



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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

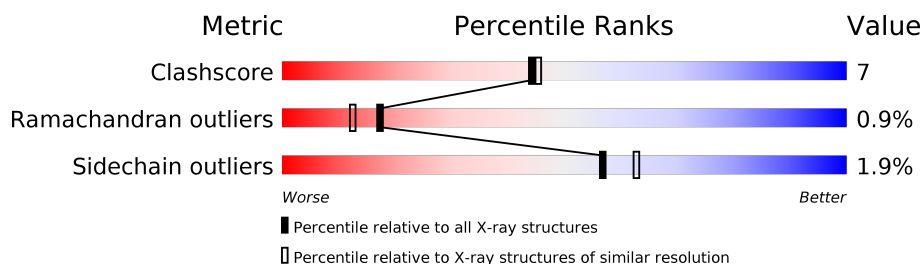
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

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	<div><div></div><div>82%17%</div><div></div></div>
1	J	221	<div><div></div><div>80%19%</div><div></div></div>
1	K	221	<div><div></div><div>84%15%</div><div></div></div>
1	L	221	<div><div></div><div>81%19%</div><div></div></div>
1	M	221	<div><div></div><div>80%19%</div><div></div></div>
1	N	221	<div><div></div><div>81%19%</div><div></div></div>
1	O	221	<div><div></div><div>79%20%</div><div></div></div>

## 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.

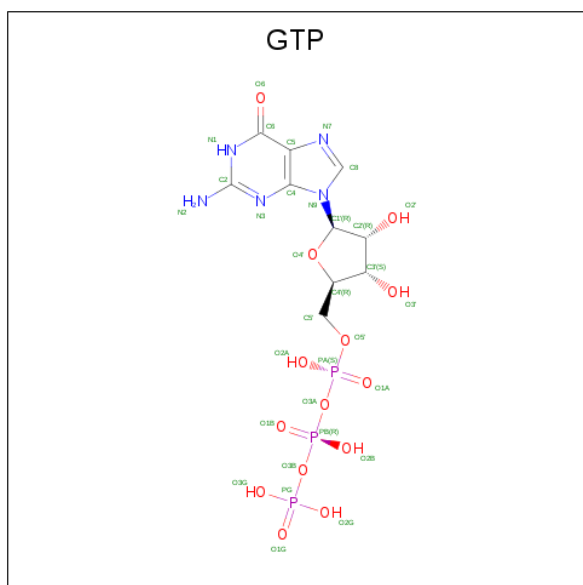
- Molecule 1 is a protein called GTP CYCLOHYDROLASE I.

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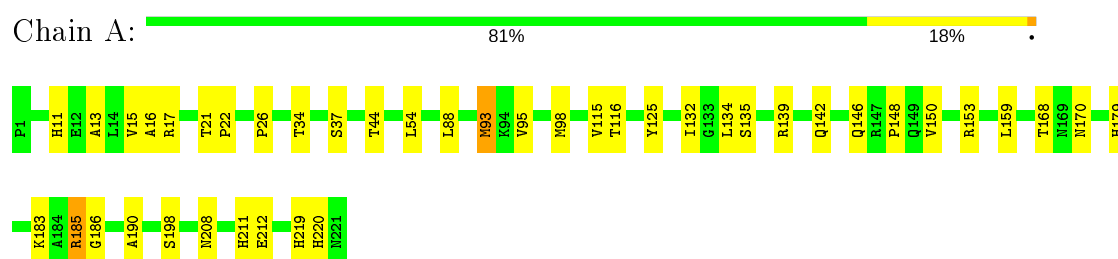
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	67	Total 67	O 67	0	0
3	J	61	Total 61	O 61	0	0
3	K	65	Total 65	O 65	0	0
3	L	65	Total 65	O 65	0	0
3	M	68	Total 68	O 68	0	0
3	N	64	Total 64	O 64	0	0
3	O	63	Total 63	O 63	0	0

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

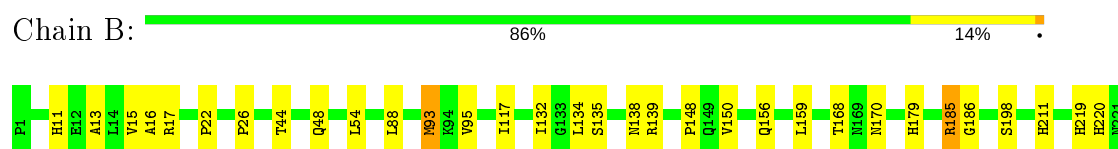
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

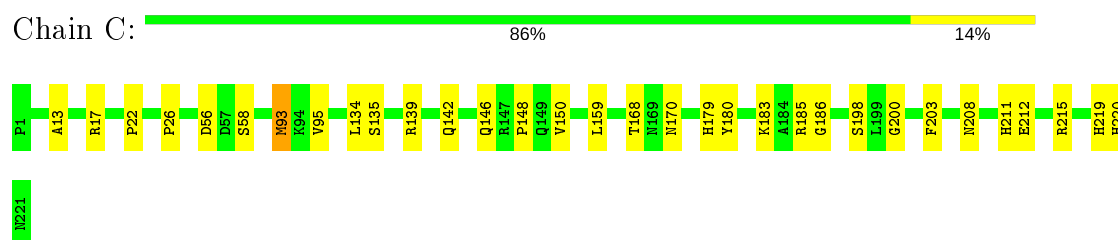
#### • Molecule 1: GTP CYCLOHYDROLASE I



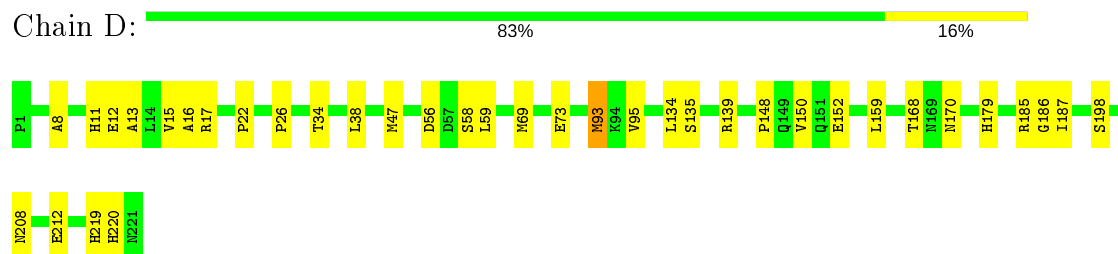
#### • Molecule 1: GTP CYCLOHYDROLASE I



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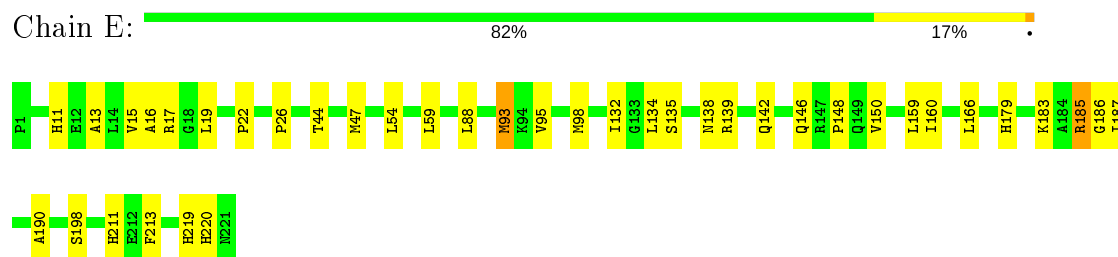


#### • Molecule 1: GTP CYCLOHYDROLASE I

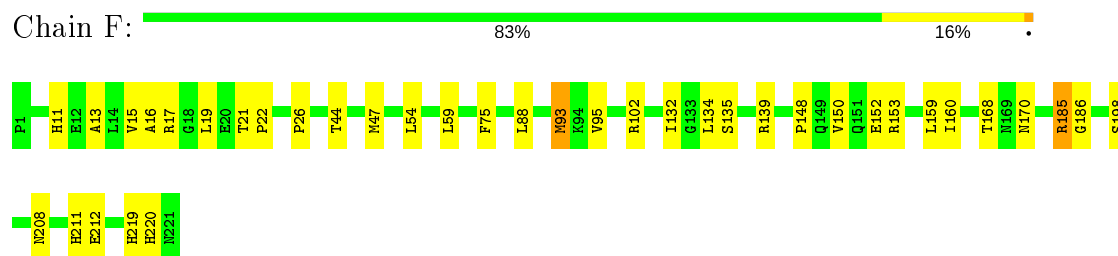


#### • Molecule 1: GTP CYCLOHYDROLASE I

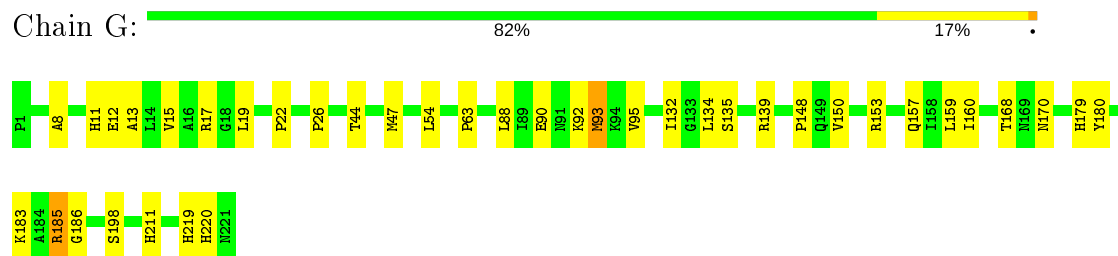




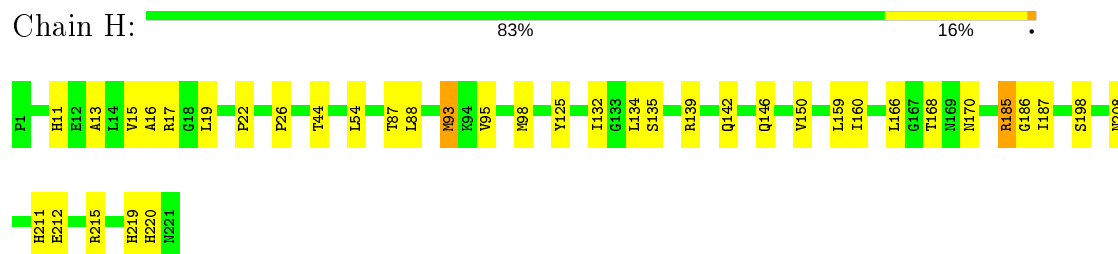
- Molecule 1: GTP CYCLOHYDROLASE I



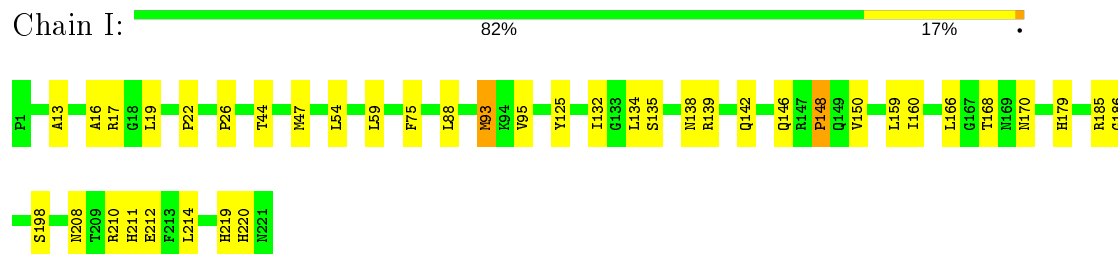
- Molecule 1: GTP CYCLOHYDROLASE I




- Molecule 1: GTP CYCLOHYDROLASE I

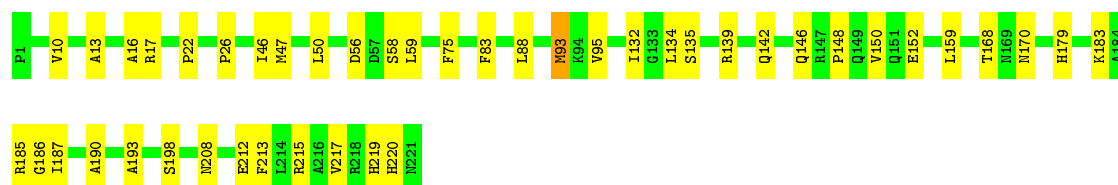


- Molecule 1: GTP CYCLOHYDROLASE I




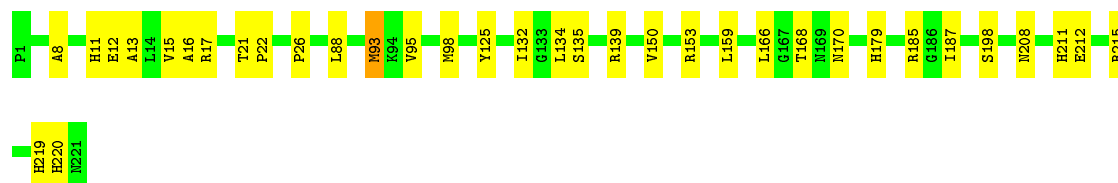
- Molecule 1: GTP CYCLOHYDROLASE I

Chain J:  80% 19%




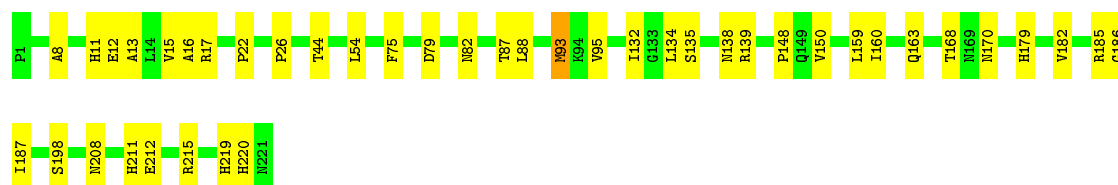
- Molecule 1: GTP CYCLOHYDROLASE I

Chain K:  84% 15%




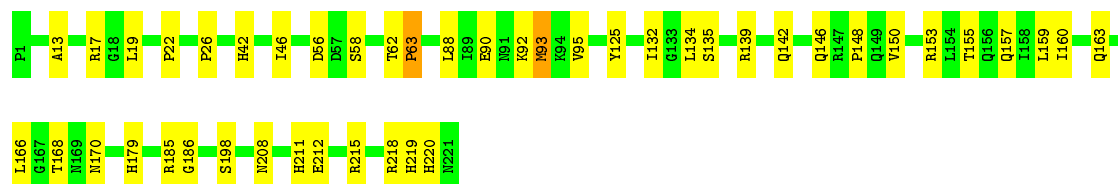
- Molecule 1: GTP CYCLOHYDROLASE I

Chain L:  81% 19%




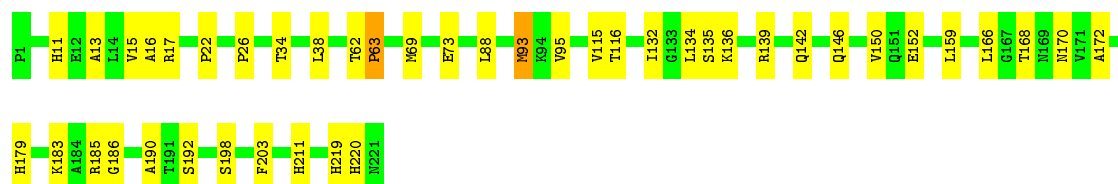
- Molecule 1: GTP CYCLOHYDROLASE I

Chain M:  80% 19%



- Molecule 1: GTP CYCLOHYDROLASE I

Chain N:  81% 19%

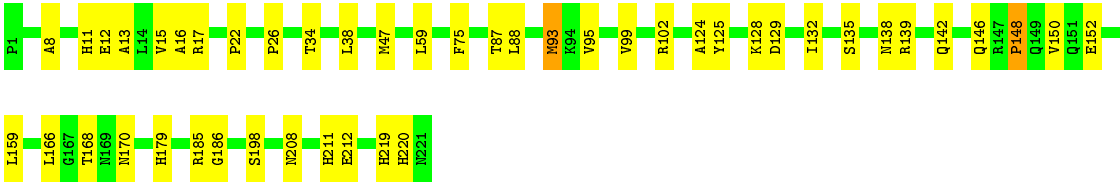


- Molecule 1: GTP CYCLOHYDROLASE I

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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.

All (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
1	G	150	VAL	N-CA-C	-6.11	94.50	111.00
1	B	150	VAL	N-CA-C	-6.02	94.75	111.00
1	M	150	VAL	N-CA-C	-6.02	94.75	111.00
1	O	150	VAL	N-CA-C	-5.93	94.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	150	VAL	N-CA-C	-5.86	95.17	111.00
1	A	150	VAL	N-CA-C	-5.83	95.27	111.00
1	N	150	VAL	N-CA-C	-5.77	95.41	111.00
1	D	148	PRO	N-CA-C	-5.67	97.35	112.10
1	M	148	PRO	N-CA-C	-5.59	97.56	112.10
1	C	148	PRO	N-CA-C	-5.57	97.63	112.10
1	I	150	VAL	N-CA-C	-5.54	96.06	111.00
1	L	150	VAL	N-CA-C	-5.51	96.12	111.00
1	E	150	VAL	N-CA-C	-5.48	96.19	111.00
1	A	148	PRO	N-CA-C	-5.40	98.06	112.10
1	I	148	PRO	N-CA-C	-5.34	98.22	112.10
1	G	148	PRO	N-CA-C	-5.30	98.33	112.10
1	E	148	PRO	N-CA-C	-5.25	98.46	112.10
1	O	148	PRO	N-CA-C	-5.21	98.55	112.10
1	B	148	PRO	N-CA-C	-5.16	98.70	112.10
1	B	117	ILE	N-CA-C	-5.01	97.47	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:13:ALA:O	1:F:17:ARG:HD3	1.91	0.70
1:G:13:ALA:O	1:G:17:ARG:HD3	1.91	0.70
1:M:179:HIS:HD2	3:M:580:HOH:O	1.76	0.69
1:J:93:MET:HB2	1:J:95:VAL:HG23	1.75	0.69
1:B:159:LEU:HD22	1:B:198:SER:HB3	1.75	0.68
1:H:135:SER:O	1:H:139:ARG:HG3	1.95	0.67
1:H:13:ALA:O	1:H:17:ARG:HD3	1.94	0.67
1:F:135:SER:O	1:F:139:ARG:HG3	1.95	0.67
1:A:13:ALA:O	1:A:17:ARG:HD3	1.94	0.67
1:K:93:MET:HB2	1:K:95:VAL:HG23	1.77	0.66
1:N:13:ALA:O	1:N:17:ARG:HD3	1.94	0.66
1:O:13:ALA:O	1:O:17:ARG:HD3	1.95	0.66
1:K:13:ALA:O	1:K:17:ARG:HD3	1.95	0.66
1:A:168:THR:HG22	1:A:170:ASN:H	1.61	0.66
1:F:159:LEU:HD22	1:F:198:SER:HB3	1.78	0.65
1:K:187:ILE:HD13	1:L:139:ARG:HG2	1.78	0.65
1:M:168:THR:HG22	1:M:170:ASN:H	1.61	0.65
1:D:93:MET:HB2	1:D:95:VAL:HG23	1.78	0.65
1:G:179:HIS:HD2	3:G:467:HOH:O	1.80	0.65
1:I:93:MET:HB2	1:I:95:VAL:HG23	1.79	0.65
1:C:179:HIS:HD2	3:C:578:HOH:O	1.78	0.64
1:M:159:LEU:HD22	1:M:198:SER:HB3	1.80	0.64
1:B:88:LEU:HD23	1:B:132:ILE:HA	1.79	0.64
1:D:168:THR:HG22	1:D:170:ASN:H	1.63	0.64
1:I:159:LEU:HD22	1:I:198:SER:HB3	1.80	0.64
1:C:93:MET:HB2	1:C:95:VAL:HG23	1.80	0.63
1:L:13:ALA:O	1:L:17:ARG:HD3	1.99	0.63
1:O:185:ARG:NH2	2:O:415:GTP:O2B	2.32	0.63
1:M:93:MET:HB2	1:M:95:VAL:HG23	1.80	0.63
1:C:135:SER:O	1:C:139:ARG:HG3	1.99	0.62
1:M:13:ALA:O	1:M:17:ARG:HD3	2.00	0.62
1:H:168:THR:HG22	1:H:170:ASN:H	1.64	0.62
1:B:13:ALA:O	1:B:17:ARG:HD3	1.98	0.62
1:K:168:THR:HG22	1:K:170:ASN:H	1.63	0.62
1:A:93:MET:HB2	1:A:95:VAL:HG23	1.81	0.62
1:J:13:ALA:O	1:J:17:ARG:HD3	1.99	0.62
1:L:168:THR:HG22	1:L:170:ASN:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:93:MET:HB2	1:N:95:VAL:HG23	1.81	0.62
1:E:13:ALA:O	1:E:17:ARG:HD3	2.00	0.61
1:F:93:MET:HB2	1:F:95:VAL:HG23	1.81	0.61
1:G:93:MET:HB2	1:G:95:VAL:HG23	1.81	0.61
1:G:168:THR:HG22	1:G:170:ASN:H	1.66	0.61
1:O:135:SER:O	1:O:139:ARG:HG3	2.01	0.61
1:D:13:ALA:O	1:D:17:ARG:HD3	2.01	0.60
1:K:11:HIS:O	1:K:15:VAL:HG23	2.01	0.60
1:B:93:MET:HB2	1:B:95:VAL:HG23	1.83	0.60
1:A:11:HIS:O	1:A:15:VAL:HG23	2.02	0.60
1:F:168:THR:HG22	1:F:170:ASN:H	1.66	0.60
1:I:135:SER:O	1:I:139:ARG:HG3	2.02	0.60
1:C:168:THR:HG22	1:C:170:ASN:H	1.68	0.59
1:I:185:ARG:HG2	1:I:186:GLY:N	2.18	0.58
1:O:168:THR:HG22	1:O:170:ASN:H	1.68	0.58
1:D:185:ARG:HG2	1:D:186:GLY:N	2.17	0.58
1:G:88:LEU:HD23	1:G:132:ILE:HA	1.86	0.58
1:I:185:ARG:NH2	2:I:409:GTP:O2B	2.37	0.58
1:E:93:MET:HB2	1:E:95:VAL:HG23	1.87	0.57
1:O:185:ARG:HG2	1:O:186:GLY:N	2.19	0.57
1:I:179:HIS:HD2	3:I:469:HOH:O	1.86	0.57
1:F:185:ARG:NH2	2:F:406:GTP:O2B	2.38	0.56
1:F:75:PHE:CE1	1:F:148:PRO:HG3	2.40	0.56
1:L:88:LEU:HD23	1:L:132:ILE:HA	1.88	0.56
1:O:179:HIS:HD2	3:O:558:HOH:O	1.88	0.56
1:A:185:ARG:HG2	1:A:186:GLY:N	2.21	0.56
1:E:132:ILE:HB	1:E:166:LEU:HD21	1.88	0.56
1:H:185:ARG:HG2	1:H:186:GLY:N	2.21	0.56
1:N:88:LEU:HD23	1:N:132:ILE:HA	1.88	0.56
1:E:159:LEU:HD22	1:E:198:SER:HB3	1.89	0.55
1:H:159:LEU:HD22	1:H:198:SER:HB3	1.88	0.55
1:J:168:THR:HG22	1:J:170:ASN:H	1.71	0.55
1:J:179:HIS:HD2	3:J:558:HOH:O	1.90	0.55
1:I:168:THR:HG22	1:I:170:ASN:H	1.73	0.54
1:K:159:LEU:HD22	1:K:198:SER:HB3	1.90	0.54
1:O:75:PHE:CE1	1:O:148:PRO:HG3	2.43	0.54
1:C:211:HIS:HB3	3:D:520:HOH:O	2.08	0.54
2:H:408:GTP:C2	1:I:134:LEU:HG	2.43	0.53
1:K:88:LEU:HD23	1:K:132:ILE:HA	1.89	0.53
1:A:88:LEU:HD23	1:A:132:ILE:HA	1.90	0.53
1:A:16:ALA:HB3	1:A:17:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HG2	1:C:186:GLY:N	2.24	0.53
1:G:211:HIS:CD2	1:H:215:ARG:HH22	2.27	0.53
1:J:185:ARG:HG2	1:J:186:GLY:N	2.23	0.53
3:K:471:HOH:O	1:O:211:HIS:HB3	2.07	0.53
1:B:168:THR:HG22	1:B:170:ASN:H	1.74	0.53
1:F:11:HIS:O	1:F:15:VAL:HG23	2.08	0.53
1:I:211:HIS:HB3	3:J:520:HOH:O	2.08	0.53
1:F:88:LEU:HD23	1:F:132:ILE:HA	1.91	0.53
1:O:185:ARG:HG2	1:O:186:GLY:H	1.74	0.53
1:D:159:LEU:HD22	1:D:198:SER:HB3	1.91	0.52
1:I:75:PHE:CE1	1:I:148:PRO:HG3	2.44	0.52
1:K:135:SER:O	1:K:139:ARG:HG3	2.09	0.52
1:M:211:HIS:HB3	3:N:520:HOH:O	2.10	0.52
1:N:135:SER:O	1:N:139:ARG:HG3	2.08	0.52
1:N:159:LEU:HD22	1:N:198:SER:HB3	1.91	0.52
1:G:211:HIS:HB3	3:G:437:HOH:O	2.09	0.52
1:N:152:GLU:HB3	1:O:95:VAL:HG21	1.90	0.52
1:G:185:ARG:HG2	1:G:186:GLY:N	2.23	0.52
1:M:185:ARG:NH2	2:M:413:GTP:O2B	2.42	0.52
1:B:135:SER:O	1:B:139:ARG:HG3	2.09	0.52
1:E:19:LEU:HD12	1:E:160:ILE:HG13	1.91	0.52
1:I:142:GLN:O	1:I:146:GLN:HG2	2.10	0.52
1:E:138:ASN:HD22	1:E:138:ASN:H	1.56	0.51
1:L:208:ASN:O	1:L:212:GLU:HG3	2.11	0.51
1:F:152:GLU:HB3	1:G:95:VAL:HG21	1.92	0.51
1:M:42:HIS:O	1:M:46:ILE:HG13	2.11	0.51
3:A:463:HOH:O	1:E:211:HIS:HB3	2.10	0.51
1:I:16:ALA:HB3	1:I:17:ARG:HH11	1.75	0.51
1:N:185:ARG:HG2	1:N:186:GLY:N	2.25	0.51
1:N:211:HIS:HB3	3:O:520:HOH:O	2.09	0.51
1:A:179:HIS:HD2	3:A:455:HOH:O	1.93	0.51
1:L:11:HIS:O	1:L:15:VAL:HG23	2.11	0.51
1:A:21:THR:HG23	1:A:153:ARG:NH1	2.26	0.50
1:C:142:GLN:O	1:C:146:GLN:HG2	2.11	0.50
1:E:179:HIS:HD2	3:E:464:HOH:O	1.93	0.50
1:L:159:LEU:HD22	1:L:198:SER:HB3	1.93	0.50
1:D:185:ARG:HG2	1:D:186:GLY:H	1.75	0.50
1:G:159:LEU:HD22	1:G:198:SER:HB3	1.92	0.50
1:O:11:HIS:O	1:O:15:VAL:HG23	2.11	0.50
1:E:88:LEU:HD23	1:E:132:ILE:HA	1.94	0.50
1:K:134:LEU:HG	2:O:415:GTP:C2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:SER:O	1:G:139:ARG:HG3	2.12	0.49
1:I:44:THR:HG23	1:I:54:LEU:HD13	1.93	0.49
1:J:159:LEU:HD22	1:J:198:SER:HB3	1.94	0.49
2:G:407:GTP:C2	1:H:134:LEU:HG	2.47	0.49
1:H:211:HIS:HB3	3:I:411:HOH:O	2.11	0.49
1:O:88:LEU:HD23	1:O:132:ILE:HA	1.94	0.49
1:O:179:HIS:CD2	3:O:558:HOH:O	2.65	0.49
1:D:135:SER:O	1:D:139:ARG:HG3	2.12	0.49
1:E:44:THR:HG23	1:E:54:LEU:HD13	1.93	0.49
1:O:125:TYR:CD2	1:O:166:LEU:HD13	2.48	0.49
2:F:406:GTP:C2	1:G:134:LEU:HG	2.48	0.49
1:A:135:SER:O	1:A:139:ARG:HG3	2.13	0.49
1:H:88:LEU:HD23	1:H:132:ILE:HA	1.93	0.49
2:L:412:GTP:C2	1:M:134:LEU:HG	2.48	0.49
1:M:135:SER:O	1:M:139:ARG:HG3	2.13	0.49
1:N:132:ILE:HB	1:N:166:LEU:HD21	1.94	0.49
1:O:208:ASN:O	1:O:212:GLU:HG3	2.13	0.49
1:G:11:HIS:O	1:G:15:VAL:HG23	2.13	0.48
1:F:95:VAL:HG21	1:J:152:GLU:HB3	1.95	0.48
1:K:98:MET:HA	1:K:125:TYR:O	2.13	0.48
1:L:212:GLU:HG2	1:L:215:ARG:NH2	2.27	0.48
1:L:212:GLU:HG2	1:L:215:ARG:HH21	1.78	0.48
1:G:180:TYR:CE2	1:G:183:LYS:HD3	2.48	0.48
1:I:88:LEU:HD23	1:I:132:ILE:HA	1.94	0.48
1:A:159:LEU:HD22	1:A:198:SER:HB3	1.96	0.48
1:B:16:ALA:HB3	1:B:17:ARG:HH11	1.79	0.48
1:B:138:ASN:H	1:B:138:ASN:HD22	1.62	0.48
1:O:168:THR:HG21	3:O:540:HOH:O	2.13	0.48
1:O:138:ASN:H	1:O:138:ASN:HD22	1.61	0.48
1:D:11:HIS:O	1:D:15:VAL:HG23	2.14	0.48
1:H:11:HIS:O	1:H:15:VAL:HG23	2.14	0.48
1:I:185:ARG:HG2	1:I:186:GLY:H	1.79	0.48
1:L:185:ARG:NH2	2:L:412:GTP:O2B	2.47	0.48
1:L:44:THR:HG23	1:L:54:LEU:HD13	1.95	0.48
1:M:159:LEU:O	1:M:163:GLN:HG3	2.14	0.48
1:F:211:HIS:HB3	3:G:409:HOH:O	2.13	0.48
1:L:138:ASN:H	1:L:138:ASN:HD22	1.61	0.47
1:J:135:SER:O	1:J:139:ARG:HG3	2.14	0.47
1:L:75:PHE:CE1	1:L:148:PRO:HG3	2.49	0.47
1:L:185:ARG:HG2	1:L:186:GLY:N	2.30	0.47
1:O:16:ALA:HB3	1:O:17:ARG:HH11	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:HIS:O	1:E:15:VAL:HG23	2.13	0.47
1:N:62:THR:HB	1:N:63:PRO:HD3	1.97	0.47
1:E:135:SER:O	1:E:139:ARG:HG3	2.14	0.47
1:D:179:HIS:HD2	3:D:577:HOH:O	1.96	0.47
1:M:132:ILE:HB	1:M:166:LEU:HD21	1.96	0.47
1:M:90:GLU:HB3	1:M:92:LYS:HE3	1.97	0.47
1:A:139:ARG:HG2	1:E:187:ILE:HD13	1.96	0.47
1:O:34:THR:O	1:O:38:LEU:HG	2.14	0.47
1:G:90:GLU:HB3	1:G:92:LYS:HE3	1.97	0.47
1:H:208:ASN:O	1:H:212:GLU:HG3	2.15	0.47
1:L:211:HIS:CD2	1:M:215:ARG:HH22	2.32	0.47
1:B:179:HIS:HD2	3:B:558:HOH:O	1.97	0.47
1:N:168:THR:HG22	1:N:170:ASN:H	1.80	0.47
1:E:183:LYS:HG3	1:E:190:ALA:HA	1.96	0.46
1:I:208:ASN:O	1:I:212:GLU:HG3	2.16	0.46
1:E:142:GLN:O	1:E:146:GLN:HG2	2.15	0.46
1:F:16:ALA:HB3	1:F:17:ARG:HH11	1.80	0.46
1:E:47:MET:CE	1:E:59:LEU:HD22	2.45	0.46
1:J:88:LEU:HD23	1:J:132:ILE:HA	1.98	0.46
1:J:56:ASP:OD2	1:J:58:SER:HB3	2.16	0.46
1:D:47:MET:CE	1:D:59:LEU:HD22	2.45	0.46
1:C:180:TYR:CE2	1:C:183:LYS:HD3	2.51	0.46
1:F:208:ASN:O	1:F:212:GLU:HG3	2.16	0.46
2:G:407:GTP:O1A	1:H:87:THR:HG21	2.15	0.46
1:H:142:GLN:O	1:H:146:GLN:HG2	2.16	0.46
1:N:11:HIS:O	1:N:15:VAL:HG23	2.15	0.46
2:C:403:GTP:C2	1:D:134:LEU:HG	2.51	0.46
1:D:208:ASN:O	1:D:212:GLU:HG3	2.15	0.46
1:F:134:LEU:HG	2:J:410:GTP:C2	2.51	0.46
1:J:142:GLN:O	1:J:146:GLN:HG2	2.15	0.46
1:L:16:ALA:HB3	1:L:17:ARG:HH11	1.81	0.46
1:M:185:ARG:HG2	1:M:186:GLY:N	2.31	0.46
2:M:413:GTP:C2	1:N:134:LEU:HG	2.51	0.46
1:D:56:ASP:OD2	1:D:58:SER:HB3	2.16	0.46
1:H:19:LEU:HD12	1:H:160:ILE:HG13	1.98	0.46
1:F:139:ARG:HG2	1:J:187:ILE:HD13	1.98	0.46
1:K:8:ALA:O	1:K:12:GLU:HG3	2.16	0.46
1:O:142:GLN:O	1:O:146:GLN:HG2	2.16	0.46
2:M:413:GTP:O3'	1:N:136:LYS:HE2	2.17	0.45
1:M:125:TYR:CD2	1:M:166:LEU:HD13	2.51	0.45
1:K:95:VAL:HG21	1:O:152:GLU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASN:O	1:C:212:GLU:HG3	2.17	0.45
1:B:179:HIS:CD2	3:B:558:HOH:O	2.69	0.45
1:E:98:MET:HE1	1:E:213:PHE:HD1	1.82	0.45
1:I:125:TYR:CD2	1:I:166:LEU:HD13	2.52	0.45
1:A:34:THR:HA	1:A:37:SER:OG	2.16	0.45
1:H:98:MET:HA	1:H:125:TYR:O	2.16	0.45
1:N:183:LYS:HG3	1:N:190:ALA:HA	1.98	0.45
1:M:208:ASN:O	1:M:212:GLU:HG3	2.17	0.45
1:O:47:MET:CE	1:O:59:LEU:HD22	2.46	0.45
1:I:19:LEU:HD12	1:I:160:ILE:HG13	1.98	0.45
1:B:211:HIS:CD2	1:C:215:ARG:HH22	2.35	0.45
2:K:411:GTP:C2	1:L:134:LEU:HG	2.52	0.45
1:M:142:GLN:O	1:M:146:GLN:HG2	2.16	0.45
1:D:185:ARG:NH2	2:D:404:GTP:O2B	2.50	0.44
1:H:16:ALA:HB3	1:H:17:ARG:HH11	1.82	0.44
1:F:44:THR:HG23	1:F:54:LEU:HD13	1.98	0.44
2:N:414:GTP:O1A	1:O:87:THR:HG21	2.17	0.44
1:K:125:TYR:CD2	1:K:166:LEU:HD13	2.53	0.44
1:A:142:GLN:O	1:A:146:GLN:HG2	2.16	0.44
1:A:211:HIS:HB3	3:B:520:HOH:O	2.17	0.44
1:B:11:HIS:O	1:B:15:VAL:HG23	2.16	0.44
1:A:179:HIS:CD2	3:A:455:HOH:O	2.69	0.44
1:C:185:ARG:HG2	1:C:186:GLY:H	1.83	0.44
1:D:8:ALA:O	1:D:12:GLU:HG3	2.17	0.44
1:E:185:ARG:HG2	1:E:186:GLY:N	2.32	0.44
1:F:19:LEU:HD12	1:F:160:ILE:HG13	2.00	0.44
1:G:8:ALA:O	1:G:12:GLU:HG3	2.17	0.44
1:I:138:ASN:HD22	1:I:138:ASN:H	1.66	0.44
1:C:179:HIS:CD2	3:C:578:HOH:O	2.62	0.44
1:D:16:ALA:HB3	1:D:17:ARG:HH11	1.82	0.44
1:I:132:ILE:HB	1:I:166:LEU:HD21	1.99	0.44
1:M:56:ASP:OD2	1:M:58:SER:HB3	2.17	0.44
2:D:404:GTP:C2	1:E:134:LEU:HG	2.52	0.44
1:N:34:THR:O	1:N:38:LEU:HG	2.18	0.44
1:B:168:THR:HG21	3:B:540:HOH:O	2.18	0.44
1:H:44:THR:HG23	1:H:54:LEU:HD13	2.00	0.44
1:K:21:THR:HG23	1:K:153:ARG:NH1	2.32	0.44
1:L:187:ILE:HD13	1:M:139:ARG:HG2	1.98	0.44
1:O:159:LEU:HD22	1:O:198:SER:HB3	1.99	0.43
1:A:208:ASN:O	1:A:212:GLU:HG3	2.18	0.43
1:M:88:LEU:HD23	1:M:132:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HG	2:E:405:GTP:C2	2.53	0.43
1:I:47:MET:CE	1:I:59:LEU:HD22	2.48	0.43
1:K:211:HIS:CD2	1:L:215:ARG:HH22	2.37	0.43
1:M:19:LEU:HD12	1:M:160:ILE:HG13	2.00	0.43
1:C:56:ASP:OD2	1:C:58:SER:HB3	2.19	0.43
1:K:16:ALA:HB3	1:K:17:ARG:HH11	1.83	0.43
1:I:210:ARG:O	1:I:214:LEU:HG	2.18	0.43
1:L:8:ALA:O	1:L:12:GLU:HG3	2.19	0.43
1:G:44:THR:HG23	1:G:54:LEU:HD13	2.00	0.43
2:K:411:GTP:O1A	1:L:87:THR:HG21	2.19	0.43
1:A:185:ARG:HG2	1:A:186:GLY:H	1.82	0.43
1:J:75:PHE:CE1	1:J:148:PRO:HG3	2.54	0.43
1:J:16:ALA:HB3	1:J:17:ARG:HH11	1.83	0.43
1:J:46:ILE:O	1:J:50:LEU:HG	2.18	0.43
1:A:168:THR:HG21	3:A:438:HOH:O	2.18	0.43
1:G:153:ARG:O	1:G:157:GLN:HG3	2.19	0.43
1:J:47:MET:CE	1:J:59:LEU:HD22	2.49	0.43
1:A:98:MET:HA	1:A:125:TYR:O	2.19	0.42
2:A:401:GTP:C2	1:B:134:LEU:HG	2.53	0.42
1:H:125:TYR:CD2	1:H:166:LEU:HD13	2.54	0.42
1:I:211:HIS:CD2	1:J:215:ARG:HH22	2.37	0.42
1:N:16:ALA:HB3	1:N:17:ARG:HH11	1.84	0.42
1:B:185:ARG:HG2	1:B:186:GLY:N	2.34	0.42
1:C:159:LEU:HD22	1:C:198:SER:HB3	2.01	0.42
1:F:21:THR:HG23	1:F:153:ARG:NH1	2.35	0.42
1:F:47:MET:CE	1:F:59:LEU:HD22	2.48	0.42
1:D:34:THR:O	1:D:38:LEU:HG	2.19	0.42
1:J:183:LYS:HG3	1:J:190:ALA:HA	2.01	0.42
1:A:44:THR:HG23	1:A:54:LEU:HD13	2.01	0.42
1:E:16:ALA:HB3	1:E:17:ARG:HH11	1.84	0.42
1:K:179:HIS:HD2	3:K:463:HOH:O	2.01	0.42
2:B:402:GTP:C2	1:C:134:LEU:HG	2.55	0.42
1:F:185:ARG:HG2	1:F:186:GLY:N	2.35	0.42
1:N:172:ALA:HB2	1:N:203:PHE:CG	2.55	0.42
1:H:168:THR:HG21	3:H:576:HOH:O	2.20	0.42
1:H:187:ILE:HD13	1:I:139:ARG:HG2	2.02	0.42
1:C:200:GLY:O	1:C:203:PHE:HB2	2.20	0.42
1:J:208:ASN:O	1:J:212:GLU:HG3	2.20	0.41
1:L:135:SER:O	1:L:139:ARG:HG3	2.19	0.41
1:L:13:ALA:HA	1:L:17:ARG:NH1	2.35	0.41
1:B:156:GLN:HG3	1:C:93:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:THR:HB	1:M:63:PRO:HD3	2.02	0.41
1:O:128:LYS:HB3	1:O:129:ASP:H	1.76	0.41
1:H:185:ARG:NH2	2:H:408:GTP:O2B	2.53	0.41
1:J:185:ARG:NH2	2:J:410:GTP:O2B	2.53	0.41
1:N:192:SER:HA	1:O:102:ARG:O	2.20	0.41
1:D:187:ILE:HD13	1:E:139:ARG:HG2	2.01	0.41
1:N:115:VAL:HG12	1:N:116:THR:N	2.36	0.41
1:N:69:MET:HA	1:N:73:GLU:OE1	2.20	0.41
1:D:152:GLU:HB3	1:E:95:VAL:HG21	2.03	0.41
1:F:102:ARG:CZ	1:J:193:ALA:HB3	2.50	0.41
1:K:208:ASN:O	1:K:212:GLU:HG3	2.20	0.41
1:L:79:ASP:HB3	1:L:82:ASN:ND2	2.36	0.41
1:A:115:VAL:HG12	1:A:116:THR:N	2.36	0.41
1:D:69:MET:HA	1:D:73:GLU:OE1	2.21	0.41
1:B:185:ARG:NH2	2:B:402:GTP:O2B	2.53	0.41
1:L:160:ILE:HA	1:L:163:GLN:HE21	1.85	0.41
1:N:179:HIS:HD2	3:N:576:HOH:O	2.02	0.41
1:J:213:PHE:O	1:J:217:VAL:HG23	2.21	0.41
1:J:10:VAL:HG21	1:J:83:PHE:CZ	2.56	0.41
1:G:19:LEU:HD12	1:G:160:ILE:HG13	2.03	0.41
1:M:155:THR:HG22	1:M:198:SER:OG	2.21	0.41
1:L:182:VAL:HG22	1:M:135:SER:HB3	2.03	0.40
1:B:44:THR:O	1:B:48:GLN:HG3	2.21	0.40
1:G:47:MET:SD	1:G:63:PRO:HG3	2.61	0.40
2:I:409:GTP:C2	1:J:134:LEU:HG	2.56	0.40
1:L:179:HIS:HD2	3:L:578:HOH:O	2.03	0.40
1:O:8:ALA:O	1:O:12:GLU:HG3	2.20	0.40
1:N:185:ARG:HG2	1:N:186:GLY:H	1.85	0.40
1:L:179:HIS:CD2	3:L:578:HOH:O	2.73	0.40
1:M:153:ARG:O	1:M:157:GLN:HG3	2.20	0.40
1:N:142:GLN:O	1:N:146:GLN:HG2	2.21	0.40
1:K:215:ARG:HH22	1:O:211:HIS:CD2	2.39	0.40
1:A:183:LYS:HG3	1:A:190:ALA:HA	2.03	0.40
1:B:44:THR:HG23	1:B:54:LEU:HD13	2.02	0.40
1:O:99:VAL:O	1:O:124:ALA:HA	2.21	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	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
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

All (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
1	A	26	PRO
1	B	26	PRO
1	C	26	PRO

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Mol	Chain	Res	Type
1	D	26	PRO
1	E	22	PRO
1	E	26	PRO
1	F	22	PRO
1	F	26	PRO
1	G	22	PRO
1	G	26	PRO
1	H	22	PRO
1	H	26	PRO
1	I	26	PRO
1	J	22	PRO
1	J	26	PRO
1	K	26	PRO
1	L	26	PRO
1	M	26	PRO
1	N	26	PRO
1	O	22	PRO
1	O	26	PRO
1	M	22	PRO
1	N	22	PRO
1	M	218	ARG
1	C	22	PRO
1	D	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
1	E	194/194 (100%)	190 (98%)	4 (2%)	53	59
1	F	194/194 (100%)	190 (98%)	4 (2%)	53	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	MET
1	A	185	ARG
1	A	219	HIS
1	A	220	HIS
1	B	93	MET
1	B	185	ARG
1	B	219	HIS
1	B	220	HIS
1	C	93	MET
1	C	219	HIS
1	C	220	HIS
1	D	93	MET
1	D	219	HIS
1	D	220	HIS
1	E	93	MET
1	E	185	ARG
1	E	219	HIS
1	E	220	HIS
1	F	93	MET
1	F	185	ARG
1	F	219	HIS
1	F	220	HIS
1	G	93	MET
1	G	185	ARG
1	G	219	HIS

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Mol	Chain	Res	Type
1	G	220	HIS
1	H	93	MET
1	H	185	ARG
1	H	219	HIS
1	H	220	HIS
1	I	93	MET
1	I	219	HIS
1	I	220	HIS
1	J	93	MET
1	J	219	HIS
1	J	220	HIS
1	K	93	MET
1	K	185	ARG
1	K	219	HIS
1	K	220	HIS
1	L	93	MET
1	L	219	HIS
1	L	220	HIS
1	M	63	PRO
1	M	93	MET
1	M	219	HIS
1	M	220	HIS
1	N	63	PRO
1	N	93	MET
1	N	219	HIS
1	N	220	HIS
1	O	93	MET
1	O	219	HIS
1	O	220	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	163	GLN
1	A	207	GLN
1	B	138	ASN
1	B	163	GLN
1	B	207	GLN
1	B	211	HIS
1	C	146	GLN
1	C	163	GLN

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Mol	Chain	Res	Type
1	C	207	GLN
1	D	146	GLN
1	D	163	GLN
1	D	207	GLN
1	E	138	ASN
1	E	207	GLN
1	F	138	ASN
1	F	163	GLN
1	F	207	GLN
1	G	138	ASN
1	G	146	GLN
1	G	163	GLN
1	G	207	GLN
1	H	138	ASN
1	H	163	GLN
1	H	207	GLN
1	I	138	ASN
1	I	163	GLN
1	I	207	GLN
1	J	138	ASN
1	J	163	GLN
1	K	42	HIS
1	K	138	ASN
1	K	146	GLN
1	K	163	GLN
1	L	138	ASN
1	L	163	GLN
1	L	207	GLN
1	M	138	ASN
1	M	163	GLN
1	M	207	GLN
1	N	42	HIS
1	N	138	ASN
1	N	163	GLN
1	N	207	GLN
1	O	138	ASN
1	O	146	GLN
1	O	163	GLN
1	O	207	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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

All (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
2	C	403	GTP	C6-N1	3.96	1.39	1.33
2	G	407	GTP	C6-N1	3.79	1.39	1.33
2	H	408	GTP	C6-N1	3.72	1.39	1.33
2	I	409	GTP	C6-N1	3.50	1.39	1.33
2	O	415	GTP	C2-N1	3.42	1.41	1.35
2	M	413	GTP	C6-N1	3.41	1.39	1.33
2	H	408	GTP	C2'-C1'	-3.39	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	410	GTP	C2-N1	3.38	1.41	1.35
2	B	402	GTP	C6-N1	3.23	1.38	1.33
2	K	411	GTP	C2'-C1'	-3.21	1.48	1.53
2	D	404	GTP	C2-N1	3.18	1.41	1.35
2	N	414	GTP	C2'-C1'	-3.11	1.49	1.53
2	M	413	GTP	C2-N1	3.11	1.40	1.35
2	M	413	GTP	C2'-C1'	-3.08	1.49	1.53
2	L	412	GTP	O4'-C4'	3.06	1.51	1.45
2	A	401	GTP	C2'-C1'	-3.00	1.49	1.53
2	N	414	GTP	C6-N1	2.99	1.38	1.33
2	C	403	GTP	C2'-C1'	-2.94	1.49	1.53
2	N	414	GTP	O4'-C4'	2.93	1.51	1.45
2	E	405	GTP	O4'-C4'	2.91	1.51	1.45
2	C	403	GTP	C2-N1	2.89	1.40	1.35
2	B	402	GTP	O4'-C4'	2.84	1.51	1.45
2	E	405	GTP	C6-N1	2.84	1.38	1.33
2	L	412	GTP	C2-N1	2.83	1.40	1.35
2	F	406	GTP	O4'-C4'	2.76	1.51	1.45
2	I	409	GTP	C2-N1	2.76	1.40	1.35
2	D	404	GTP	C2'-C1'	-2.73	1.49	1.53
2	M	413	GTP	C6-C5	2.71	1.46	1.41
2	G	407	GTP	C2-N1	2.70	1.40	1.35
2	A	401	GTP	C6-N1	2.66	1.37	1.33
2	I	409	GTP	PB-O2B	-2.62	1.43	1.55
2	O	415	GTP	O4'-C4'	2.61	1.50	1.45
2	L	412	GTP	C2'-C1'	-2.56	1.49	1.53
2	I	409	GTP	O4'-C4'	2.55	1.50	1.45
2	I	409	GTP	O4'-C1'	2.51	1.44	1.41
2	K	411	GTP	O6-C6	-2.51	1.18	1.24
2	H	408	GTP	O4'-C4'	2.50	1.50	1.45
2	F	406	GTP	C2-N1	2.49	1.39	1.35
2	E	405	GTP	C2-N1	2.47	1.39	1.35
2	I	409	GTP	C2'-C1'	-2.45	1.50	1.53
2	G	407	GTP	C2'-C1'	-2.40	1.50	1.53
2	H	408	GTP	C2-N1	2.39	1.39	1.35
2	O	415	GTP	O4'-C1'	2.36	1.44	1.41
2	D	404	GTP	C4-N3	2.36	1.39	1.35
2	E	405	GTP	O6-C6	-2.35	1.18	1.24
2	D	404	GTP	C6-C5	2.35	1.45	1.41
2	F	406	GTP	O6-C6	-2.33	1.18	1.24
2	J	410	GTP	O4'-C4'	2.32	1.50	1.45
2	G	407	GTP	O4'-C4'	2.32	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	404	GTP	O2'-C2'	2.27	1.48	1.43
2	H	408	GTP	PB-O2B	-2.25	1.44	1.55
2	I	409	GTP	O6-C6	-2.24	1.18	1.24
2	G	407	GTP	C6-C5	2.22	1.45	1.41
2	G	407	GTP	O2'-C2'	2.22	1.48	1.43
2	C	403	GTP	C8-N7	-2.21	1.30	1.34
2	H	408	GTP	O2'-C2'	2.21	1.48	1.43
2	L	412	GTP	PB-O2B	-2.21	1.45	1.55
2	K	411	GTP	O4'-C4'	2.19	1.49	1.45
2	C	403	GTP	PB-O2B	-2.19	1.45	1.55
2	C	403	GTP	O4'-C1'	2.18	1.44	1.41
2	B	402	GTP	C2'-C1'	-2.18	1.50	1.53
2	A	401	GTP	O6-C6	-2.16	1.19	1.24
2	C	403	GTP	O2'-C2'	2.16	1.48	1.43
2	M	413	GTP	O4'-C4'	2.14	1.49	1.45
2	A	401	GTP	PB-O2B	-2.13	1.45	1.55
2	H	408	GTP	PB-O1B	-2.12	1.43	1.50
2	B	402	GTP	PB-O2B	-2.11	1.45	1.55
2	M	413	GTP	O6-C6	-2.11	1.19	1.24
2	B	402	GTP	PA-O2A	-2.10	1.45	1.55
2	G	407	GTP	O6-C6	-2.10	1.19	1.24
2	E	405	GTP	PB-O2B	-2.08	1.45	1.55
2	L	412	GTP	O2'-C2'	2.02	1.47	1.43
2	G	407	GTP	O4'-C1'	2.01	1.43	1.41
2	M	413	GTP	C8-N7	-2.00	1.31	1.34

All (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
2	I	409	GTP	C5-C6-N1	-7.34	113.39	123.43
2	C	403	GTP	C5-C6-N1	-7.29	113.46	123.43
2	E	405	GTP	C5-C6-N1	-7.29	113.46	123.43
2	J	410	GTP	C5-C6-N1	-7.26	113.50	123.43
2	O	415	GTP	C5-C6-N1	-7.20	113.58	123.43
2	N	414	GTP	C5-C6-N1	-7.18	113.62	123.43
2	G	407	GTP	C5-C6-N1	-7.18	113.62	123.43
2	F	406	GTP	C5-C6-N1	-7.07	113.76	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GTP	C5-C6-N1	-6.96	113.91	123.43
2	K	411	GTP	C5-C6-N1	-6.96	113.91	123.43
2	H	408	GTP	C6-N1-C2	5.61	124.84	115.93
2	K	411	GTP	C6-N1-C2	5.57	124.79	115.93
2	E	405	GTP	C6-N1-C2	5.57	124.79	115.93
2	L	412	GTP	C6-N1-C2	5.46	124.61	115.93
2	C	403	GTP	C6-N1-C2	5.44	124.58	115.93
2	I	409	GTP	C6-N1-C2	5.41	124.53	115.93
2	N	414	GTP	C6-N1-C2	5.38	124.47	115.93
2	D	404	GTP	C6-N1-C2	5.31	124.37	115.93
2	A	401	GTP	C6-N1-C2	5.25	124.27	115.93
2	B	402	GTP	C6-N1-C2	5.25	124.26	115.93
2	M	413	GTP	C6-N1-C2	5.23	124.24	115.93
2	O	415	GTP	C6-N1-C2	5.17	124.15	115.93
2	F	406	GTP	C6-N1-C2	5.17	124.14	115.93
2	G	407	GTP	C6-N1-C2	5.03	123.92	115.93
2	J	410	GTP	C6-N1-C2	4.87	123.67	115.93
2	O	415	GTP	N3-C2-N1	-4.35	121.42	127.22
2	C	403	GTP	N3-C2-N1	-4.29	121.50	127.22
2	J	410	GTP	N3-C2-N1	-4.25	121.55	127.22
2	E	405	GTP	N3-C2-N1	-4.16	121.67	127.22
2	L	412	GTP	N3-C2-N1	-4.09	121.77	127.22
2	I	409	GTP	N3-C2-N1	-4.08	121.78	127.22
2	F	406	GTP	N3-C2-N1	-4.03	121.84	127.22
2	K	411	GTP	N3-C2-N1	-3.97	121.93	127.22
2	H	408	GTP	O4'-C4'-C5'	3.91	122.22	109.37
2	N	414	GTP	N3-C2-N1	-3.89	122.03	127.22
2	N	414	GTP	O4'-C4'-C5'	3.88	122.13	109.37
2	E	405	GTP	O4'-C4'-C5'	3.84	122.02	109.37
2	D	404	GTP	O4'-C4'-C5'	3.76	121.75	109.37
2	H	408	GTP	N3-C2-N1	-3.71	122.28	127.22
2	L	412	GTP	O4'-C4'-C5'	3.70	121.56	109.37
2	J	410	GTP	O4'-C4'-C5'	3.69	121.50	109.37
2	D	404	GTP	N3-C2-N1	-3.69	122.31	127.22
2	M	413	GTP	O4'-C4'-C5'	3.68	121.48	109.37
2	G	407	GTP	O4'-C4'-C5'	3.68	121.48	109.37
2	G	407	GTP	N3-C2-N1	-3.67	122.33	127.22
2	B	402	GTP	N3-C2-N1	-3.65	122.35	127.22
2	F	406	GTP	O4'-C4'-C5'	3.61	121.25	109.37
2	A	401	GTP	O4'-C4'-C5'	3.56	121.10	109.37
2	B	402	GTP	O4'-C4'-C5'	3.56	121.07	109.37
2	I	409	GTP	O4'-C4'-C5'	3.55	121.05	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	413	GTP	N3-C2-N1	-3.54	122.50	127.22
2	A	401	GTP	N3-C2-N1	-3.52	122.53	127.22
2	C	403	GTP	O4'-C4'-C5'	3.47	120.80	109.37
2	K	411	GTP	O4'-C4'-C5'	3.38	120.51	109.37
2	O	415	GTP	O4'-C4'-C5'	3.31	120.27	109.37
2	O	415	GTP	C3'-C2'-C1'	-3.16	96.23	100.98
2	L	412	GTP	C3'-C2'-C1'	-3.14	96.25	100.98
2	H	408	GTP	C3'-C2'-C1'	-3.05	96.39	100.98
2	D	404	GTP	C3'-C2'-C1'	-2.98	96.50	100.98
2	I	409	GTP	C3'-C2'-C1'	-2.92	96.58	100.98
2	C	403	GTP	C3'-C2'-C1'	-2.91	96.59	100.98
2	K	411	GTP	C3'-C2'-C1'	-2.86	96.67	100.98
2	E	405	GTP	C5'-C4'-C3'	-2.85	104.51	115.18
2	F	406	GTP	PB-O3B-PG	-2.81	123.17	132.83
2	H	408	GTP	C5'-C4'-C3'	-2.78	104.78	115.18
2	A	401	GTP	C6-C5-C4	-2.76	118.17	120.80
2	M	413	GTP	C3'-C2'-C1'	-2.73	96.86	100.98
2	J	410	GTP	C1'-N9-C4	-2.67	121.95	126.64
2	C	403	GTP	C5'-C4'-C3'	-2.65	105.24	115.18
2	N	414	GTP	C5'-C4'-C3'	-2.64	105.27	115.18
2	C	403	GTP	O5'-PA-O1A	-2.64	98.76	109.07
2	G	407	GTP	C1'-N9-C4	-2.64	122.01	126.64
2	F	406	GTP	C6-C5-C4	-2.63	118.29	120.80
2	O	415	GTP	C5'-C4'-C3'	-2.62	105.37	115.18
2	K	411	GTP	C6-C5-C4	-2.60	118.31	120.80
2	N	414	GTP	C3'-C2'-C1'	-2.60	97.07	100.98
2	I	409	GTP	C5'-C4'-C3'	-2.59	105.46	115.18
2	M	413	GTP	C1'-N9-C4	-2.57	122.13	126.64
2	M	413	GTP	C5'-C4'-C3'	-2.57	105.56	115.18
2	L	412	GTP	C5'-C4'-C3'	-2.56	105.58	115.18
2	J	410	GTP	C5'-C4'-C3'	-2.55	105.63	115.18
2	I	409	GTP	C6-C5-C4	-2.55	118.37	120.80
2	I	409	GTP	PB-O3B-PG	-2.52	124.18	132.83
2	D	404	GTP	C5'-C4'-C3'	-2.50	105.81	115.18
2	D	404	GTP	C1'-N9-C4	-2.50	122.25	126.64
2	B	402	GTP	C5'-C4'-C3'	-2.49	105.86	115.18
2	F	406	GTP	C1'-N9-C4	-2.48	122.29	126.64
2	G	407	GTP	C5'-C4'-C3'	-2.46	105.96	115.18
2	C	403	GTP	C6-C5-C4	-2.46	118.45	120.80
2	F	406	GTP	C5'-C4'-C3'	-2.46	105.97	115.18
2	A	401	GTP	C5'-C4'-C3'	-2.45	105.99	115.18
2	F	406	GTP	C3'-C2'-C1'	-2.45	97.29	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	412	GTP	C6-C5-C4	-2.45	118.46	120.80
2	J	410	GTP	O5'-C5'-C4'	-2.44	100.58	108.99
2	M	413	GTP	O5'-PA-O1A	-2.44	99.54	109.07
2	M	413	GTP	O2A-PA-O1A	2.44	124.28	112.24
2	J	410	GTP	C3'-C2'-C1'	-2.42	97.33	100.98
2	L	412	GTP	C1'-N9-C4	-2.42	122.39	126.64
2	M	413	GTP	C6-C5-C4	-2.42	118.49	120.80
2	I	409	GTP	O5'-PA-O1A	-2.41	99.66	109.07
2	E	405	GTP	O5'-PA-O1A	-2.40	99.69	109.07
2	K	411	GTP	C1'-N9-C4	-2.38	122.46	126.64
2	G	407	GTP	C6-C5-C4	-2.37	118.53	120.80
2	I	409	GTP	C1'-N9-C4	-2.37	122.48	126.64
2	L	412	GTP	PB-O3B-PG	-2.36	124.73	132.83
2	M	413	GTP	O2G-PG-O3B	2.34	112.47	104.64
2	G	407	GTP	C3'-C2'-C1'	-2.33	97.46	100.98
2	E	405	GTP	PB-O3B-PG	-2.33	124.82	132.83
2	K	411	GTP	C5'-C4'-C3'	-2.33	106.44	115.18
2	C	403	GTP	C1'-N9-C4	-2.31	122.58	126.64
2	D	404	GTP	C6-C5-C4	-2.30	118.60	120.80
2	B	402	GTP	C6-C5-C4	-2.30	118.60	120.80
2	D	404	GTP	PB-O3B-PG	-2.29	124.96	132.83
2	H	408	GTP	C6-C5-C4	-2.28	118.62	120.80
2	B	402	GTP	C3'-C2'-C1'	-2.28	97.54	100.98
2	F	406	GTP	O5'-C5'-C4'	-2.28	101.14	108.99
2	O	415	GTP	PB-O3B-PG	-2.26	125.07	132.83
2	O	415	GTP	O5'-C5'-C4'	-2.26	101.22	108.99
2	I	409	GTP	O2A-PA-O1A	2.25	123.35	112.24
2	E	405	GTP	O2G-PG-O1G	2.25	119.48	110.68
2	E	405	GTP	O5'-C5'-C4'	-2.24	101.28	108.99
2	L	412	GTP	O2'-C2'-C3'	2.23	119.05	111.82
2	H	408	GTP	PB-O3B-PG	-2.23	125.18	132.83
2	N	414	GTP	C1'-N9-C4	-2.22	122.73	126.64
2	M	413	GTP	PB-O3B-PG	-2.22	125.20	132.83
2	I	409	GTP	O2G-PG-O1G	2.21	119.33	110.68
2	C	403	GTP	O2A-PA-O1A	2.21	123.15	112.24
2	A	401	GTP	O5'-C5'-C4'	-2.20	101.43	108.99
2	I	409	GTP	O5'-C5'-C4'	-2.20	101.43	108.99
2	O	415	GTP	C1'-N9-C4	-2.19	122.80	126.64
2	L	412	GTP	O2G-PG-O1G	2.19	119.25	110.68
2	N	414	GTP	C6-C5-C4	-2.19	118.71	120.80
2	K	411	GTP	O2G-PG-O3B	2.18	111.96	104.64
2	L	412	GTP	PA-O3A-PB	-2.18	125.34	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	407	GTP	O2G-PG-O3B	2.17	111.91	104.64
2	E	405	GTP	C6-C5-C4	-2.17	118.73	120.80
2	I	409	GTP	O2'-C2'-C3'	2.16	118.80	111.82
2	O	415	GTP	O2'-C2'-C3'	2.16	118.80	111.82
2	M	413	GTP	O5'-C5'-C4'	-2.15	101.58	108.99
2	O	415	GTP	C6-C5-C4	-2.15	118.74	120.80
2	G	407	GTP	O2A-PA-O1A	2.14	122.82	112.24
2	G	407	GTP	O5'-C5'-C4'	-2.13	101.64	108.99
2	K	411	GTP	O3'-C3'-C2'	2.13	118.72	111.82
2	C	403	GTP	O5'-C5'-C4'	-2.13	101.66	108.99
2	C	403	GTP	O2G-PG-O3B	2.12	111.75	104.64
2	F	406	GTP	O2A-PA-O1A	2.12	122.72	112.24
2	A	401	GTP	C1'-N9-C4	-2.12	122.92	126.64
2	A	401	GTP	O2A-PA-O1A	2.11	122.67	112.24
2	N	414	GTP	O5'-C5'-C4'	-2.09	101.79	108.99
2	O	415	GTP	O2A-PA-O1A	2.09	122.55	112.24
2	J	410	GTP	O2G-PG-O1G	2.08	118.84	110.68
2	B	402	GTP	O4'-C1'-C2'	2.08	109.97	106.93
2	E	405	GTP	C1'-N9-C4	-2.07	123.00	126.64
2	K	411	GTP	PB-O3B-PG	-2.07	125.73	132.83
2	B	402	GTP	PB-O3B-PG	-2.07	125.74	132.83
2	O	415	GTP	O2G-PG-O1G	2.06	118.75	110.68
2	H	408	GTP	O2'-C2'-C3'	2.06	118.49	111.82
2	K	411	GTP	O2'-C2'-C3'	2.06	118.48	111.82
2	M	413	GTP	O2'-C2'-C3'	2.04	118.44	111.82
2	H	408	GTP	C1'-N9-C4	-2.04	123.05	126.64
2	G	407	GTP	PB-O3B-PG	-2.04	125.82	132.83
2	D	404	GTP	O2A-PA-O1A	2.04	122.32	112.24
2	L	412	GTP	O5'-C5'-C4'	-2.04	101.98	108.99
2	D	404	GTP	O2'-C2'-C3'	2.03	118.40	111.82
2	E	405	GTP	C3'-C2'-C1'	-2.03	97.92	100.98
2	E	405	GTP	O2A-PA-O1A	2.01	122.19	112.24
2	A	401	GTP	PB-O3B-PG	-2.00	125.95	132.83

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
2	N	414	GTP	O4'-C4'-C5'-O5'
2	E	405	GTP	PB-O3B-PG-O2G
2	L	412	GTP	O4'-C4'-C5'-O5'
2	F	406	GTP	O4'-C4'-C5'-O5'
2	M	413	GTP	PB-O3B-PG-O2G
2	A	401	GTP	O4'-C4'-C5'-O5'
2	J	410	GTP	O4'-C4'-C5'-O5'
2	D	404	GTP	O4'-C4'-C5'-O5'
2	N	414	GTP	C3'-C4'-C5'-O5'
2	E	405	GTP	O4'-C4'-C5'-O5'
2	H	408	GTP	O4'-C4'-C5'-O5'
2	G	407	GTP	O4'-C4'-C5'-O5'
2	B	402	GTP	O4'-C4'-C5'-O5'
2	M	413	GTP	O4'-C4'-C5'-O5'
2	O	415	GTP	C3'-C4'-C5'-O5'
2	L	412	GTP	C3'-C4'-C5'-O5'
2	C	403	GTP	O4'-C4'-C5'-O5'
2	I	409	GTP	O4'-C4'-C5'-O5'
2	F	406	GTP	C3'-C4'-C5'-O5'
2	D	404	GTP	C3'-C4'-C5'-O5'
2	H	408	GTP	C3'-C4'-C5'-O5'
2	K	411	GTP	O4'-C4'-C5'-O5'
2	B	402	GTP	C3'-C4'-C5'-O5'
2	J	410	GTP	C3'-C4'-C5'-O5'
2	K	411	GTP	PB-O3B-PG-O1G
2	A	401	GTP	PB-O3B-PG-O1G
2	G	407	GTP	PB-O3B-PG-O1G
2	L	412	GTP	PB-O3B-PG-O2G
2	C	403	GTP	PB-O3B-PG-O2G
2	G	407	GTP	PB-O3B-PG-O2G
2	E	405	GTP	C3'-C4'-C5'-O5'
2	M	413	GTP	C3'-C4'-C5'-O5'
2	N	414	GTP	PB-O3B-PG-O1G
2	E	405	GTP	PB-O3B-PG-O1G
2	M	413	GTP	PB-O3B-PG-O1G
2	C	403	GTP	C3'-C4'-C5'-O5'
2	A	401	GTP	C3'-C4'-C5'-O5'
2	I	409	GTP	C3'-C4'-C5'-O5'
2	G	407	GTP	C3'-C4'-C5'-O5'
2	L	412	GTP	PB-O3B-PG-O1G
2	C	403	GTP	PB-O3B-PG-O1G
2	J	410	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
2	D	404	GTP	PB-O3B-PG-O2G
2	H	408	GTP	PB-O3B-PG-O2G
2	G	407	GTP	PB-O3B-PG-O3G
2	B	402	GTP	PB-O3B-PG-O2G
2	K	411	GTP	C3'-C4'-C5'-O5'

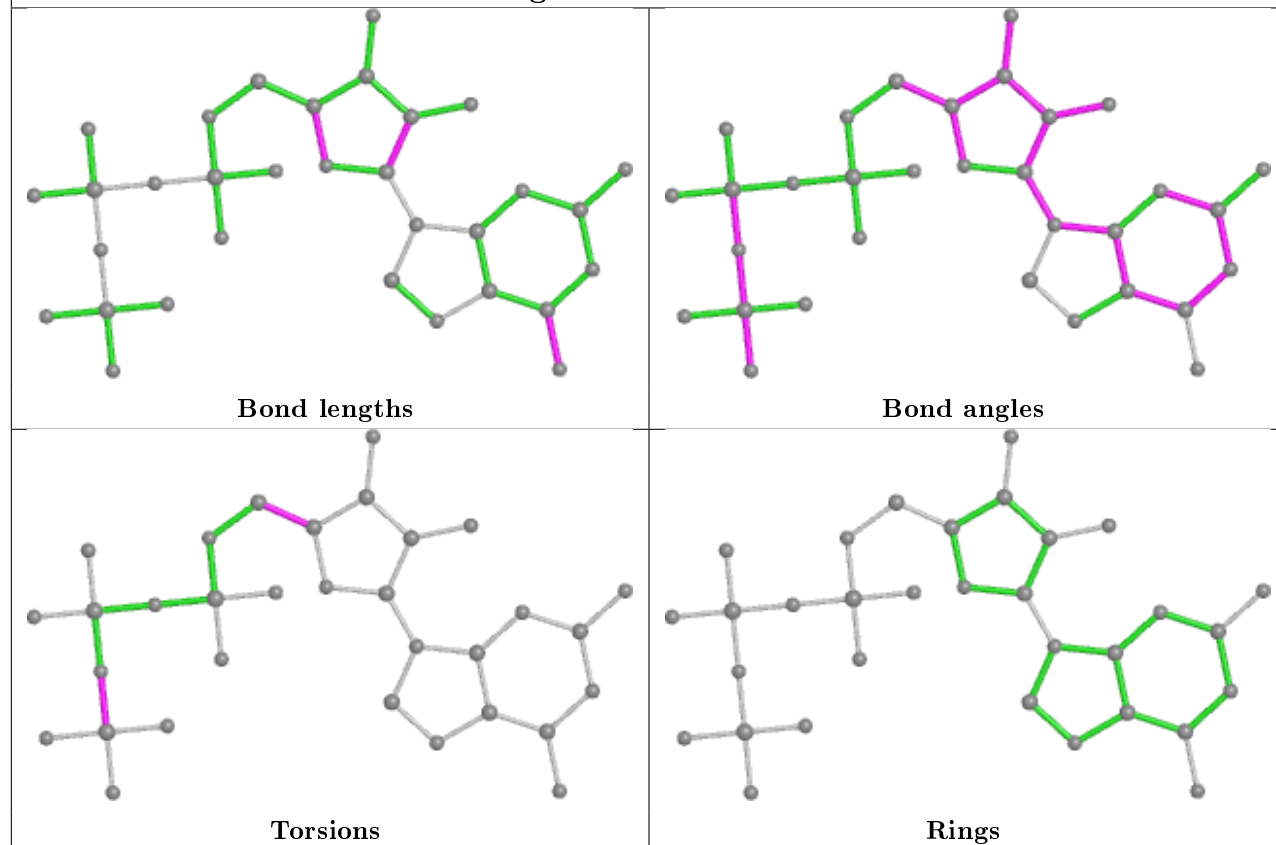
There are no ring outliers.

15 monomers are involved in 27 short contacts:

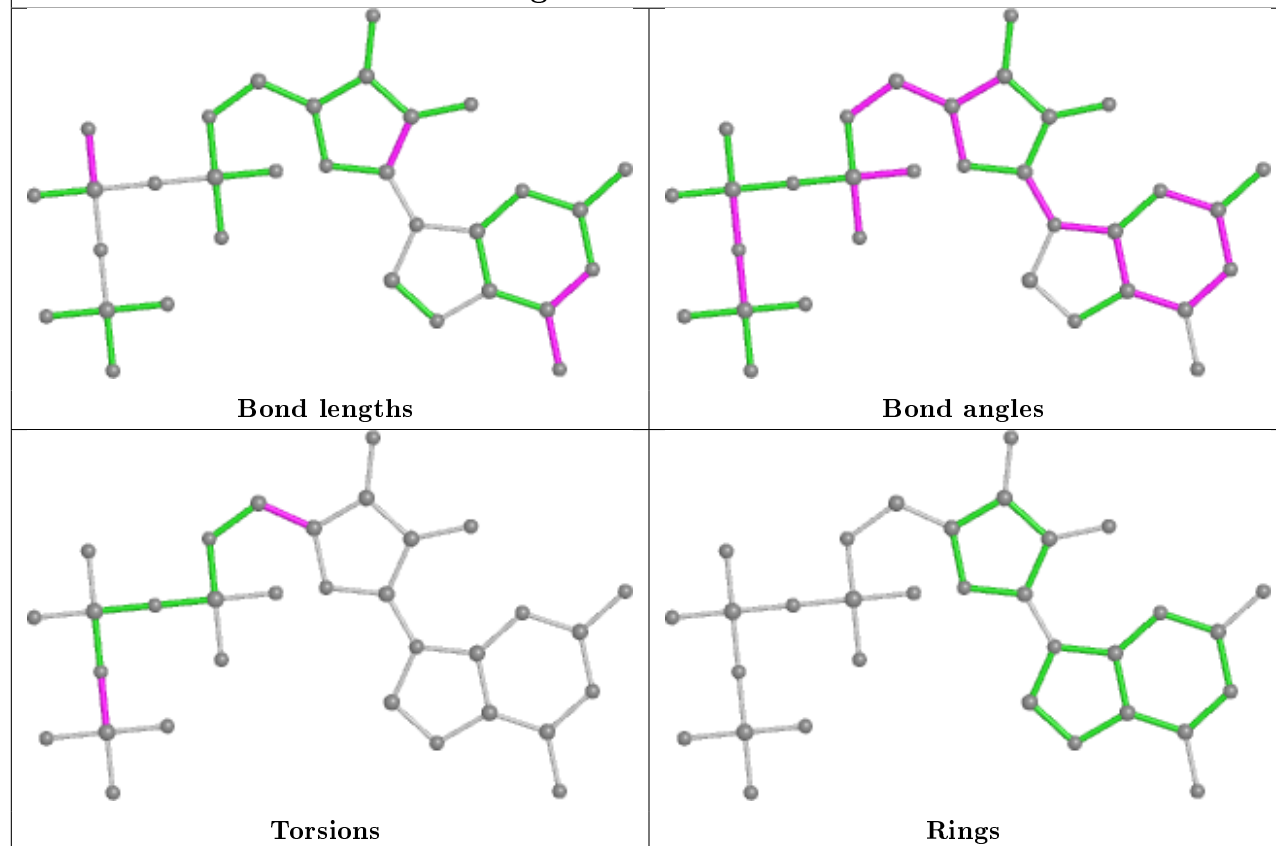
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	411	GTP	2	0
2	A	401	GTP	1	0
2	O	415	GTP	2	0
2	G	407	GTP	2	0
2	J	410	GTP	2	0
2	D	404	GTP	2	0
2	E	405	GTP	1	0
2	L	412	GTP	2	0
2	C	403	GTP	1	0
2	I	409	GTP	2	0
2	N	414	GTP	1	0
2	B	402	GTP	2	0
2	F	406	GTP	2	0
2	H	408	GTP	2	0
2	M	413	GTP	3	0

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.

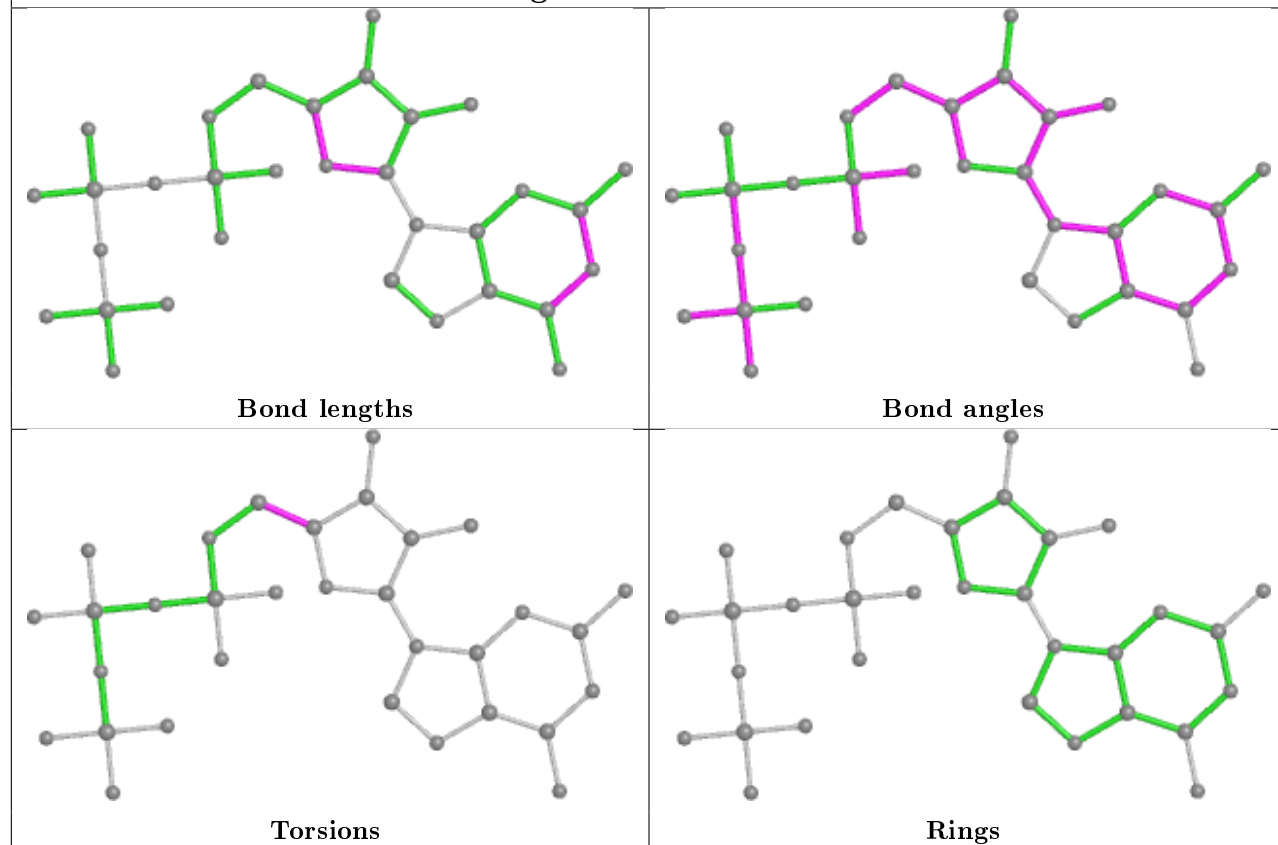
## Ligand GTP K 411



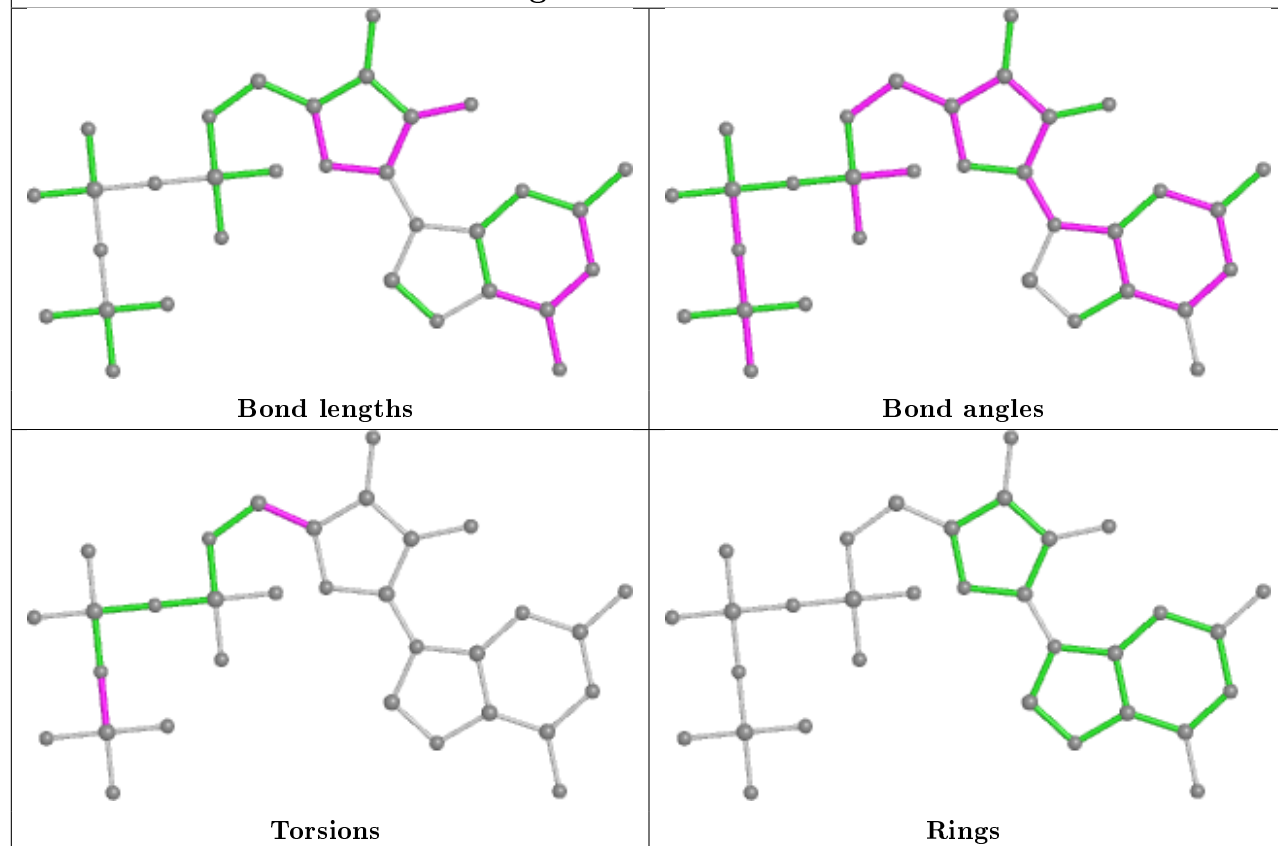
## Ligand GTP A 401



## Ligand GTP O 415

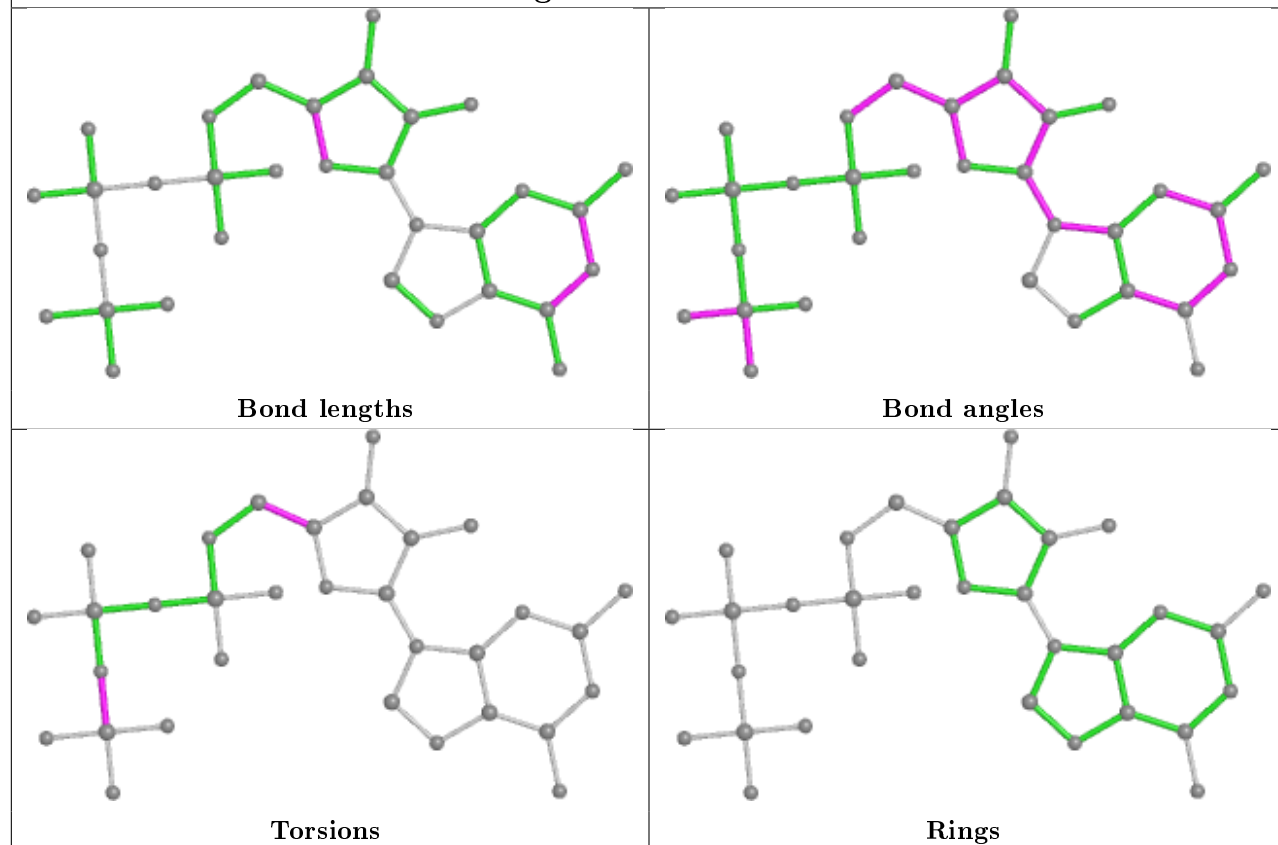


## Ligand GTP G 407

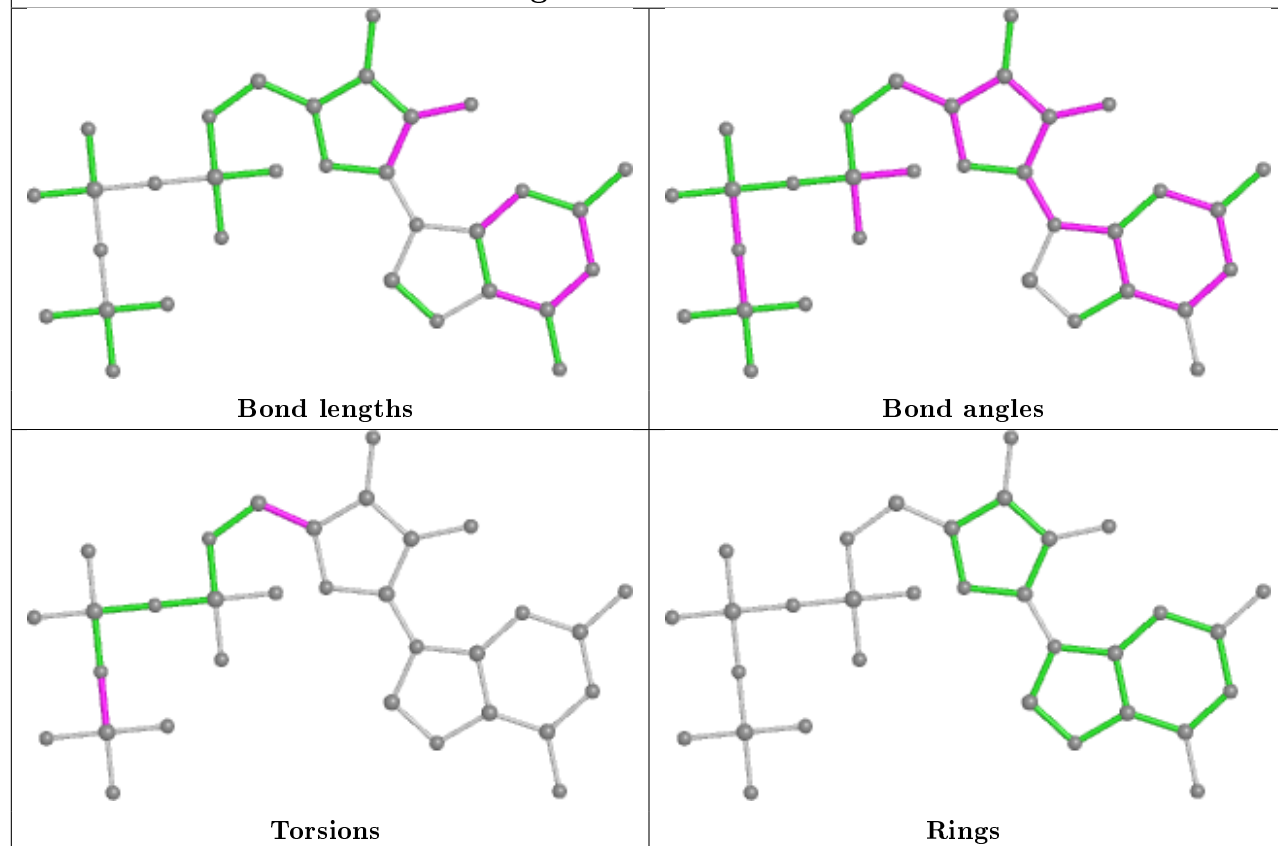




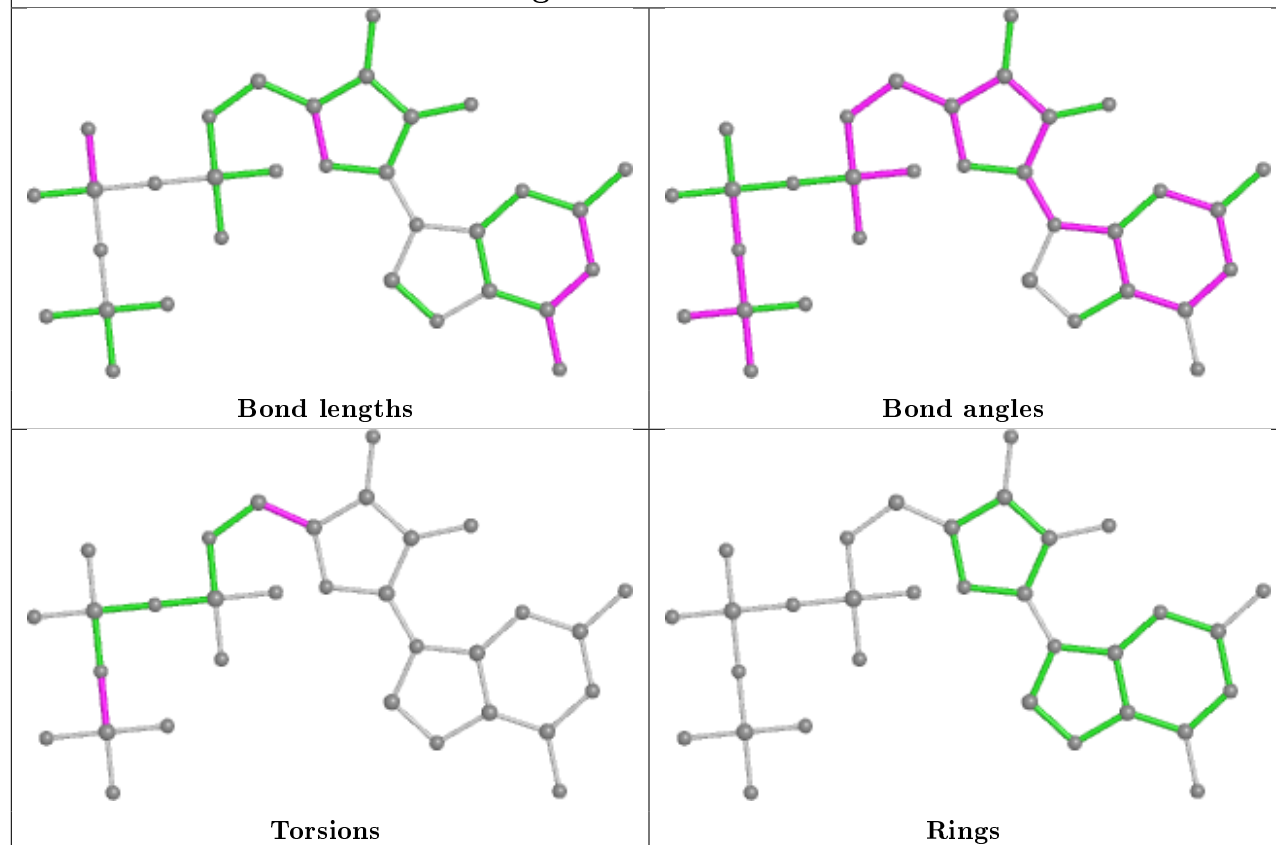
## Ligand GTP J 410



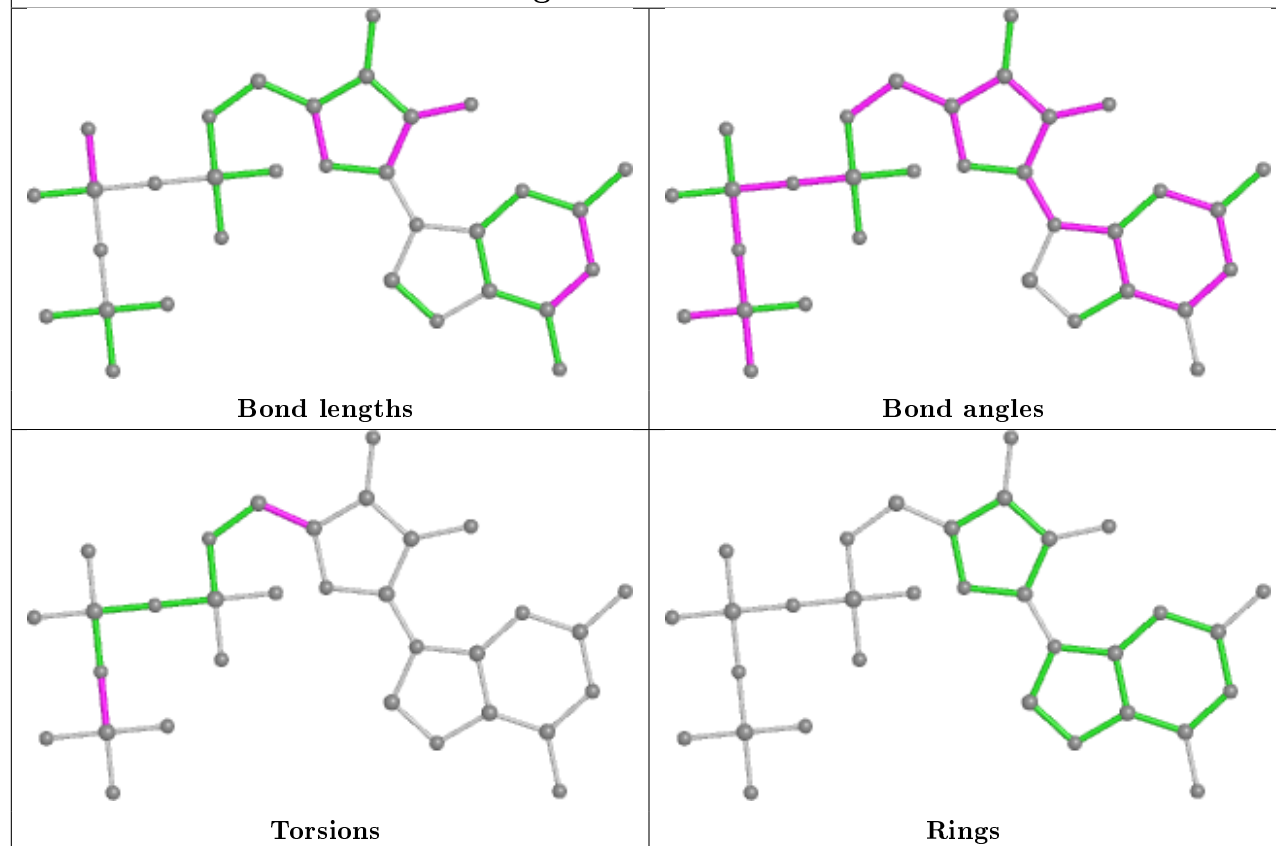
## Ligand GTP D 404



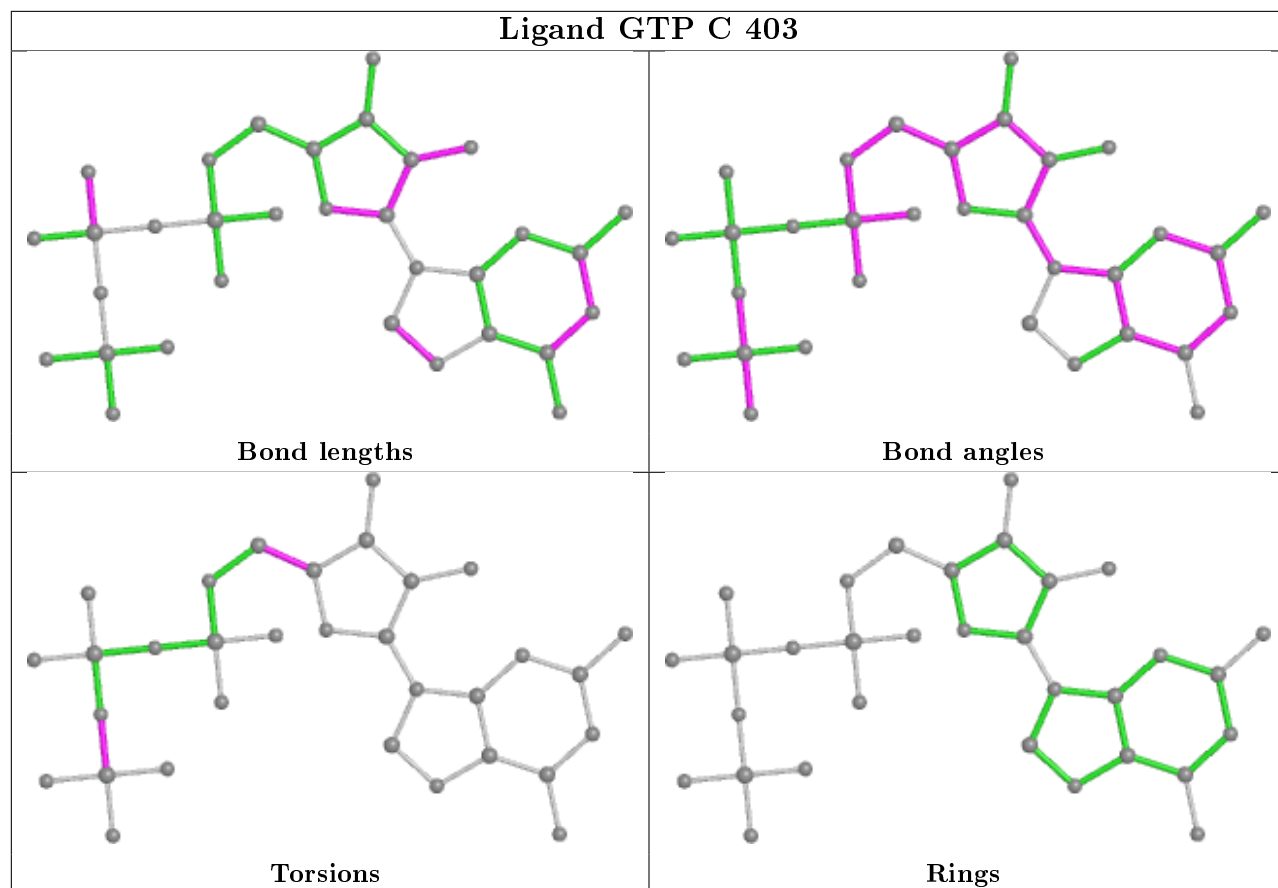
## Ligand GTP E 405



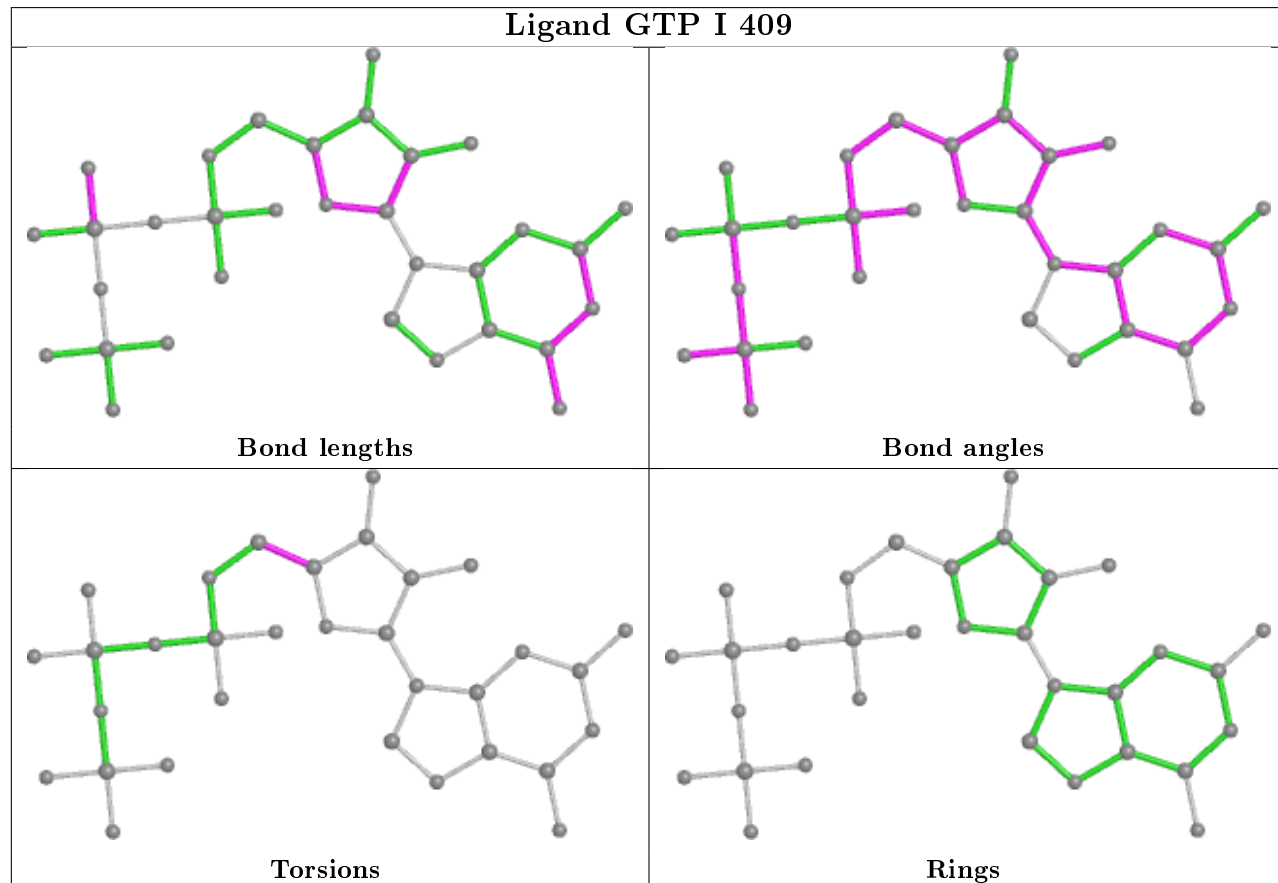
## Ligand GTP L 412



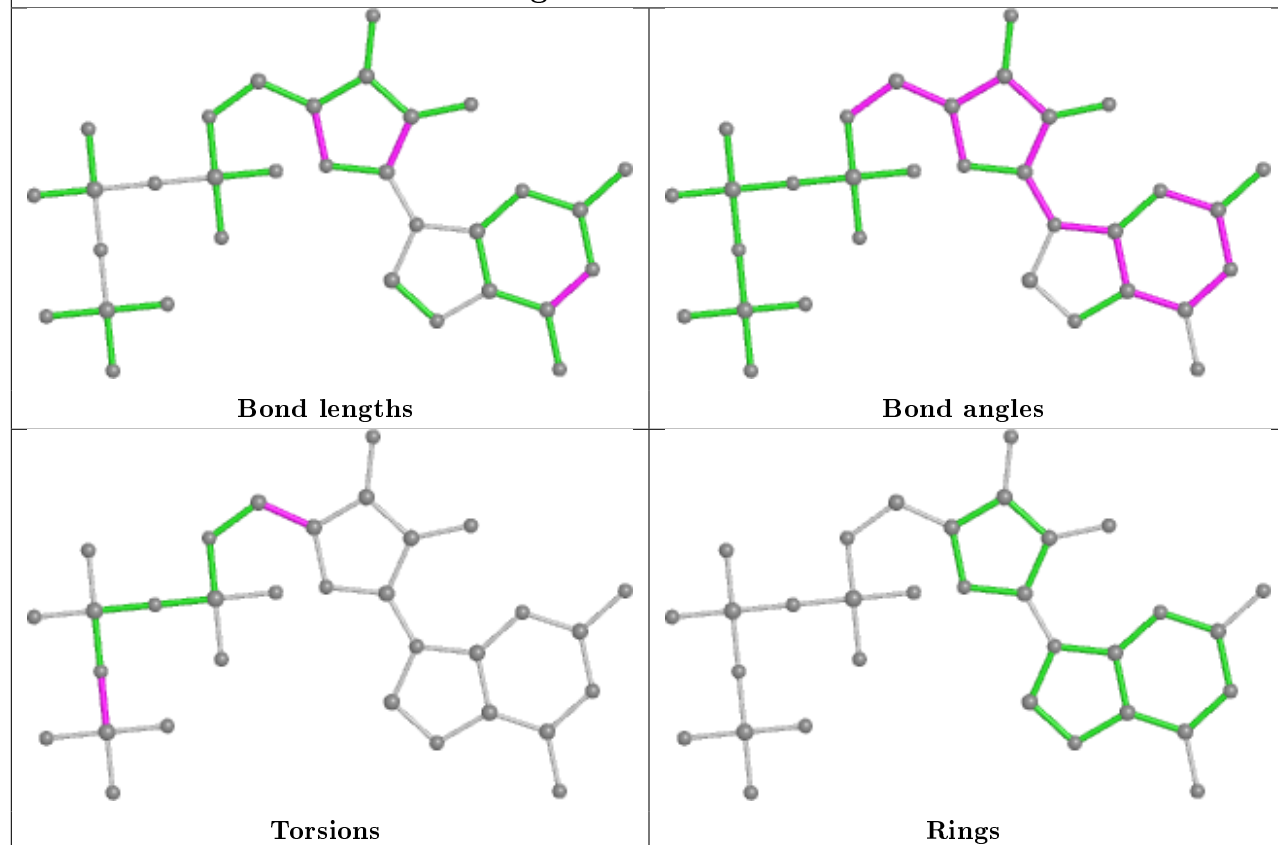
## Ligand GTP C 403



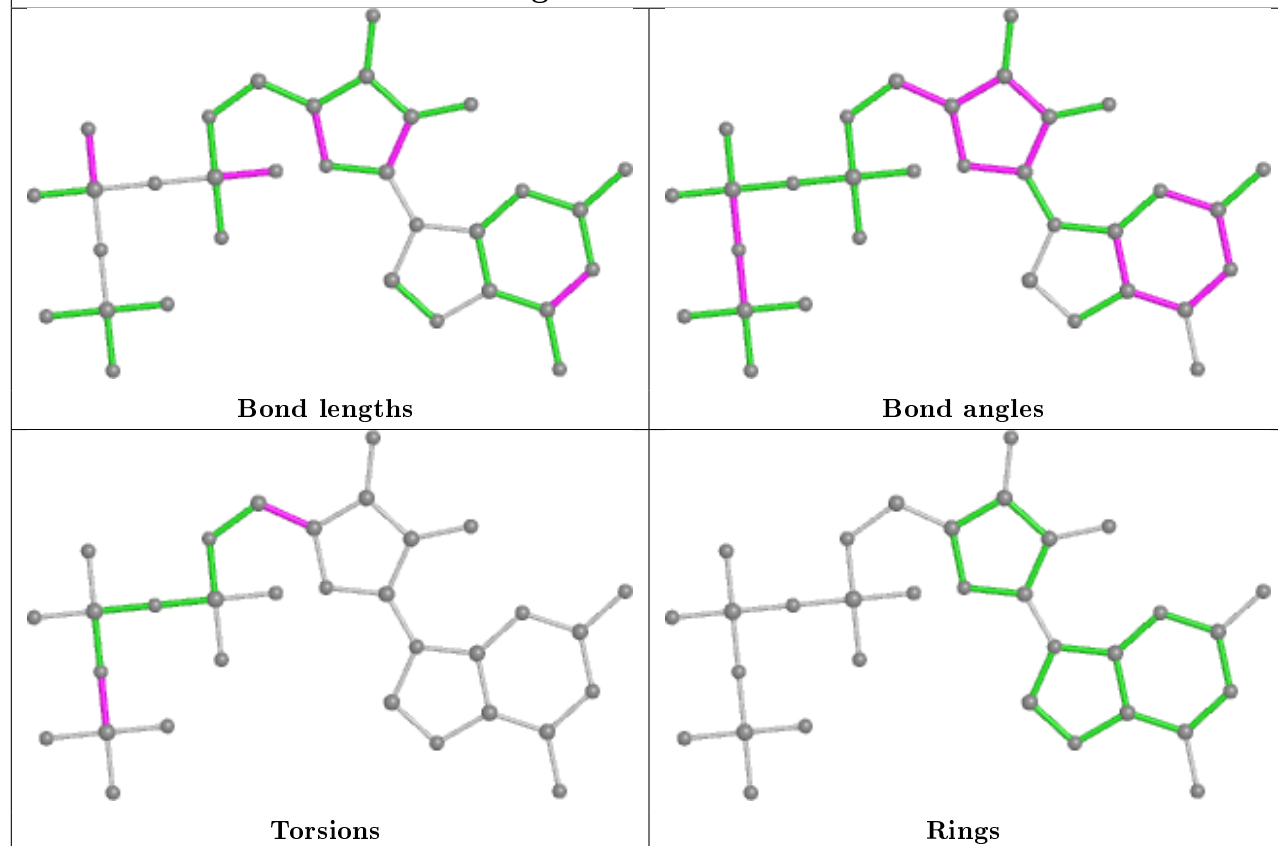
## Ligand GTP I 409



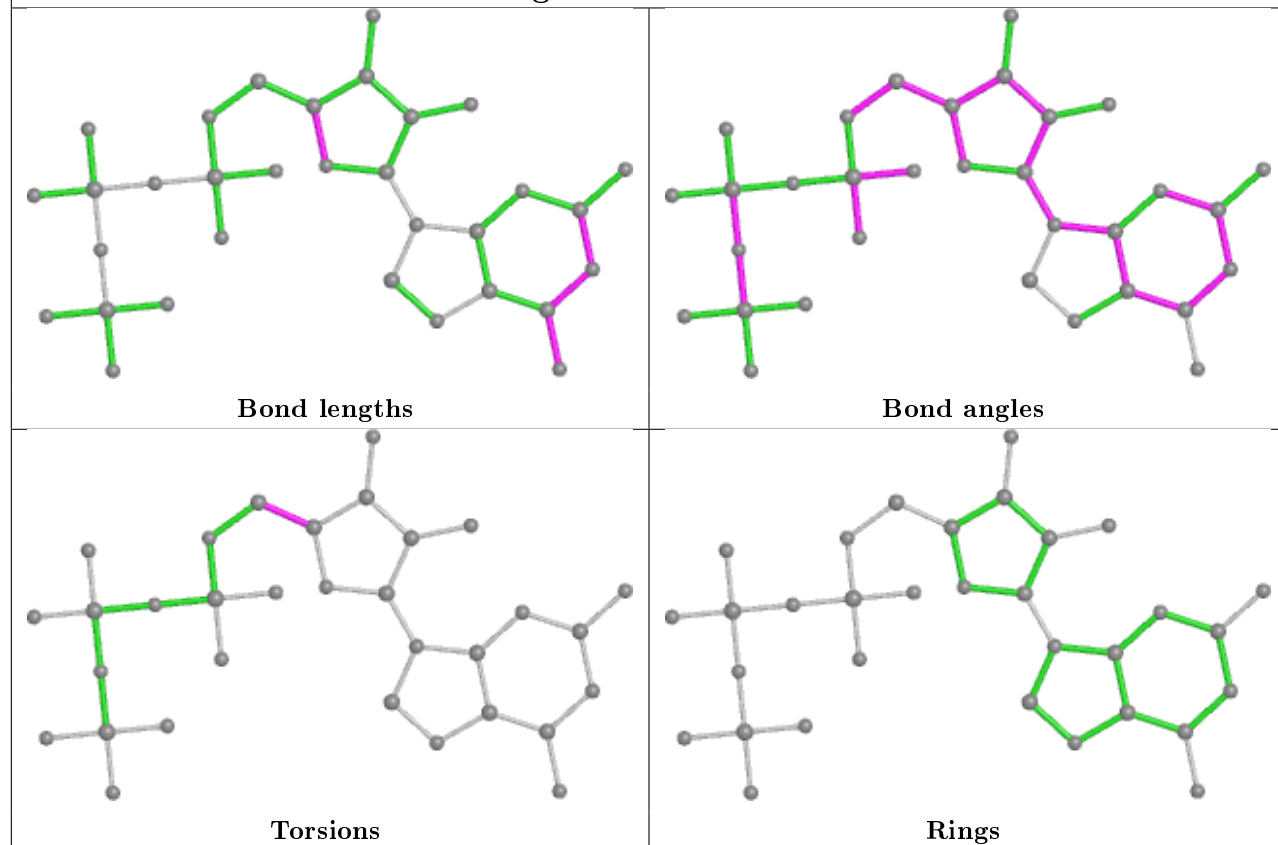
## Ligand GTP N 414



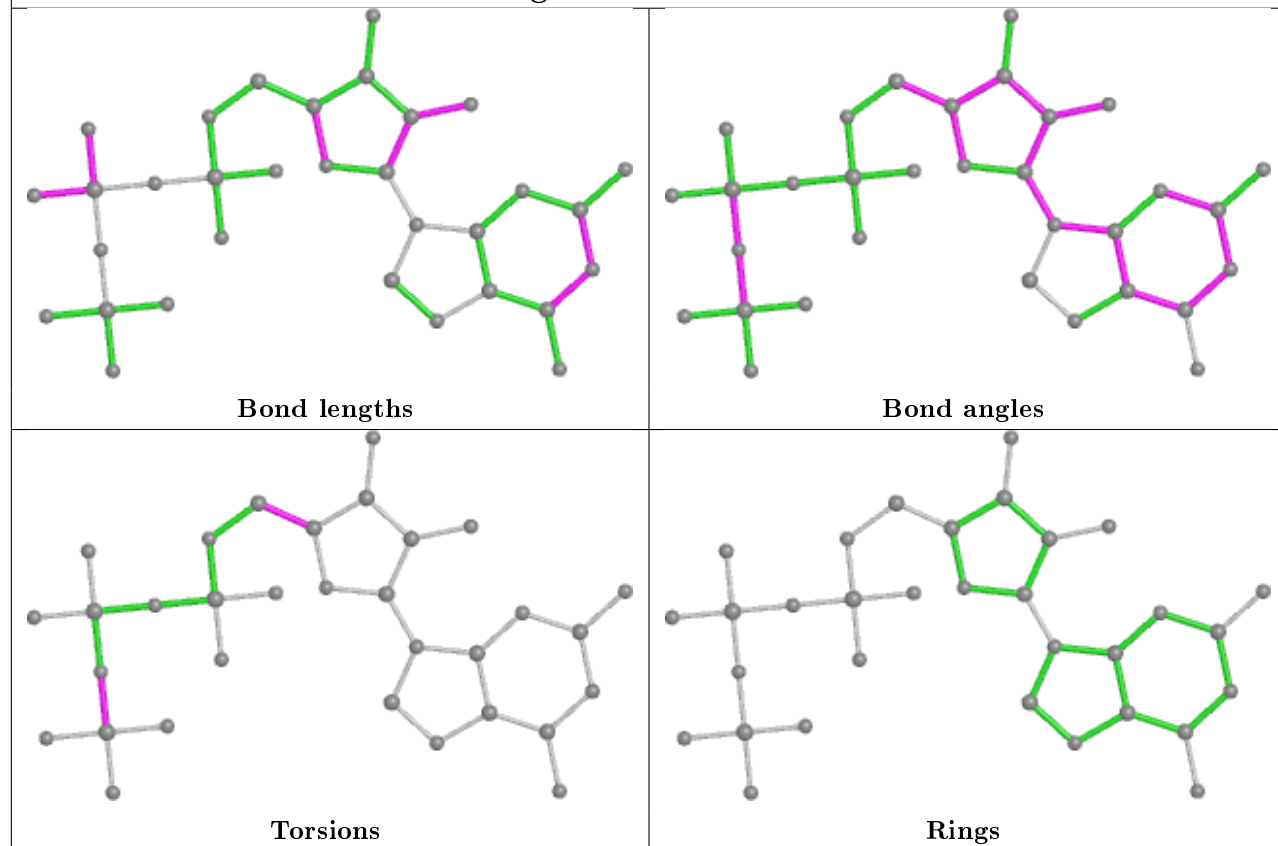
## Ligand GTP B 402

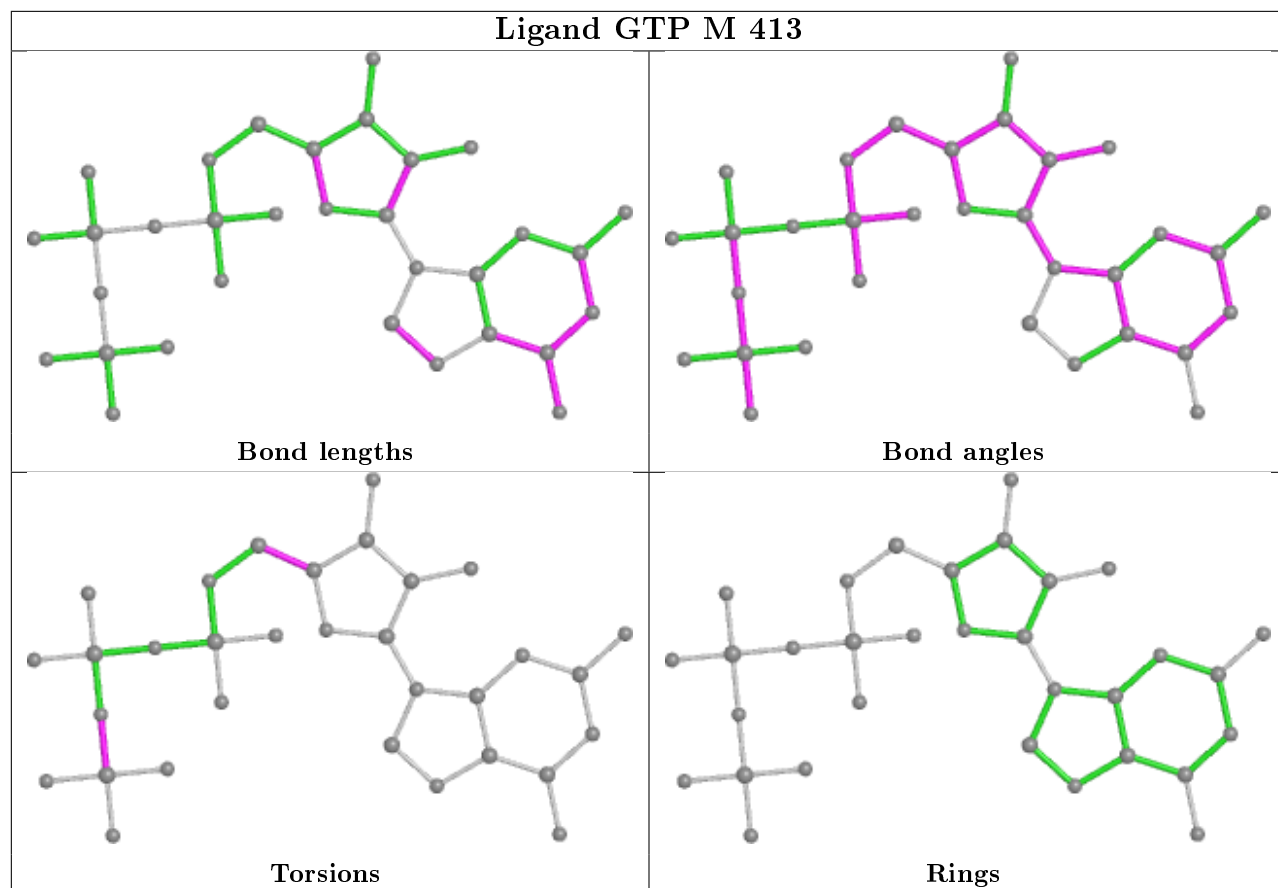


## Ligand GTP F 406



## 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.