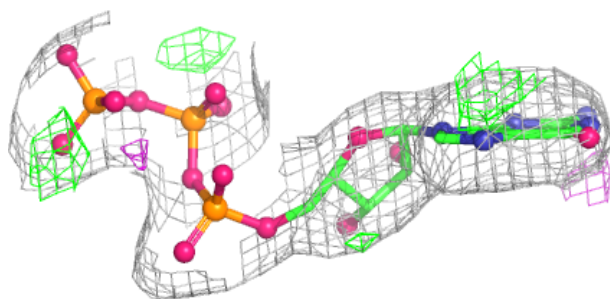
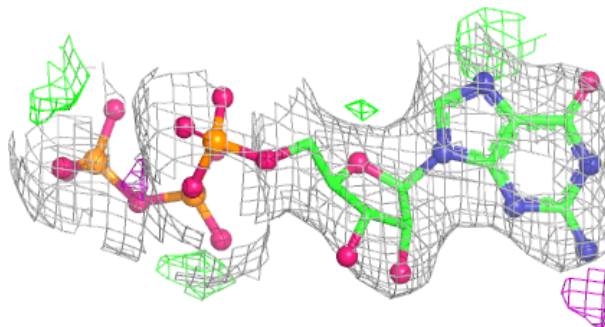
**Electron density around GTP E 401:**

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

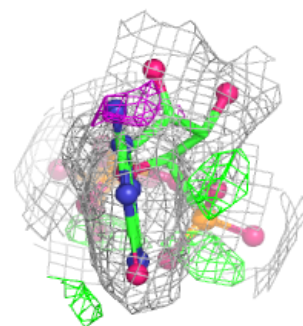
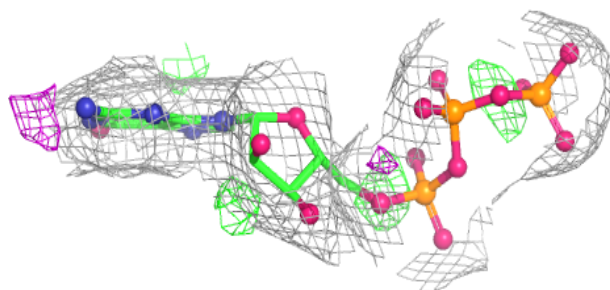
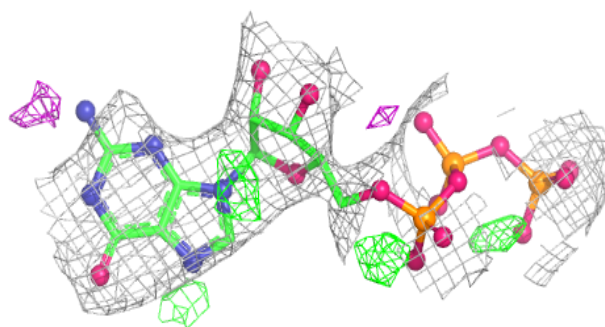


Electron density around GTP A 401:

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

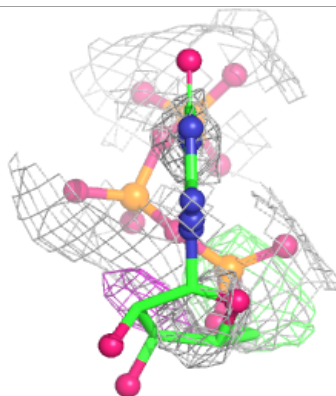
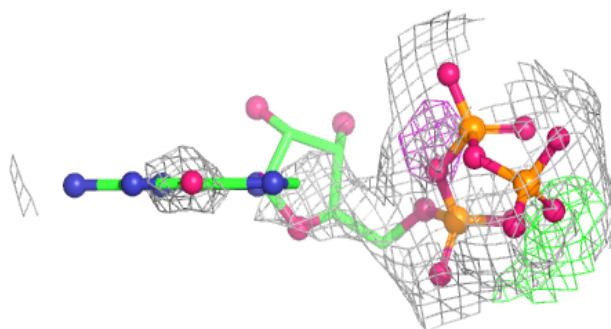
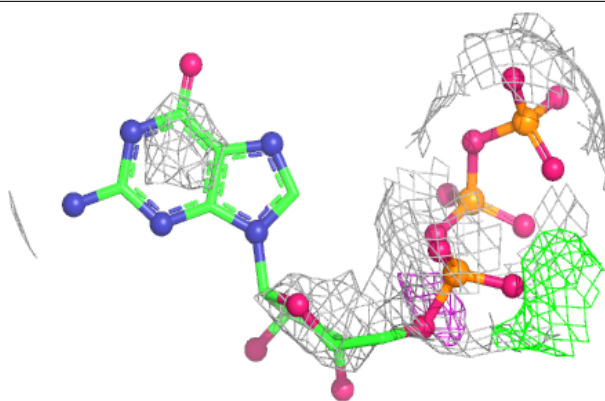
**Electron density around GTP P 401:**

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

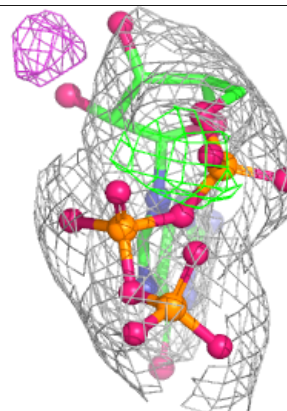
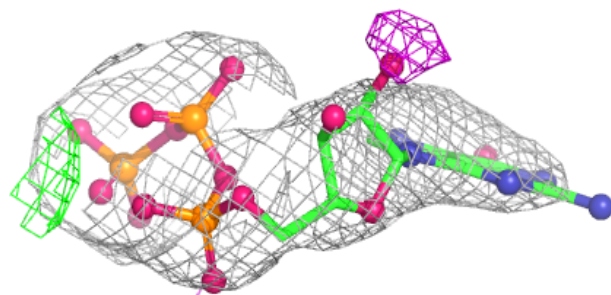
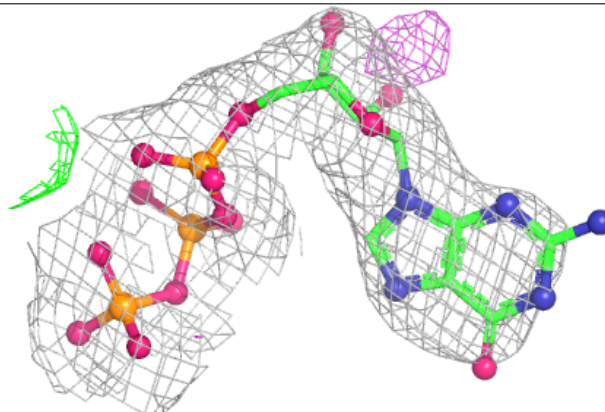


Electron density around GTP F 301:

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

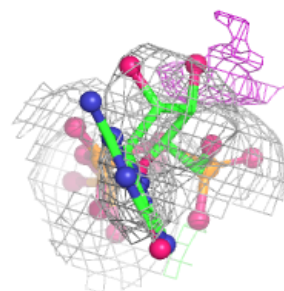
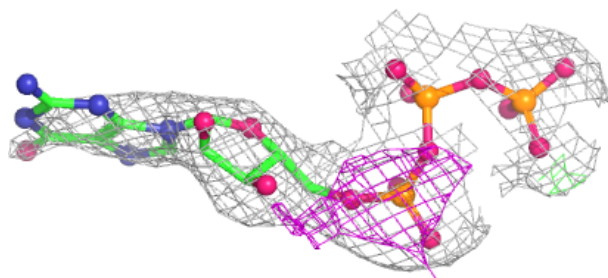
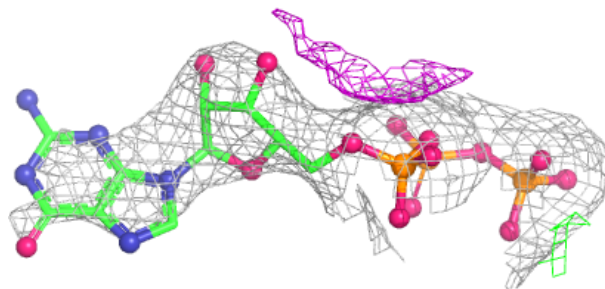
**Electron density around GTP D 301:**

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

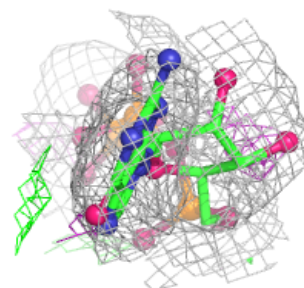
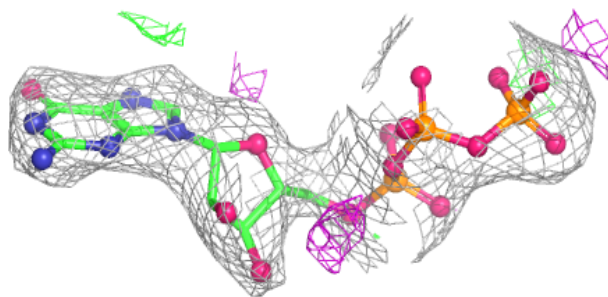
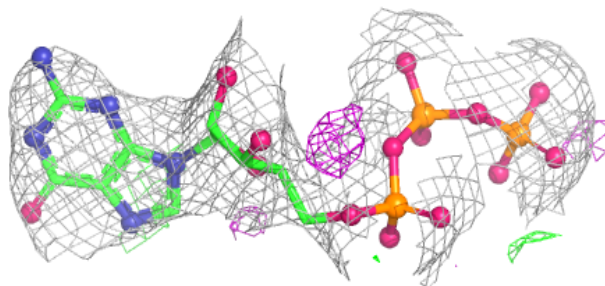


Electron density around GTP C 401:

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

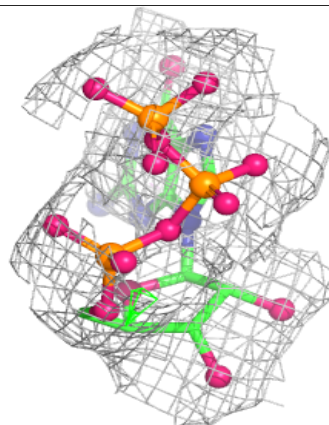
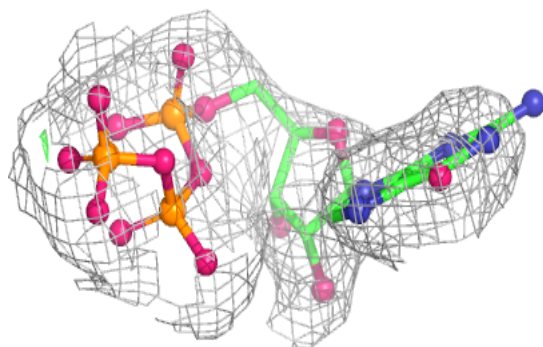
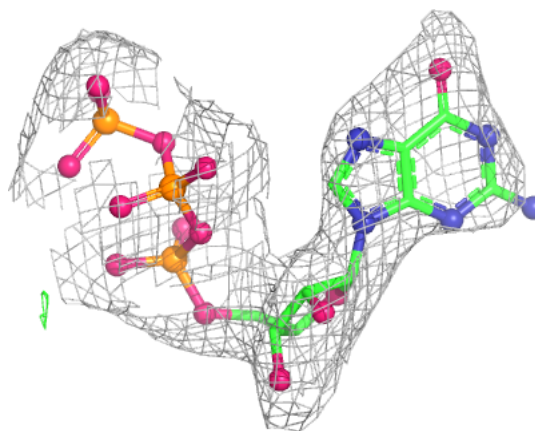
**Electron density around GTP I 401:**

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

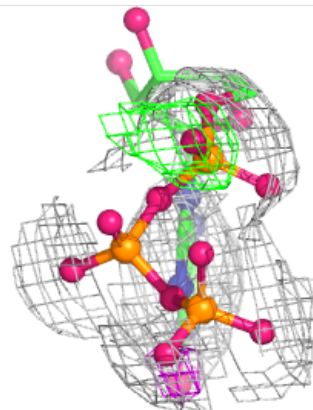
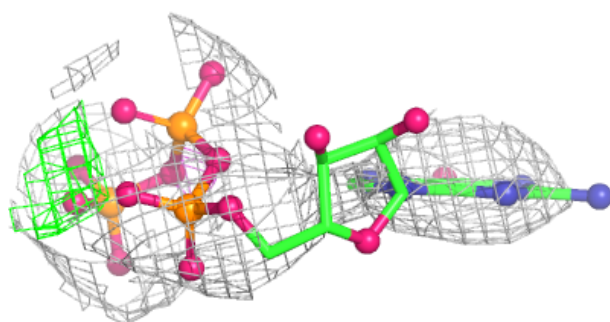
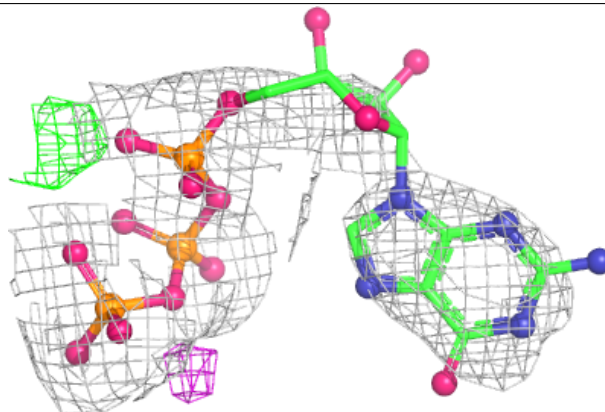


Electron density around GTP O 406:

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and green (positive)

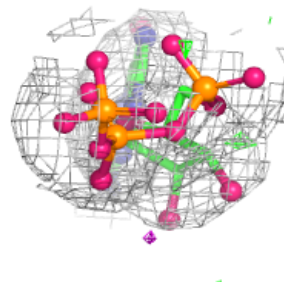
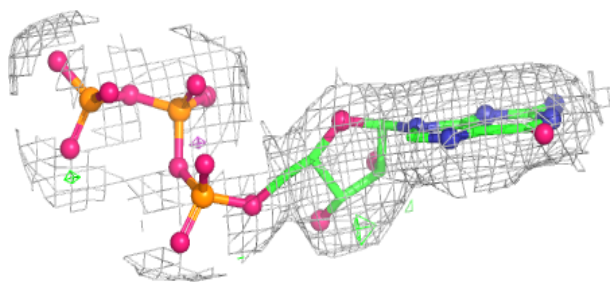
**Electron density around GTP G 402:**

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and green (positive)

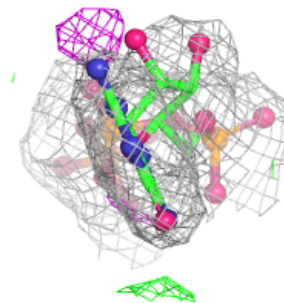
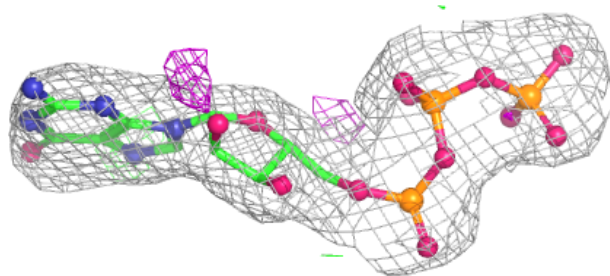
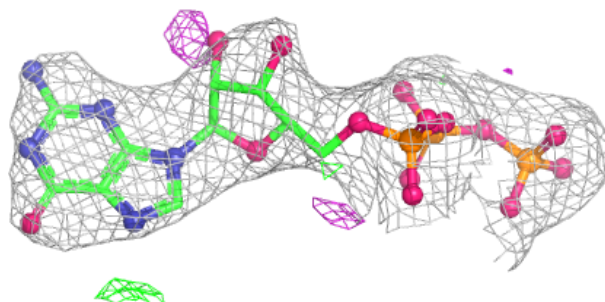


Electron density around GTP G 401:

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and green (positive)

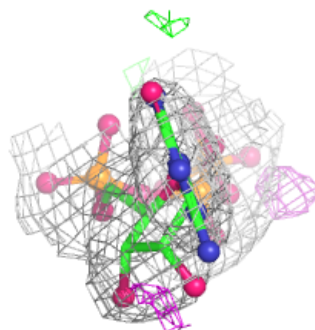
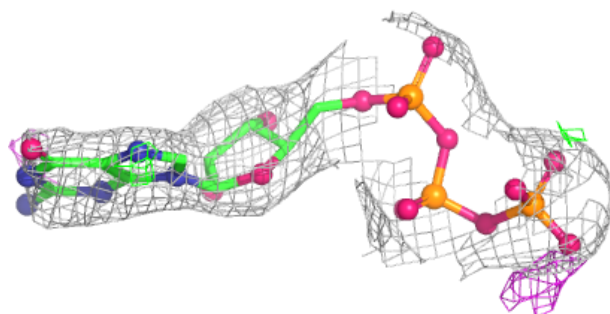
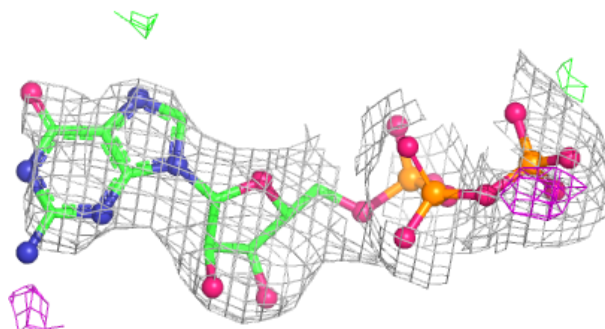
**Electron density around GTP M 401:**

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

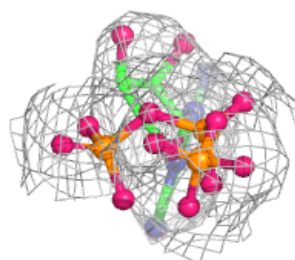
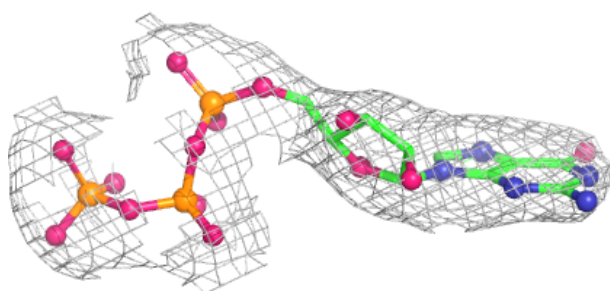
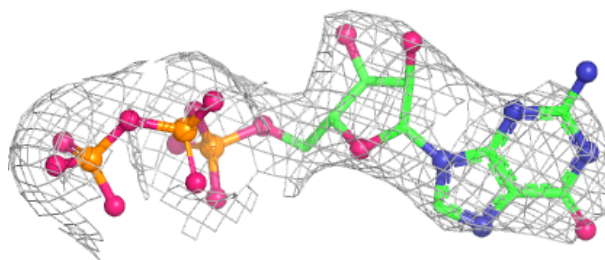


Electron density around GTP F 303:

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

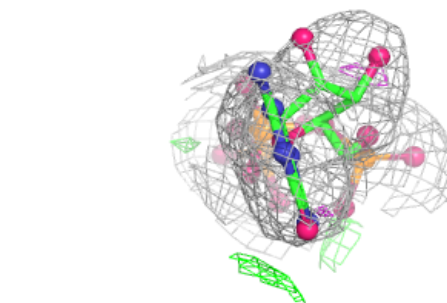
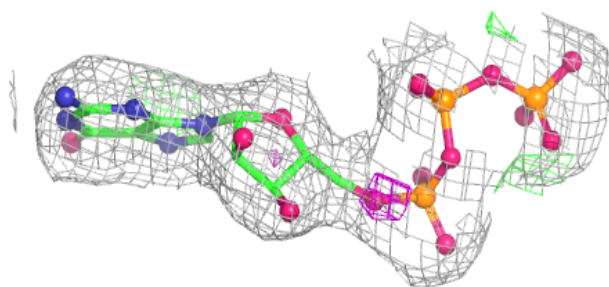
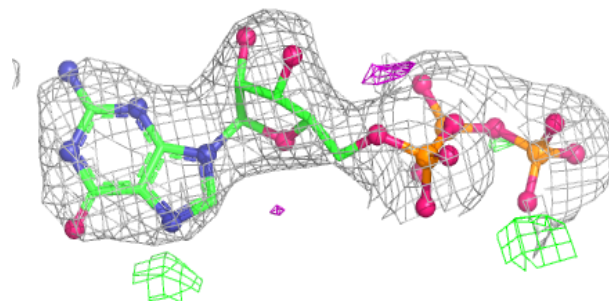
**Electron density around GTP B 401:**

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

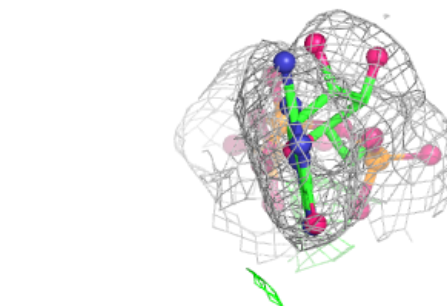
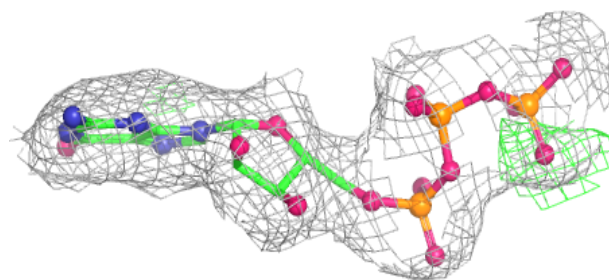
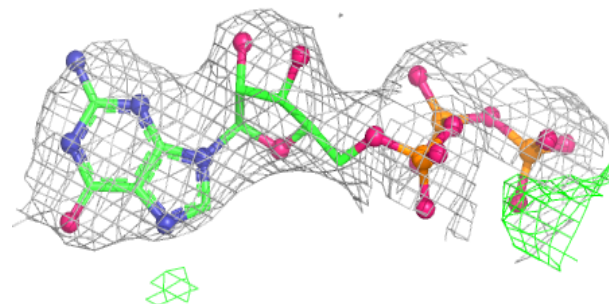


Electron density around GTP D 302:

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

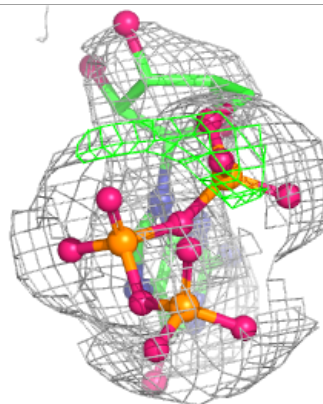
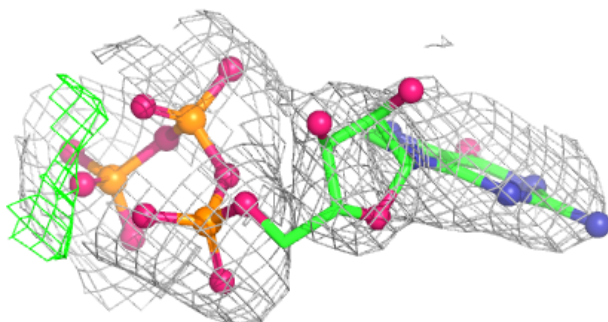
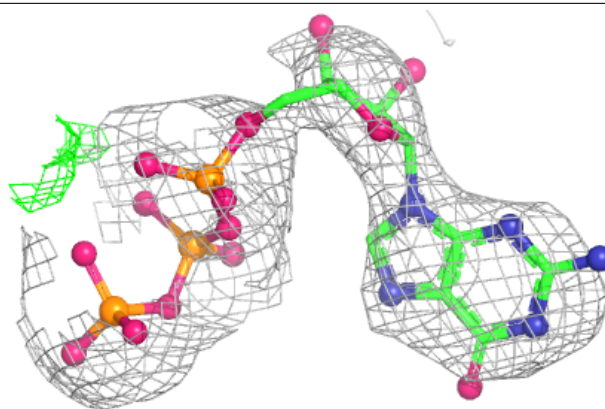
**Electron density around GTP H 401:**

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

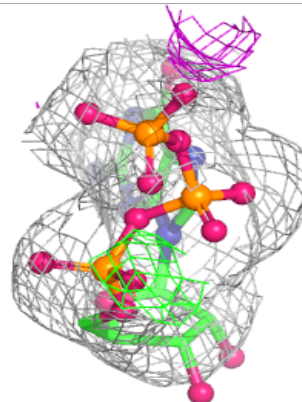
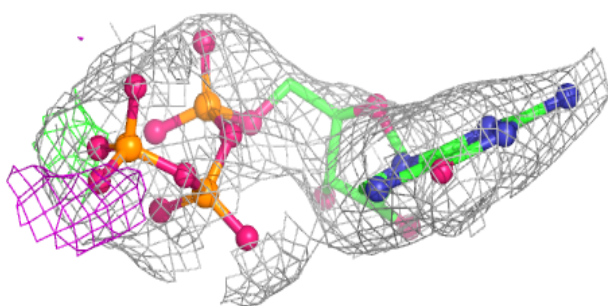
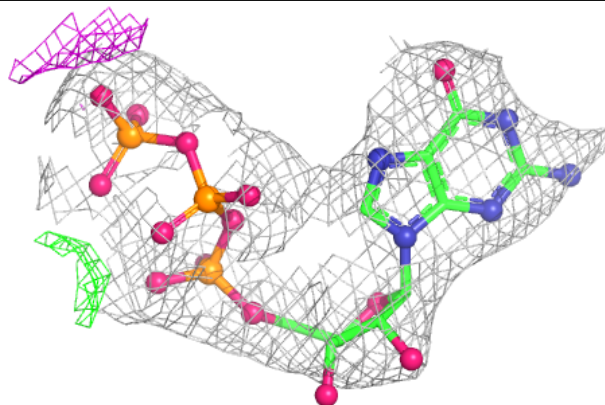


Electron density around GTP A 402:

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

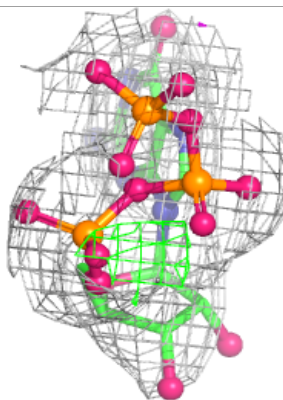
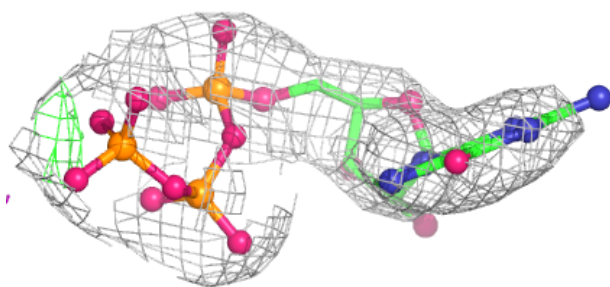
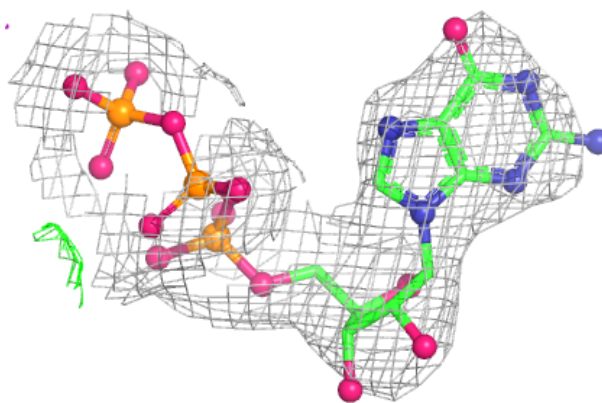
**Electron density around GTP I 402:**

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

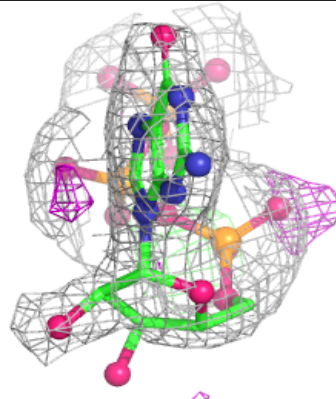
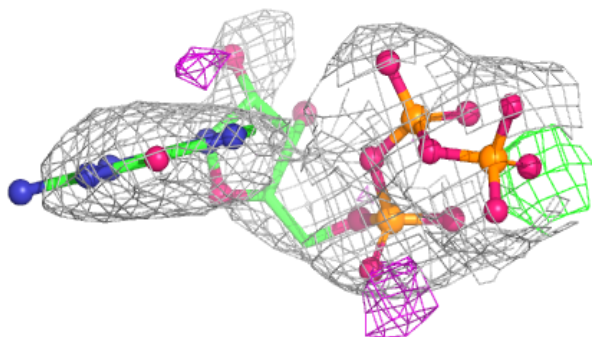
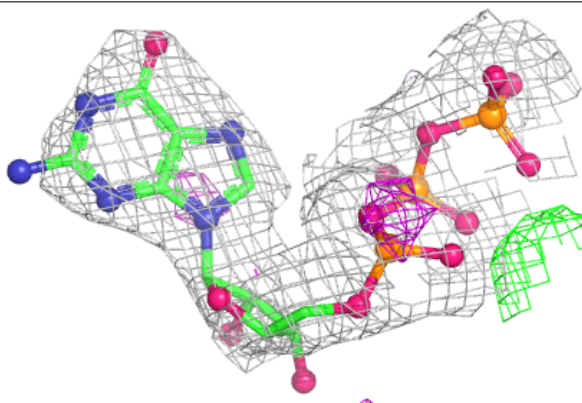


Electron density around GTP E 404:

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

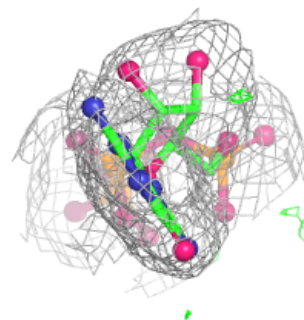
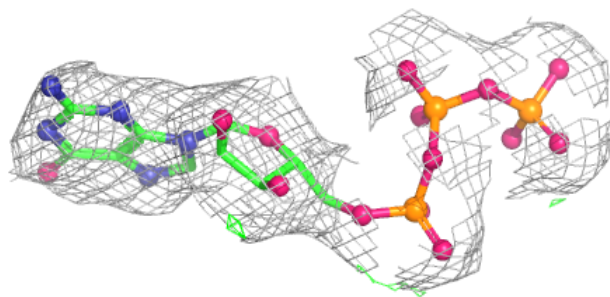
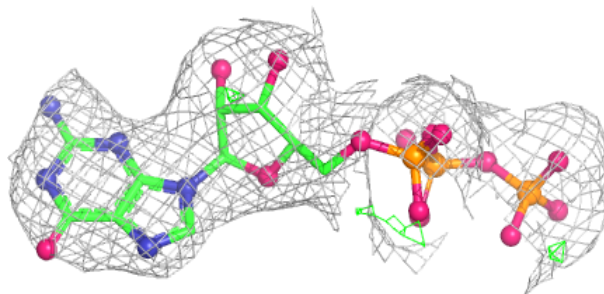
**Electron density around GTP C 405:**

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

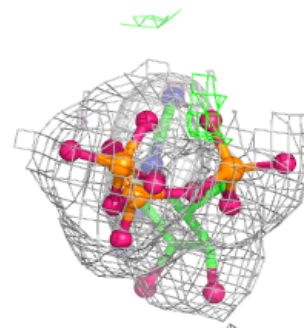
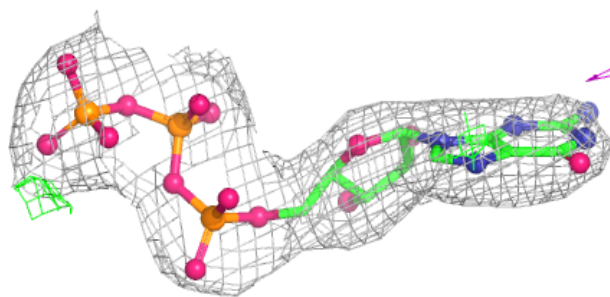
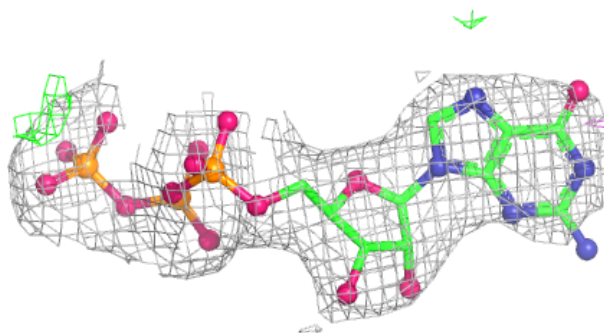


Electron density around GTP L 303:

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

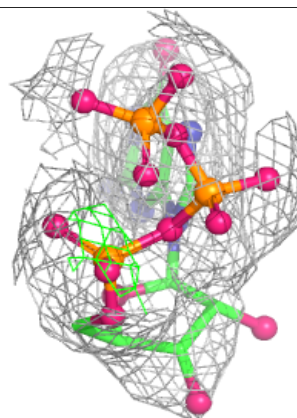
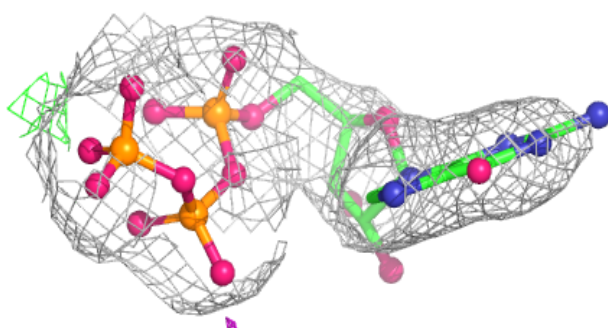
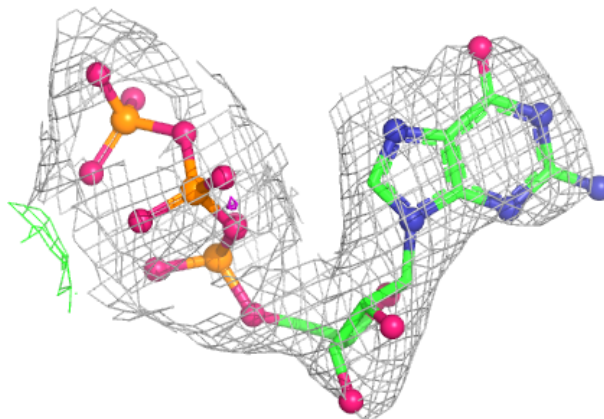
**Electron density around GTP J 401:**

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

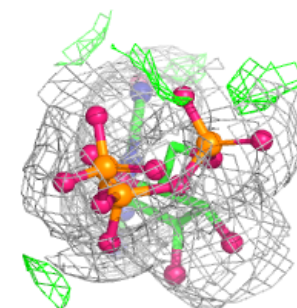
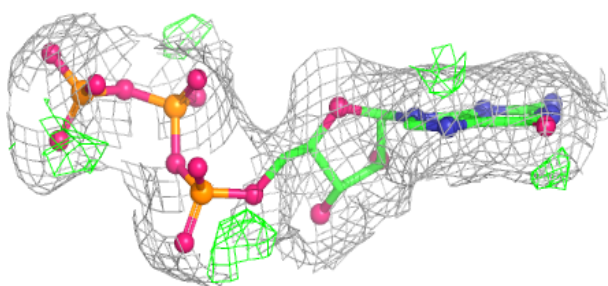
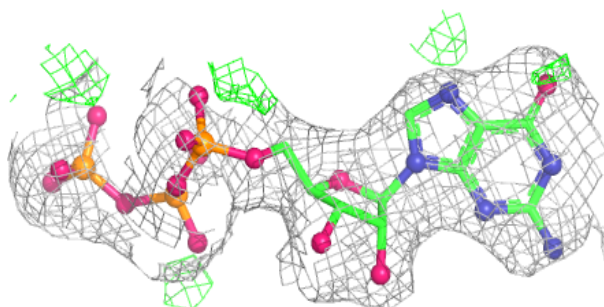


Electron density around GTP M 402:

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

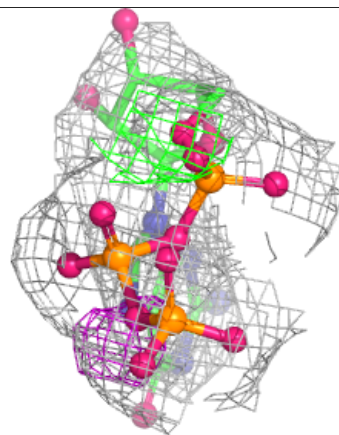
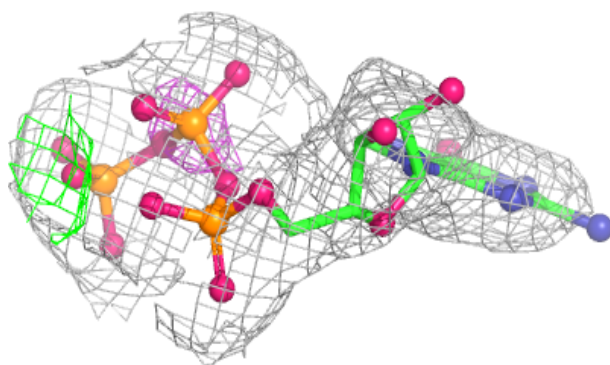
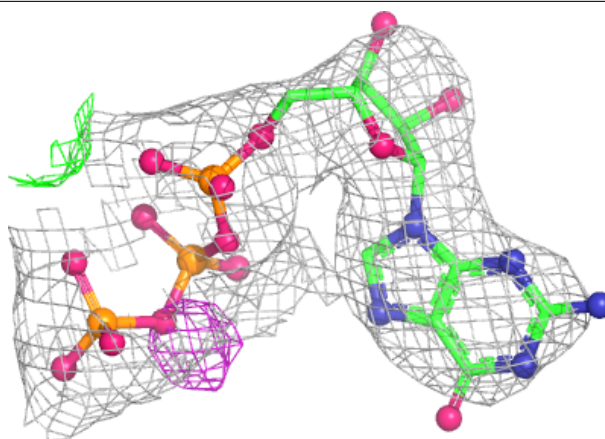
**Electron density around GTP N 401:**

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

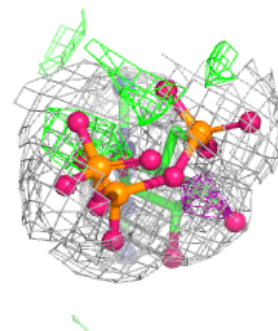
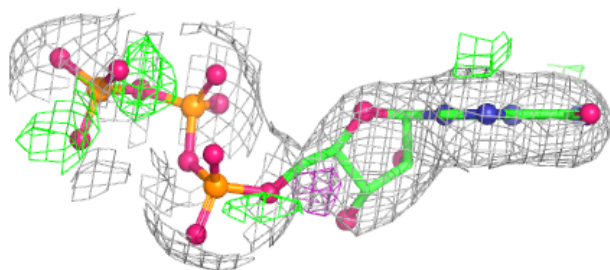
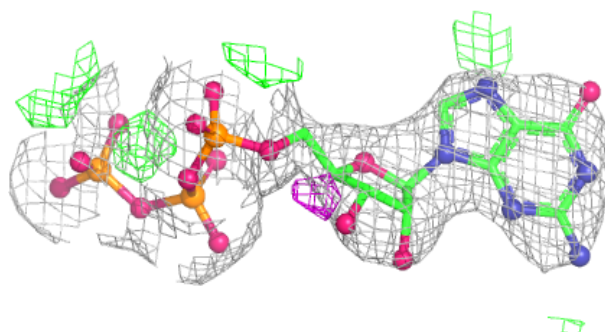


Electron density around GTP N 402:

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

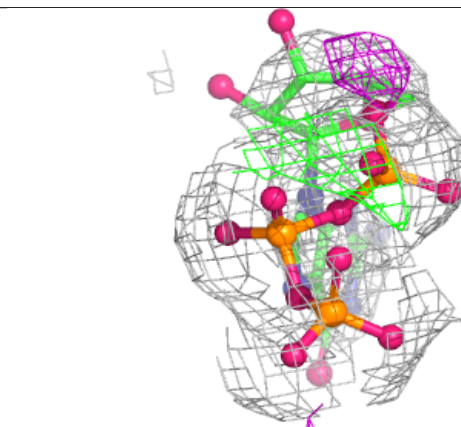
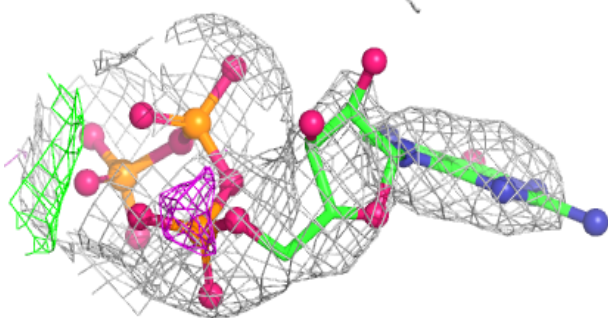
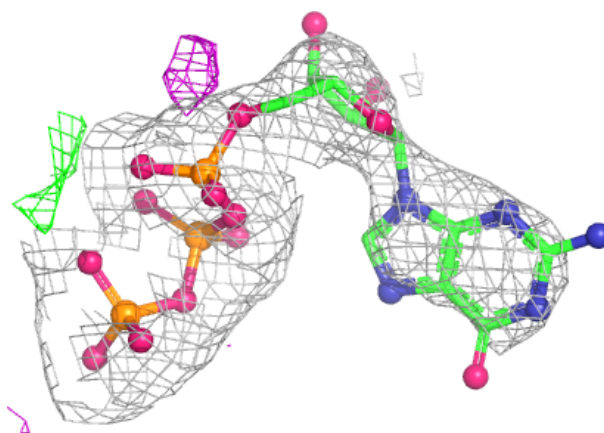
**Electron density around GTP O 401:**

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

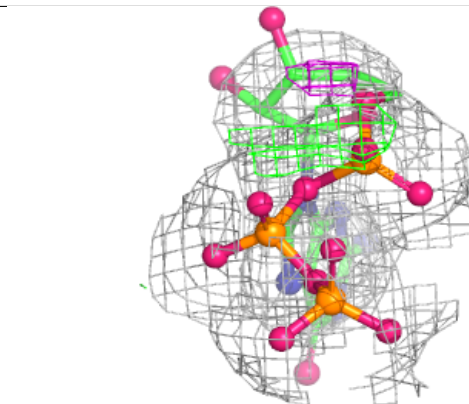
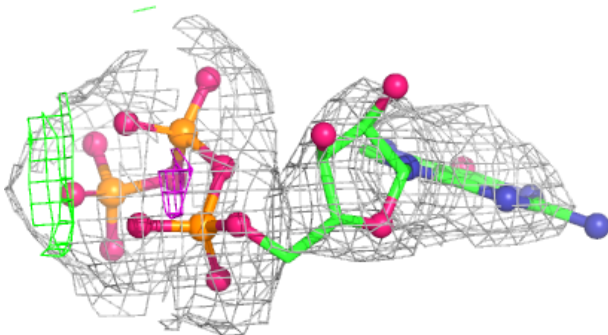
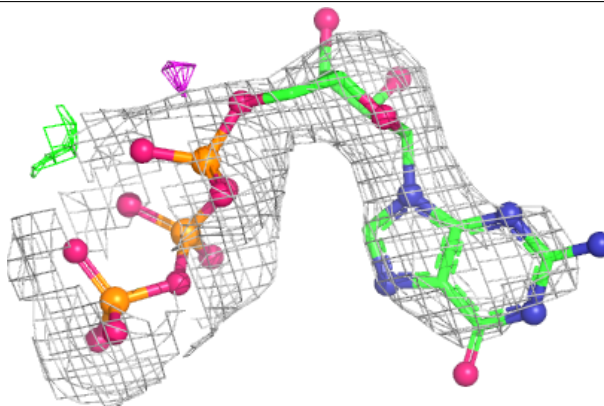


Electron density around GTP O 402:

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

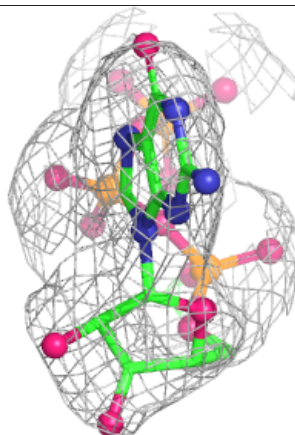
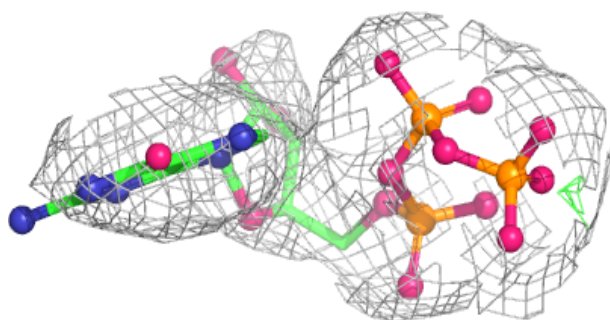
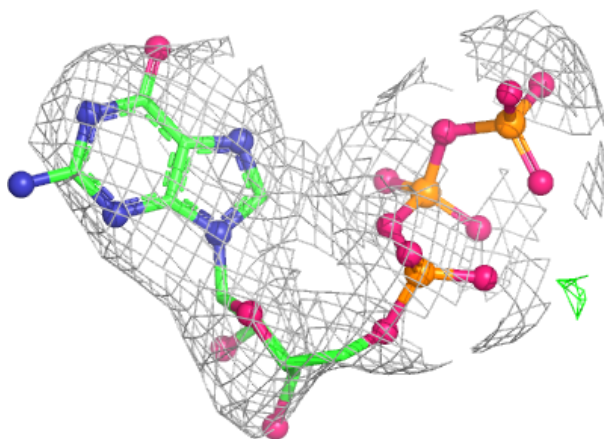
**Electron density around GTP J 402:**

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



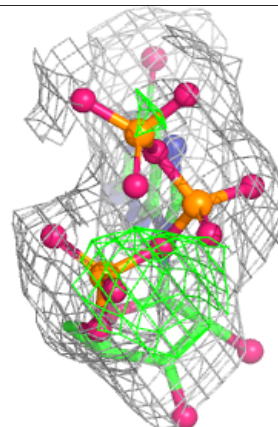
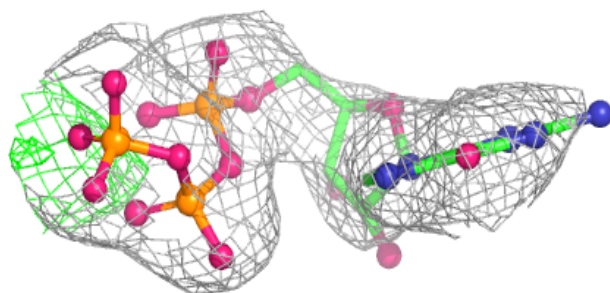
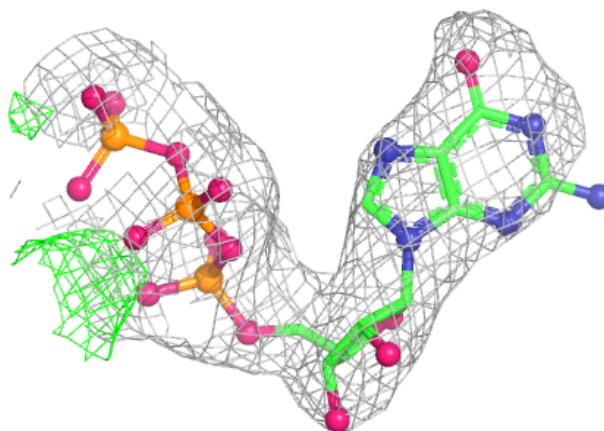
Electron density around GTP B 402:

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

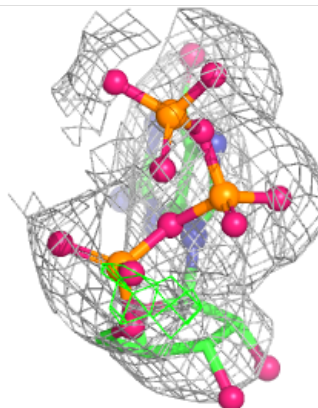
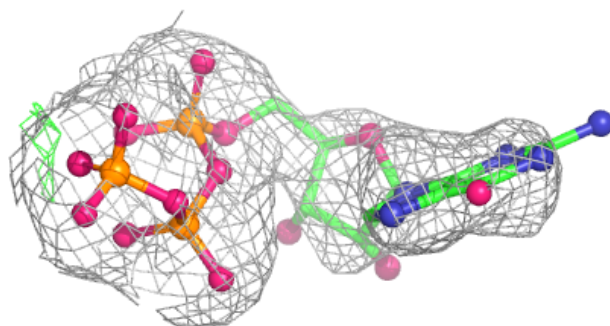
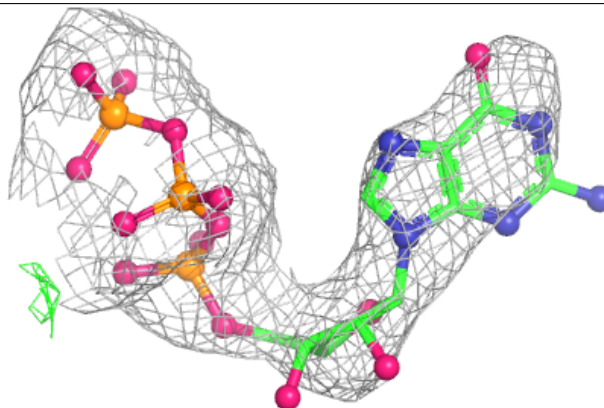


Electron density around GTP H 402:

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

**Electron density around GTP L 304:**

$2mF_o-DF_c$ (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.