



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:17 pm BST

PDB ID : 1A8R
Title : GTP CYCLOHYDROLASE I (H112S MUTANT) IN COMPLEX WITH GTP
Authors : Auerbach, G.; Nar, H.; Bracher, A.; Bacher, A.; Huber, R.
Deposited on : 1998-03-27
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

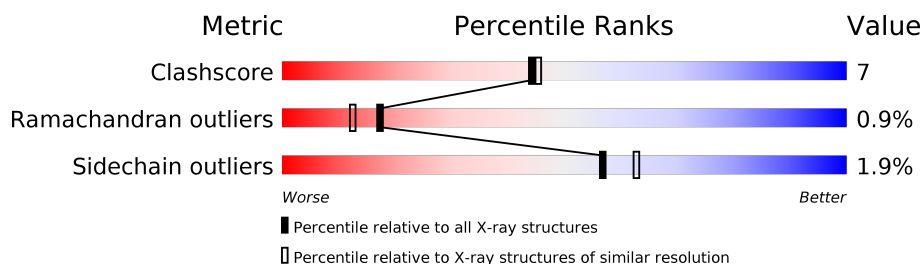
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	
1	H	221	

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Mol	Chain	Length	Quality of chain
1	I	221	 82% 17% .
1	J	221	 80% 19% .
1	K	221	 84% 15% .
1	L	221	 81% 19% .
1	M	221	 80% 19% .
1	N	221	 81% 19% .
1	O	221	 79% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27375 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.

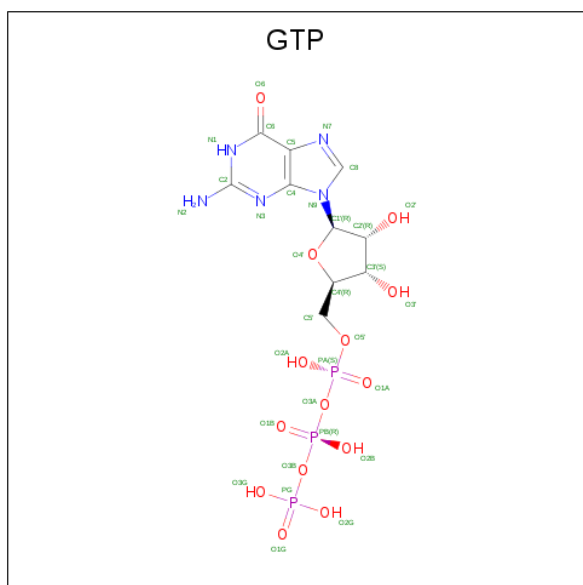
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	B	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	C	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	D	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	E	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	F	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	G	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	H	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	I	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	J	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	K	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	L	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	M	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	N	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			
1	O	221	Total	C	N	O	S	148	0	0
			1728	1085	307	327	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
B	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
C	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
D	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
E	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
F	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
G	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
H	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
I	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
J	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
K	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
L	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
M	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
N	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5
O	112	SER	HIS	ENGINEERED MUTATION	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	64	Total	O	0	0
			64	64		
3	C	66	Total	O	0	0
			66	66		
3	D	66	Total	O	0	0
			66	66		
3	E	63	Total	O	0	0
			63	63		
3	F	66	Total	O	0	0
			66	66		
3	G	67	Total	O	0	0
			67	67		
3	H	64	Total	O	0	0
			64	64		

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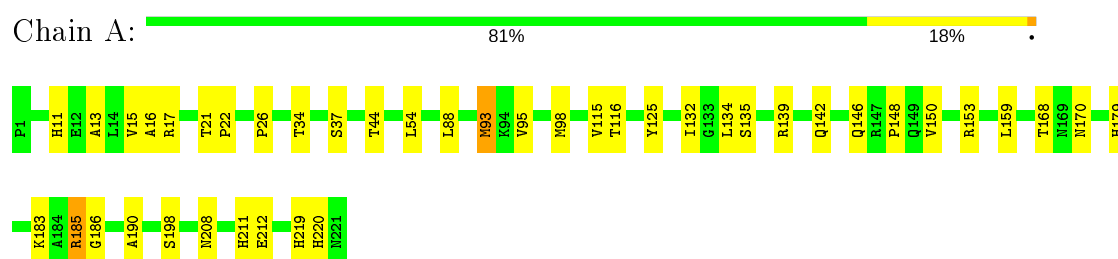
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	67	Total 67	O 67	0	0
3	J	61	Total 61	O 61	0	0
3	K	65	Total 65	O 65	0	0
3	L	65	Total 65	O 65	0	0
3	M	68	Total 68	O 68	0	0
3	N	64	Total 64	O 64	0	0
3	O	63	Total 63	O 63	0	0

3 Residue-property plots

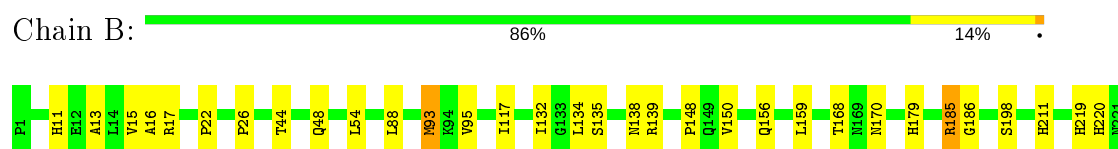
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

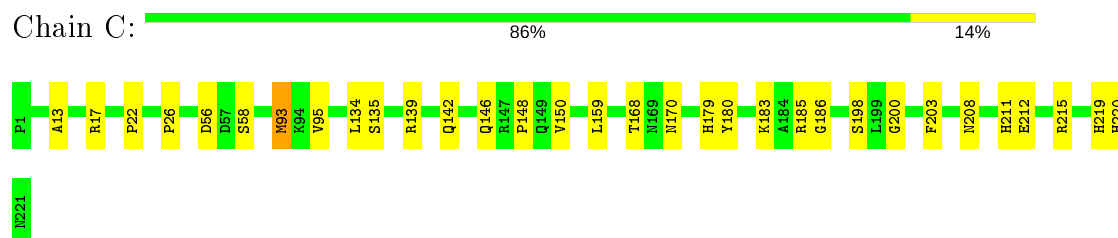
• Molecule 1: GTP CYCLOHYDROLASE I



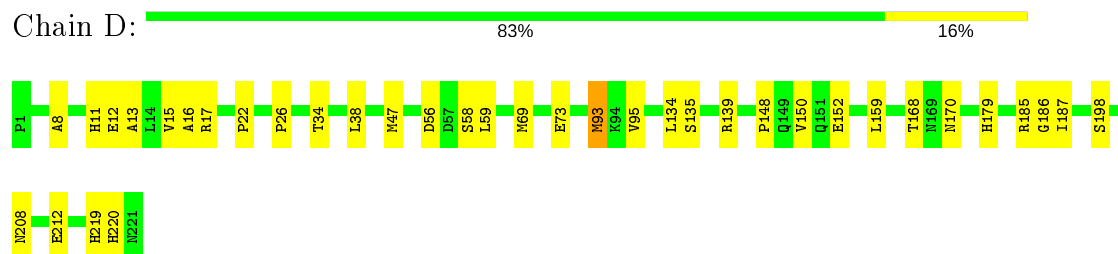
• Molecule 1: GTP CYCLOHYDROLASE I



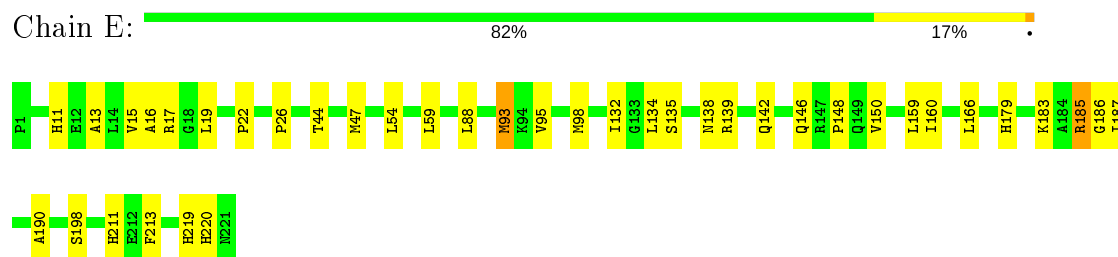
• Molecule 1: GTP CYCLOHYDROLASE I



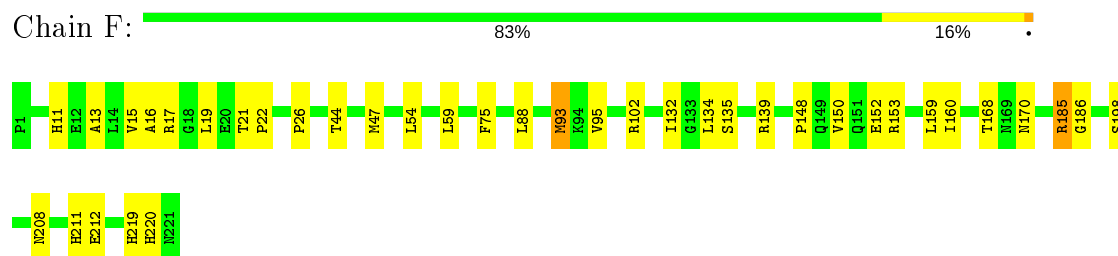
• Molecule 1: GTP CYCLOHYDROLASE I



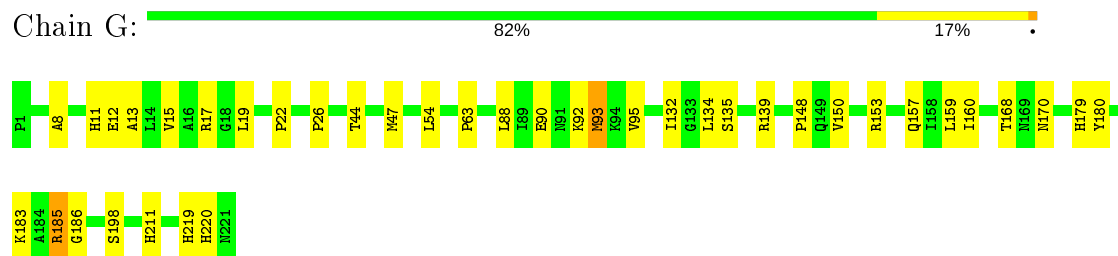
• Molecule 1: GTP CYCLOHYDROLASE I



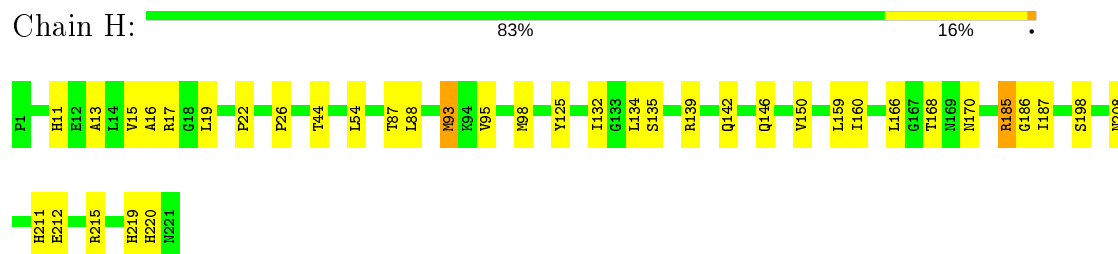
- Molecule 1: GTP CYCLOHYDROLASE I



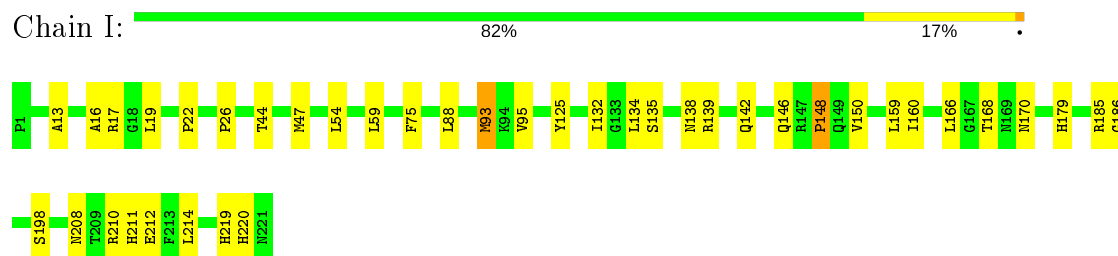
- Molecule 1: GTP CYCLOHYDROLASE I



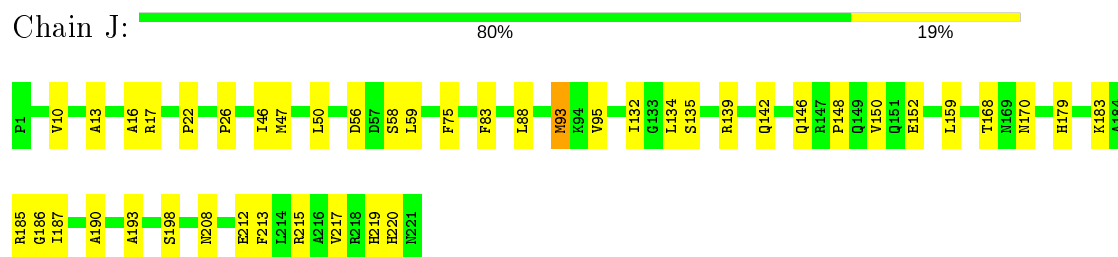
- Molecule 1: GTP CYCLOHYDROLASE I



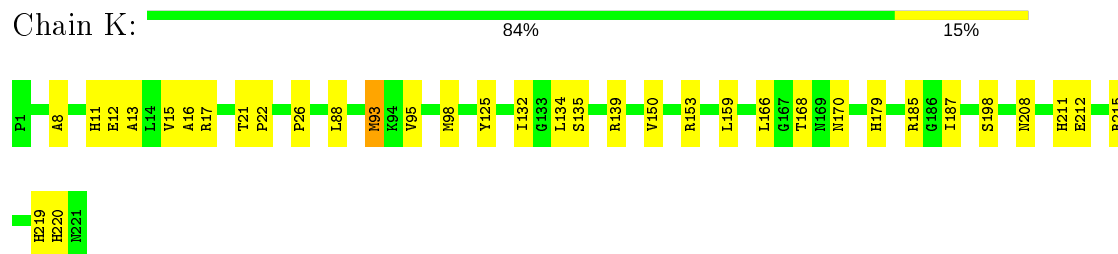
- Molecule 1: GTP CYCLOHYDROLASE I



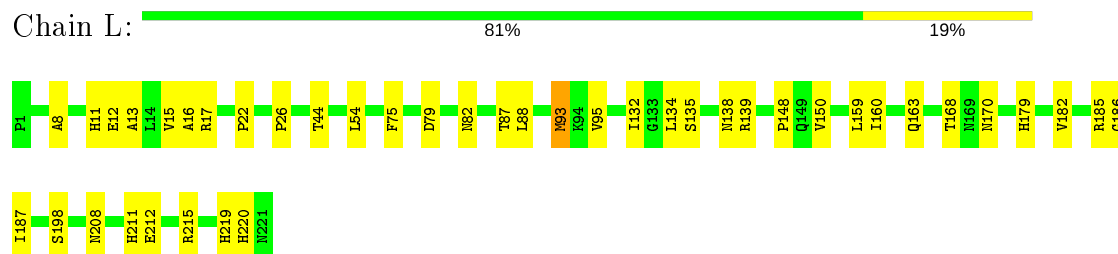
- Molecule 1: GTP CYCLOHYDROLASE I



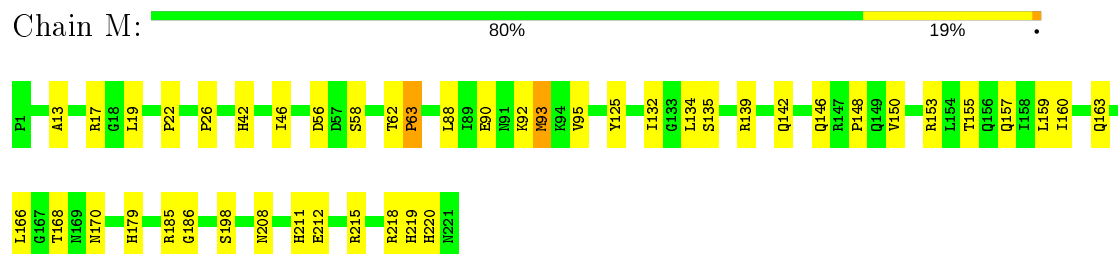
- Molecule 1: GTP CYCLOHYDROLASE I



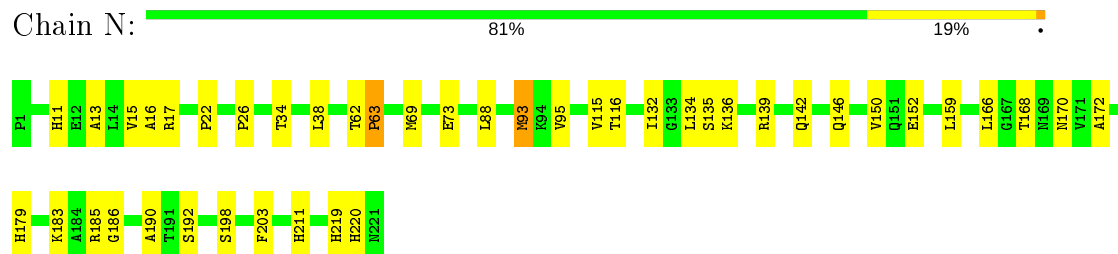
- Molecule 1: GTP CYCLOHYDROLASE I



- Molecule 1: GTP CYCLOHYDROLASE I



- Molecule 1: GTP CYCLOHYDROLASE I

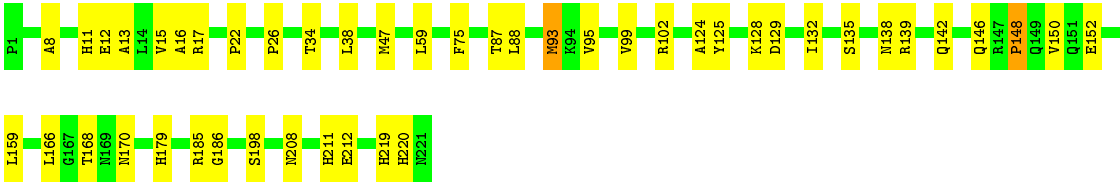


- Molecule 1: GTP CYCLOHYDROLASE I

Chain O:

79%

20%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	314.95Å 219.14Å 131.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.4 (8.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.200 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27375	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	0/1755	0.82	2/2377 (0.1%)
1	B	0.53	0/1755	0.82	3/2377 (0.1%)
1	C	0.53	0/1755	0.82	2/2377 (0.1%)
1	D	0.53	0/1755	0.82	2/2377 (0.1%)
1	E	0.51	0/1755	0.79	2/2377 (0.1%)
1	F	0.50	0/1755	0.77	1/2377 (0.0%)
1	G	0.50	0/1755	0.79	2/2377 (0.1%)
1	H	0.51	0/1755	0.81	1/2377 (0.0%)
1	I	0.52	0/1755	0.80	2/2377 (0.1%)
1	J	0.54	0/1755	0.81	1/2377 (0.0%)
1	K	0.53	0/1755	0.82	1/2377 (0.0%)
1	L	0.49	0/1755	0.79	1/2377 (0.0%)
1	M	0.51	0/1755	0.81	2/2377 (0.1%)
1	N	0.52	0/1755	0.80	1/2377 (0.0%)
1	O	0.50	0/1755	0.79	2/2377 (0.1%)
All	All	0.52	0/26325	0.80	25/35655 (0.1%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	150	VAL	N-CA-C	-6.28	94.05	111.00
1	C	150	VAL	N-CA-C	-6.25	94.12	111.00
1	D	150	VAL	N-CA-C	-6.23	94.19	111.00
1	H	150	VAL	N-CA-C	-6.16	94.36	111.00
1	K	150	VAL	N-CA-C	-6.15	94.40	111.00

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	1728	0	1766	24	0
1	B	1728	0	1766	19	0
1	C	1728	0	1766	18	0
1	D	1728	0	1766	20	0
1	E	1728	0	1766	22	0
1	F	1728	0	1766	22	0
1	G	1728	0	1766	20	0
1	H	1728	0	1766	22	0
1	I	1728	0	1766	25	0
1	J	1728	0	1766	24	0
1	K	1728	0	1766	19	0
1	L	1728	0	1766	29	0
1	M	1728	0	1766	26	0
1	N	1728	0	1766	24	0
1	O	1728	0	1766	30	0
2	A	32	0	12	1	0
2	B	32	0	12	2	0
2	C	32	0	12	1	0
2	D	32	0	12	2	0
2	E	32	0	12	1	0
2	F	32	0	12	2	0
2	G	32	0	12	2	0
2	H	32	0	12	2	0
2	I	32	0	12	2	0
2	J	32	0	12	2	0
2	K	32	0	12	2	0
2	L	32	0	12	2	0
2	M	32	0	12	3	0
2	N	32	0	12	1	0
2	O	32	0	12	2	0
3	A	66	0	0	4	0
3	B	64	0	0	4	0
3	C	66	0	0	2	0
3	D	66	0	0	2	0
3	E	63	0	0	1	0
3	F	66	0	0	0	0
3	G	67	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	64	0	0	1	0
3	I	67	0	0	2	0
3	J	61	0	0	2	0
3	K	65	0	0	2	0
3	L	65	0	0	2	0
3	M	68	0	0	1	0
3	N	64	0	0	2	0
3	O	63	0	0	4	0
All	All	27375	0	26670	323	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 323 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:I:13:ALA:O	1:I:17:ARG:HD3	1.83	0.78
1:O:93:MET:HB2	1:O:95:VAL:HG23	1.72	0.71
1:C:13:ALA:O	1:C:17:ARG:HD3	1.90	0.71
1:H:93:MET:HB2	1:H:95:VAL:HG23	1.71	0.71
1:L:93:MET:HB2	1:L:95:VAL:HG23	1.73	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
1	B	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
1	C	219/221 (99%)	211 (96%)	6 (3%)	2 (1%)	17	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	17	12
1	E	219/221 (99%)	208 (95%)	9 (4%)	2 (1%)	17	12
1	F	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	17	12
1	G	219/221 (99%)	206 (94%)	11 (5%)	2 (1%)	17	12
1	H	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
1	I	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
1	J	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	17	12
1	K	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
1	L	219/221 (99%)	205 (94%)	12 (6%)	2 (1%)	17	12
1	M	219/221 (99%)	208 (95%)	8 (4%)	3 (1%)	11	6
1	N	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
1	O	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	17	12
All	All	3285/3315 (99%)	3114 (95%)	140 (4%)	31 (1%)	17	12

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	PRO
1	I	22	PRO
1	K	22	PRO
1	L	22	PRO
1	A	22	PRO

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	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	B	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	C	194/194 (100%)	191 (98%)	3 (2%)	65	71
1	D	194/194 (100%)	191 (98%)	3 (2%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	F	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	G	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	H	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	I	194/194 (100%)	191 (98%)	3 (2%)	65	71
1	J	194/194 (100%)	191 (98%)	3 (2%)	65	71
1	K	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	L	194/194 (100%)	191 (98%)	3 (2%)	65	71
1	M	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	N	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	O	194/194 (100%)	191 (98%)	3 (2%)	65	71
All	All	2910/2910 (100%)	2856 (98%)	54 (2%)	57	63

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	219	HIS
1	I	93	MET
1	N	219	HIS
1	G	220	HIS
1	H	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	207	GLN
1	I	163	GLN
1	O	138	ASN
1	H	138	ASN
1	H	207	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GTP	K	411	-	26,34,34	1.36	3 (11%)	33,54,54	2.32	12 (36%)
2	GTP	A	401	-	26,34,34	1.41	4 (15%)	33,54,54	2.24	10 (30%)
2	GTP	O	415	-	26,34,34	1.70	4 (15%)	33,54,54	2.34	13 (39%)
2	GTP	G	407	-	26,34,34	1.62	8 (30%)	33,54,54	2.28	12 (36%)
2	GTP	J	410	-	26,34,34	1.59	3 (11%)	33,54,54	2.28	9 (27%)
2	GTP	D	404	-	26,34,34	1.76	6 (23%)	33,54,54	2.36	11 (33%)
2	GTP	E	405	-	26,34,34	1.44	5 (19%)	33,54,54	2.38	13 (39%)
2	GTP	L	412	-	26,34,34	1.64	6 (23%)	33,54,54	2.41	13 (39%)
2	GTP	C	403	-	26,34,34	1.73	7 (26%)	33,54,54	2.38	12 (36%)
2	GTP	I	409	-	26,34,34	1.64	7 (26%)	33,54,54	2.42	14 (42%)
2	GTP	N	414	-	26,34,34	1.46	3 (11%)	33,54,54	2.29	9 (27%)
2	GTP	B	402	-	26,34,34	1.44	5 (19%)	33,54,54	2.22	9 (27%)
2	GTP	F	406	-	26,34,34	1.59	4 (15%)	33,54,54	2.34	11 (33%)
2	GTP	H	408	-	26,34,34	1.60	7 (26%)	33,54,54	2.39	10 (30%)
2	GTP	M	413	-	26,34,34	1.67	7 (26%)	33,54,54	2.40	14 (42%)

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	K	411	-	-	4/18/38/38	0/3/3/3
2	GTP	A	401	-	-	4/18/38/38	0/3/3/3
2	GTP	O	415	-	-	2/18/38/38	0/3/3/3
2	GTP	G	407	-	-	5/18/38/38	0/3/3/3
2	GTP	J	410	-	-	3/18/38/38	0/3/3/3
2	GTP	D	404	-	-	3/18/38/38	0/3/3/3
2	GTP	E	405	-	-	4/18/38/38	0/3/3/3
2	GTP	L	412	-	-	4/18/38/38	0/3/3/3
2	GTP	C	403	-	-	4/18/38/38	0/3/3/3
2	GTP	I	409	-	-	2/18/38/38	0/3/3/3
2	GTP	N	414	-	-	4/18/38/38	0/3/3/3
2	GTP	B	402	-	-	3/18/38/38	0/3/3/3
2	GTP	F	406	-	-	2/18/38/38	0/3/3/3
2	GTP	H	408	-	-	3/18/38/38	0/3/3/3
2	GTP	M	413	-	-	4/18/38/38	0/3/3/3

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	404	GTP	C6-N1	4.99	1.41	1.33
2	J	410	GTP	C6-N1	4.38	1.40	1.33
2	F	406	GTP	C6-N1	4.09	1.40	1.33
2	O	415	GTP	C6-N1	4.08	1.40	1.33
2	L	412	GTP	C6-N1	4.06	1.40	1.33

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	408	GTP	C5-C6-N1	-7.82	112.74	123.43
2	L	412	GTP	C5-C6-N1	-7.57	113.07	123.43
2	D	404	GTP	C5-C6-N1	-7.52	113.14	123.43
2	M	413	GTP	C5-C6-N1	-7.49	113.19	123.43
2	B	402	GTP	C5-C6-N1	-7.36	113.37	123.43

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	411	GTP	PB-O3B-PG-O2G
2	A	401	GTP	PB-O3B-PG-O2G
2	O	415	GTP	O4'-C4'-C5'-O5'
2	N	414	GTP	PB-O3B-PG-O2G
2	N	414	GTP	O4'-C4'-C5'-O5'

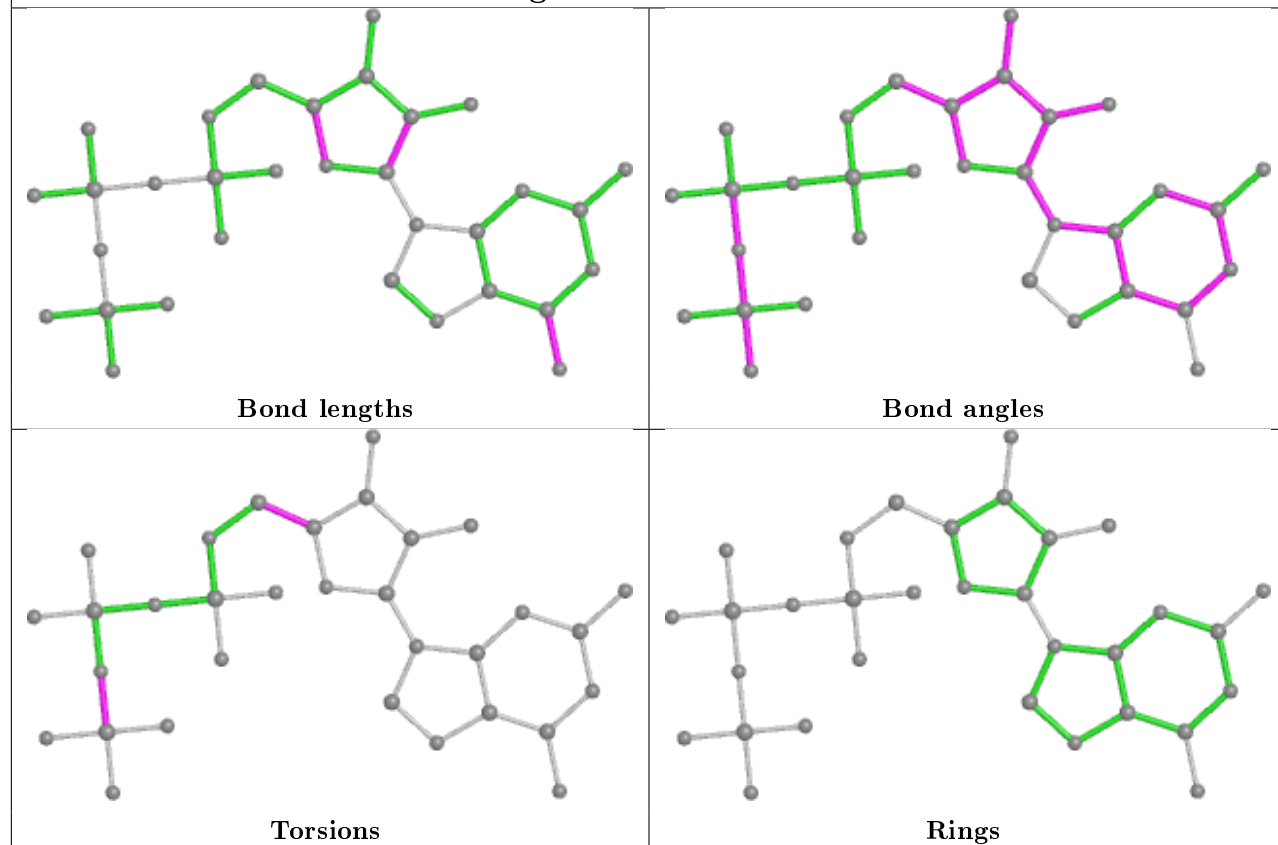
There are no ring outliers.

15 monomers are involved in 27 short contacts:

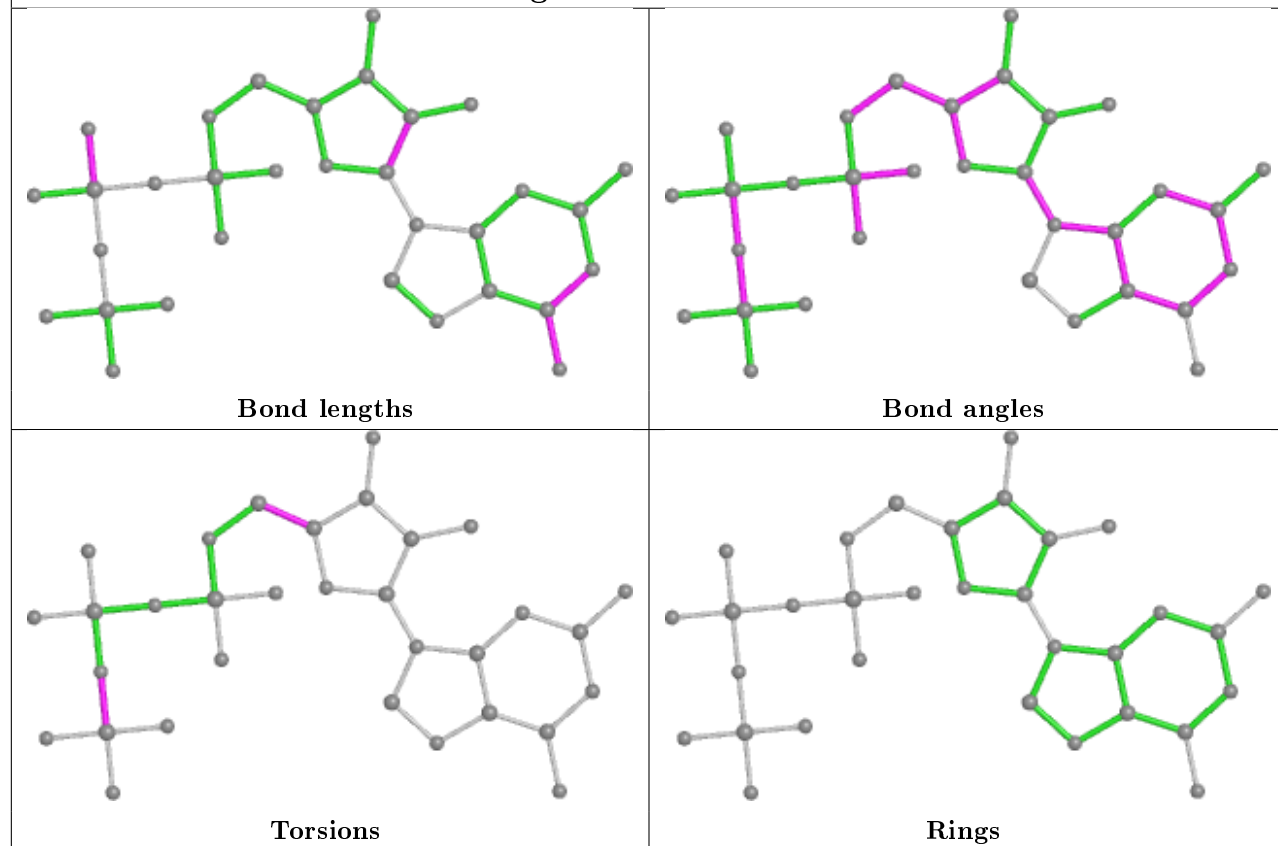
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	411	GTP	2	0
2	A	401	GTP	1	0
2	O	415	GTP	2	0
2	G	407	GTP	2	0
2	J	410	GTP	2	0
2	D	404	GTP	2	0
2	E	405	GTP	1	0
2	L	412	GTP	2	0
2	C	403	GTP	1	0
2	I	409	GTP	2	0
2	N	414	GTP	1	0
2	B	402	GTP	2	0
2	F	406	GTP	2	0
2	H	408	GTP	2	0
2	M	413	GTP	3	0

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.

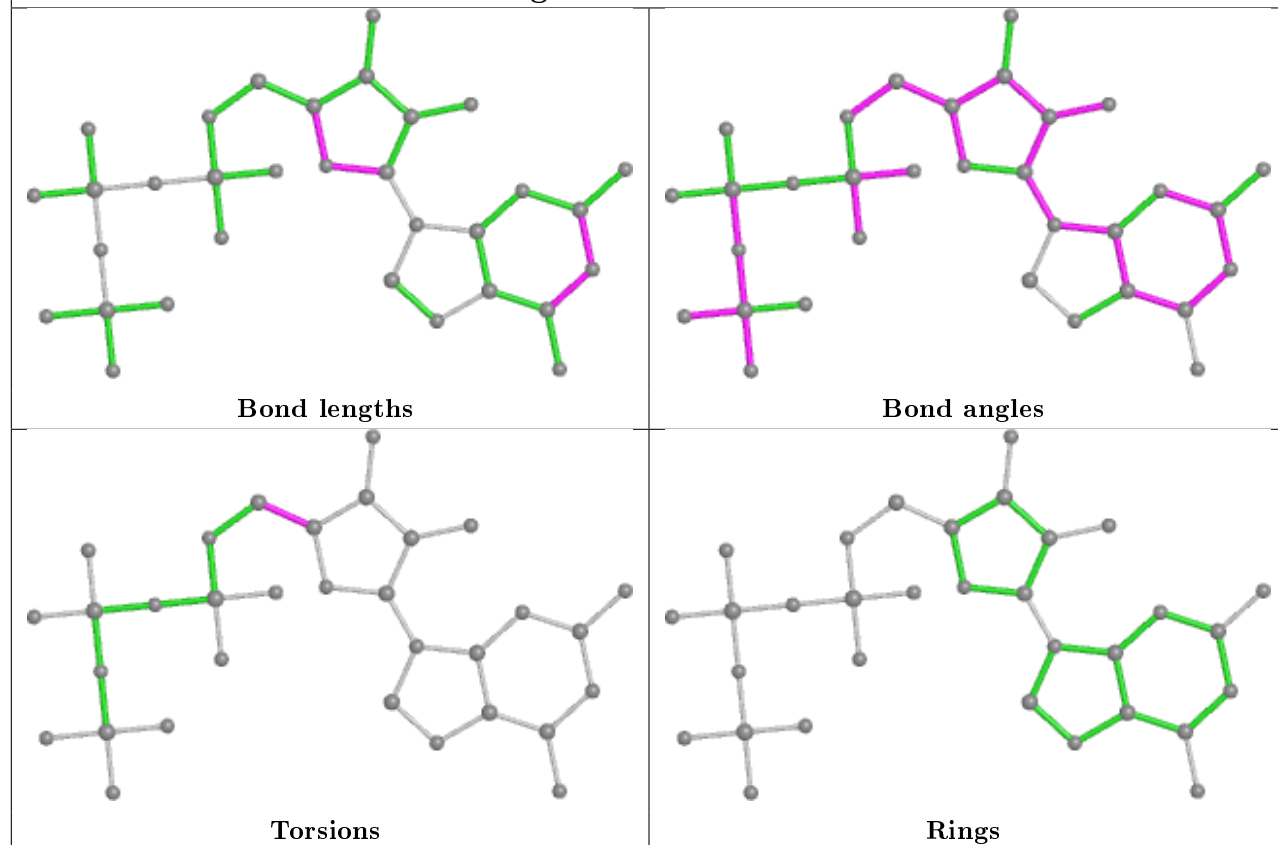
Ligand GTP K 411



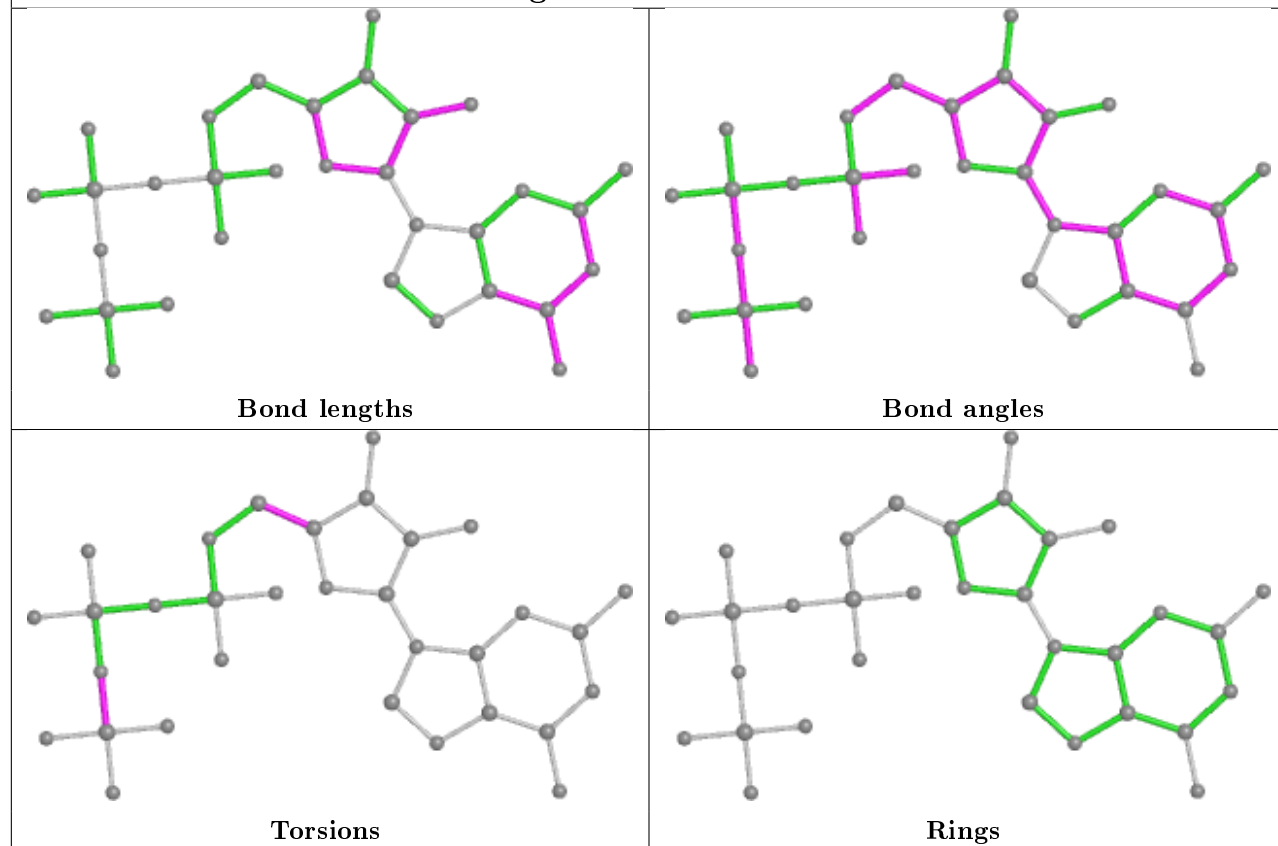
Ligand GTP A 401



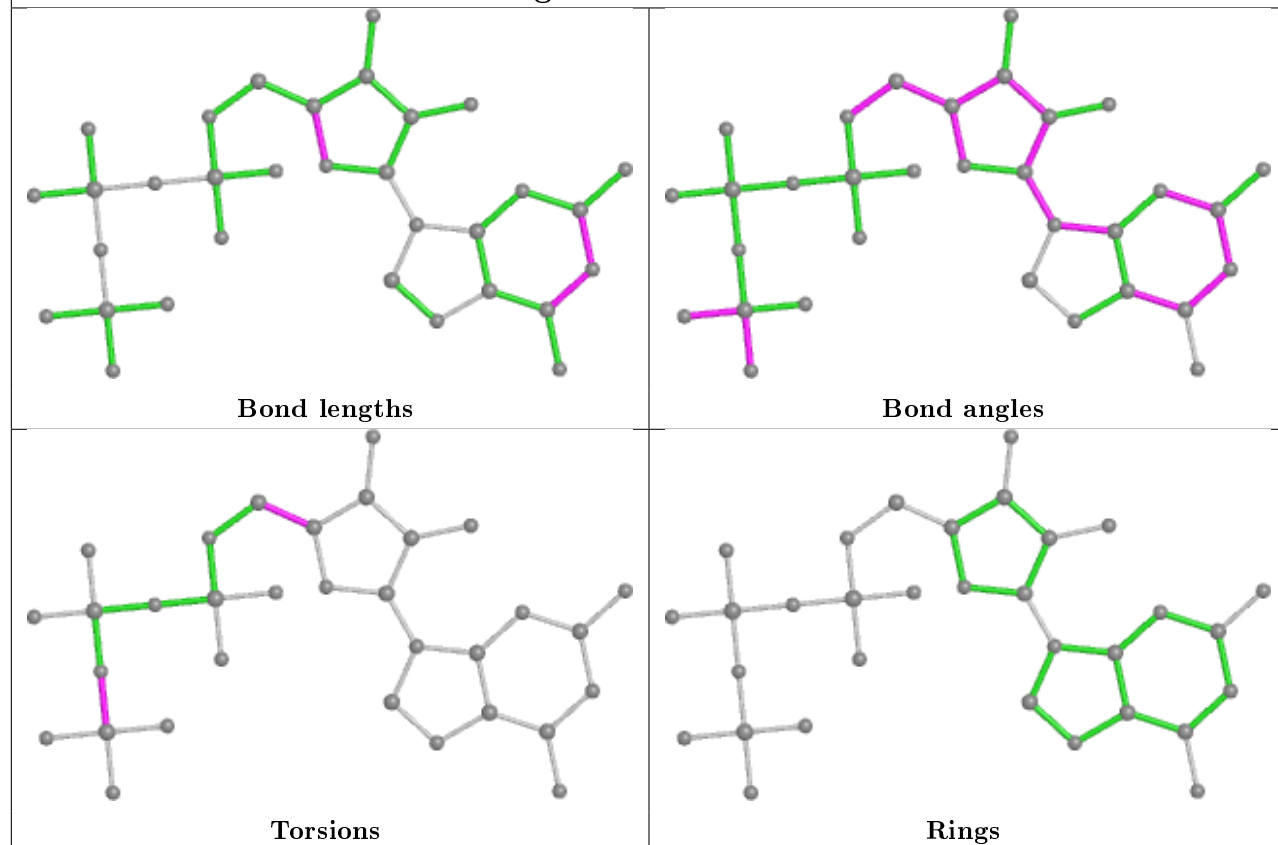
Ligand GTP O 415



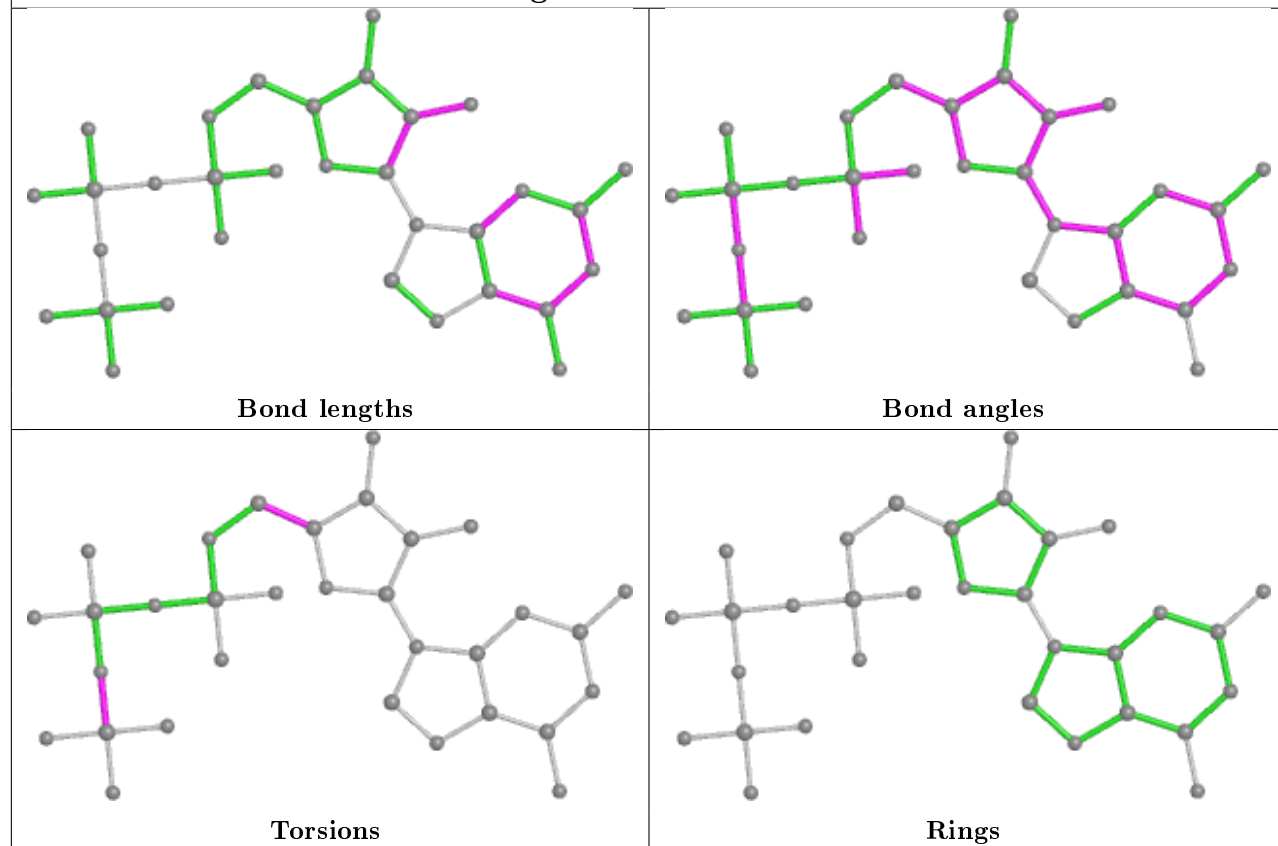
Ligand GTP G 407



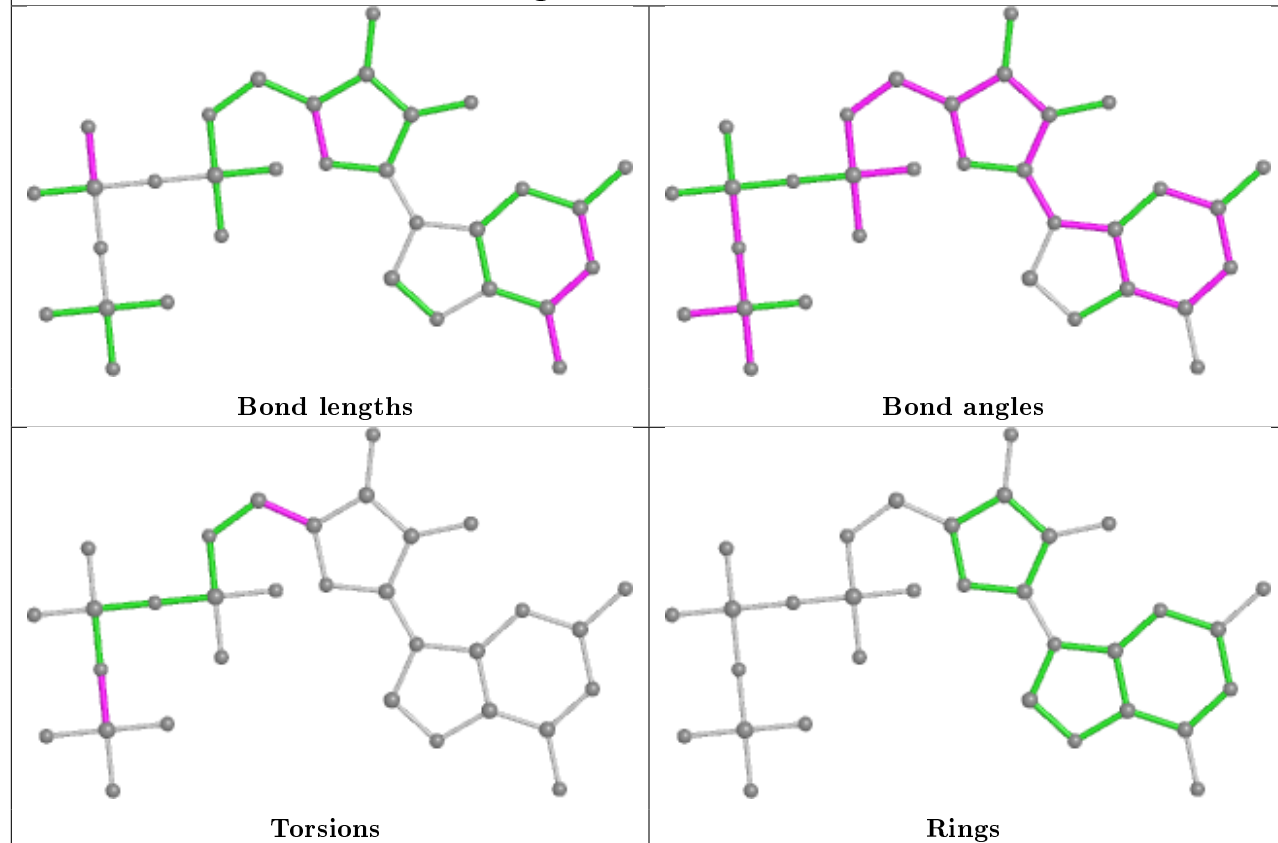
Ligand GTP J 410



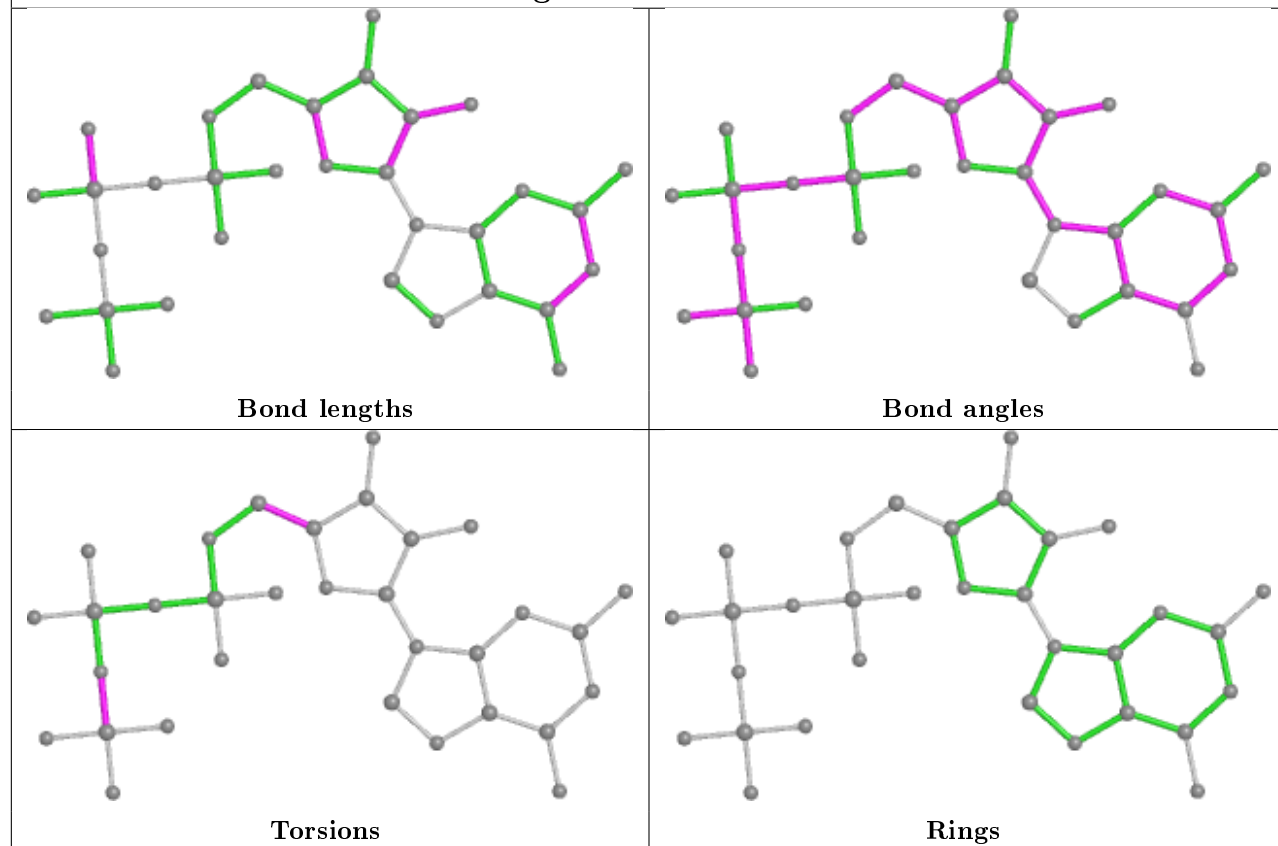
Ligand GTP D 404



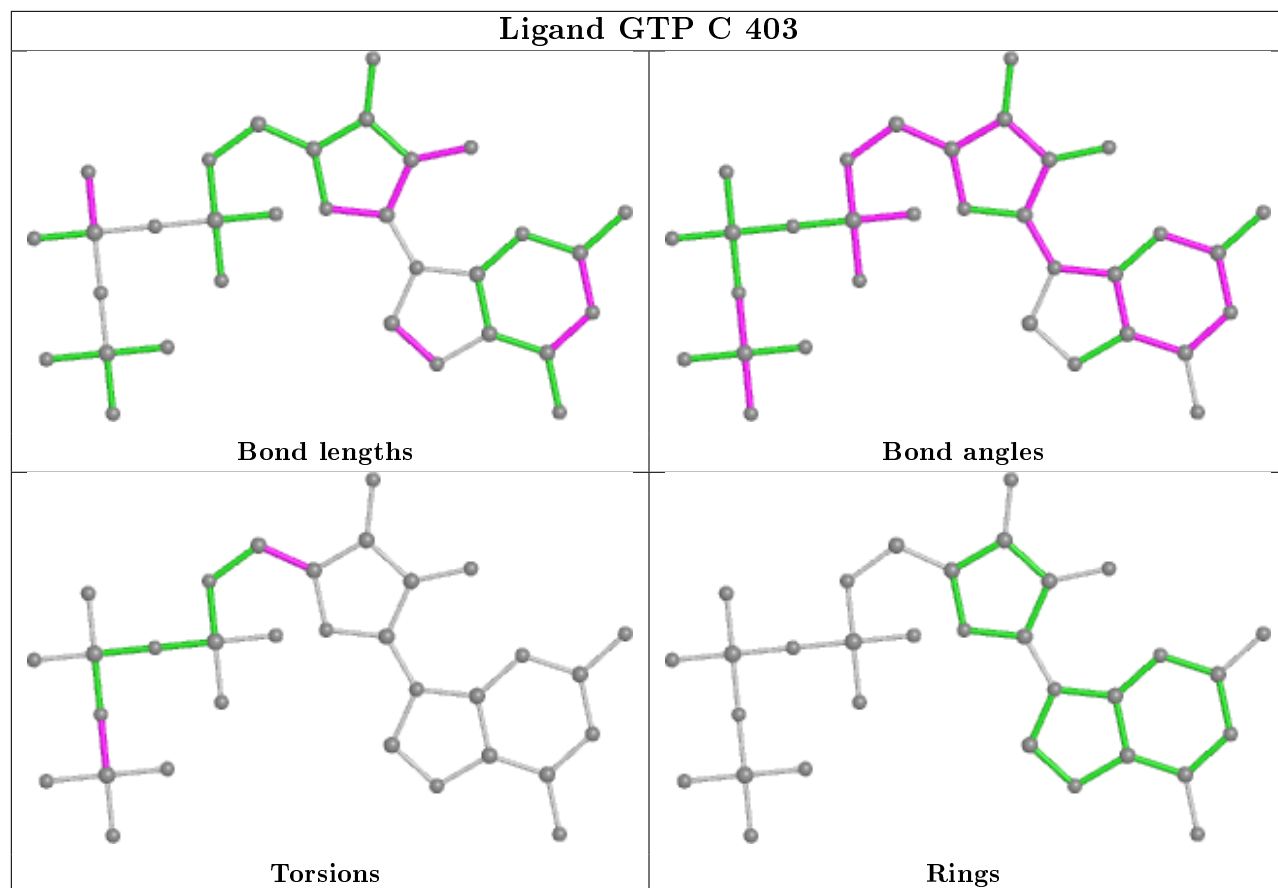
Ligand GTP E 405



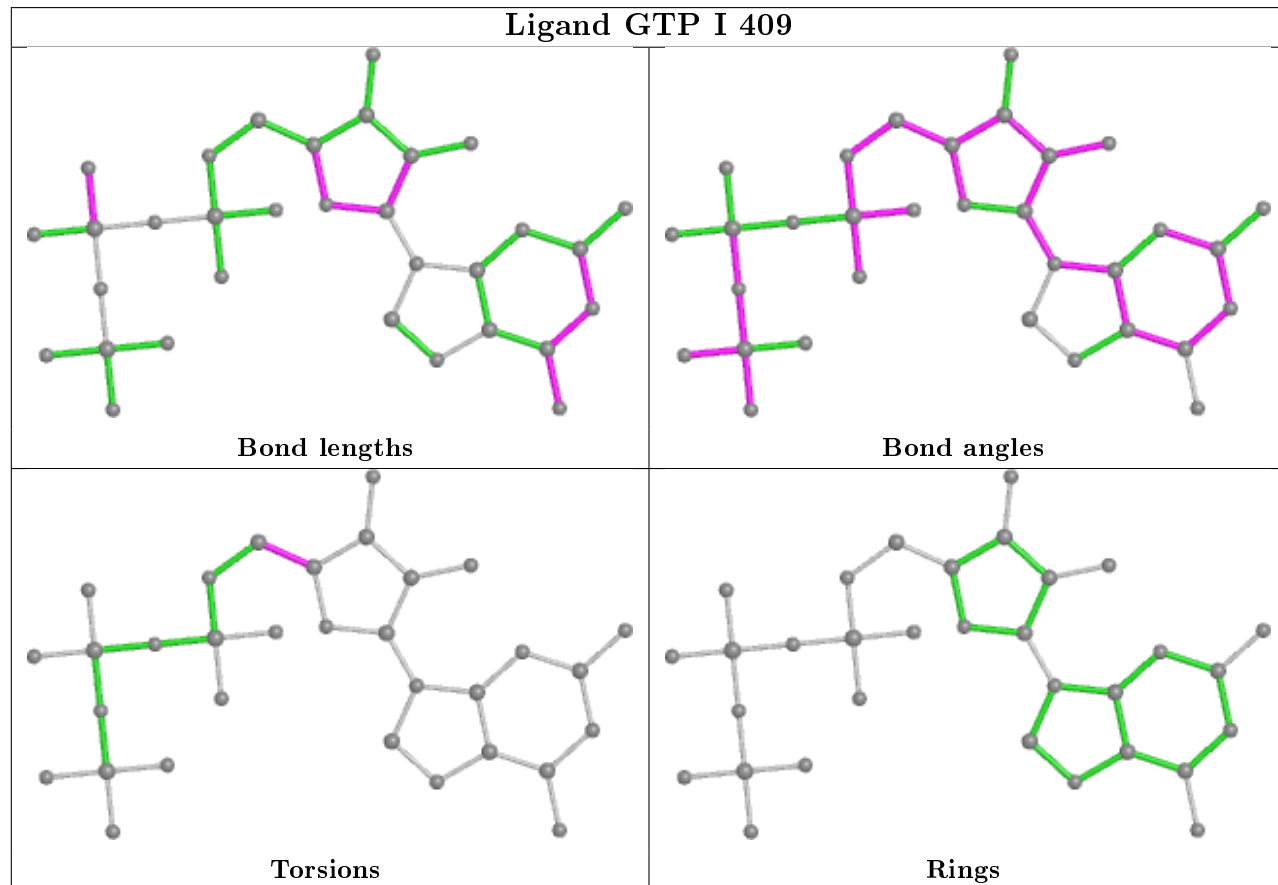
Ligand GTP L 412

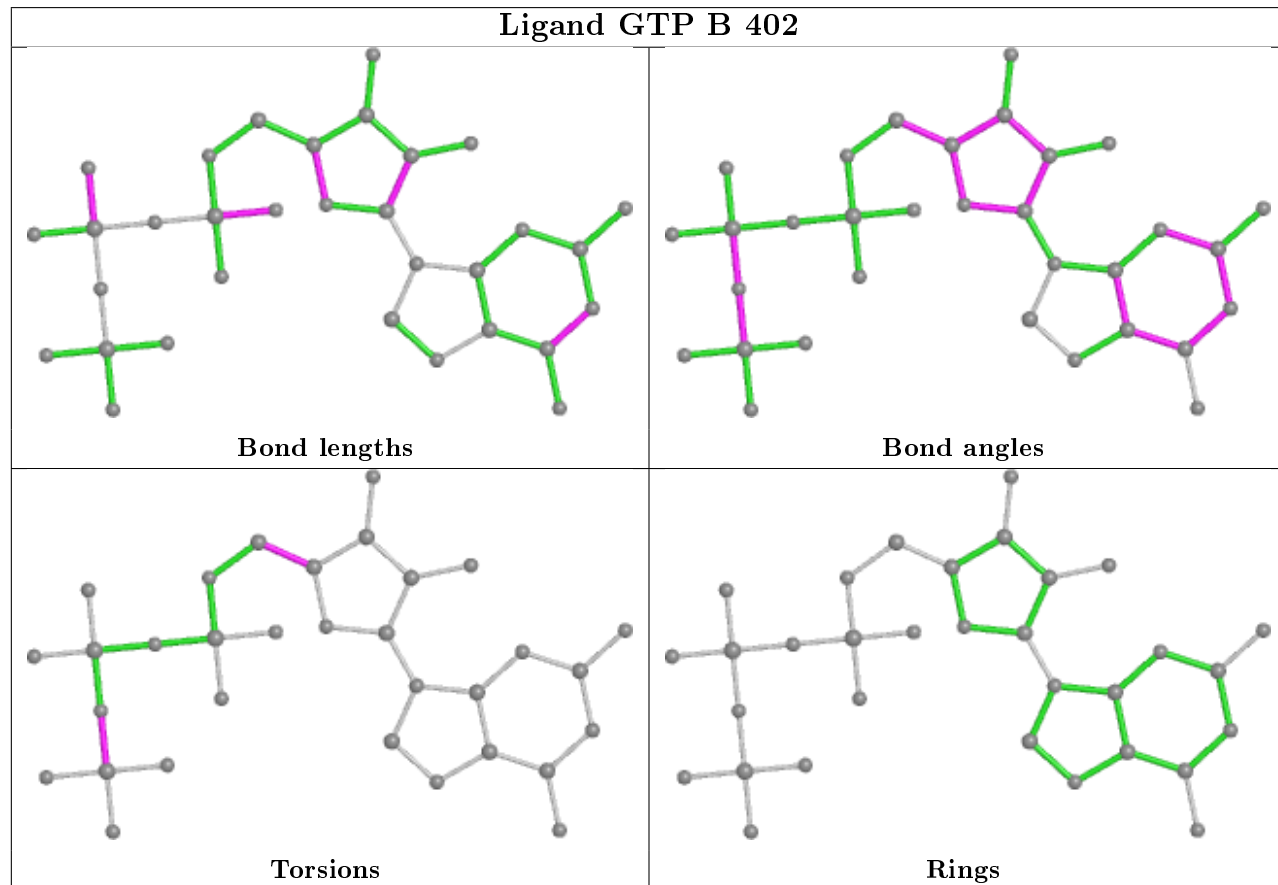
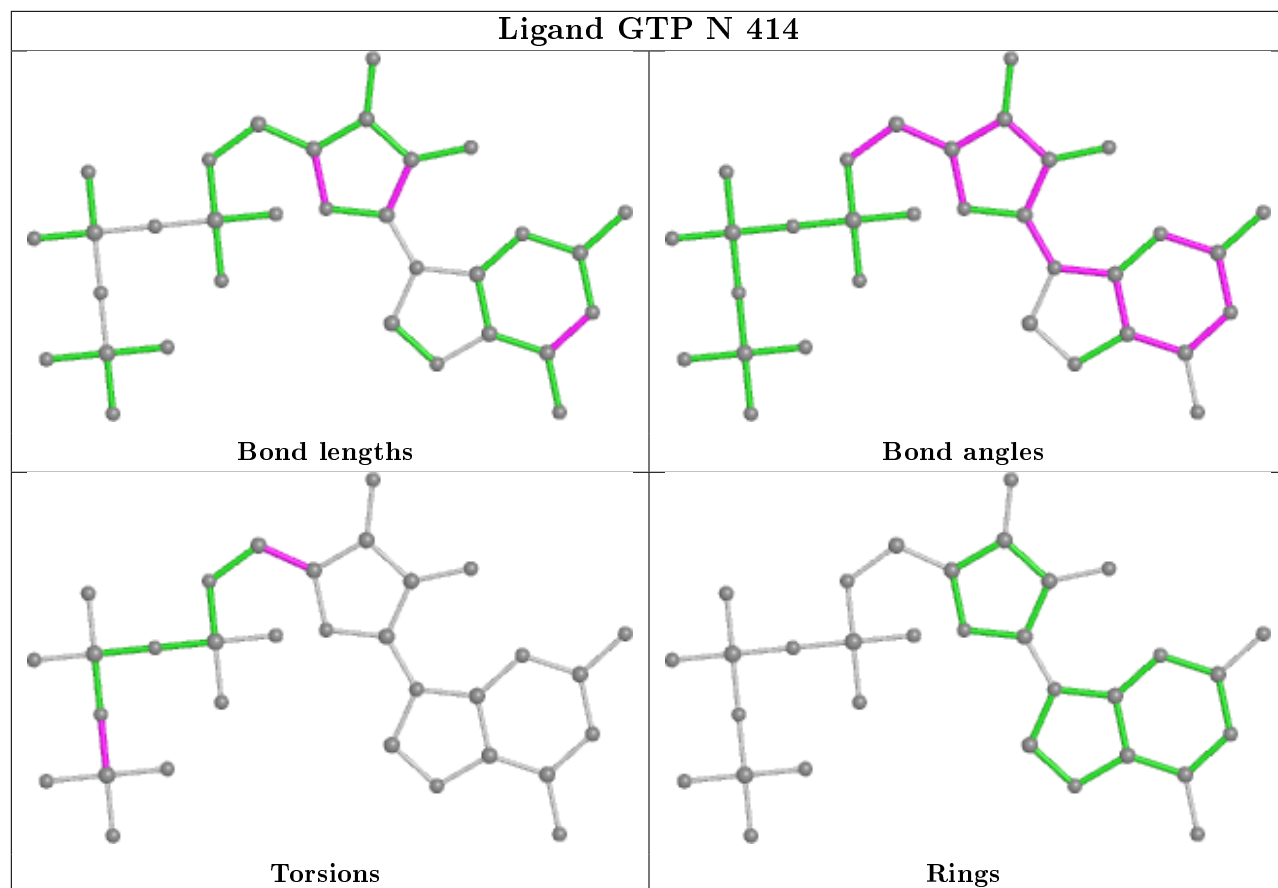


Ligand GTP C 403

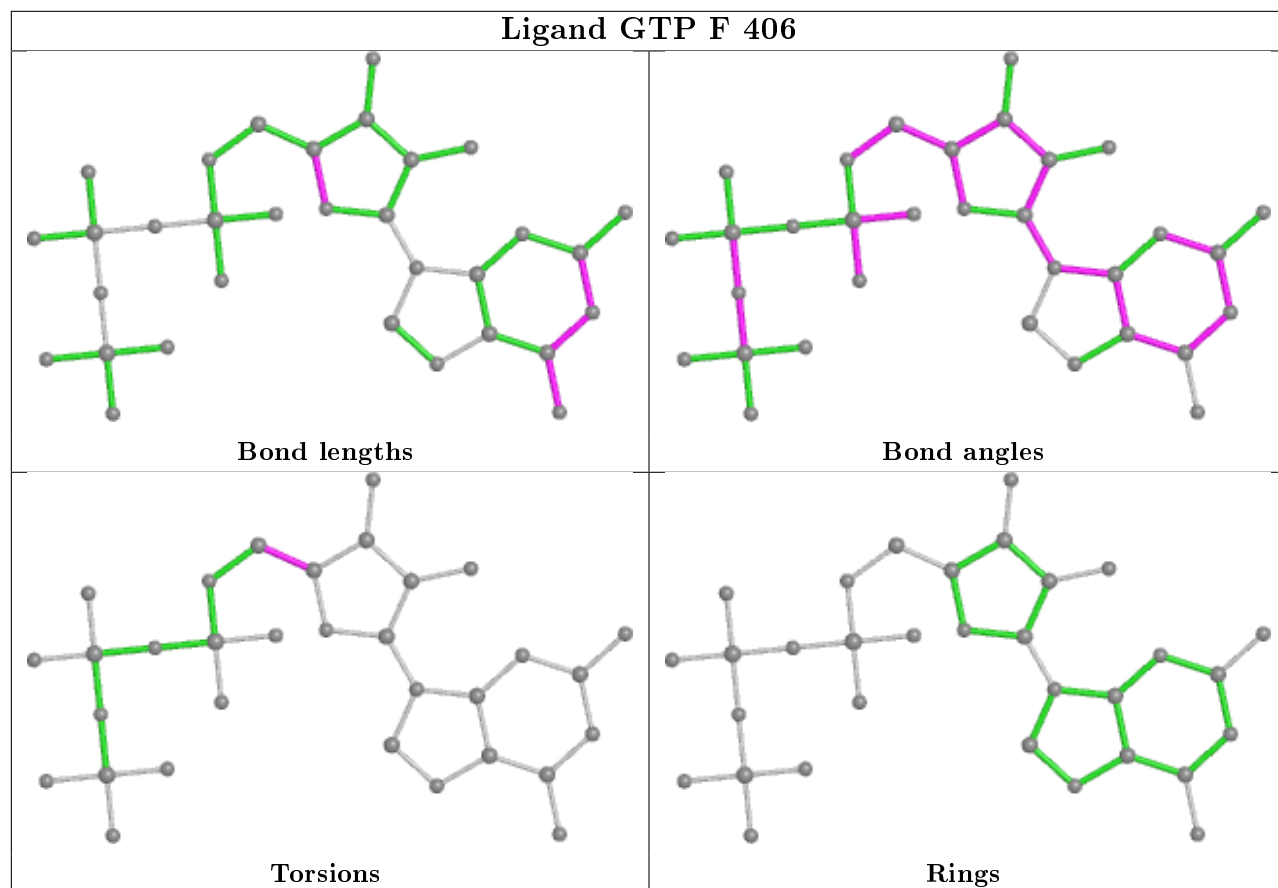


Ligand GTP I 409

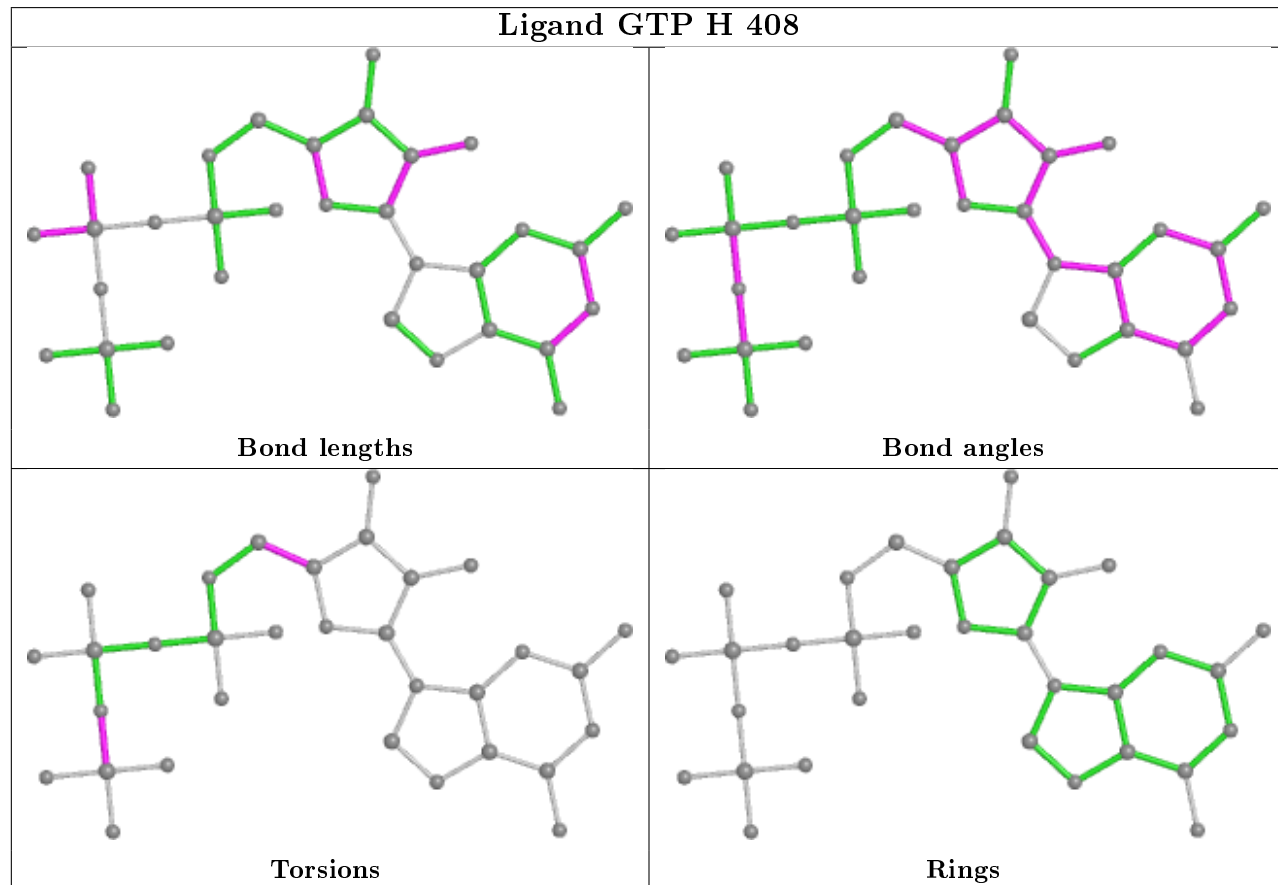


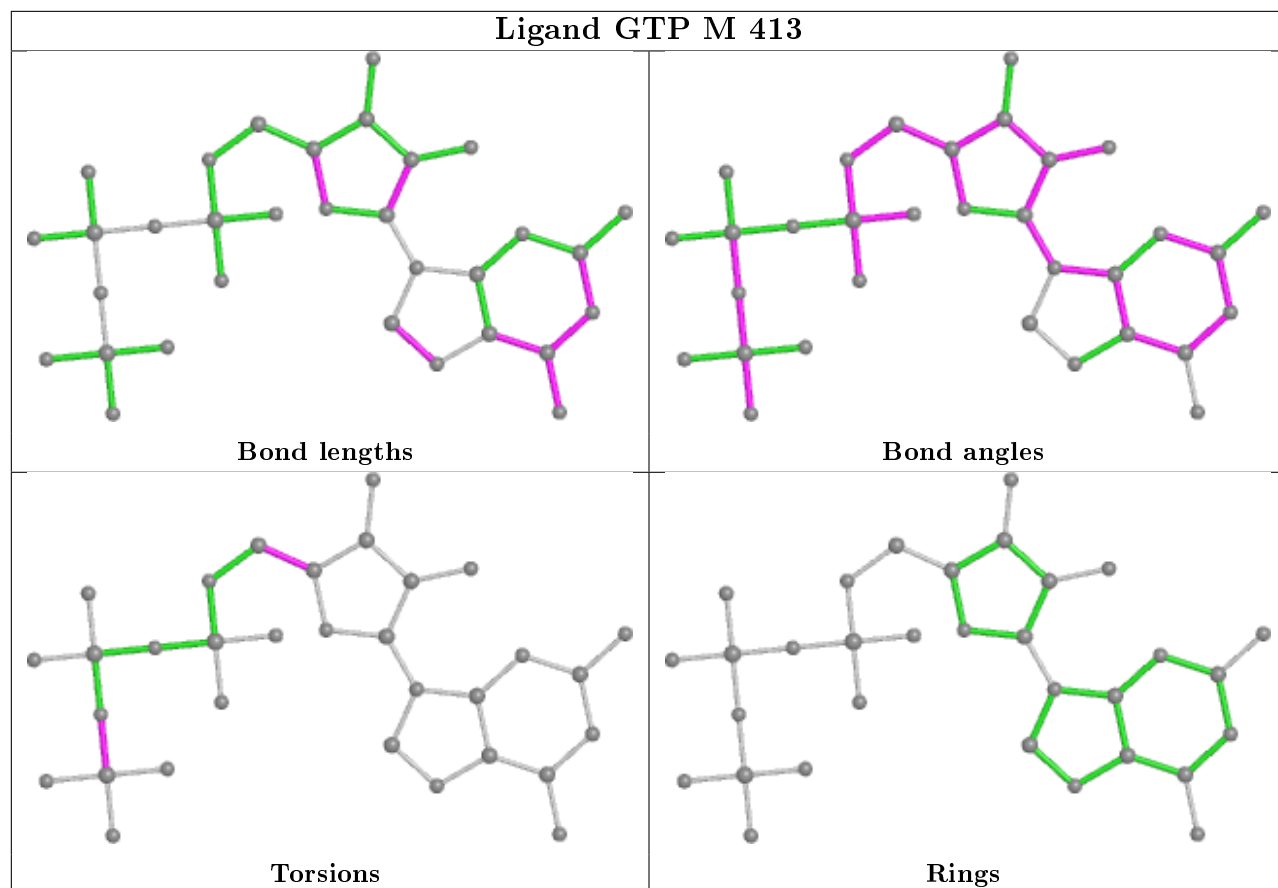


Ligand GTP F 406



Ligand GTP H 408





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.