



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2026 – 06:27 PM JST

PDB ID : 9UVK / pdb_00009uvk
Title : Crystal structure of UMPK from *S. aureus* in complex with GTP
Authors : Gao, Y.; Niu, L.W.
Deposited on : 2025-05-10
Resolution : 2.88 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

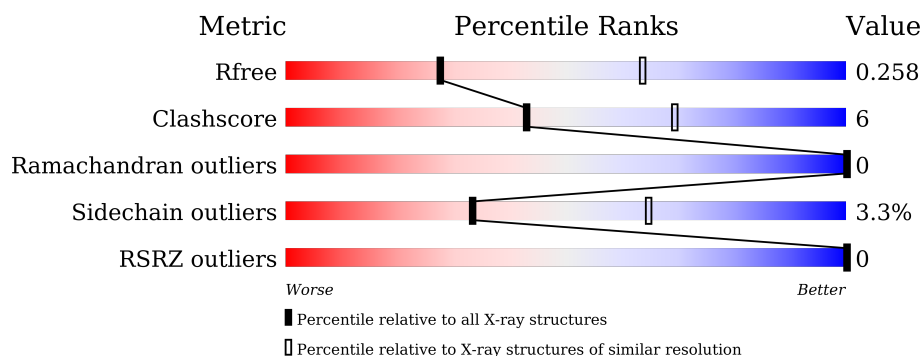
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	248	
1	B	248	
1	C	248	
1	D	248	
1	E	248	
1	F	248	

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Mol	Chain	Length	Quality of chain
1	G	248	 83% 12% .
1	H	248	 77% 18% . .
1	I	248	 81% 15% . .
1	J	248	 83% 12% . 5%
1	K	248	 77% 18% 5%
1	L	248	 78% 17% .
1	M	248	 79% 16% 5%
1	N	248	 75% 20% . .
1	O	248	 78% 17% . .
1	P	248	 77% 18% .
1	Q	248	 79% 16% . .
1	R	248	 81% 15% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33341 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 Uridylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	239	Total	C	N	O	S	0	0	0
			1815	1138	314	348	15			
1	A	239	Total	C	N	O	S	0	0	0
			1815	1138	314	348	15			
1	B	239	Total	C	N	O	S	0	0	0
			1815	1138	314	348	15			
1	D	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			
1	E	236	Total	C	N	O	S	0	0	0
			1793	1124	310	344	15			
1	F	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			
1	G	239	Total	C	N	O	S	0	0	0
			1815	1138	314	348	15			
1	H	239	Total	C	N	O	S	0	0	0
			1815	1138	314	348	15			
1	I	238	Total	C	N	O	S	0	0	0
			1810	1135	313	347	15			
1	J	236	Total	C	N	O	S	0	0	0
			1793	1124	310	344	15			
1	K	236	Total	C	N	O	S	0	0	0
			1793	1124	310	344	15			
1	L	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			
1	M	236	Total	C	N	O	S	0	0	0
			1793	1124	310	344	15			
1	N	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			
1	O	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			
1	P	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			
1	R	237	Total	C	N	O	S	0	0	0
			1801	1130	311	345	15			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	initiating methionine	UNP Q2FZ22
C	-6	GLY	-	expression tag	UNP Q2FZ22
C	-5	HIS	-	expression tag	UNP Q2FZ22
C	-4	HIS	-	expression tag	UNP Q2FZ22
C	-3	HIS	-	expression tag	UNP Q2FZ22
C	-2	HIS	-	expression tag	UNP Q2FZ22
C	-1	HIS	-	expression tag	UNP Q2FZ22
C	0	HIS	-	expression tag	UNP Q2FZ22
A	-7	MET	-	initiating methionine	UNP Q2FZ22
A	-6	GLY	-	expression tag	UNP Q2FZ22
A	-5	HIS	-	expression tag	UNP Q2FZ22
A	-4	HIS	-	expression tag	UNP Q2FZ22
A	-3	HIS	-	expression tag	UNP Q2FZ22
A	-2	HIS	-	expression tag	UNP Q2FZ22
A	-1	HIS	-	expression tag	UNP Q2FZ22
A	0	HIS	-	expression tag	UNP Q2FZ22
B	-7	MET	-	initiating methionine	UNP Q2FZ22
B	-6	GLY	-	expression tag	UNP Q2FZ22
B	-5	HIS	-	expression tag	UNP Q2FZ22
B	-4	HIS	-	expression tag	UNP Q2FZ22
B	-3	HIS	-	expression tag	UNP Q2FZ22
B	-2	HIS	-	expression tag	UNP Q2FZ22
B	-1	HIS	-	expression tag	UNP Q2FZ22
B	0	HIS	-	expression tag	UNP Q2FZ22
D	-7	MET	-	initiating methionine	UNP Q2FZ22
D	-6	GLY	-	expression tag	UNP Q2FZ22
D	-5	HIS	-	expression tag	UNP Q2FZ22
D	-4	HIS	-	expression tag	UNP Q2FZ22
D	-3	HIS	-	expression tag	UNP Q2FZ22
D	-2	HIS	-	expression tag	UNP Q2FZ22
D	-1	HIS	-	expression tag	UNP Q2FZ22
D	0	HIS	-	expression tag	UNP Q2FZ22
E	-7	MET	-	initiating methionine	UNP Q2FZ22
E	-6	GLY	-	expression tag	UNP Q2FZ22

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q2FZ22
E	-4	HIS	-	expression tag	UNP Q2FZ22
E	-3	HIS	-	expression tag	UNP Q2FZ22
E	-2	HIS	-	expression tag	UNP Q2FZ22
E	-1	HIS	-	expression tag	UNP Q2FZ22
E	0	HIS	-	expression tag	UNP Q2FZ22
F	-7	MET	-	initiating methionine	UNP Q2FZ22
F	-6	GLY	-	expression tag	UNP Q2FZ22
F	-5	HIS	-	expression tag	UNP Q2FZ22
F	-4	HIS	-	expression tag	UNP Q2FZ22
F	-3	HIS	-	expression tag	UNP Q2FZ22
F	-2	HIS	-	expression tag	UNP Q2FZ22
F	-1	HIS	-	expression tag	UNP Q2FZ22
F	0	HIS	-	expression tag	UNP Q2FZ22
G	-7	MET	-	initiating methionine	UNP Q2FZ22
G	-6	GLY	-	expression tag	UNP Q2FZ22
G	-5	HIS	-	expression tag	UNP Q2FZ22
G	-4	HIS	-	expression tag	UNP Q2FZ22
G	-3	HIS	-	expression tag	UNP Q2FZ22
G	-2	HIS	-	expression tag	UNP Q2FZ22
G	-1	HIS	-	expression tag	UNP Q2FZ22
G	0	HIS	-	expression tag	UNP Q2FZ22
H	-7	MET	-	initiating methionine	UNP Q2FZ22
H	-6	GLY	-	expression tag	UNP Q2FZ22
H	-5	HIS	-	expression tag	UNP Q2FZ22
H	-4	HIS	-	expression tag	UNP Q2FZ22
H	-3	HIS	-	expression tag	UNP Q2FZ22
H	-2	HIS	-	expression tag	UNP Q2FZ22
H	-1	HIS	-	expression tag	UNP Q2FZ22
H	0	HIS	-	expression tag	UNP Q2FZ22
I	-7	MET	-	initiating methionine	UNP Q2FZ22
I	-6	GLY	-	expression tag	UNP Q2FZ22
I	-5	HIS	-	expression tag	UNP Q2FZ22
I	-4	HIS	-	expression tag	UNP Q2FZ22
I	-3	HIS	-	expression tag	UNP Q2FZ22
I	-2	HIS	-	expression tag	UNP Q2FZ22
I	-1	HIS	-	expression tag	UNP Q2FZ22
I	0	HIS	-	expression tag	UNP Q2FZ22
J	-7	MET	-	initiating methionine	UNP Q2FZ22
J	-6	GLY	-	expression tag	UNP Q2FZ22
J	-5	HIS	-	expression tag	UNP Q2FZ22
J	-4	HIS	-	expression tag	UNP Q2FZ22

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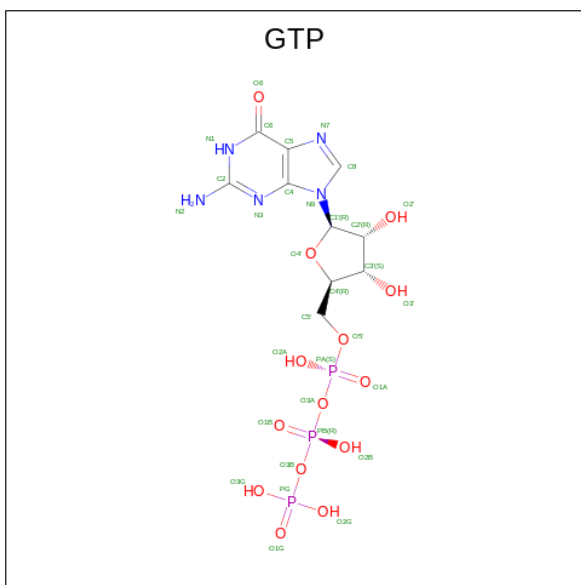
Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	HIS	-	expression tag	UNP Q2FZ22
J	-2	HIS	-	expression tag	UNP Q2FZ22
J	-1	HIS	-	expression tag	UNP Q2FZ22
J	0	HIS	-	expression tag	UNP Q2FZ22
K	-7	MET	-	initiating methionine	UNP Q2FZ22
K	-6	GLY	-	expression tag	UNP Q2FZ22
K	-5	HIS	-	expression tag	UNP Q2FZ22
K	-4	HIS	-	expression tag	UNP Q2FZ22
K	-3	HIS	-	expression tag	UNP Q2FZ22
K	-2	HIS	-	expression tag	UNP Q2FZ22
K	-1	HIS	-	expression tag	UNP Q2FZ22
K	0	HIS	-	expression tag	UNP Q2FZ22
L	-7	MET	-	initiating methionine	UNP Q2FZ22
L	-6	GLY	-	expression tag	UNP Q2FZ22
L	-5	HIS	-	expression tag	UNP Q2FZ22
L	-4	HIS	-	expression tag	UNP Q2FZ22
L	-3	HIS	-	expression tag	UNP Q2FZ22
L	-2	HIS	-	expression tag	UNP Q2FZ22
L	-1	HIS	-	expression tag	UNP Q2FZ22
L	0	HIS	-	expression tag	UNP Q2FZ22
M	-7	MET	-	initiating methionine	UNP Q2FZ22
M	-6	GLY	-	expression tag	UNP Q2FZ22
M	-5	HIS	-	expression tag	UNP Q2FZ22
M	-4	HIS	-	expression tag	UNP Q2FZ22
M	-3	HIS	-	expression tag	UNP Q2FZ22
M	-2	HIS	-	expression tag	UNP Q2FZ22
M	-1	HIS	-	expression tag	UNP Q2FZ22
M	0	HIS	-	expression tag	UNP Q2FZ22
N	-7	MET	-	initiating methionine	UNP Q2FZ22
N	-6	GLY	-	expression tag	UNP Q2FZ22
N	-5	HIS	-	expression tag	UNP Q2FZ22
N	-4	HIS	-	expression tag	UNP Q2FZ22
N	-3	HIS	-	expression tag	UNP Q2FZ22
N	-2	HIS	-	expression tag	UNP Q2FZ22
N	-1	HIS	-	expression tag	UNP Q2FZ22
N	0	HIS	-	expression tag	UNP Q2FZ22
O	-7	MET	-	initiating methionine	UNP Q2FZ22
O	-6	GLY	-	expression tag	UNP Q2FZ22
O	-5	HIS	-	expression tag	UNP Q2FZ22
O	-4	HIS	-	expression tag	UNP Q2FZ22
O	-3	HIS	-	expression tag	UNP Q2FZ22
O	-2	HIS	-	expression tag	UNP Q2FZ22

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	HIS	-	expression tag	UNP Q2FZ22
O	0	HIS	-	expression tag	UNP Q2FZ22
P	-7	MET	-	initiating methionine	UNP Q2FZ22
P	-6	GLY	-	expression tag	UNP Q2FZ22
P	-5	HIS	-	expression tag	UNP Q2FZ22
P	-4	HIS	-	expression tag	UNP Q2FZ22
P	-3	HIS	-	expression tag	UNP Q2FZ22
P	-2	HIS	-	expression tag	UNP Q2FZ22
P	-1	HIS	-	expression tag	UNP Q2FZ22
P	0	HIS	-	expression tag	UNP Q2FZ22
Q	-7	MET	-	initiating methionine	UNP Q2FZ22
Q	-6	GLY	-	expression tag	UNP Q2FZ22
Q	-5	HIS	-	expression tag	UNP Q2FZ22
Q	-4	HIS	-	expression tag	UNP Q2FZ22
Q	-3	HIS	-	expression tag	UNP Q2FZ22
Q	-2	HIS	-	expression tag	UNP Q2FZ22
Q	-1	HIS	-	expression tag	UNP Q2FZ22
Q	0	HIS	-	expression tag	UNP Q2FZ22
R	-7	MET	-	initiating methionine	UNP Q2FZ22
R	-6	GLY	-	expression tag	UNP Q2FZ22
R	-5	HIS	-	expression tag	UNP Q2FZ22
R	-4	HIS	-	expression tag	UNP Q2FZ22
R	-3	HIS	-	expression tag	UNP Q2FZ22
R	-2	HIS	-	expression tag	UNP Q2FZ22
R	-1	HIS	-	expression tag	UNP Q2FZ22
R	0	HIS	-	expression tag	UNP Q2FZ22

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



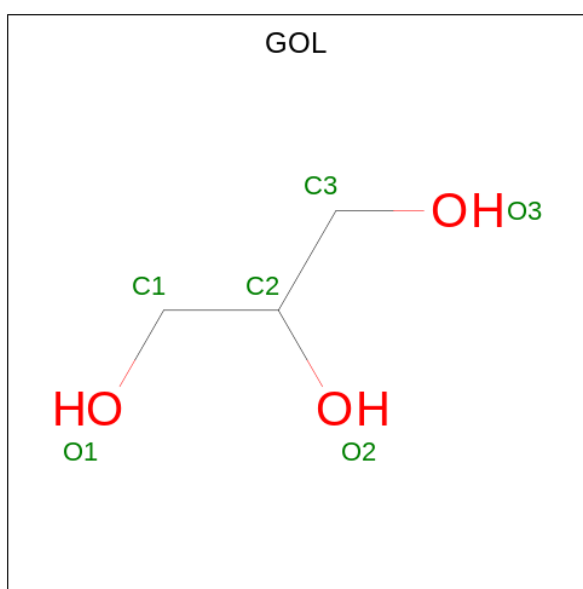
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	F	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	G	1	Total 32	C 10	N 5	O 14	P 3	0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

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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	P	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	Q	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	R	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		

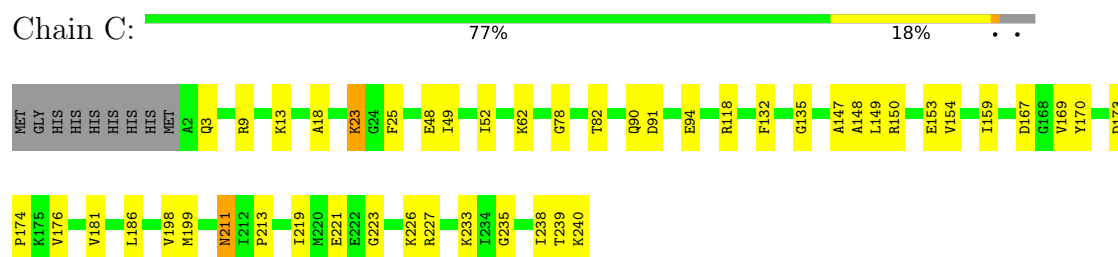
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	9	Total O 9 9	0	0
4	A	11	Total O 11 11	0	0
4	B	11	Total O 11 11	0	0
4	D	9	Total O 9 9	0	0
4	E	8	Total O 8 8	0	0
4	F	10	Total O 10 10	0	0
4	G	8	Total O 8 8	0	0
4	H	4	Total O 4 4	0	0
4	I	9	Total O 9 9	0	0
4	J	8	Total O 8 8	0	0
4	K	7	Total O 7 7	0	0
4	L	8	Total O 8 8	0	0
4	M	9	Total O 9 9	0	0
4	N	4	Total O 4 4	0	0
4	O	7	Total O 7 7	0	0
4	P	8	Total O 8 8	0	0
4	Q	3	Total O 3 3	0	0
4	R	11	Total O 11 11	0	0

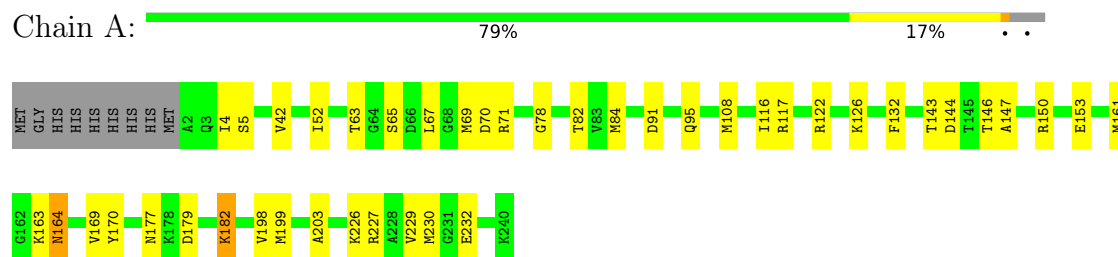
3 Residue-property plots

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.

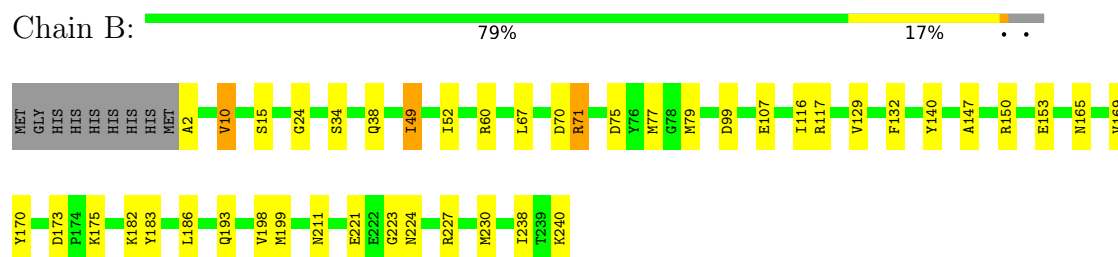
• Molecule 1: Uridylate kinase



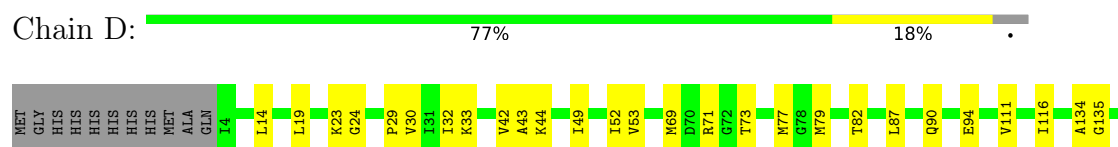
• Molecule 1: Uridylate kinase



• Molecule 1: Uridylate kinase



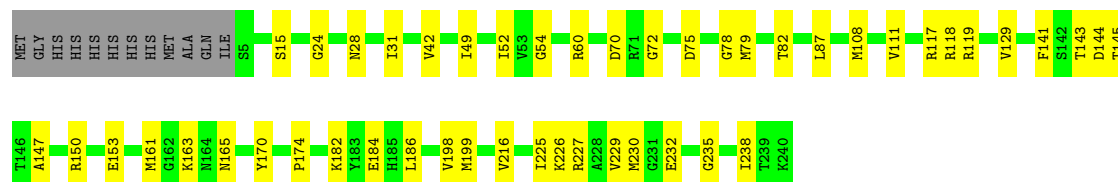
• Molecule 1: Uridylate kinase





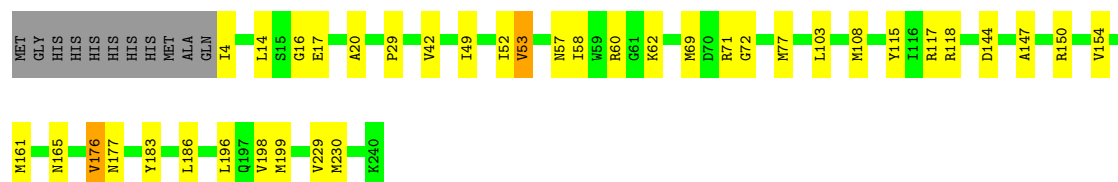
- Molecule 1: Uridylate kinase

Chain E: 76% 19% 5%



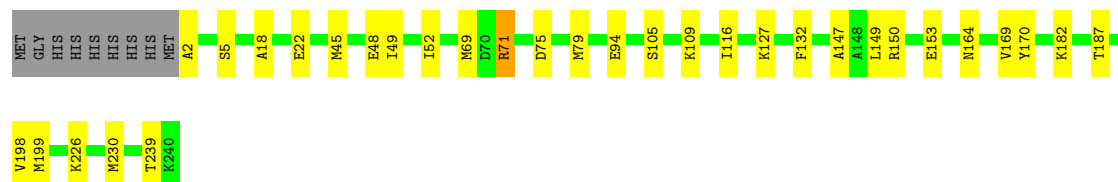
- Molecule 1: Uridylate kinase

Chain F: 80% 15% ..



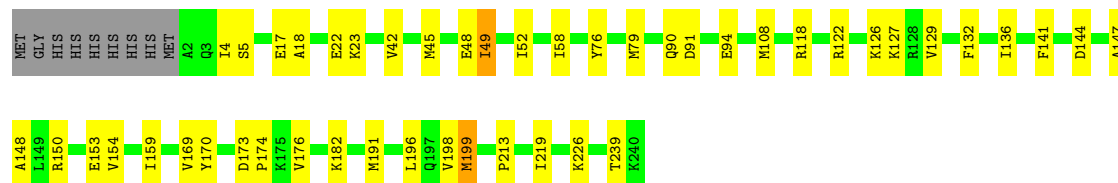
- Molecule 1: Uridylate kinase

Chain G: 83% 12% .



- Molecule 1: Uridylate kinase

Chain H: 77% 18% ..



- Molecule 1: Uridylate kinase

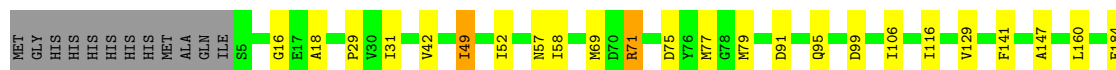
Chain I: 81% 15% ..





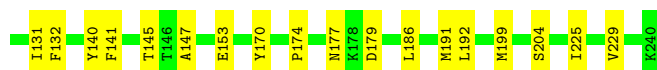
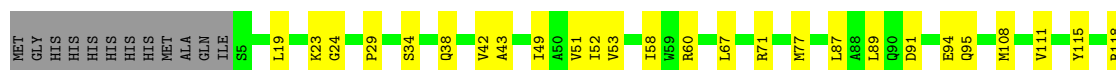
- Molecule 1: Uridylate kinase

Chain J: 83% 12% 5%



- Molecule 1: Uridylate kinase

Chain K: 77% 18% 5%



- Molecule 1: Uridylate kinase

Chain L: 78% 17% 5%



- Molecule 1: Uridylate kinase

Chain M: 79% 16% 5%



- Molecule 1: Uridylate kinase

Chain N: 75% 20% 5%





- Molecule 1: Uridylate kinase

Chain O: 78% 17%



- Molecule 1: Uridylate kinase

Chain P: 77% 18%



- Molecule 1: Uridylate kinase

Chain Q: 79% 16%



- Molecule 1: Uridylate kinase

Chain R: 81% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	194.26Å 194.26Å 116.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	13.14 – 2.88 13.14 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (13.14-2.88) 87.2 (13.14-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.89Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.203 , 0.257 0.204 , 0.258	Depositor DCC
R_{free} test set	5481 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.016 for h,-h-k,-l 0.148 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	33341	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2430e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/1835	0.33	0/2471
1	B	0.12	0/1835	0.32	0/2471
1	C	0.13	0/1835	0.33	0/2471
1	D	0.13	0/1821	0.32	0/2452
1	E	0.13	0/1813	0.33	0/2441
1	F	0.14	0/1821	0.35	0/2452
1	G	0.13	0/1835	0.32	0/2471
1	H	0.12	0/1835	0.34	0/2471
1	I	0.13	0/1830	0.33	0/2464
1	J	0.14	0/1813	0.33	0/2441
1	K	0.13	0/1813	0.32	0/2441
1	L	0.15	0/1821	0.33	0/2452
1	M	0.13	0/1813	0.32	0/2441
1	N	0.12	0/1821	0.31	0/2452
1	O	0.13	0/1821	0.32	0/2452
1	P	0.14	0/1821	0.33	0/2452
1	Q	0.12	0/1821	0.35	0/2452
1	R	0.13	0/1821	0.33	0/2452
All	All	0.13	0/32825	0.33	0/44199

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1815	0	1863	26	0
1	B	1815	0	1863	28	0
1	C	1815	0	1863	26	0
1	D	1801	0	1850	25	0
1	E	1793	0	1839	32	0
1	F	1801	0	1850	30	0
1	G	1815	0	1863	19	0
1	H	1815	0	1863	27	0
1	I	1810	0	1858	19	0
1	J	1793	0	1839	20	0
1	K	1793	0	1839	27	0
1	L	1801	0	1850	24	0
1	M	1793	0	1839	24	0
1	N	1801	0	1850	29	0
1	O	1801	0	1850	27	0
1	P	1801	0	1850	31	0
1	Q	1801	0	1850	23	0
1	R	1801	0	1850	16	0
2	A	32	0	11	0	0
2	B	32	0	11	0	0
2	C	32	0	11	0	0
2	D	32	0	11	0	0
2	E	32	0	11	1	0
2	F	32	0	11	0	0
2	G	32	0	11	1	0
2	H	32	0	11	1	0
2	I	32	0	11	0	0
2	J	32	0	11	0	0
2	K	32	0	11	0	0
2	L	32	0	11	1	0
2	M	32	0	11	0	0
2	N	32	0	11	2	0
2	O	32	0	11	1	0
2	P	32	0	11	1	0
2	Q	32	0	11	0	0
2	R	32	0	11	0	0
3	A	18	0	24	1	0
3	C	12	0	16	1	0
3	D	12	0	16	1	0
3	E	24	0	32	2	0
3	F	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	J	12	0	16	0	0
3	K	6	0	8	0	0
3	L	18	0	24	2	0
3	O	6	0	8	0	0
3	P	12	0	16	2	0
3	Q	12	0	16	3	0
4	A	11	0	0	0	0
4	B	11	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
4	E	8	0	0	0	0
4	F	10	0	0	0	0
4	G	8	0	0	0	0
4	H	4	0	0	0	0
4	I	9	0	0	0	0
4	J	8	0	0	1	0
4	K	7	0	0	0	0
4	L	8	0	0	0	0
4	M	9	0	0	0	0
4	N	4	0	0	0	0
4	O	7	0	0	0	0
4	P	8	0	0	0	0
4	Q	3	0	0	0	0
4	R	11	0	0	0	0
All	All	33341	0	33735	414	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 6.

All (414) 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:E:144:ASP:HB3	1:E:199:MET:HE2	1.65	0.77
1:P:6:LYS:HD2	1:P:231:GLY:HA3	1.69	0.75
1:A:144:ASP:HB3	1:A:199:MET:HE3	1.70	0.74
1:O:6:LYS:HD2	1:O:231:GLY:HA3	1.67	0.74
1:E:161:MET:HE1	1:E:199:MET:HE3	1.69	0.73
1:R:144:ASP:HB3	1:R:199:MET:HE2	1.71	0.71
1:D:135:GLY:HA3	3:D:302:GOL:H11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ARG:NH1	1:J:210:ASN:OD1	2.25	0.69
1:L:108:MET:HE2	1:M:108:MET:HG2	1.75	0.69
1:K:52:ILE:HG12	1:K:132:PHE:HB2	1.75	0.68
1:D:52:ILE:HD12	1:D:147:ALA:HA	1.75	0.68
1:P:13:LYS:HD2	1:P:161:MET:HE2	1.75	0.68
1:H:144:ASP:HB3	1:H:199:MET:HE3	1.74	0.67
1:L:6:LYS:HD3	1:L:231:GLY:HA3	1.76	0.67
1:N:42:VAL:HA	1:N:45:MET:HE2	1.76	0.67
1:A:52:ILE:HG12	1:A:132:PHE:HB2	1.76	0.66
1:L:144:ASP:HB3	1:L:199:MET:HE3	1.78	0.66
1:I:52:ILE:HD12	1:I:147:ALA:HA	1.77	0.66
1:L:199:MET:HE2	1:L:203:ALA:HB1	1.75	0.66
1:B:52:ILE:HD12	1:B:147:ALA:HA	1.78	0.65
1:M:6:LYS:HD3	1:M:231:GLY:HA3	1.80	0.64
1:Q:78:GLY:HA3	3:Q:303:GOL:H12	1.80	0.64
1:O:4:ILE:HG12	1:O:5:SER:H	1.63	0.64
1:N:116:ILE:HB	1:N:119:ARG:HB2	1.80	0.63
1:D:177:ASN:HD21	1:D:179:ASP:HB3	1.64	0.63
1:F:60:ARG:HD3	1:F:62:LYS:HE2	1.78	0.63
1:Q:52:ILE:HD12	1:Q:147:ALA:HA	1.80	0.63
1:M:52:ILE:HG12	1:M:132:PHE:HB2	1.81	0.62
1:N:141:PHE:HD1	1:N:145:THR:HG21	1.63	0.62
1:D:42:VAL:HG11	1:D:229:VAL:HG21	1.81	0.62
1:M:42:VAL:HG13	1:M:229:VAL:HG11	1.80	0.62
1:F:144:ASP:HB3	1:F:199:MET:HE2	1.81	0.62
1:R:87:LEU:HD11	1:R:111:VAL:HG13	1.83	0.61
1:P:173:ASP:HB3	1:P:176:VAL:HB	1.83	0.61
1:O:198:VAL:HG23	1:O:199:MET:HG3	1.83	0.61
1:E:52:ILE:HD12	1:E:147:ALA:HA	1.82	0.61
1:A:52:ILE:HD12	1:A:147:ALA:HA	1.82	0.60
1:F:20:ALA:HB2	1:F:57:ASN:HB2	1.83	0.60
1:J:52:ILE:HD12	1:J:147:ALA:HA	1.82	0.60
1:J:42:VAL:HG13	1:J:229:VAL:HG11	1.84	0.60
1:O:150:ARG:NH1	1:O:153:GLU:OE1	2.35	0.60
1:I:144:ASP:HB3	1:I:199:MET:HE2	1.83	0.60
1:C:52:ILE:HD12	1:C:147:ALA:HA	1.84	0.59
1:N:6:LYS:HD2	1:N:231:GLY:HA3	1.84	0.59
1:A:199:MET:HE2	1:A:203:ALA:HB1	1.85	0.59
1:I:172:ALA:HB1	1:I:177:ASN:HD21	1.68	0.59
1:Q:144:ASP:HB3	1:Q:199:MET:HE2	1.85	0.59
2:L:301:GTP:H4'	1:P:118:ARG:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:144:ASP:HB3	1:M:199:MET:HE2	1.85	0.58
1:K:43:ALA:HA	1:K:49:ILE:HD13	1.86	0.58
1:K:58:ILE:HG22	1:O:84:MET:HE1	1.85	0.58
1:E:198:VAL:HG23	1:E:199:MET:HG2	1.84	0.58
1:O:52:ILE:HG12	1:O:132:PHE:HB2	1.85	0.58
1:P:71:ARG:HH21	1:P:140:TYR:HA	1.69	0.57
1:Q:42:VAL:HA	1:Q:45:MET:HE2	1.87	0.57
1:D:42:VAL:HG12	1:D:49:ILE:HD11	1.85	0.57
1:M:42:VAL:HG11	1:M:229:VAL:HG21	1.85	0.57
1:H:18:ALA:HB1	1:H:219:ILE:HD11	1.87	0.57
1:B:2:ALA:HA	1:B:230:MET:SD	2.44	0.57
1:F:42:VAL:HG11	1:F:229:VAL:HG21	1.87	0.56
1:F:198:VAL:HG23	1:F:199:MET:HG3	1.86	0.56
1:P:75:ASP:HA	3:P:303:GOL:H31	1.86	0.56
1:P:170:TYR:CE2	1:P:182:LYS:HB2	2.39	0.56
1:K:87:LEU:HD11	1:K:111:VAL:HG13	1.88	0.56
1:Q:42:VAL:HG13	1:Q:229:VAL:HG11	1.87	0.56
1:G:52:ILE:HD12	1:G:147:ALA:HA	1.86	0.56
1:H:170:TYR:CE2	1:H:182:LYS:HB2	2.41	0.56
1:K:52:ILE:HD12	1:K:147:ALA:HA	1.87	0.56
1:K:71:ARG:HD3	1:K:140:TYR:CE2	2.41	0.56
1:L:71:ARG:HH22	1:L:140:TYR:HA	1.71	0.55
1:B:150:ARG:NH1	1:B:153:GLU:OE1	2.38	0.55
1:C:213:PRO:HB3	1:C:239:THR:HG22	1.88	0.55
1:D:199:MET:HE2	1:D:203:ALA:HB1	1.89	0.55
1:E:143:THR:HB	3:E:302:GOL:H2	1.87	0.55
1:F:29:PRO:HG3	1:P:63:THR:HG23	1.89	0.55
1:A:164:ASN:OD1	1:A:164:ASN:N	2.39	0.55
1:F:52:ILE:HD12	1:F:147:ALA:HA	1.87	0.55
1:K:51:VAL:HB	1:K:131:ILE:HG12	1.89	0.55
1:H:52:ILE:HG12	1:H:132:PHE:HB2	1.88	0.54
1:G:198:VAL:HG23	1:G:199:MET:HG3	1.89	0.54
1:P:59:TRP:HE1	3:P:303:GOL:H12	1.72	0.54
1:Q:52:ILE:HG12	1:Q:132:PHE:HB2	1.89	0.54
1:I:29:PRO:O	1:I:33:LYS:HG2	2.08	0.54
1:I:52:ILE:HG12	1:I:132:PHE:HB2	1.88	0.54
1:R:169:VAL:HB	1:R:236:THR:HG21	1.89	0.54
1:M:6:LYS:HE2	1:M:7:TYR:CZ	2.43	0.53
1:H:52:ILE:HD12	1:H:147:ALA:HA	1.91	0.53
1:M:161:MET:HE2	1:M:163:LYS:HE3	1.89	0.53
1:D:19:LEU:HD22	1:D:32:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:ASP:HA	1:I:218:SER:HB2	1.91	0.53
1:K:225:ILE:O	1:K:229:VAL:HG23	2.08	0.53
1:O:165:ASN:OD1	1:O:165:ASN:N	2.41	0.53
1:N:167:ASP:HA	1:N:218:SER:HB2	1.91	0.53
1:C:149:LEU:HD22	1:D:141:PHE:HE2	1.74	0.53
1:D:43:ALA:HA	1:D:49:ILE:HD13	1.90	0.53
1:N:52:ILE:HG12	1:N:132:PHE:HB2	1.91	0.52
1:R:14:LEU:HD22	1:R:219:ILE:HD13	1.92	0.52
1:K:19:LEU:HD11	1:K:53:VAL:HG21	1.92	0.52
1:M:170:TYR:CE2	1:M:182:LYS:HB2	2.44	0.52
1:P:226:LYS:HG2	1:P:230:MET:HE2	1.90	0.52
1:C:52:ILE:HG12	1:C:132:PHE:HB2	1.92	0.52
1:H:17:GLU:OE1	1:H:17:GLU:N	2.35	0.52
1:G:2:ALA:HA	1:G:230:MET:SD	2.49	0.51
1:R:23:LYS:HG3	1:R:25:PHE:H	1.73	0.51
1:Q:169:VAL:HB	1:Q:236:THR:HG21	1.91	0.51
1:D:170:TYR:CE2	1:D:182:LYS:HB2	2.45	0.51
1:D:87:LEU:HD11	1:D:111:VAL:HG13	1.93	0.51
1:P:167:ASP:HA	1:P:218:SER:HB2	1.92	0.51
1:M:213:PRO:HB3	1:M:239:THR:HG22	1.93	0.51
1:L:170:TYR:CE2	1:L:182:LYS:HB2	2.46	0.51
1:G:52:ILE:HG12	1:G:132:PHE:HB2	1.93	0.51
1:G:169:VAL:HG22	1:G:198:VAL:HG11	1.93	0.51
1:J:69:MET:HA	1:N:91:ASP:OD2	2.11	0.51
1:O:29:PRO:O	1:O:33:LYS:HG2	2.11	0.51
1:C:23:LYS:HG2	1:C:25:PHE:HD2	1.76	0.51
1:B:169:VAL:HG22	1:B:198:VAL:HG11	1.93	0.50
1:H:150:ARG:NH1	1:H:153:GLU:OE1	2.43	0.50
1:I:213:PRO:HB3	1:I:239:THR:HG22	1.93	0.50
1:B:211:ASN:HB2	1:B:240:LYS:NZ	2.26	0.50
1:N:170:TYR:CE2	1:N:182:LYS:HB2	2.47	0.50
1:C:170:TYR:CG	1:C:174:PRO:HG3	2.46	0.50
1:D:90:GLN:O	1:D:94:GLU:HG3	2.11	0.50
1:D:79:MET:HB3	1:D:134:ALA:HA	1.93	0.50
1:D:144:ASP:HB3	1:D:199:MET:HE3	1.92	0.50
1:F:42:VAL:CG1	1:F:229:VAL:HG11	2.40	0.50
1:F:183:TYR:HE1	1:F:196:LEU:HD11	1.76	0.50
1:C:150:ARG:O	1:C:154:VAL:HG22	2.12	0.50
1:M:87:LEU:HD11	1:M:111:VAL:HG13	1.94	0.50
1:A:122:ARG:HG3	1:A:126:LYS:HE3	1.94	0.50
1:H:122:ARG:HG3	1:H:126:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:TYR:CG	1:H:174:PRO:HG3	2.47	0.50
1:J:18:ALA:O	1:J:31:ILE:HG21	2.12	0.50
1:E:42:VAL:HG13	1:E:229:VAL:HG11	1.94	0.49
1:P:167:ASP:O	1:P:235:GLY:HA2	2.12	0.49
1:G:48:GLU:OE2	1:G:127:LYS:NZ	2.45	0.49
1:B:117:ARG:NH1	1:F:72:GLY:HA3	2.27	0.49
1:D:42:VAL:HG13	1:D:229:VAL:HG11	1.93	0.49
1:E:79:MET:HG2	3:E:303:GOL:H2	1.94	0.49
1:F:77:MET:HE3	1:P:84:MET:HB3	1.95	0.49
1:I:21:GLY:HA3	1:I:23:LYS:HE3	1.95	0.49
1:K:170:TYR:CD2	1:K:174:PRO:HG3	2.48	0.49
1:M:52:ILE:HD12	1:M:147:ALA:HA	1.94	0.49
1:R:150:ARG:O	1:R:154:VAL:HG22	2.11	0.49
1:A:227:ARG:HG2	1:A:232:GLU:OE1	2.13	0.49
1:F:161:MET:HE1	1:F:199:MET:HG2	1.95	0.49
1:Q:161:MET:HE1	1:Q:199:MET:HE3	1.94	0.49
1:H:49:ILE:HG23	1:H:129:VAL:HG22	1.95	0.49
1:I:91:ASP:O	1:I:95:GLN:HG3	2.13	0.49
1:B:67:LEU:HA	1:I:33:LYS:HZ1	1.78	0.48
1:L:45:MET:HE1	1:L:230:MET:HG2	1.95	0.48
1:I:161:MET:HE1	1:I:199:MET:HE3	1.95	0.48
1:A:42:VAL:HG11	1:A:229:VAL:HG21	1.96	0.48
1:O:103:LEU:HA	1:O:113:GLU:O	2.14	0.48
1:F:4:ILE:HG22	1:F:230:MET:HE1	1.95	0.48
1:H:148:ALA:HA	1:H:159:ILE:HD11	1.95	0.48
1:K:177:ASN:HD21	1:K:179:ASP:HB3	1.78	0.48
1:M:42:VAL:CG1	1:M:229:VAL:HG11	2.43	0.48
1:E:24:GLY:O	1:E:60:ARG:NH2	2.47	0.48
1:I:18:ALA:HB1	1:I:219:ILE:HD11	1.95	0.48
1:N:49:ILE:HG23	1:N:129:VAL:HG22	1.96	0.48
1:Q:71:ARG:HD3	1:Q:140:TYR:CE2	2.49	0.48
1:E:225:ILE:O	1:E:229:VAL:HG23	2.14	0.48
1:F:71:ARG:HH21	1:F:71:ARG:HG2	1.78	0.48
1:B:71:ARG:HG2	1:B:140:TYR:CE2	2.49	0.48
1:G:150:ARG:NH1	1:G:153:GLU:OE1	2.47	0.48
1:F:42:VAL:HG13	1:F:229:VAL:HG11	1.94	0.47
1:B:183:TYR:CD2	1:B:186:LEU:HD21	2.49	0.47
1:J:160:LEU:HD22	1:J:228:ALA:HB1	1.96	0.47
1:R:170:TYR:CE2	1:R:182:LYS:HB2	2.49	0.47
1:B:24:GLY:O	1:B:60:ARG:NH2	2.48	0.47
1:E:150:ARG:NH1	1:E:153:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:GLY:HA3	1:N:182:LYS:HE2	1.96	0.47
1:P:6:LYS:HD3	1:P:7:TYR:CZ	2.49	0.47
1:P:148:ALA:HA	1:P:159:ILE:HD11	1.95	0.47
1:E:75:ASP:O	1:E:79:MET:HG3	2.14	0.47
1:E:119:ARG:HG2	2:H:301:GTP:H5''	1.97	0.47
1:R:4:ILE:HD13	1:R:5:SER:H	1.79	0.47
1:E:141:PHE:HD1	1:E:145:THR:HG21	1.80	0.47
1:L:105:SER:OG	1:L:135:GLY:O	2.26	0.47
1:L:165:ASN:OD1	1:L:165:ASN:N	2.47	0.47
1:Q:90:GLN:O	1:Q:94:GLU:HG3	2.14	0.47
1:J:49:ILE:HG23	1:J:129:VAL:HG22	1.97	0.47
1:K:115:TYR:OH	1:K:153:GLU:OE1	2.32	0.47
1:H:118:ARG:HG3	2:O:301:GTP:H4'	1.96	0.47
1:H:213:PRO:HB3	1:H:239:THR:HG22	1.95	0.47
1:I:223:GLY:O	1:I:227:ARG:HG3	2.15	0.47
1:P:17:GLU:OE1	1:P:17:GLU:N	2.43	0.47
1:I:150:ARG:NH1	1:I:153:GLU:OE1	2.47	0.47
1:C:23:LYS:HE3	1:C:25:PHE:HB2	1.95	0.47
1:C:90:GLN:O	1:C:94:GLU:HG2	2.14	0.47
1:C:150:ARG:NH1	1:C:153:GLU:OE1	2.48	0.47
1:H:48:GLU:OE2	1:H:127:LYS:NZ	2.47	0.47
1:L:42:VAL:HG13	1:L:229:VAL:HG11	1.97	0.47
1:Q:150:ARG:O	1:Q:154:VAL:HG22	2.15	0.47
1:R:18:ALA:HB1	1:R:219:ILE:HD11	1.97	0.47
1:J:91:ASP:O	1:J:95:GLN:HG3	2.15	0.46
1:Q:170:TYR:CE2	1:Q:182:LYS:HB2	2.49	0.46
1:H:76:TYR:HA	1:H:79:MET:HE3	1.96	0.46
1:J:42:VAL:HG11	1:J:229:VAL:HG21	1.98	0.46
1:K:34:SER:O	1:K:38:GLN:HG3	2.16	0.46
1:C:78:GLY:O	1:C:82:THR:HG23	2.15	0.46
1:C:135:GLY:HA3	3:C:302:GOL:H32	1.97	0.46
1:G:5:SER:HB2	1:G:45:MET:HE2	1.98	0.46
1:P:141:PHE:HD1	1:P:145:THR:HG21	1.81	0.46
1:F:103:LEU:HD23	1:F:115:TYR:HA	1.97	0.46
1:K:141:PHE:HD1	1:K:145:THR:HG21	1.79	0.46
1:K:186:LEU:HD13	1:K:191:MET:HG2	1.98	0.46
1:P:71:ARG:HG2	1:P:140:TYR:CE2	2.50	0.46
1:R:42:VAL:HG13	1:R:229:VAL:HG11	1.96	0.46
1:H:118:ARG:HA	1:H:118:ARG:HD2	1.76	0.46
1:N:170:TYR:CZ	1:N:182:LYS:HD3	2.50	0.46
1:C:169:VAL:HG22	1:C:198:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:VAL:HG13	1:F:177:ASN:H	1.81	0.46
1:I:187:THR:HA	1:I:239:THR:O	2.16	0.46
1:K:91:ASP:OD2	1:O:69:MET:HA	2.16	0.46
1:N:42:VAL:HG11	1:N:229:VAL:HG21	1.98	0.46
1:M:233:LYS:HD3	1:M:233:LYS:HA	1.47	0.46
1:O:49:ILE:HG23	1:O:129:VAL:HG22	1.98	0.46
1:R:167:ASP:O	1:R:235:GLY:HA2	2.16	0.46
1:J:16:GLY:O	1:J:57:ASN:HB3	2.16	0.46
1:H:90:GLN:O	1:H:94:GLU:HG3	2.15	0.46
1:O:213:PRO:HB3	1:O:239:THR:HG22	1.97	0.46
1:B:77:MET:HE3	1:B:77:MET:HB3	1.88	0.46
1:B:170:TYR:CE2	1:B:182:LYS:HB2	2.51	0.46
1:E:170:TYR:CG	1:E:174:PRO:HG3	2.51	0.46
1:F:16:GLY:O	1:F:57:ASN:HB3	2.16	0.45
1:G:116:ILE:HD13	2:N:301:GTP:C6	2.51	0.45
1:L:150:ARG:O	1:L:154:VAL:HG22	2.16	0.45
1:A:143:THR:OG1	3:A:303:GOL:H31	2.16	0.45
1:B:221:GLU:HB3	1:B:224:ASN:ND2	2.30	0.45
1:D:44:LYS:HE2	1:D:44:LYS:HB2	1.73	0.45
1:G:149:LEU:HD22	1:J:141:PHE:HE2	1.81	0.45
1:H:136:ILE:HD11	1:H:141:PHE:CD2	2.51	0.45
1:J:77:MET:HE3	1:N:84:MET:HB3	1.98	0.45
1:G:105:SER:OG	1:G:150:ARG:NH2	2.49	0.45
1:L:167:ASP:HA	1:L:218:SER:HB2	1.99	0.45
1:O:150:ARG:O	1:O:154:VAL:HG22	2.16	0.45
1:F:150:ARG:O	1:F:154:VAL:HG22	2.16	0.45
1:Q:135:GLY:HA3	3:Q:302:GOL:H11	1.98	0.45
1:R:188:HIS:HB3	1:R:208:MET:HE2	1.98	0.45
1:C:13:LYS:HG3	1:C:147:ALA:HB2	1.98	0.45
1:O:122:ARG:HG3	1:O:126:LYS:HE2	1.97	0.45
1:B:75:ASP:O	1:B:79:MET:HG3	2.17	0.45
1:B:198:VAL:HG23	1:B:199:MET:HG3	1.99	0.45
1:G:170:TYR:CE2	1:G:182:LYS:HB2	2.51	0.45
1:H:169:VAL:HG22	1:H:198:VAL:HG11	1.99	0.45
1:J:106:ILE:HG23	1:N:110:GLN:OE1	2.17	0.45
1:C:223:GLY:O	1:C:227:ARG:HG3	2.17	0.45
1:A:161:MET:SD	1:A:163:LYS:HE3	2.57	0.45
1:J:71:ARG:NH2	4:J:401:HOH:O	2.45	0.45
1:A:69:MET:HA	1:H:91:ASP:OD2	2.16	0.44
1:B:70:ASP:CG	1:F:117:ARG:HH12	2.25	0.44
1:O:144:ASP:HB3	1:O:199:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:NH1	1:A:153:GLU:OE1	2.50	0.44
1:L:42:VAL:HG11	1:L:229:VAL:HG21	1.98	0.44
1:M:223:GLY:O	1:M:227:ARG:HG3	2.17	0.44
1:B:173:ASP:OD2	1:B:175:LYS:HB2	2.17	0.44
1:G:226:LYS:HG2	1:G:230:MET:HE2	1.99	0.44
1:Q:136:ILE:HD11	1:Q:141:PHE:CD2	2.52	0.44
1:E:49:ILE:CG2	1:E:129:VAL:HG22	2.47	0.44
1:H:150:ARG:O	1:H:154:VAL:HG22	2.17	0.44
1:O:199:MET:HE2	1:O:203:ALA:HB1	2.00	0.44
1:A:84:MET:HE1	1:H:58:ILE:HG22	2.00	0.44
1:F:69:MET:HA	1:P:91:ASP:OD2	2.17	0.44
1:I:118:ARG:HD2	1:I:118:ARG:HA	1.72	0.44
1:J:91:ASP:OD2	1:N:69:MET:HA	2.18	0.44
1:L:19:LEU:HD22	1:L:32:ILE:HD13	2.00	0.44
1:M:198:VAL:HG23	1:M:199:MET:HG3	2.00	0.44
1:J:186:LEU:O	1:J:238:ILE:HA	2.16	0.44
1:K:91:ASP:O	1:K:95:GLN:HG3	2.18	0.44
1:L:28:ASN:OD1	1:L:30:VAL:HG12	2.17	0.44
1:B:52:ILE:HG12	1:B:132:PHE:HB2	2.00	0.44
1:E:226:LYS:O	1:E:230:MET:HG2	2.18	0.44
1:J:75:ASP:O	1:J:79:MET:HG3	2.18	0.44
1:J:77:MET:HE2	1:J:77:MET:HB3	1.87	0.44
1:A:91:ASP:O	1:A:95:GLN:HG3	2.17	0.44
1:E:28:ASN:HB3	1:E:31:ILE:HB	1.99	0.44
1:C:9:ARG:NH2	1:C:48:GLU:OE1	2.46	0.43
1:C:186:LEU:O	1:C:238:ILE:HA	2.18	0.43
1:A:169:VAL:HG22	1:A:198:VAL:HG11	1.98	0.43
1:K:29:PRO:HA	1:O:67:LEU:HD21	2.00	0.43
1:O:71:ARG:HG2	1:O:140:TYR:CE2	2.53	0.43
1:P:49:ILE:HG23	1:P:129:VAL:HG22	2.00	0.43
1:Q:49:ILE:HG23	1:Q:129:VAL:HG22	1.99	0.43
1:F:42:VAL:HG12	1:F:49:ILE:HD11	2.00	0.43
1:N:6:LYS:HD3	1:N:7:TYR:CZ	2.53	0.43
1:Q:79:MET:O	1:Q:82:THR:OG1	2.33	0.43
1:C:91:ASP:OD2	1:G:69:MET:HA	2.19	0.43
1:A:78:GLY:O	1:A:82:THR:HG23	2.18	0.43
1:B:34:SER:O	1:B:38:GLN:HG3	2.17	0.43
1:B:186:LEU:O	1:B:238:ILE:HA	2.18	0.43
1:M:31:ILE:O	1:M:35:VAL:HG23	2.18	0.43
1:H:4:ILE:HG12	1:H:5:SER:H	1.84	0.43
1:C:18:ALA:HB1	1:C:219:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:MET:O	1:D:82:THR:OG1	2.33	0.43
1:D:226:LYS:HG2	1:D:230:MET:HE2	2.01	0.43
1:I:70:ASP:CG	1:L:117:ARG:HH22	2.27	0.43
1:K:77:MET:HE3	1:O:84:MET:HB3	1.99	0.43
1:K:89:LEU:HD12	1:K:89:LEU:HA	1.84	0.43
1:P:165:ASN:OD1	1:P:165:ASN:N	2.52	0.43
1:B:10:VAL:HG12	1:B:49:ILE:HD12	2.01	0.43
1:D:186:LEU:HD13	1:D:191:MET:HG2	2.00	0.43
1:N:117:ARG:HH12	1:Q:70:ASP:CG	2.27	0.43
1:N:214:LEU:O	1:N:237:LEU:HD12	2.18	0.43
1:P:197:GLN:HG2	1:P:199:MET:O	2.19	0.43
1:H:173:ASP:HB3	1:H:176:VAL:HG12	2.00	0.43
1:L:143:THR:OG1	3:L:303:GOL:H11	2.19	0.43
1:P:14:LEU:HD22	1:P:219:ILE:HD13	2.01	0.43
1:A:52:ILE:HD11	1:A:150:ARG:HG3	2.01	0.43
1:B:49:ILE:HG23	1:B:129:VAL:HG22	2.01	0.43
1:E:118:ARG:HD2	1:E:118:ARG:HA	1.76	0.43
1:K:23:LYS:HD2	1:O:25:PHE:CE2	2.53	0.43
1:N:198:VAL:HG23	1:N:199:MET:HG3	2.00	0.43
1:C:233:LYS:HD2	1:F:186:LEU:HD23	2.01	0.43
1:O:52:ILE:HD12	1:O:147:ALA:HA	2.00	0.43
1:A:4:ILE:HG12	1:A:5:SER:H	1.84	0.42
1:E:170:TYR:CE2	1:E:182:LYS:HB2	2.54	0.42
1:E:186:LEU:O	1:E:238:ILE:HA	2.19	0.42
1:N:150:ARG:O	1:N:154:VAL:HG22	2.19	0.42
1:A:70:ASP:CG	1:E:117:ARG:HH22	2.28	0.42
1:E:216:VAL:O	1:E:235:GLY:HA3	2.18	0.42
1:H:42:VAL:HA	1:H:45:MET:HE2	2.00	0.42
1:M:7:TYR:HD2	1:M:229:VAL:O	2.02	0.42
1:N:103:LEU:HA	1:N:113:GLU:O	2.20	0.42
1:Q:75:ASP:HA	3:Q:303:GOL:H11	2.00	0.42
1:D:29:PRO:HA	1:Q:67:LEU:HD21	2.01	0.42
1:F:20:ALA:HB2	1:F:57:ASN:CB	2.48	0.42
1:J:29:PRO:HA	1:N:67:LEU:HD21	2.02	0.42
1:K:77:MET:HE2	1:K:77:MET:HB3	1.76	0.42
1:L:67:LEU:HD21	1:M:29:PRO:HA	2.00	0.42
1:E:227:ARG:HG2	1:E:232:GLU:OE1	2.19	0.42
1:B:116:ILE:HD13	2:P:301:GTP:C6	2.54	0.42
1:E:49:ILE:HG23	1:E:129:VAL:HG22	2.02	0.42
1:L:13:LYS:NZ	3:L:302:GOL:H32	2.34	0.42
1:R:31:ILE:O	1:R:35:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:HG2	1:A:230:MET:HE2	2.00	0.42
1:B:107:GLU:OE2	1:P:109:LYS:HE2	2.19	0.42
1:K:199:MET:HE3	1:K:204:SER:HA	2.01	0.42
1:L:58:ILE:HB	1:L:81:ALA:HB1	2.01	0.42
1:E:141:PHE:CD1	1:E:145:THR:HG21	2.55	0.42
1:M:166:VAL:O	1:M:218:SER:HB2	2.20	0.42
1:N:19:LEU:HD22	1:N:32:ILE:HD12	2.02	0.42
1:N:165:ASN:OD1	1:N:165:ASN:N	2.47	0.42
1:A:170:TYR:CE2	1:A:182:LYS:HB2	2.54	0.42
1:I:62:LYS:HE2	1:I:66:ASP:OD2	2.20	0.42
1:L:135:GLY:HA2	1:L:146:THR:HG21	2.02	0.42
1:N:148:ALA:HB1	1:N:206:PHE:CD1	2.54	0.42
1:C:211:ASN:OD1	1:C:240:LYS:HD2	2.20	0.42
1:E:230:MET:HG3	1:E:232:GLU:HG3	2.02	0.42
1:K:24:GLY:O	1:K:60:ARG:NH2	2.43	0.42
1:E:54:GLY:C	1:E:82:THR:HG22	2.45	0.41
1:F:14:LEU:HB2	1:F:53:VAL:HG13	2.01	0.41
1:I:99:ASP:HB3	1:I:128:ARG:HG2	2.01	0.41
1:O:168:GLY:HA3	1:O:182:LYS:HE2	2.02	0.41
1:R:9:ARG:HA	1:R:48:GLU:O	2.20	0.41
1:R:226:LYS:O	1:R:230:MET:HB2	2.20	0.41
1:C:3:GLN:NE2	1:B:193:GLN:O	2.52	0.41
1:F:58:ILE:HG22	1:P:84:MET:HE1	2.02	0.41
1:K:67:LEU:HD21	1:O:29:PRO:HA	2.03	0.41
1:Q:71:ARG:NH2	1:Q:75:ASP:OD2	2.53	0.41
1:B:117:ARG:HH12	1:F:72:GLY:HA3	1.85	0.41
1:D:69:MET:HA	1:Q:91:ASP:OD2	2.21	0.41
2:E:301:GTP:C6	1:O:116:ILE:HD13	2.56	0.41
1:F:77:MET:HE2	1:F:77:MET:HB3	1.94	0.41
1:K:170:TYR:CG	1:K:174:PRO:HG3	2.55	0.41
1:O:73:THR:O	1:O:77:MET:HG2	2.20	0.41
1:A:170:TYR:CZ	1:A:182:LYS:HB2	2.54	0.41
1:L:91:ASP:O	1:L:95:GLN:HG3	2.19	0.41
1:Q:9:ARG:HA	1:Q:48:GLU:O	2.20	0.41
1:Q:198:VAL:HG23	1:Q:199:MET:HG3	2.03	0.41
1:G:187:THR:HA	1:G:239:THR:O	2.20	0.41
1:L:211:ASN:OD1	1:L:240:LYS:HD2	2.20	0.41
1:M:169:VAL:HB	1:M:236:THR:HG21	2.02	0.41
1:O:42:VAL:HA	1:O:45:MET:HE2	2.01	0.41
1:R:211:ASN:CG	1:R:240:LYS:HD2	2.46	0.41
1:E:165:ASN:OD1	1:E:165:ASN:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:ILE:HG22	1:N:84:MET:HE1	2.02	0.41
1:B:223:GLY:O	1:B:227:ARG:HG3	2.20	0.41
1:C:148:ALA:HA	1:C:159:ILE:HD11	2.03	0.41
1:C:167:ASP:O	1:C:235:GLY:HA2	2.21	0.41
1:D:14:LEU:O	1:D:53:VAL:HA	2.21	0.41
1:D:23:LYS:HG3	1:D:24:GLY:H	1.85	0.41
1:E:161:MET:SD	1:E:163:LYS:HE3	2.61	0.41
1:F:118:ARG:HD2	1:F:118:ARG:HA	1.90	0.41
1:G:75:ASP:O	1:G:79:MET:HG3	2.21	0.41
1:K:42:VAL:CG1	1:K:229:VAL:HG11	2.51	0.41
1:M:71:ARG:HG2	1:M:140:TYR:CE2	2.56	0.41
1:N:186:LEU:O	1:N:238:ILE:HA	2.21	0.41
1:P:52:ILE:HG12	1:P:132:PHE:HB2	2.03	0.41
1:H:191:MET:HB3	1:H:196:LEU:O	2.21	0.41
1:C:198:VAL:HG23	1:C:199:MET:HG3	2.03	0.40
1:B:165:ASN:OD1	1:B:165:ASN:N	2.48	0.40
1:E:78:GLY:O	1:E:82:THR:HG23	2.22	0.40
1:O:23:LYS:HB2	1:O:25:PHE:CE2	2.56	0.40
1:P:150:ARG:O	1:P:154:VAL:HG22	2.21	0.40
1:P:232:GLU:O	1:P:234:ILE:HG22	2.21	0.40
1:A:52:ILE:HD13	1:A:146:THR:HG22	2.03	0.40
1:A:63:THR:O	1:A:67:LEU:HG	2.21	0.40
1:E:87:LEU:HD11	1:E:111:VAL:HG13	2.02	0.40
1:G:18:ALA:HA	1:G:164:ASN:HD21	1.87	0.40
1:L:232:GLU:O	1:L:234:ILE:HG22	2.21	0.40
1:N:13:LYS:HE3	1:N:144:ASP:OD1	2.20	0.40
1:P:144:ASP:HB3	1:P:199:MET:HE2	2.02	0.40
1:P:199:MET:HE2	1:P:199:MET:HB3	1.92	0.40
1:C:173:ASP:HB3	1:C:176:VAL:HB	2.02	0.40
1:A:108:MET:HG2	1:H:108:MET:HG2	2.02	0.40
1:D:73:THR:O	1:D:77:MET:HG2	2.22	0.40
1:F:108:MET:HG2	1:P:108:MET:HG2	2.03	0.40
1:G:109:LYS:O	2:G:301:GTP:N1	2.52	0.40
1:M:187:THR:HA	1:M:239:THR:O	2.21	0.40
1:M:214:LEU:O	1:M:237:LEU:HD12	2.21	0.40
1:D:77:MET:HE3	1:D:77:MET:HB3	1.93	0.40
1:A:117:ARG:NH1	1:E:72:GLY:HA3	2.37	0.40
1:N:109:LYS:O	2:N:301:GTP:N1	2.51	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	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
1	B	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
1	C	237/248 (96%)	231 (98%)	6 (2%)	0	100	100
1	D	235/248 (95%)	231 (98%)	4 (2%)	0	100	100
1	E	234/248 (94%)	226 (97%)	8 (3%)	0	100	100
1	F	235/248 (95%)	230 (98%)	5 (2%)	0	100	100
1	G	237/248 (96%)	232 (98%)	5 (2%)	0	100	100
1	H	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
1	I	236/248 (95%)	229 (97%)	7 (3%)	0	100	100
1	J	234/248 (94%)	228 (97%)	6 (3%)	0	100	100
1	K	234/248 (94%)	228 (97%)	6 (3%)	0	100	100
1	L	235/248 (95%)	230 (98%)	5 (2%)	0	100	100
1	M	234/248 (94%)	231 (99%)	3 (1%)	0	100	100
1	N	235/248 (95%)	225 (96%)	10 (4%)	0	100	100
1	O	235/248 (95%)	229 (97%)	6 (3%)	0	100	100
1	P	235/248 (95%)	228 (97%)	7 (3%)	0	100	100
1	Q	235/248 (95%)	230 (98%)	5 (2%)	0	100	100
1	R	235/248 (95%)	230 (98%)	5 (2%)	0	100	100
All	All	4237/4464 (95%)	4128 (97%)	109 (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	195/203 (96%)	188 (96%)	7 (4%)	31	63
1	B	195/203 (96%)	190 (97%)	5 (3%)	40	71
1	C	195/203 (96%)	187 (96%)	8 (4%)	27	59
1	D	194/203 (96%)	185 (95%)	9 (5%)	24	55
1	E	193/203 (95%)	189 (98%)	4 (2%)	47	75
1	F	194/203 (96%)	190 (98%)	4 (2%)	47	75
1	G	195/203 (96%)	191 (98%)	4 (2%)	47	75
1	H	195/203 (96%)	190 (97%)	5 (3%)	40	71
1	I	195/203 (96%)	186 (95%)	9 (5%)	24	55
1	J	193/203 (95%)	186 (96%)	7 (4%)	31	63
1	K	193/203 (95%)	189 (98%)	4 (2%)	47	75
1	L	194/203 (96%)	188 (97%)	6 (3%)	35	66
1	M	193/203 (95%)	187 (97%)	6 (3%)	35	66
1	N	194/203 (96%)	182 (94%)	12 (6%)	16	43
1	O	194/203 (96%)	187 (96%)	7 (4%)	31	63
1	P	194/203 (96%)	190 (98%)	4 (2%)	47	75
1	Q	194/203 (96%)	185 (95%)	9 (5%)	24	55
1	R	194/203 (96%)	187 (96%)	7 (4%)	31	63
All	All	3494/3654 (96%)	3377 (97%)	117 (3%)	33	65

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LYS
1	C	49	ILE
1	C	62	LYS
1	C	118	ARG
1	C	181	VAL
1	C	211	ASN
1	C	221	GLU
1	C	226	LYS
1	A	65	SER
1	A	71	ARG
1	A	116	ILE

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	177	ASN
1	A	179	ASP
1	A	182	LYS
1	B	10	VAL
1	B	15	SER
1	B	49	ILE
1	B	71	ARG
1	B	99	ASP
1	D	30	VAL
1	D	33	LYS
1	D	71	ARG
1	D	116	ILE
1	D	164	ASN
1	D	189	ILE
1	D	199	MET
1	D	201	SER
1	D	240	LYS
1	E	15	SER
1	E	70	ASP
1	E	108	MET
1	E	184	GLU
1	F	17	GLU
1	F	53	VAL
1	F	165	ASN
1	F	176	VAL
1	G	22	GLU
1	G	49	ILE
1	G	71	ARG
1	G	94	GLU
1	H	22	GLU
1	H	23	LYS
1	H	49	ILE
1	H	199	MET
1	H	226	LYS
1	I	8	LYS
1	I	10	VAL
1	I	15	SER
1	I	23	LYS
1	I	49	ILE
1	I	70	ASP
1	I	94	GLU

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Mol	Chain	Res	Type
1	I	178	LYS
1	I	240	LYS
1	J	49	ILE
1	J	71	ARG
1	J	99	ASP
1	J	116	ILE
1	J	184	GLU
1	J	199	MET
1	J	237	LEU
1	K	94	GLU
1	K	108	MET
1	K	118	ARG
1	K	192	LEU
1	L	4	ILE
1	L	30	VAL
1	L	49	ILE
1	L	109	LYS
1	L	113	GLU
1	L	176	VAL
1	M	10	VAL
1	M	15	SER
1	M	32	ILE
1	M	49	ILE
1	M	94	GLU
1	M	233	LYS
1	N	23	LYS
1	N	32	ILE
1	N	33	LYS
1	N	49	ILE
1	N	94	GLU
1	N	109	LYS
1	N	177	ASN
1	N	184	GLU
1	N	196	LEU
1	N	197	GLN
1	N	221	GLU
1	N	240	LYS
1	O	13	LYS
1	O	22	GLU
1	O	23	LYS
1	O	30	VAL
1	O	32	ILE

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Mol	Chain	Res	Type
1	O	49	ILE
1	O	109	LYS
1	P	8	LYS
1	P	70	ASP
1	P	94	GLU
1	P	161	MET
1	Q	6	LYS
1	Q	15	SER
1	Q	32	ILE
1	Q	49	ILE
1	Q	109	LYS
1	Q	177	ASN
1	Q	199	MET
1	Q	233	LYS
1	Q	234	ILE
1	R	4	ILE
1	R	15	SER
1	R	52	ILE
1	R	94	GLU
1	R	99	ASP
1	R	178	LYS
1	R	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	C	90	GLN
1	A	3	GLN
1	B	3	GLN
1	D	164	ASN
1	D	190	GLN
1	E	197	GLN
1	G	177	ASN
1	H	3	GLN
1	H	224	ASN
1	J	138	ASN
1	J	211	ASN
1	K	38	GLN
1	K	165	ASN
1	M	197	GLN
1	N	197	GLN

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Mol	Chain	Res	Type
1	O	38	GLN
1	O	110	GLN
1	O	177	ASN
1	P	177	ASN
1	Q	188	HIS
1	R	165	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](#)

44 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	H	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.67	10 (21%)
3	GOL	E	302	-	5,5,5	0.38	0	5,5,5	0.33	0
2	GTP	R	301	-	30,34,34	3.20	13 (43%)	46,54,54	1.74	13 (28%)
3	GOL	C	303	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	D	302	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	A	303	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	F	303	-	5,5,5	0.42	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	O	302	-	5,5,5	0.42	0	5,5,5	0.17	0
2	GTP	F	301	-	30,34,34	3.22	13 (43%)	46,54,54	1.70	12 (26%)
2	GTP	L	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.66	10 (21%)
2	GTP	M	301	-	30,34,34	3.21	13 (43%)	46,54,54	1.70	11 (23%)
2	GTP	K	301	-	30,34,34	3.22	13 (43%)	46,54,54	1.69	12 (26%)
2	GTP	N	301	-	30,34,34	3.21	13 (43%)	46,54,54	1.65	11 (23%)
3	GOL	E	304	-	5,5,5	0.39	0	5,5,5	0.27	0
2	GTP	I	301	-	30,34,34	3.21	13 (43%)	46,54,54	1.72	12 (26%)
2	GTP	D	301	-	30,34,34	3.21	13 (43%)	46,54,54	1.70	10 (21%)
3	GOL	E	305	-	5,5,5	0.39	0	5,5,5	0.27	0
3	GOL	J	303	-	5,5,5	0.40	0	5,5,5	0.19	0
2	GTP	G	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.72	11 (23%)
3	GOL	Q	302	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	K	302	-	5,5,5	0.38	0	5,5,5	0.28	0
2	GTP	P	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.69	11 (23%)
3	GOL	D	303	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	J	302	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	G	302	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GOL	P	303	-	5,5,5	0.40	0	5,5,5	0.26	0
2	GTP	A	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.72	12 (26%)
3	GOL	C	302	-	5,5,5	0.37	0	5,5,5	0.41	0
3	GOL	H	302	-	5,5,5	0.41	0	5,5,5	0.22	0
3	GOL	L	304	-	5,5,5	0.37	0	5,5,5	0.38	0
3	GOL	F	302	-	5,5,5	0.39	0	5,5,5	0.21	0
3	GOL	L	303	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	L	302	-	5,5,5	0.41	0	5,5,5	0.23	0
3	GOL	A	302	-	5,5,5	0.38	0	5,5,5	0.32	0
2	GTP	O	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.67	11 (23%)
2	GTP	J	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.76	11 (23%)
3	GOL	Q	303	-	5,5,5	0.39	0	5,5,5	0.34	0
2	GTP	E	301	-	30,34,34	3.24	13 (43%)	46,54,54	1.69	10 (21%)
2	GTP	Q	301	-	30,34,34	3.23	13 (43%)	46,54,54	1.65	11 (23%)
3	GOL	A	304	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	E	303	-	5,5,5	0.40	0	5,5,5	0.34	0
2	GTP	B	301	-	30,34,34	3.22	13 (43%)	46,54,54	1.67	10 (21%)
2	GTP	C	301	-	30,34,34	3.21	13 (43%)	46,54,54	1.71	11 (23%)
3	GOL	P	302	-	5,5,5	0.40	0	5,5,5	0.31	0

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	H	301	-	-	5/22/38/38	0/3/3/3
3	GOL	E	302	-	-	1/4/4/4	-
2	GTP	R	301	-	-	5/22/38/38	0/3/3/3
3	GOL	C	303	-	-	4/4/4/4	-
3	GOL	D	302	-	-	4/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-
3	GOL	F	303	-	-	2/4/4/4	-
3	GOL	O	302	-	-	0/4/4/4	-
2	GTP	F	301	-	-	5/22/38/38	0/3/3/3
2	GTP	L	301	-	-	6/22/38/38	0/3/3/3
2	GTP	M	301	-	-	6/22/38/38	0/3/3/3
2	GTP	K	301	-	-	2/22/38/38	0/3/3/3
2	GTP	N	301	-	-	5/22/38/38	0/3/3/3
3	GOL	E	304	-	-	2/4/4/4	-
2	GTP	I	301	-	-	7/22/38/38	0/3/3/3
2	GTP	D	301	-	-	6/22/38/38	0/3/3/3
3	GOL	E	305	-	-	4/4/4/4	-
3	GOL	J	303	-	-	2/4/4/4	-
2	GTP	G	301	-	-	4/22/38/38	0/3/3/3
3	GOL	Q	302	-	-	0/4/4/4	-
3	GOL	K	302	-	-	2/4/4/4	-
2	GTP	P	301	-	-	8/22/38/38	0/3/3/3
3	GOL	D	303	-	-	4/4/4/4	-
3	GOL	J	302	-	-	0/4/4/4	-
3	GOL	G	302	-	-	4/4/4/4	-
3	GOL	P	303	-	-	2/4/4/4	-
2	GTP	A	301	-	-	3/22/38/38	0/3/3/3
3	GOL	C	302	-	-	2/4/4/4	-
3	GOL	H	302	-	-	4/4/4/4	-
3	GOL	L	304	-	-	0/4/4/4	-
3	GOL	F	302	-	-	4/4/4/4	-
3	GOL	L	303	-	-	4/4/4/4	-
3	GOL	L	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	302	-	-	2/4/4/4	-
2	GTP	O	301	-	-	4/22/38/38	0/3/3/3
2	GTP	J	301	-	-	4/22/38/38	0/3/3/3
3	GOL	Q	303	-	-	2/4/4/4	-
2	GTP	E	301	-	-	3/22/38/38	0/3/3/3
2	GTP	Q	301	-	-	3/22/38/38	0/3/3/3
3	GOL	A	304	-	-	0/4/4/4	-
3	GOL	E	303	-	-	4/4/4/4	-
2	GTP	B	301	-	-	6/22/38/38	0/3/3/3
2	GTP	C	301	-	-	6/22/38/38	0/3/3/3
3	GOL	P	302	-	-	2/4/4/4	-

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	GTP	C3'-C4'	-8.94	1.30	1.53
2	J	301	GTP	C3'-C4'	-8.93	1.30	1.53
2	P	301	GTP	C3'-C4'	-8.71	1.30	1.53
2	O	301	GTP	C3'-C4'	-8.71	1.30	1.53
2	Q	301	GTP	C3'-C4'	-8.70	1.30	1.53
2	F	301	GTP	C3'-C4'	-8.69	1.30	1.53
2	I	301	GTP	C3'-C4'	-8.67	1.30	1.53
2	E	301	GTP	C3'-C4'	-8.66	1.30	1.53
2	L	301	GTP	C3'-C4'	-8.66	1.30	1.53
2	C	301	GTP	C3'-C4'	-8.64	1.30	1.53
2	A	301	GTP	C3'-C4'	-8.63	1.30	1.53
2	K	301	GTP	C3'-C4'	-8.63	1.30	1.53
2	D	301	GTP	C3'-C4'	-8.63	1.30	1.53
2	G	301	GTP	C3'-C4'	-8.61	1.31	1.53
2	M	301	GTP	C3'-C4'	-8.61	1.31	1.53
2	B	301	GTP	C3'-C4'	-8.58	1.31	1.53
2	N	301	GTP	C3'-C4'	-8.55	1.31	1.53
2	R	301	GTP	C3'-C4'	-8.53	1.31	1.53
2	N	301	GTP	O4'-C4'	8.12	1.63	1.45
2	G	301	GTP	O4'-C4'	8.08	1.63	1.45
2	A	301	GTP	O4'-C4'	8.07	1.63	1.45
2	E	301	GTP	O4'-C4'	8.07	1.63	1.45
2	Q	301	GTP	O4'-C4'	8.06	1.63	1.45
2	L	301	GTP	O4'-C4'	8.01	1.62	1.45
2	B	301	GTP	O4'-C4'	8.01	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	GTP	O4'-C4'	8.00	1.62	1.45
2	M	301	GTP	O4'-C4'	7.98	1.62	1.45
2	O	301	GTP	O4'-C4'	7.98	1.62	1.45
2	F	301	GTP	O4'-C4'	7.95	1.62	1.45
2	D	301	GTP	O4'-C4'	7.94	1.62	1.45
2	C	301	GTP	O4'-C4'	7.93	1.62	1.45
2	I	301	GTP	O4'-C4'	7.91	1.62	1.45
2	P	301	GTP	O4'-C4'	7.90	1.62	1.45
2	H	301	GTP	O4'-C4'	7.85	1.62	1.45
2	R	301	GTP	O4'-C4'	7.81	1.62	1.45
2	J	301	GTP	O4'-C4'	7.67	1.62	1.45
2	O	301	GTP	C4-N3	6.29	1.49	1.34
2	R	301	GTP	C4-N3	6.27	1.49	1.34
2	B	301	GTP	C4-N3	6.26	1.49	1.34
2	D	301	GTP	C4-N3	6.25	1.49	1.34
2	E	301	GTP	C4-N3	6.24	1.49	1.34
2	J	301	GTP	C4-N3	6.23	1.49	1.34
2	K	301	GTP	C4-N3	6.23	1.49	1.34
2	I	301	GTP	C4-N3	6.20	1.49	1.34
2	A	301	GTP	C4-N3	6.19	1.49	1.34
2	L	301	GTP	C4-N3	6.19	1.49	1.34
2	P	301	GTP	C4-N3	6.18	1.48	1.34
2	M	301	GTP	C4-N3	6.18	1.48	1.34
2	Q	301	GTP	C4-N3	6.17	1.48	1.34
2	C	301	GTP	C4-N3	6.17	1.48	1.34
2	G	301	GTP	C4-N3	6.16	1.48	1.34
2	H	301	GTP	C4-N3	6.14	1.48	1.34
2	N	301	GTP	C4-N3	6.13	1.48	1.34
2	F	301	GTP	C4-N3	6.10	1.48	1.34
2	E	301	GTP	C2-N3	5.42	1.46	1.33
2	Q	301	GTP	C2-N3	5.39	1.46	1.33
2	R	301	GTP	C2-N3	5.38	1.46	1.33
2	M	301	GTP	C2-N3	5.38	1.46	1.33
2	H	301	GTP	C2-N3	5.36	1.46	1.33
2	O	301	GTP	C2-N3	5.36	1.46	1.33
2	B	301	GTP	C2-N3	5.36	1.46	1.33
2	K	301	GTP	C2-N3	5.35	1.46	1.33
2	D	301	GTP	C2-N3	5.34	1.46	1.33
2	L	301	GTP	C2-N3	5.32	1.46	1.33
2	A	301	GTP	C2-N3	5.32	1.46	1.33
2	G	301	GTP	C2-N3	5.31	1.46	1.33
2	J	301	GTP	C2-N3	5.31	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	GTP	C2-N3	5.31	1.46	1.33
2	P	301	GTP	C2-N3	5.30	1.46	1.33
2	I	301	GTP	C2-N3	5.29	1.45	1.33
2	N	301	GTP	C2-N3	5.27	1.45	1.33
2	F	301	GTP	C2-N3	5.24	1.45	1.33
2	K	301	GTP	C2-N2	4.68	1.45	1.34
2	H	301	GTP	C2-N2	4.67	1.45	1.34
2	C	301	GTP	C2-N2	4.67	1.45	1.34
2	F	301	GTP	C2-N2	4.67	1.45	1.34
2	Q	301	GTP	C2-N2	4.66	1.45	1.34
2	D	301	GTP	C2-N2	4.66	1.45	1.34
2	E	301	GTP	C2-N2	4.65	1.45	1.34
2	R	301	GTP	C2-N2	4.65	1.45	1.34
2	G	301	GTP	C2-N2	4.65	1.45	1.34
2	L	301	GTP	C2-N2	4.64	1.45	1.34
2	I	301	GTP	C2-N2	4.63	1.45	1.34
2	P	301	GTP	C2-N2	4.63	1.45	1.34
2	J	301	GTP	C2-N2	4.63	1.45	1.34
2	A	301	GTP	C2-N2	4.61	1.45	1.34
2	B	301	GTP	C2-N2	4.61	1.45	1.34
2	O	301	GTP	C2-N2	4.61	1.45	1.34
2	M	301	GTP	C2-N2	4.60	1.45	1.34
2	N	301	GTP	C2-N2	4.56	1.45	1.34
2	A	301	GTP	O4'-C1'	-4.52	1.31	1.42
2	J	301	GTP	O4'-C1'	-4.50	1.31	1.42
2	G	301	GTP	O4'-C1'	-4.46	1.31	1.42
2	I	301	GTP	O4'-C1'	-4.46	1.31	1.42
2	E	301	GTP	O4'-C1'	-4.45	1.31	1.42
2	B	301	GTP	O4'-C1'	-4.42	1.31	1.42
2	F	301	GTP	O4'-C1'	-4.41	1.31	1.42
2	D	301	GTP	O4'-C1'	-4.41	1.31	1.42
2	L	301	GTP	O4'-C1'	-4.41	1.31	1.42
2	C	301	GTP	O4'-C1'	-4.37	1.31	1.42
2	O	301	GTP	O4'-C1'	-4.36	1.31	1.42
2	R	301	GTP	O4'-C1'	-4.35	1.31	1.42
2	P	301	GTP	O4'-C1'	-4.35	1.31	1.42
2	M	301	GTP	O4'-C1'	-4.33	1.31	1.42
2	K	301	GTP	O4'-C1'	-4.27	1.31	1.42
2	H	301	GTP	O4'-C1'	-4.25	1.31	1.42
2	N	301	GTP	O4'-C1'	-4.22	1.32	1.42
2	Q	301	GTP	O4'-C1'	-4.20	1.32	1.42
2	Q	301	GTP	O3'-C3'	3.37	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	GTP	O3'-C3'	3.33	1.50	1.43
2	P	301	GTP	O3'-C3'	3.29	1.50	1.43
2	R	301	GTP	O3'-C3'	3.27	1.50	1.43
2	O	301	GTP	O3'-C3'	3.26	1.50	1.43
2	B	301	GTP	O3'-C3'	3.25	1.50	1.43
2	G	301	GTP	O3'-C3'	3.25	1.50	1.43
2	K	301	GTP	O3'-C3'	3.24	1.50	1.43
2	L	301	GTP	O3'-C3'	3.23	1.50	1.43
2	C	301	GTP	O3'-C3'	3.22	1.50	1.43
2	M	301	GTP	O3'-C3'	3.21	1.50	1.43
2	F	301	GTP	O3'-C3'	3.19	1.50	1.43
2	H	301	GTP	O3'-C3'	3.19	1.50	1.43
2	D	301	GTP	O3'-C3'	3.19	1.50	1.43
2	E	301	GTP	O3'-C3'	3.19	1.50	1.43
2	I	301	GTP	O3'-C3'	3.17	1.50	1.43
2	J	301	GTP	O3'-C3'	3.15	1.50	1.43
2	A	301	GTP	O3'-C3'	3.15	1.50	1.43
2	H	301	GTP	C5-N7	-3.05	1.33	1.39
2	M	301	GTP	C5-N7	-3.05	1.33	1.39
2	C	301	GTP	C5-N7	-3.04	1.33	1.39
2	N	301	GTP	C5-N7	-3.04	1.33	1.39
2	J	301	GTP	C5-N7	-3.01	1.33	1.39
2	G	301	GTP	C5-N7	-3.00	1.33	1.39
2	B	301	GTP	C5-N7	-3.00	1.33	1.39
2	E	301	GTP	C5-N7	-3.00	1.33	1.39
2	O	301	GTP	C5-N7	-3.00	1.33	1.39
2	P	301	GTP	O2'-C2'	-2.99	1.35	1.43
2	F	301	GTP	C5-N7	-2.99	1.33	1.39
2	A	301	GTP	C5-N7	-2.99	1.33	1.39
2	P	301	GTP	C5-N7	-2.98	1.33	1.39
2	Q	301	GTP	C5-N7	-2.95	1.33	1.39
2	L	301	GTP	C5-N7	-2.94	1.33	1.39
2	R	301	GTP	C5-N7	-2.92	1.33	1.39
2	D	301	GTP	C5-N7	-2.89	1.33	1.39
2	I	301	GTP	C5-N7	-2.88	1.33	1.39
2	K	301	GTP	C5-N7	-2.88	1.33	1.39
2	B	301	GTP	O2'-C2'	-2.86	1.36	1.43
2	E	301	GTP	O2'-C2'	-2.86	1.36	1.43
2	M	301	GTP	O2'-C2'	-2.85	1.36	1.43
2	J	301	GTP	O2'-C2'	-2.85	1.36	1.43
2	H	301	GTP	O2'-C2'	-2.84	1.36	1.43
2	I	301	GTP	O2'-C2'	-2.83	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	301	GTP	O2'-C2'	-2.83	1.36	1.43
2	G	301	GTP	O2'-C2'	-2.82	1.36	1.43
2	A	301	GTP	O2'-C2'	-2.82	1.36	1.43
2	C	301	GTP	O2'-C2'	-2.80	1.36	1.43
2	L	301	GTP	O2'-C2'	-2.80	1.36	1.43
2	Q	301	GTP	O2'-C2'	-2.78	1.36	1.43
2	F	301	GTP	O2'-C2'	-2.78	1.36	1.43
2	R	301	GTP	O2'-C2'	-2.76	1.36	1.43
2	D	301	GTP	O2'-C2'	-2.75	1.36	1.43
2	G	301	GTP	C2-N1	2.75	1.44	1.37
2	F	301	GTP	C2-N1	2.74	1.44	1.37
2	K	301	GTP	O2'-C2'	-2.73	1.36	1.43
2	N	301	GTP	O2'-C2'	-2.72	1.36	1.43
2	H	301	GTP	C2-N1	2.72	1.44	1.37
2	P	301	GTP	C2-N1	2.70	1.44	1.37
2	C	301	GTP	C2-N1	2.67	1.44	1.37
2	N	301	GTP	C2-N1	2.66	1.44	1.37
2	M	301	GTP	C2-N1	2.66	1.44	1.37
2	K	301	GTP	C2-N1	2.65	1.44	1.37
2	A	301	GTP	C2-N1	2.64	1.44	1.37
2	L	301	GTP	C2-N1	2.64	1.44	1.37
2	R	301	GTP	C2-N1	2.63	1.44	1.37
2	I	301	GTP	C2-N1	2.63	1.44	1.37
2	Q	301	GTP	C2-N1	2.62	1.44	1.37
2	J	301	GTP	C2-N1	2.62	1.44	1.37
2	O	301	GTP	C2-N1	2.61	1.44	1.37
2	J	301	GTP	O6-C6	-2.61	1.18	1.23
2	D	301	GTP	C2-N1	2.60	1.44	1.37
2	E	301	GTP	C2-N1	2.60	1.44	1.37
2	Q	301	GTP	C5-C6	2.59	1.54	1.44
2	R	301	GTP	C5-C6	2.59	1.54	1.44
2	B	301	GTP	O6-C6	-2.58	1.18	1.23
2	I	301	GTP	C5-C6	2.57	1.53	1.44
2	D	301	GTP	O6-C6	-2.56	1.18	1.23
2	L	301	GTP	O6-C6	-2.56	1.18	1.23
2	B	301	GTP	C2-N1	2.55	1.44	1.37
2	E	301	GTP	O6-C6	-2.55	1.18	1.23
2	G	301	GTP	C5-C6	2.55	1.53	1.44
2	O	301	GTP	C5-C6	2.54	1.53	1.44
2	K	301	GTP	C5-C6	2.53	1.53	1.44
2	C	301	GTP	O6-C6	-2.52	1.18	1.23
2	A	301	GTP	C5-C6	2.52	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	GTP	C5-C6	2.52	1.53	1.44
2	P	301	GTP	C5-C6	2.50	1.53	1.44
2	N	301	GTP	C5-C6	2.49	1.53	1.44
2	F	301	GTP	O6-C6	-2.49	1.18	1.23
2	M	301	GTP	O6-C6	-2.48	1.18	1.23
2	N	301	GTP	O6-C6	-2.48	1.18	1.23
2	M	301	GTP	C5-C6	2.48	1.53	1.44
2	B	301	GTP	C5-C6	2.48	1.53	1.44
2	A	301	GTP	O6-C6	-2.47	1.18	1.23
2	E	301	GTP	C5-C6	2.47	1.53	1.44
2	L	301	GTP	C5-C6	2.47	1.53	1.44
2	H	301	GTP	O6-C6	-2.47	1.18	1.23
2	O	301	GTP	O6-C6	-2.47	1.18	1.23
2	G	301	GTP	C6-N1	2.46	1.43	1.38
2	F	301	GTP	C5-C6	2.46	1.53	1.44
2	K	301	GTP	O6-C6	-2.46	1.18	1.23
2	H	301	GTP	C5-C6	2.45	1.53	1.44
2	P	301	GTP	O6-C6	-2.44	1.18	1.23
2	Q	301	GTP	O6-C6	-2.43	1.19	1.23
2	R	301	GTP	O6-C6	-2.43	1.19	1.23
2	C	301	GTP	C5-C6	2.43	1.53	1.44
2	I	301	GTP	O6-C6	-2.42	1.19	1.23
2	J	301	GTP	C5-C6	2.40	1.53	1.44
2	F	301	GTP	C6-N1	2.39	1.43	1.38
2	P	301	GTP	C6-N1	2.37	1.43	1.38
2	G	301	GTP	O6-C6	-2.36	1.19	1.23
2	I	301	GTP	C6-N1	2.34	1.43	1.38
2	L	301	GTP	C6-N1	2.33	1.43	1.38
2	O	301	GTP	C6-N1	2.33	1.43	1.38
2	H	301	GTP	C6-N1	2.32	1.43	1.38
2	C	301	GTP	C6-N1	2.32	1.43	1.38
2	R	301	GTP	C6-N1	2.31	1.43	1.38
2	K	301	GTP	C6-N1	2.30	1.43	1.38
2	A	301	GTP	C6-N1	2.28	1.43	1.38
2	Q	301	GTP	C6-N1	2.28	1.43	1.38
2	J	301	GTP	C6-N1	2.27	1.43	1.38
2	N	301	GTP	C6-N1	2.26	1.43	1.38
2	M	301	GTP	C6-N1	2.26	1.43	1.38
2	D	301	GTP	C6-N1	2.25	1.43	1.38
2	E	301	GTP	C6-N1	2.21	1.42	1.38
2	B	301	GTP	C6-N1	2.18	1.42	1.38

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	GTP	C5-C4-N3	-4.86	120.57	128.46
2	M	301	GTP	C5-C4-N3	-4.85	120.60	128.46
2	Q	301	GTP	C5-C4-N3	-4.82	120.64	128.46
2	H	301	GTP	C5-C4-N3	-4.81	120.66	128.46
2	N	301	GTP	C5-C4-N3	-4.73	120.79	128.46
2	C	301	GTP	C5-C4-N3	-4.71	120.81	128.46
2	B	301	GTP	C5-C4-N3	-4.70	120.83	128.46
2	R	301	GTP	C5-C4-N3	-4.68	120.87	128.46
2	J	301	GTP	C5-C4-N3	-4.67	120.88	128.46
2	O	301	GTP	C5-C4-N3	-4.66	120.91	128.46
2	P	301	GTP	C5-C4-N3	-4.62	120.96	128.46
2	A	301	GTP	C5-C4-N3	-4.60	120.99	128.46
2	G	301	GTP	C5-C4-N3	-4.58	121.04	128.46
2	K	301	GTP	C5-C4-N3	-4.53	121.11	128.46
2	D	301	GTP	C5-C4-N3	-4.49	121.17	128.46
2	F	301	GTP	C5-C4-N3	-4.49	121.18	128.46
2	I	301	GTP	C5-C4-N3	-4.44	121.26	128.46
2	L	301	GTP	C5-C4-N3	-4.40	121.32	128.46
2	Q	301	GTP	C2-N3-C4	3.92	119.28	112.30
2	E	301	GTP	C2-N3-C4	3.91	119.27	112.30
2	C	301	GTP	C2-N3-C4	3.89	119.23	112.30
2	J	301	GTP	C2-N3-C4	3.86	119.18	112.30
2	M	301	GTP	C2-N3-C4	3.85	119.15	112.30
2	D	301	GTP	C2-N3-C4	3.84	119.15	112.30
2	O	301	GTP	C2-N3-C4	3.83	119.13	112.30
2	R	301	GTP	C2-N3-C4	3.82	119.10	112.30
2	H	301	GTP	C2-N3-C4	3.82	119.10	112.30
2	P	301	GTP	C2-N3-C4	3.81	119.09	112.30
2	B	301	GTP	C2-N3-C4	3.80	119.07	112.30
2	G	301	GTP	C2-N3-C4	3.80	119.07	112.30
2	I	301	GTP	C2-N3-C4	3.79	119.05	112.30
2	K	301	GTP	C2-N3-C4	3.78	119.03	112.30
2	L	301	GTP	C2-N3-C4	3.77	119.02	112.30
2	N	301	GTP	C2-N3-C4	3.76	119.00	112.30
2	F	301	GTP	C2-N3-C4	3.76	119.00	112.30
2	A	301	GTP	C2-N3-C4	3.75	118.98	112.30
2	I	301	GTP	PB-O3B-PG	-3.68	120.18	132.83
2	P	301	GTP	C1'-N9-C4	-3.41	116.36	126.50
2	K	301	GTP	C1'-N9-C4	-3.40	116.41	126.50
2	L	301	GTP	C1'-N9-C4	-3.37	116.50	126.50
2	D	301	GTP	C1'-N9-C4	-3.35	116.56	126.50
2	F	301	GTP	C1'-N9-C4	-3.33	116.60	126.50
2	J	301	GTP	C1'-N9-C4	-3.27	116.80	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	301	GTP	C1'-N9-C4	-3.22	116.92	126.50
2	G	301	GTP	C1'-N9-C4	-3.22	116.93	126.50
2	D	301	GTP	PB-O3B-PG	-3.22	121.79	132.83
2	M	301	GTP	C1'-N9-C4	-3.22	116.95	126.50
2	C	301	GTP	PB-O3B-PG	-3.21	121.82	132.83
2	A	301	GTP	C1'-N9-C4	-3.20	117.00	126.50
2	I	301	GTP	C1'-N9-C4	-3.20	117.01	126.50
2	J	301	GTP	PB-O3B-PG	-3.16	122.00	132.83
2	K	301	GTP	N9-C8-N7	-3.15	107.45	113.39
2	H	301	GTP	C1'-N9-C4	-3.13	117.21	126.50
2	J	301	GTP	N9-C4-N3	3.09	132.15	125.94
2	G	301	GTP	PB-O3B-PG	-3.08	122.25	132.83
2	E	301	GTP	N9-C4-N3	3.08	132.12	125.94
2	M	301	GTP	N9-C4-N3	3.07	132.10	125.94
2	H	301	GTP	C2-N1-C6	-3.07	119.50	125.10
2	O	301	GTP	C1'-N9-C4	-3.06	117.42	126.50
2	Q	301	GTP	N9-C4-N3	3.05	132.06	125.94
2	H	301	GTP	N9-C4-N3	3.04	132.05	125.94
2	J	301	GTP	C2-N1-C6	-3.04	119.56	125.10
2	M	301	GTP	C2-N1-C6	-3.04	119.56	125.10
2	B	301	GTP	C1'-N9-C4	-3.03	117.49	126.50
2	N	301	GTP	C2-N1-C6	-3.03	119.58	125.10
2	G	301	GTP	N9-C8-N7	-3.02	107.70	113.39
2	E	301	GTP	C1'-N9-C4	-3.01	117.57	126.50
2	C	301	GTP	C2-N1-C6	-3.00	119.63	125.10
2	E	301	GTP	C2-N1-C6	-3.00	119.63	125.10
2	J	301	GTP	N9-C8-N7	-3.00	107.75	113.39
2	Q	301	GTP	C2-N1-C6	-2.99	119.64	125.10
2	R	301	GTP	N9-C8-N7	-2.98	107.78	113.39
2	C	301	GTP	N9-C4-N3	2.97	131.91	125.94
2	F	301	GTP	N9-C8-N7	-2.97	107.80	113.39
2	Q	301	GTP	N9-C8-N7	-2.97	107.80	113.39
2	B	301	GTP	N9-C4-N3	2.97	131.90	125.94
2	A	301	GTP	C2-N1-C6	-2.96	119.70	125.10
2	C	301	GTP	C1'-N9-C4	-2.96	117.72	126.50
2	O	301	GTP	C2-N1-C6	-2.95	119.72	125.10
2	O	301	GTP	N9-C4-N3	2.95	131.85	125.94
2	M	301	GTP	N9-C8-N7	-2.95	107.84	113.39
2	N	301	GTP	C1'-N9-C4	-2.94	117.76	126.50
2	P	301	GTP	C2-N1-C6	-2.94	119.74	125.10
2	N	301	GTP	N9-C4-N3	2.94	131.84	125.94
2	P	301	GTP	N9-C8-N7	-2.94	107.86	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	GTP	N9-C8-N7	-2.94	107.86	113.39
2	B	301	GTP	C2-N1-C6	-2.92	119.78	125.10
2	F	301	GTP	C2-N1-C6	-2.92	119.78	125.10
2	P	301	GTP	C1'-N9-C8	2.91	134.97	126.70
2	D	301	GTP	N9-C8-N7	-2.90	107.93	113.39
2	Q	301	GTP	C1'-N9-C4	-2.89	117.93	126.50
2	G	301	GTP	C2-N1-C6	-2.88	119.85	125.10
2	R	301	GTP	N9-C4-N3	2.87	131.71	125.94
2	L	301	GTP	C2-N1-C6	-2.87	119.86	125.10
2	I	301	GTP	N9-C8-N7	-2.87	107.98	113.39
2	O	301	GTP	N9-C8-N7	-2.86	108.00	113.39
2	P	301	GTP	N9-C4-N3	2.86	131.68	125.94
2	N	301	GTP	N9-C8-N7	-2.84	108.05	113.39
2	K	301	GTP	N9-C4-N3	2.84	131.64	125.94
2	K	301	GTP	C2-N1-C6	-2.84	119.93	125.10
2	A	301	GTP	N9-C8-N7	-2.82	108.08	113.39
2	D	301	GTP	C1'-N9-C8	2.82	134.72	126.70
2	R	301	GTP	PB-O3B-PG	-2.80	123.22	132.83
2	B	301	GTP	N9-C8-N7	-2.79	108.13	113.39
2	R	301	GTP	C2-N1-C6	-2.79	120.01	125.10
2	H	301	GTP	PB-O3B-PG	-2.79	123.26	132.83
2	F	301	GTP	C1'-N9-C8	2.79	134.62	126.70
2	L	301	GTP	C1'-N9-C8	2.78	134.61	126.70
2	K	301	GTP	C1'-N9-C8	2.78	134.60	126.70
2	H	301	GTP	N9-C8-N7	-2.77	108.17	113.39
2	A	301	GTP	N9-C4-N3	2.77	131.50	125.94
2	D	301	GTP	C2-N1-C6	-2.77	120.05	125.10
2	G	301	GTP	N9-C4-N3	2.76	131.49	125.94
2	I	301	GTP	C2-N1-C6	-2.76	120.08	125.10
2	L	301	GTP	N9-C4-N3	2.75	131.46	125.94
2	A	301	GTP	C1'-N9-C8	2.75	134.52	126.70
2	D	301	GTP	N9-C4-N3	2.74	131.45	125.94
2	F	301	GTP	N9-C4-N3	2.74	131.44	125.94
2	J	301	GTP	PA-O3A-PB	-2.72	123.50	132.83
2	C	301	GTP	N9-C8-N7	-2.72	108.28	113.39
2	I	301	GTP	C1'-N9-C8	2.71	134.42	126.70
2	E	301	GTP	N9-C8-N7	-2.71	108.29	113.39
2	L	301	GTP	PB-O3B-PG	-2.71	123.54	132.83
2	M	301	GTP	C1'-N9-C8	2.70	134.40	126.70
2	G	301	GTP	C1'-N9-C8	2.70	134.39	126.70
2	R	301	GTP	C1'-N9-C8	2.70	134.38	126.70
2	H	301	GTP	C1'-N9-C8	2.69	134.35	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GTP	PB-O3B-PG	-2.67	123.67	132.83
2	R	301	GTP	PA-O3A-PB	-2.65	123.75	132.83
2	J	301	GTP	C1'-N9-C8	2.63	134.17	126.70
2	J	301	GTP	C5-C6-N1	2.62	119.84	113.19
2	J	301	GTP	O6-C6-C5	-2.62	119.66	126.60
2	I	301	GTP	N9-C4-N3	2.59	131.15	125.94
2	E	301	GTP	C1'-N9-C8	2.58	134.04	126.70
2	E	301	GTP	C5-C6-N1	2.58	119.74	113.19
2	L	301	GTP	C5-C6-N1	2.56	119.70	113.19
2	O	301	GTP	C5-C6-N1	2.56	119.69	113.19
2	B	301	GTP	C5-C6-N1	2.55	119.68	113.19
2	C	301	GTP	C5-C6-N1	2.55	119.67	113.19
2	C	301	GTP	O6-C6-C5	-2.55	119.84	126.60
2	B	301	GTP	C1'-N9-C8	2.55	133.94	126.70
2	D	301	GTP	C5-C6-N1	2.54	119.65	113.19
2	O	301	GTP	C1'-N9-C8	2.54	133.93	126.70
2	A	301	GTP	C5-C6-N1	2.51	119.57	113.19
2	B	301	GTP	PB-O3B-PG	-2.51	124.21	132.83
2	C	301	GTP	C1'-N9-C8	2.51	133.84	126.70
2	H	301	GTP	O6-C6-C5	-2.50	119.97	126.60
2	Q	301	GTP	C5-C6-N1	2.50	119.54	113.19
2	F	301	GTP	O6-C6-C5	-2.49	119.98	126.60
2	O	301	GTP	PB-O3B-PG	-2.49	124.28	132.83
2	M	301	GTP	C5-C6-N1	2.49	119.51	113.19
2	H	301	GTP	C5-C6-N1	2.48	119.48	113.19
2	K	301	GTP	PA-O3A-PB	-2.48	124.33	132.83
2	K	301	GTP	C5-C6-N1	2.47	119.46	113.19
2	P	301	GTP	C5-C6-N1	2.47	119.46	113.19
2	M	301	GTP	O6-C6-C5	-2.47	120.06	126.60
2	N	301	GTP	C5-C6-N1	2.46	119.44	113.19
2	N	301	GTP	C1'-N9-C8	2.46	133.69	126.70
2	I	301	GTP	C5-C6-N1	2.45	119.41	113.19
2	P	301	GTP	O6-C6-C5	-2.44	120.11	126.60
2	F	301	GTP	C5-C6-N1	2.44	119.40	113.19
2	E	301	GTP	O6-C6-C5	-2.42	120.19	126.60
2	R	301	GTP	C5-C6-N1	2.42	119.33	113.19
2	F	301	GTP	PB-O3B-PG	-2.39	124.62	132.83
2	G	301	GTP	C5-C6-N1	2.39	119.26	113.19
2	A	301	GTP	O6-C6-C5	-2.38	120.28	126.60
2	L	301	GTP	O6-C6-C5	-2.37	120.32	126.60
2	G	301	GTP	O6-C6-C5	-2.35	120.36	126.60
2	Q	301	GTP	C1'-N9-C8	2.35	133.37	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	301	GTP	O6-C6-C5	-2.34	120.41	126.60
2	I	301	GTP	PA-O3A-PB	-2.32	124.87	132.83
2	A	301	GTP	PA-O3A-PB	-2.31	124.89	132.83
2	R	301	GTP	C2'-C3'-C4'	2.31	107.12	102.64
2	K	301	GTP	PB-O3B-PG	-2.30	124.92	132.83
2	B	301	GTP	O6-C6-C5	-2.28	120.55	126.60
2	O	301	GTP	O6-C6-C5	-2.27	120.56	126.60
2	E	301	GTP	PB-O3B-PG	-2.25	125.11	132.83
2	G	301	GTP	C8-N7-C5	2.23	108.28	104.24
2	K	301	GTP	O6-C6-C5	-2.23	120.69	126.60
2	P	301	GTP	PB-O3B-PG	-2.22	125.22	132.83
2	D	301	GTP	O6-C6-C5	-2.21	120.73	126.60
2	Q	301	GTP	PB-O3B-PG	-2.20	125.26	132.83
2	R	301	GTP	C8-N7-C5	2.20	108.23	104.24
2	K	301	GTP	C8-N7-C5	2.19	108.21	104.24
2	Q	301	GTP	C8-N7-C5	2.18	108.18	104.24
2	Q	301	GTP	O6-C6-C5	-2.17	120.84	126.60
2	I	301	GTP	O6-C6-C5	-2.16	120.86	126.60
2	N	301	GTP	PB-O3B-PG	-2.16	125.42	132.83
2	R	301	GTP	O6-C6-C5	-2.13	120.94	126.60
2	M	301	GTP	C8-N7-C5	2.12	108.08	104.24
2	F	301	GTP	O2G-PG-O3B	2.08	111.60	104.64
2	C	301	GTP	PA-O3A-PB	-2.08	125.70	132.83
2	O	301	GTP	C8-N7-C5	2.07	107.98	104.24
2	I	301	GTP	C8-N7-C5	2.06	107.97	104.24
2	P	301	GTP	C8-N7-C5	2.04	107.94	104.24
2	N	301	GTP	C8-N7-C5	2.04	107.93	104.24
2	M	301	GTP	PA-O3A-PB	-2.04	125.82	132.83
2	F	301	GTP	C8-N7-C5	2.04	107.93	104.24
2	A	301	GTP	C8-N7-C5	2.02	107.89	104.24

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	GTP	C5'-O5'-PA-O3A
2	C	301	GTP	C5'-O5'-PA-O2A
2	C	301	GTP	O4'-C4'-C5'-O5'
2	C	301	GTP	C3'-C4'-C5'-O5'
2	A	301	GTP	O4'-C4'-C5'-O5'
2	B	301	GTP	C5'-O5'-PA-O3A
2	B	301	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	301	GTP	C5'-O5'-PA-O2A
2	B	301	GTP	O4'-C4'-C5'-O5'
2	B	301	GTP	C3'-C4'-C5'-O5'
2	D	301	GTP	C5'-O5'-PA-O3A
2	D	301	GTP	O4'-C4'-C5'-O5'
2	E	301	GTP	O4'-C4'-C5'-O5'
2	H	301	GTP	C5'-O5'-PA-O3A
2	H	301	GTP	C5'-O5'-PA-O1A
2	I	301	GTP	C5'-O5'-PA-O3A
2	I	301	GTP	O4'-C4'-C5'-O5'
2	I	301	GTP	C3'-C4'-C5'-O5'
2	J	301	GTP	PB-O3A-PA-O5'
2	J	301	GTP	C5'-O5'-PA-O3A
2	M	301	GTP	C5'-O5'-PA-O3A
2	N	301	GTP	C5'-O5'-PA-O1A
2	O	301	GTP	PB-O3B-PG-O2G
2	P	301	GTP	C5'-O5'-PA-O3A
2	P	301	GTP	C5'-O5'-PA-O1A
2	Q	301	GTP	O4'-C4'-C5'-O5'
2	R	301	GTP	C5'-O5'-PA-O3A
2	R	301	GTP	C5'-O5'-PA-O2A
2	R	301	GTP	O4'-C4'-C5'-O5'
3	A	302	GOL	O1-C1-C2-C3
3	A	303	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-C3
3	D	303	GOL	C1-C2-C3-O3
3	D	303	GOL	O2-C2-C3-O3
3	E	303	GOL	O1-C1-C2-C3
3	E	303	GOL	C1-C2-C3-O3
3	E	303	GOL	O2-C2-C3-O3
3	E	304	GOL	O1-C1-C2-O2
3	E	304	GOL	O1-C1-C2-C3
3	E	305	GOL	O1-C1-C2-C3
3	E	305	GOL	C1-C2-C3-O3
3	F	302	GOL	C1-C2-C3-O3
3	F	303	GOL	O1-C1-C2-O2
3	F	303	GOL	O1-C1-C2-C3
3	H	302	GOL	O1-C1-C2-C3
3	J	303	GOL	O1-C1-C2-C3
3	K	302	GOL	O1-C1-C2-C3
3	L	302	GOL	O1-C1-C2-C3
3	P	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	P	303	GOL	O1-C1-C2-C3
3	Q	303	GOL	C1-C2-C3-O3
2	A	301	GTP	C3'-C4'-C5'-O5'
2	D	301	GTP	C3'-C4'-C5'-O5'
2	E	301	GTP	C3'-C4'-C5'-O5'
2	K	301	GTP	O4'-C4'-C5'-O5'
2	O	301	GTP	O4'-C4'-C5'-O5'
2	O	301	GTP	C3'-C4'-C5'-O5'
2	P	301	GTP	O4'-C4'-C5'-O5'
2	Q	301	GTP	C3'-C4'-C5'-O5'
2	R	301	GTP	C3'-C4'-C5'-O5'
3	J	303	GOL	O1-C1-C2-O2
3	L	303	GOL	O1-C1-C2-O2
2	F	301	GTP	O4'-C4'-C5'-O5'
2	K	301	GTP	C3'-C4'-C5'-O5'
3	E	302	GOL	O1-C1-C2-C3
3	F	302	GOL	O1-C1-C2-C3
3	G	302	GOL	O1-C1-C2-C3
3	G	302	GOL	C1-C2-C3-O3
3	L	303	GOL	O1-C1-C2-C3
3	L	303	GOL	C1-C2-C3-O3
3	A	303	GOL	O2-C2-C3-O3
3	D	302	GOL	O1-C1-C2-O2
3	E	303	GOL	O1-C1-C2-O2
3	E	305	GOL	O1-C1-C2-O2
3	F	302	GOL	O2-C2-C3-O3
3	G	302	GOL	O1-C1-C2-O2
3	G	302	GOL	O2-C2-C3-O3
3	H	302	GOL	O1-C1-C2-O2
3	K	302	GOL	O1-C1-C2-O2
3	P	302	GOL	O1-C1-C2-O2
3	P	303	GOL	O1-C1-C2-O2
2	F	301	GTP	C3'-C4'-C5'-O5'
3	A	302	GOL	O1-C1-C2-O2
2	O	301	GTP	PB-O3B-PG-O1G
2	Q	301	GTP	PG-O3B-PB-O3A
2	A	301	GTP	PB-O3A-PA-O1A
2	G	301	GTP	PB-O3A-PA-O1A
2	L	301	GTP	PG-O3B-PB-O1B
2	J	301	GTP	O4'-C4'-C5'-O5'
2	M	301	GTP	O4'-C4'-C5'-O5'
2	F	301	GTP	PG-O3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
3	C	302	GOL	O1-C1-C2-O2
3	D	303	GOL	O1-C1-C2-O2
3	E	305	GOL	O2-C2-C3-O3
3	F	302	GOL	O1-C1-C2-O2
3	L	303	GOL	O2-C2-C3-O3
3	Q	303	GOL	O2-C2-C3-O3
2	L	301	GTP	O4'-C4'-C5'-O5'
2	G	301	GTP	PB-O3A-PA-O5'
2	M	301	GTP	PB-O3A-PA-O5'
2	P	301	GTP	PB-O3B-PG-O1G
2	G	301	GTP	C5'-O5'-PA-O3A
2	N	301	GTP	C5'-O5'-PA-O3A
3	C	303	GOL	O1-C1-C2-O2
3	H	302	GOL	O2-C2-C3-O3
3	L	302	GOL	O1-C1-C2-O2
2	P	301	GTP	C3'-C4'-C5'-O5'
2	H	301	GTP	PA-O3A-PB-O1B
2	H	301	GTP	PB-O3A-PA-O1A
2	N	301	GTP	PG-O3B-PB-O2B
2	P	301	GTP	PB-O3A-PA-O1A
2	R	301	GTP	PA-O3A-PB-O1B
3	C	303	GOL	O1-C1-C2-C3
3	D	302	GOL	C1-C2-C3-O3
2	C	301	GTP	C5'-O5'-PA-O1A
2	D	301	GTP	C5'-O5'-PA-O1A
2	D	301	GTP	C5'-O5'-PA-O2A
2	G	301	GTP	C5'-O5'-PA-O2A
2	I	301	GTP	C5'-O5'-PA-O1A
2	I	301	GTP	C5'-O5'-PA-O2A
2	J	301	GTP	C5'-O5'-PA-O1A
2	M	301	GTP	C5'-O5'-PA-O2A
2	N	301	GTP	C5'-O5'-PA-O2A
2	L	301	GTP	C3'-C4'-C5'-O5'
2	B	301	GTP	PG-O3B-PB-O3A
2	C	301	GTP	PB-O3A-PA-O2A
2	D	301	GTP	PB-O3A-PA-O1A
2	E	301	GTP	PB-O3A-PA-O1A
2	I	301	GTP	PB-O3A-PA-O2A
2	M	301	GTP	C3'-C4'-C5'-O5'
2	F	301	GTP	PB-O3B-PG-O1G
2	L	301	GTP	PA-O3A-PB-O2B
2	P	301	GTP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	C	303	GOL	C1-C2-C3-O3
3	D	303	GOL	O1-C1-C2-C3
3	C	303	GOL	O2-C2-C3-O3
3	D	302	GOL	O2-C2-C3-O3
2	H	301	GTP	O4'-C4'-C5'-O5'
2	I	301	GTP	PB-O3A-PA-O1A
2	L	301	GTP	PB-O3A-PA-O2A
2	M	301	GTP	PB-O3A-PA-O2A
2	N	301	GTP	PB-O3A-PA-O2A
3	C	302	GOL	O1-C1-C2-C3
3	H	302	GOL	C1-C2-C3-O3
2	P	301	GTP	C4'-C5'-O5'-PA
2	F	301	GTP	C5'-O5'-PA-O1A
2	L	301	GTP	C5'-O5'-PA-O1A

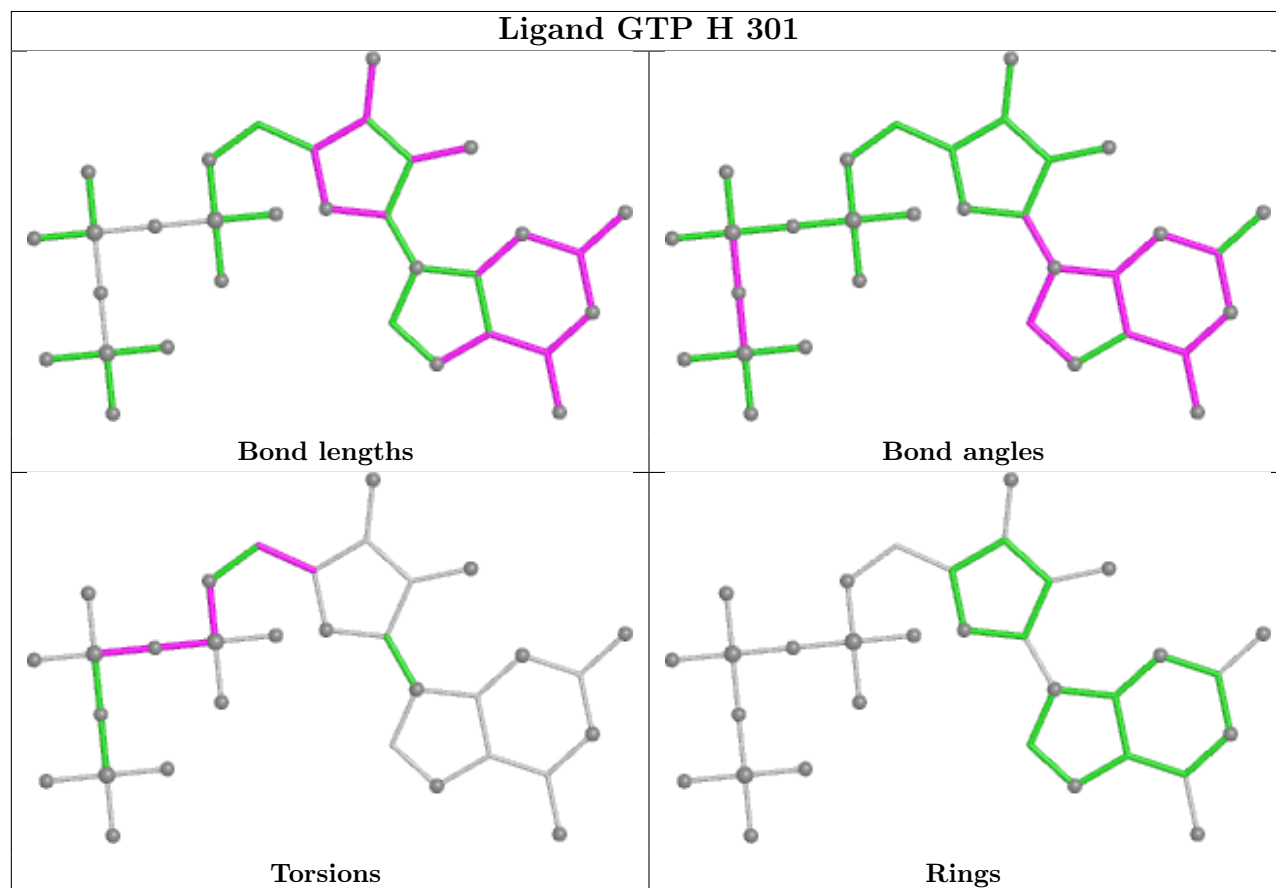
There are no ring outliers.

17 monomers are involved in 20 short contacts:

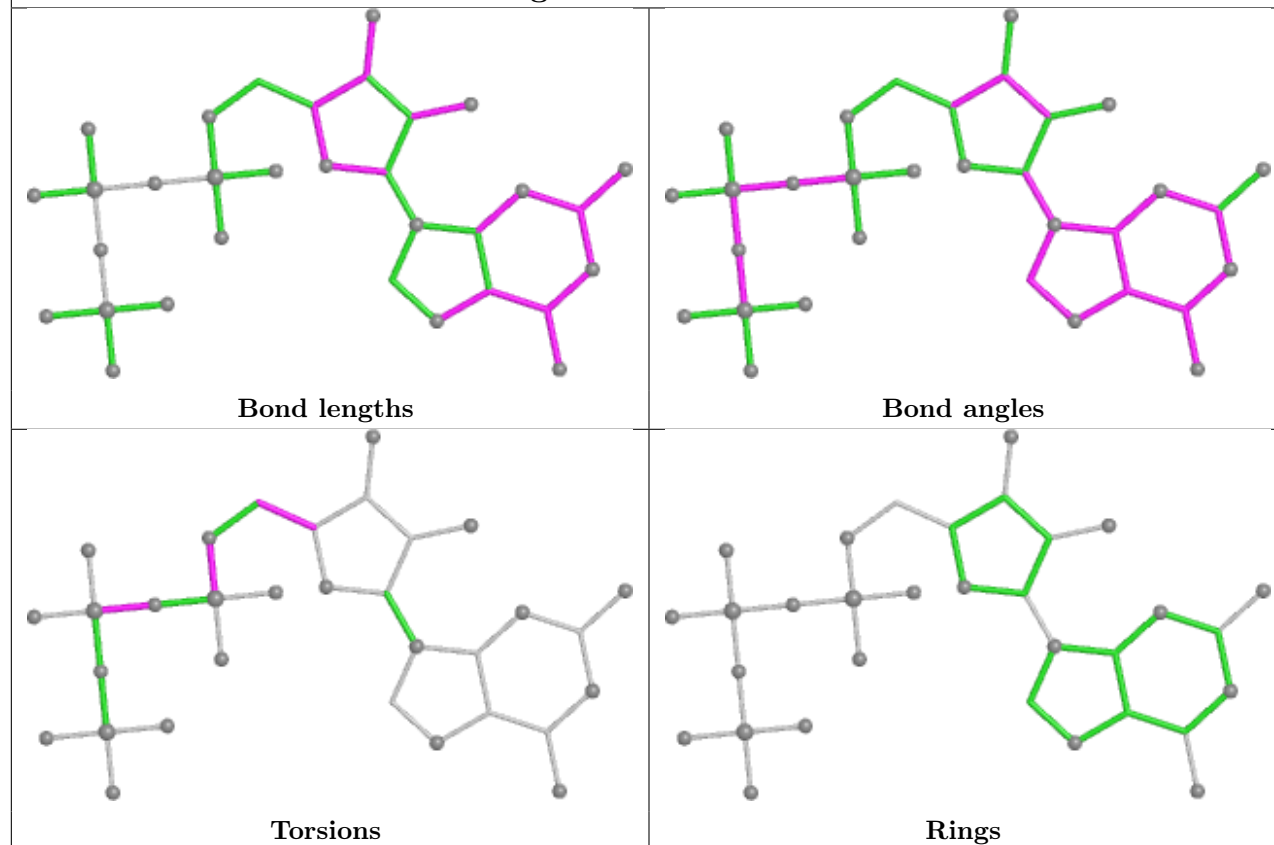
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	GTP	1	0
3	E	302	GOL	1	0
3	D	302	GOL	1	0
3	A	303	GOL	1	0
2	L	301	GTP	1	0
2	N	301	GTP	2	0
2	G	301	GTP	1	0
3	Q	302	GOL	1	0
2	P	301	GTP	1	0
3	P	303	GOL	2	0
3	C	302	GOL	1	0
3	L	303	GOL	1	0
3	L	302	GOL	1	0
2	O	301	GTP	1	0
3	Q	303	GOL	2	0
2	E	301	GTP	1	0
3	E	303	GOL	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.

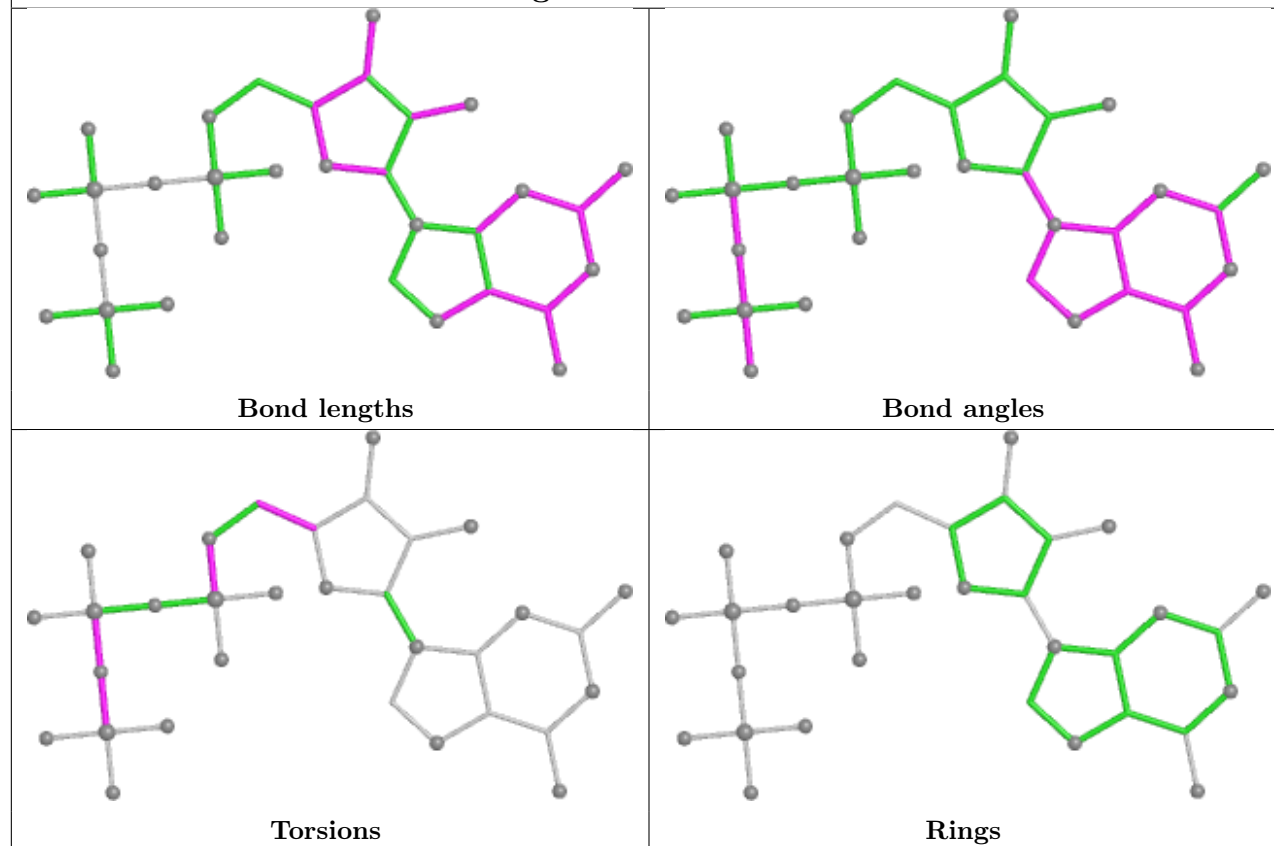
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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



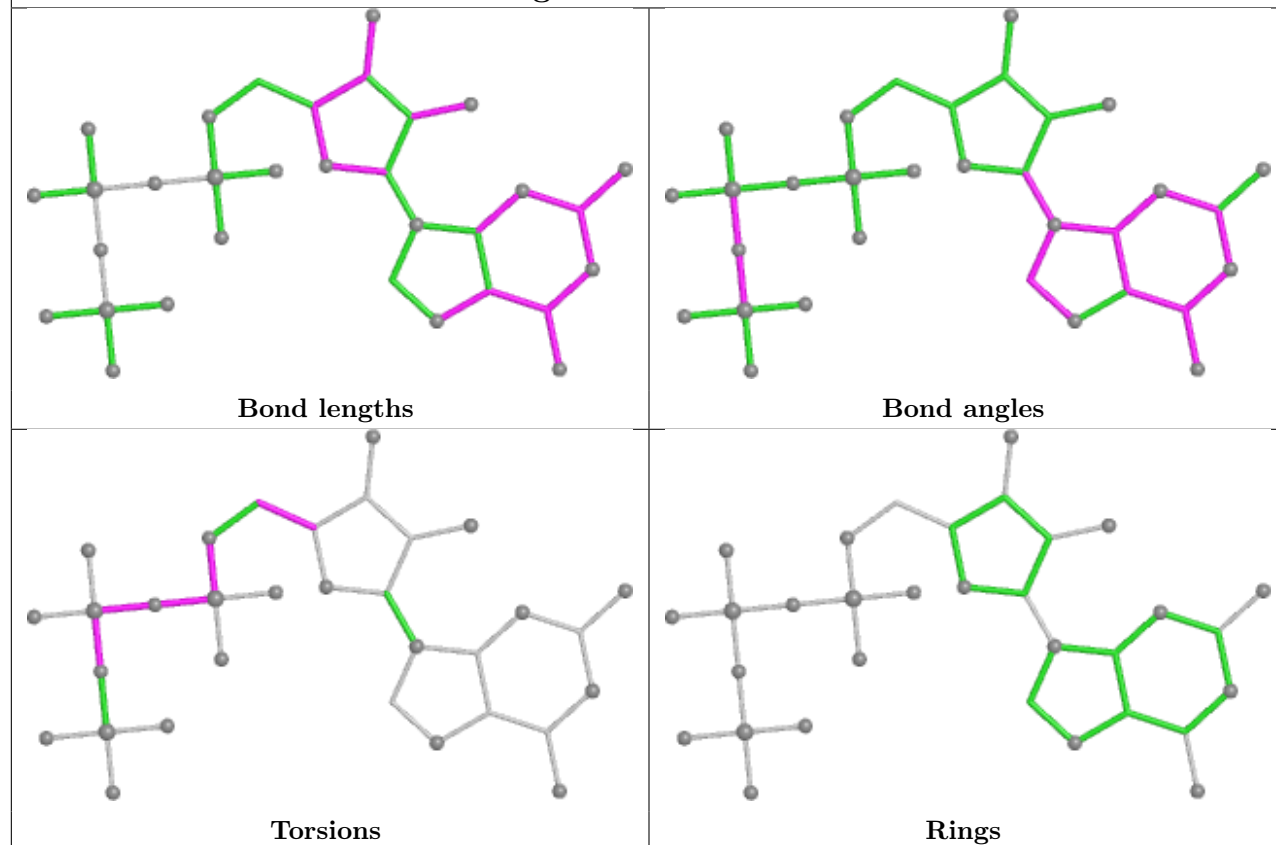
Ligand GTP R 301



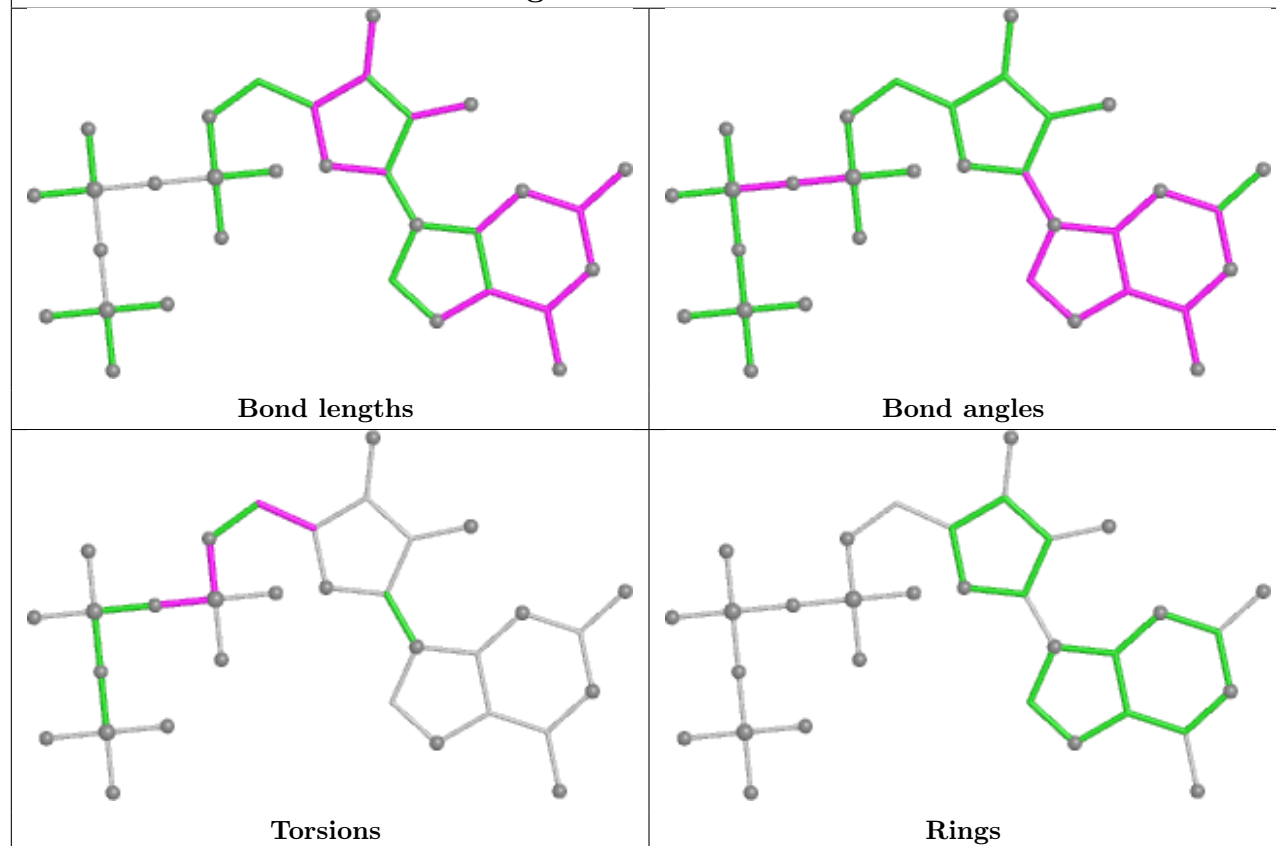
Ligand GTP F 301

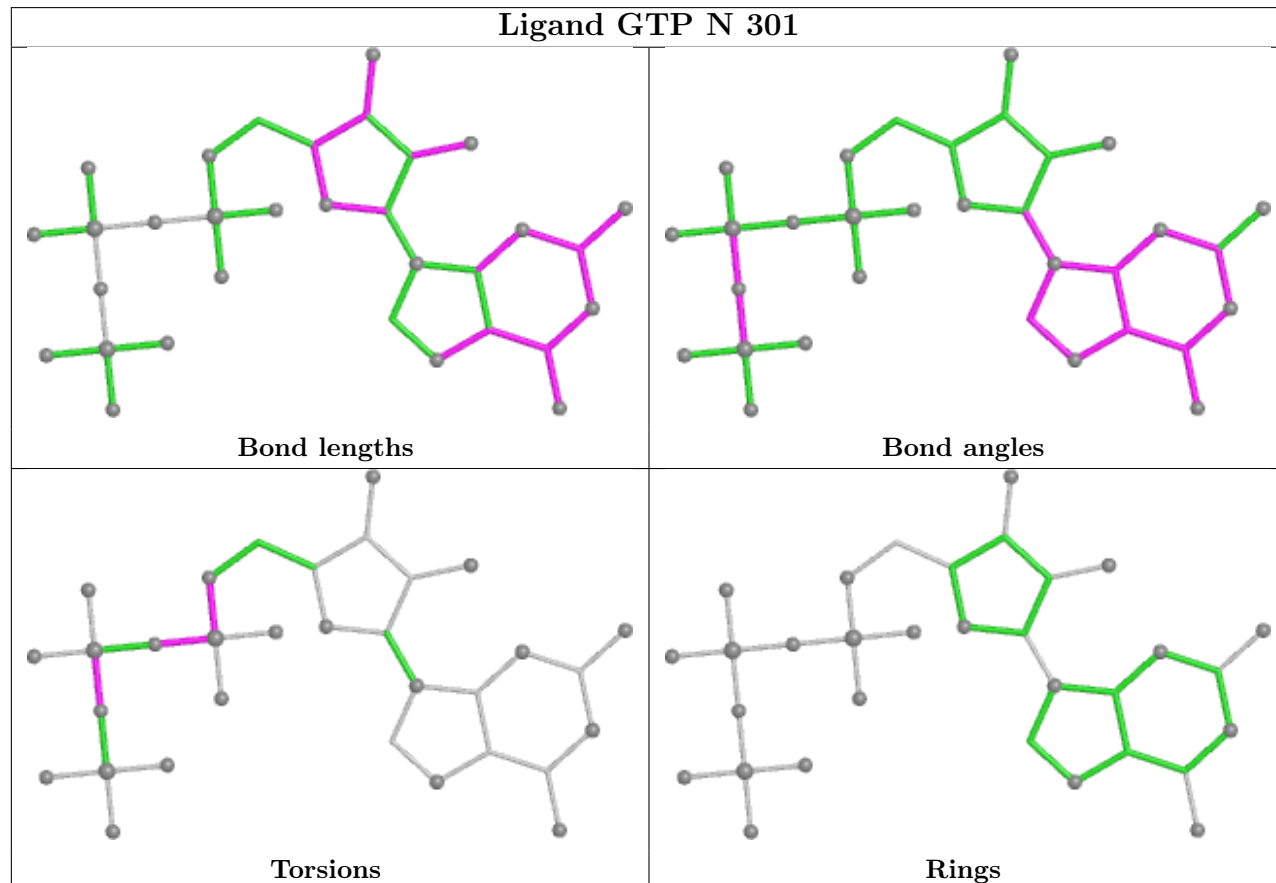
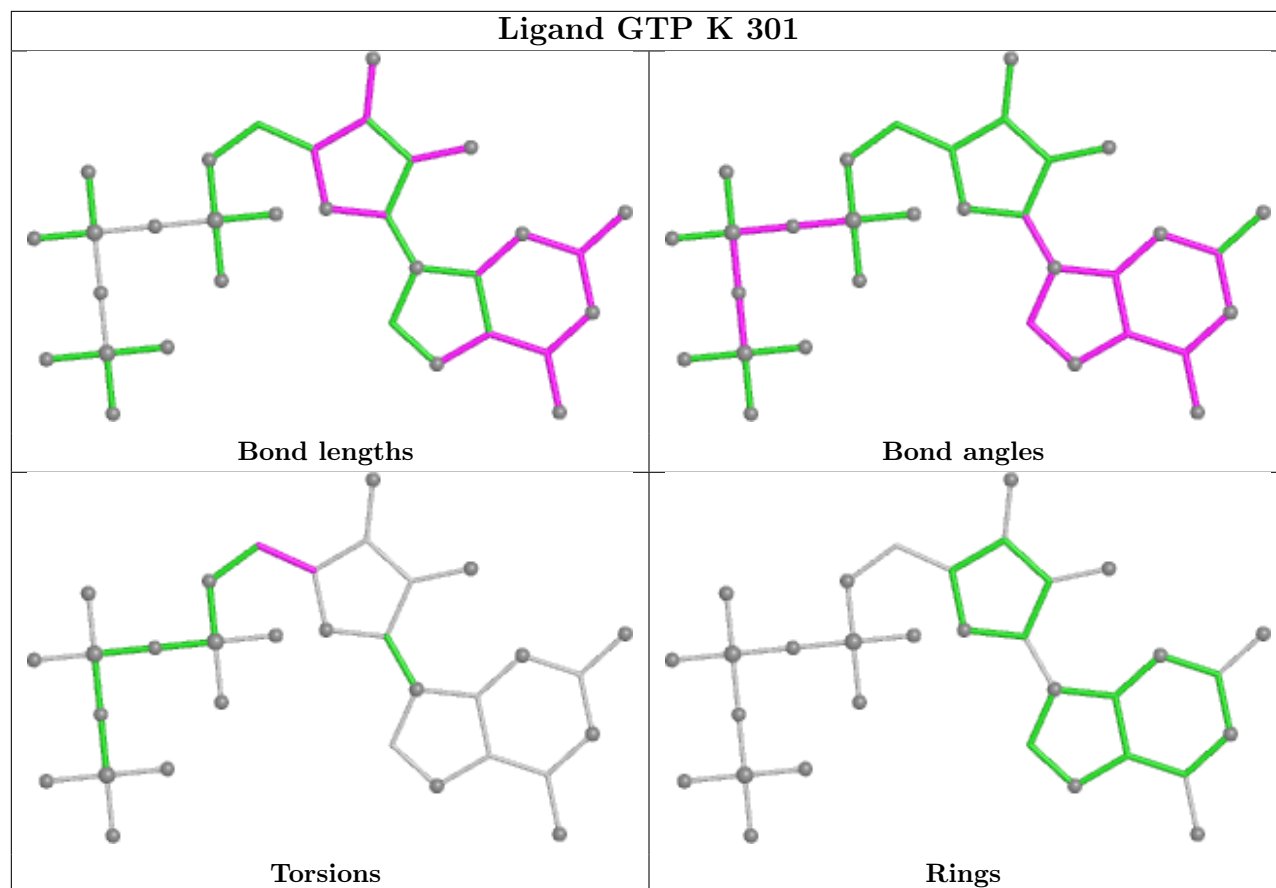


Ligand GTP L 301

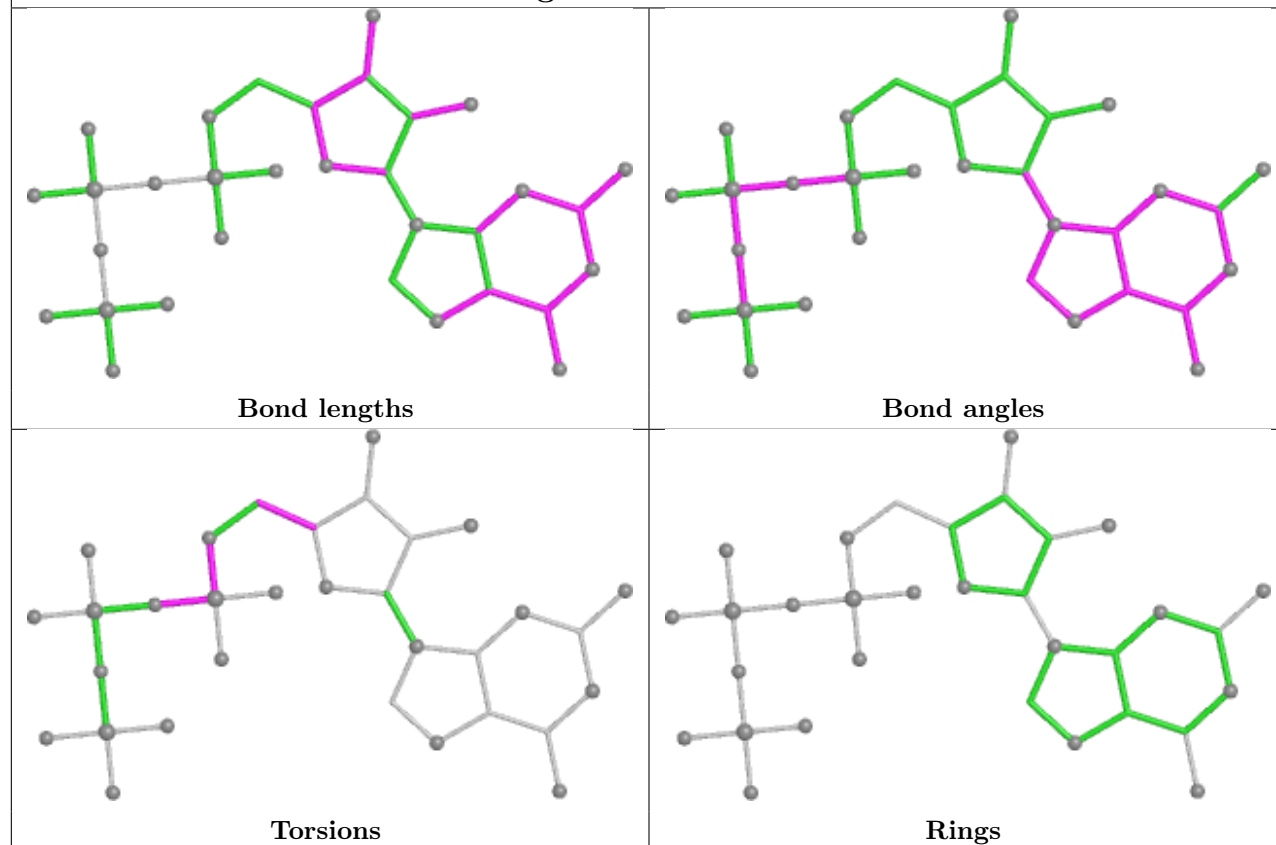


Ligand GTP M 301

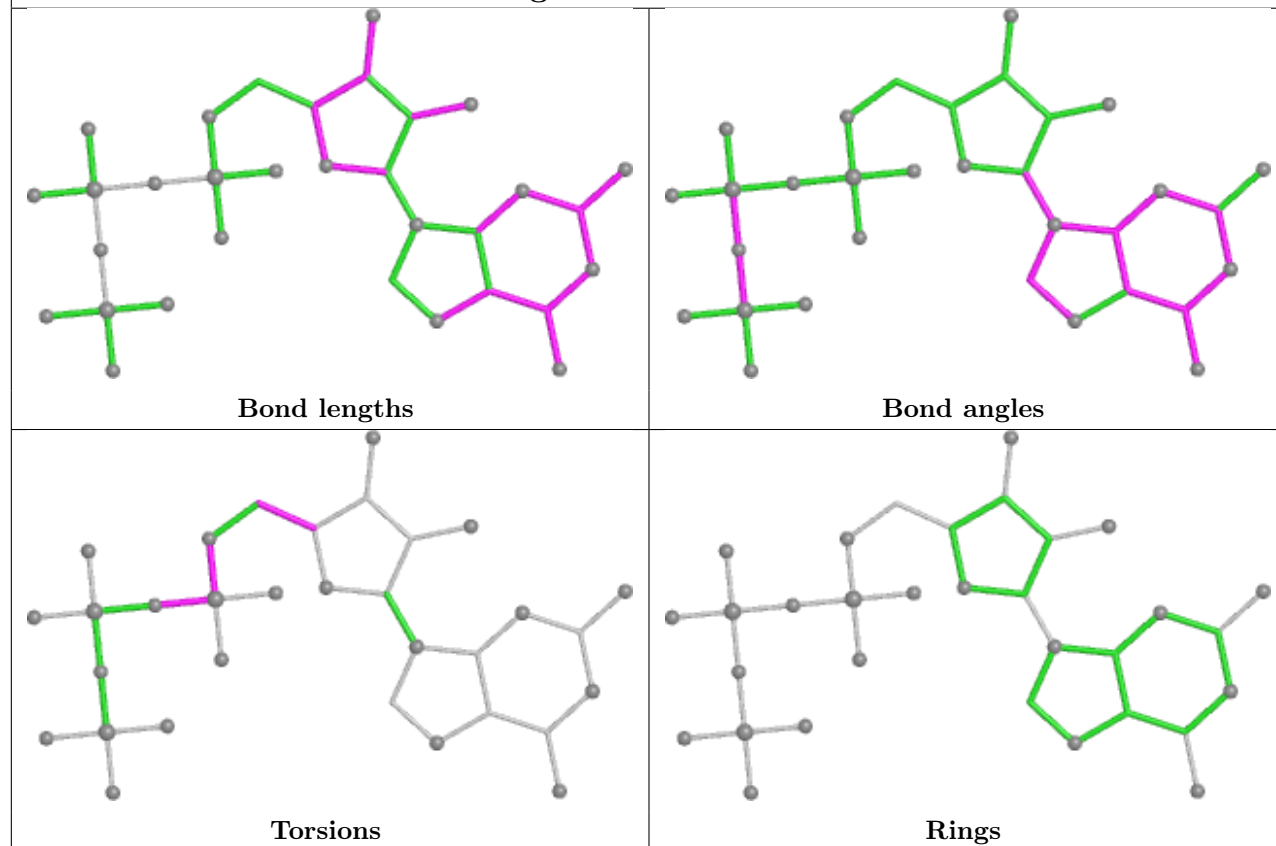


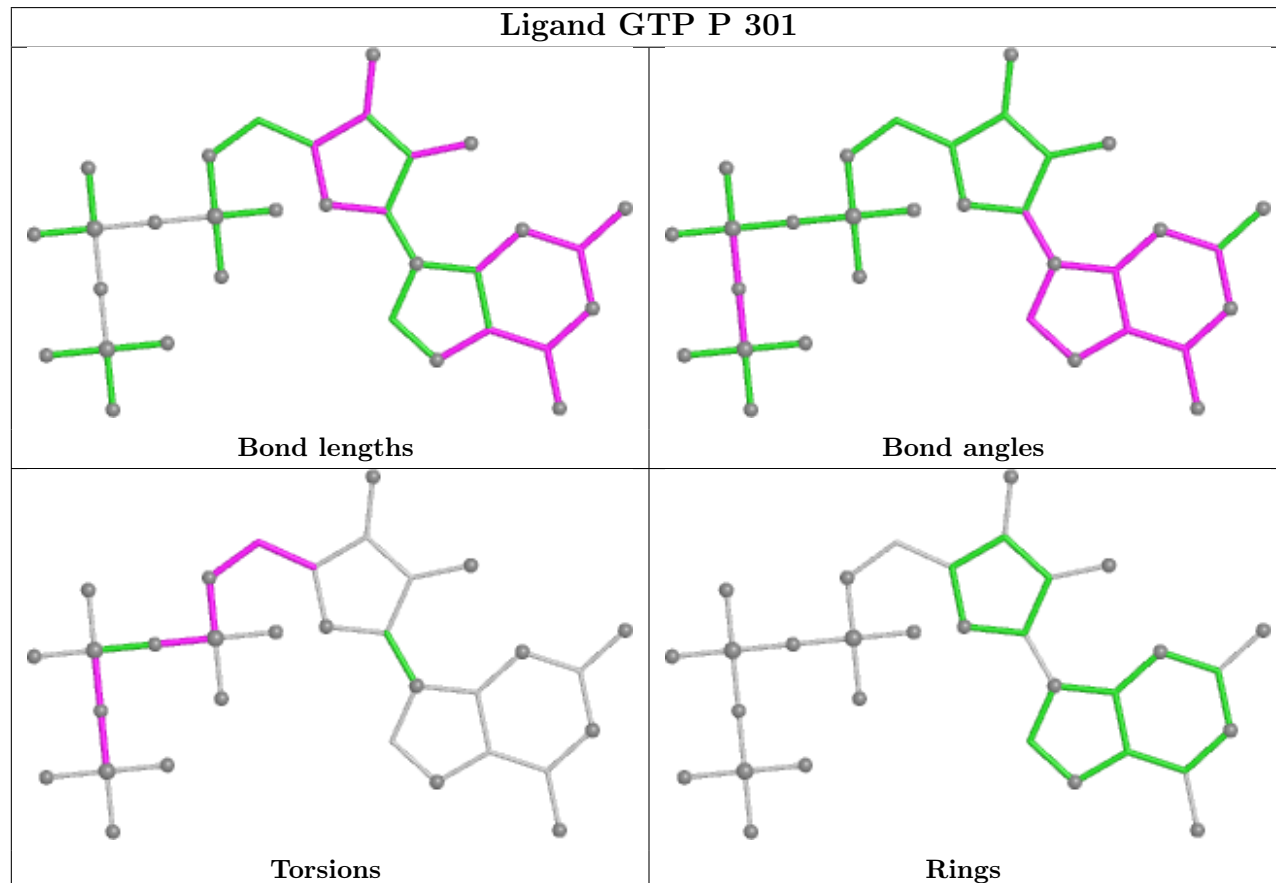
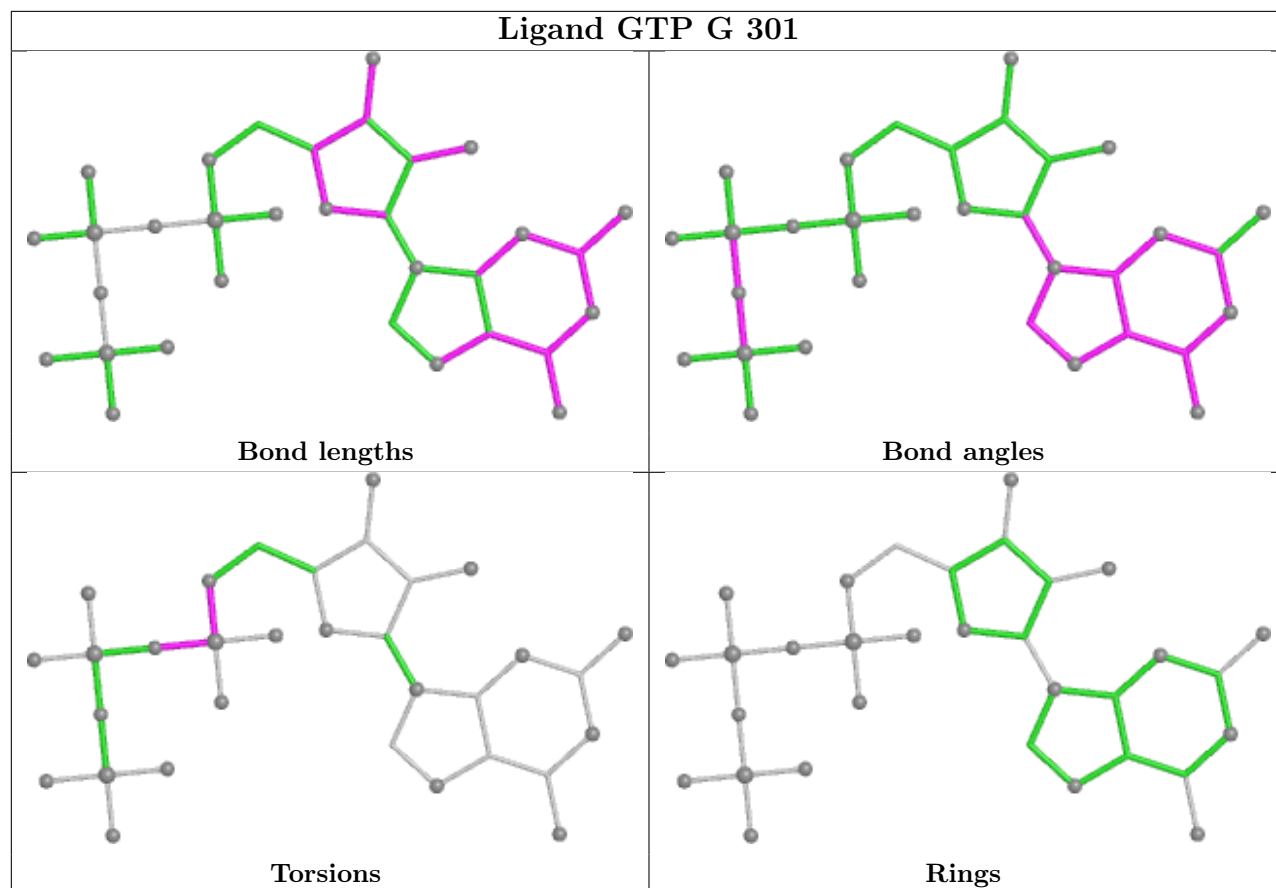


Ligand GTP I 301

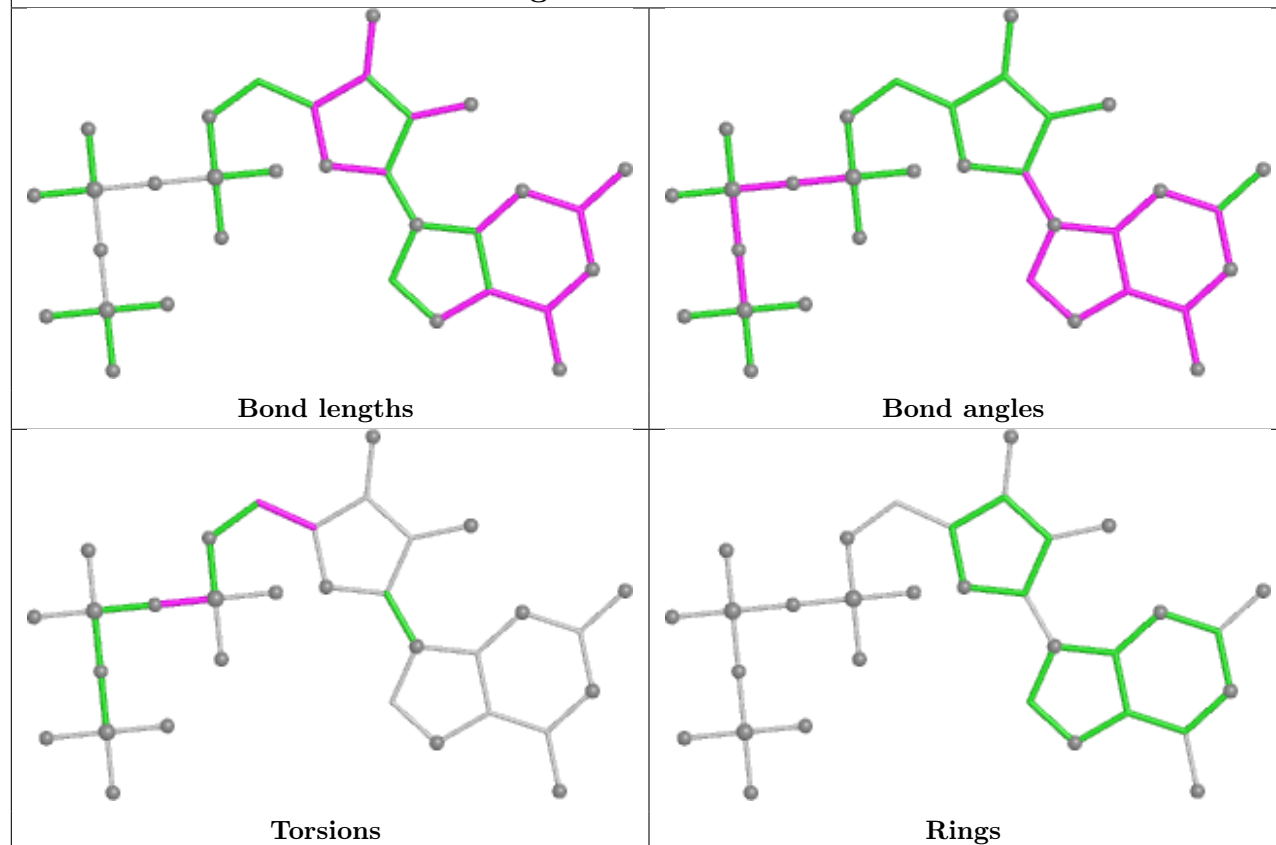


Ligand GTP D 301

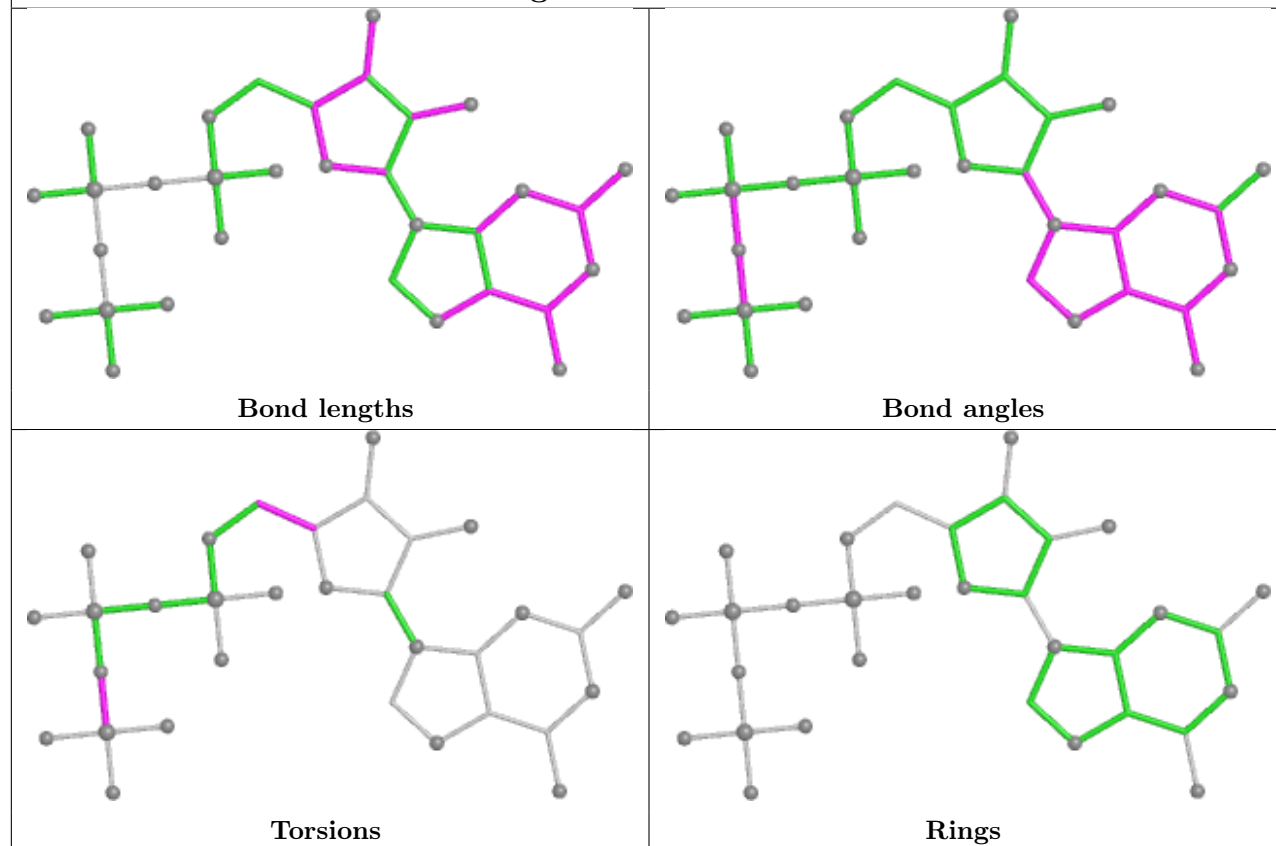




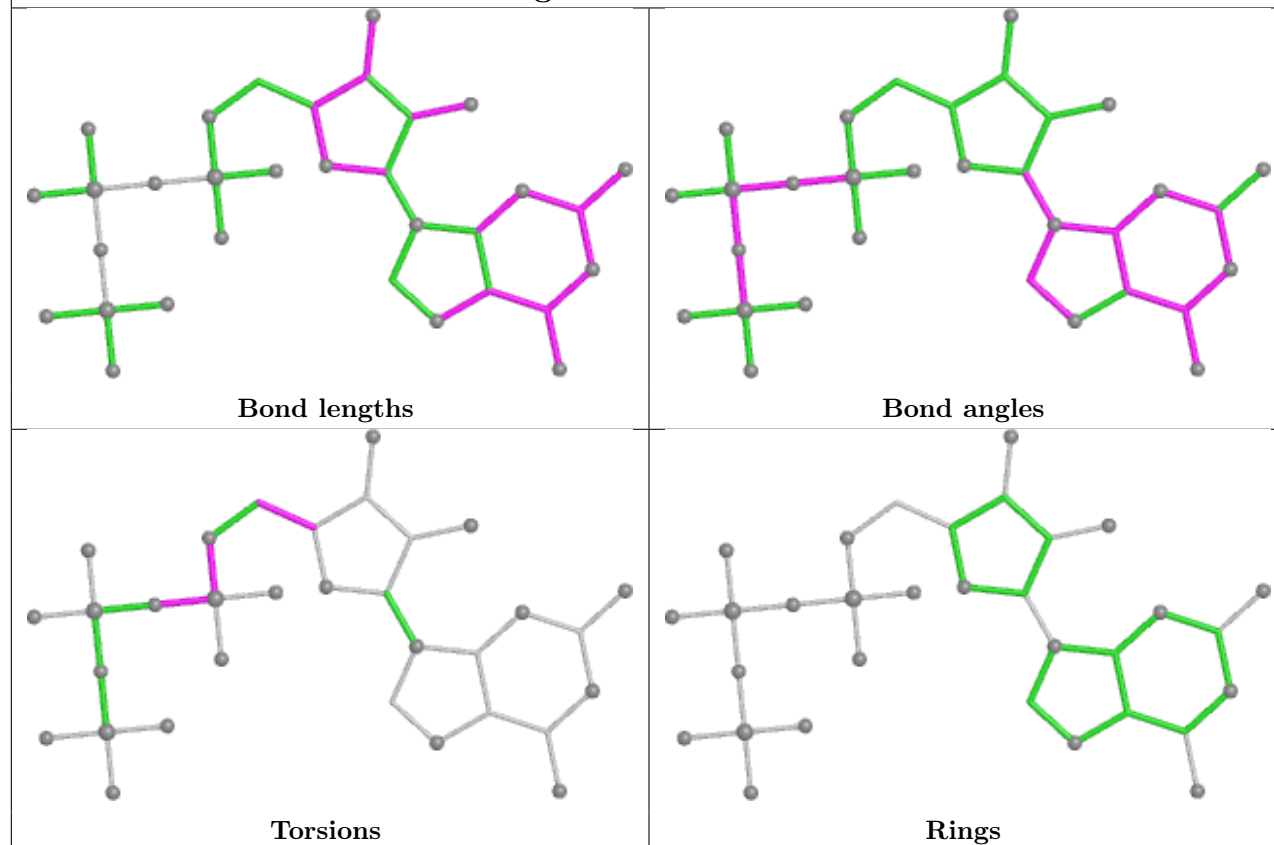
Ligand GTP A 301



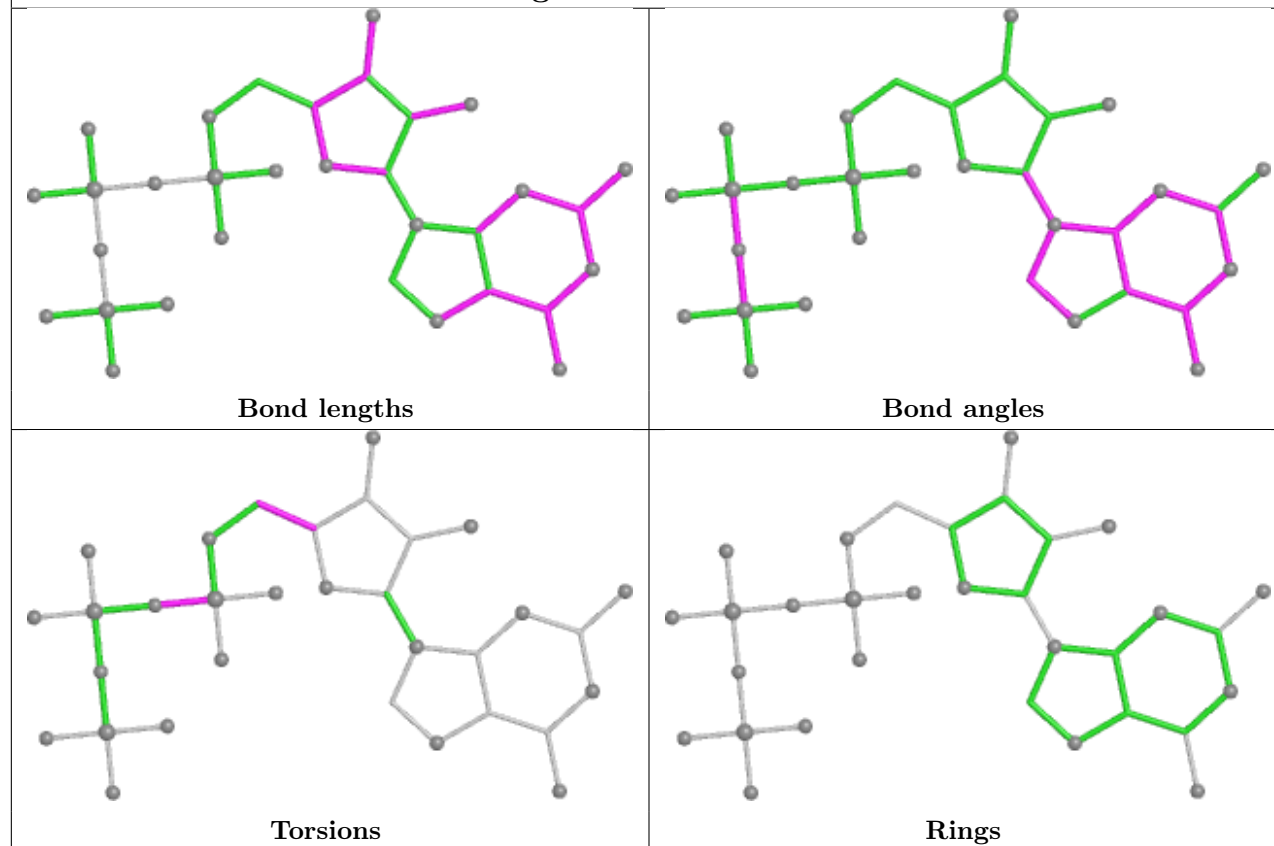
Ligand GTP O 301

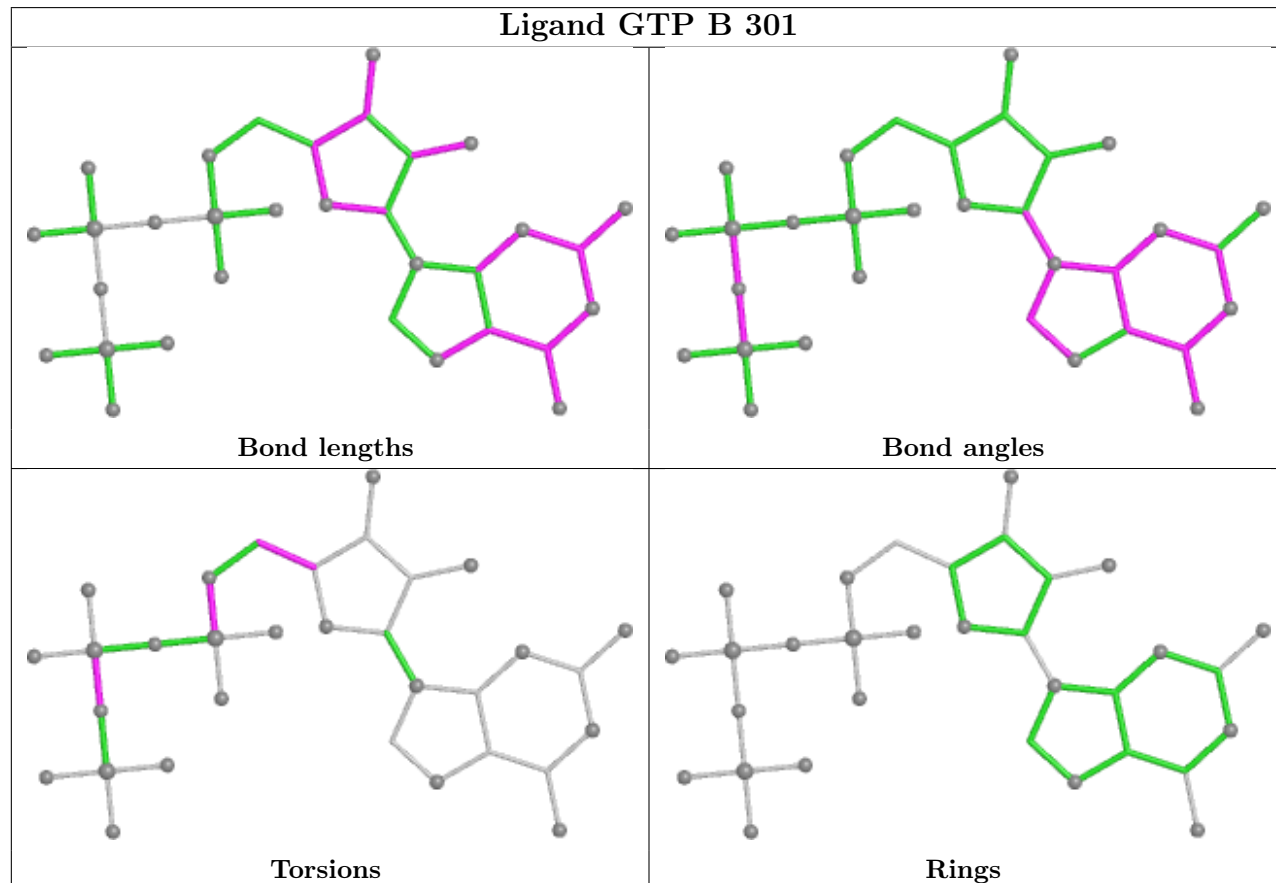
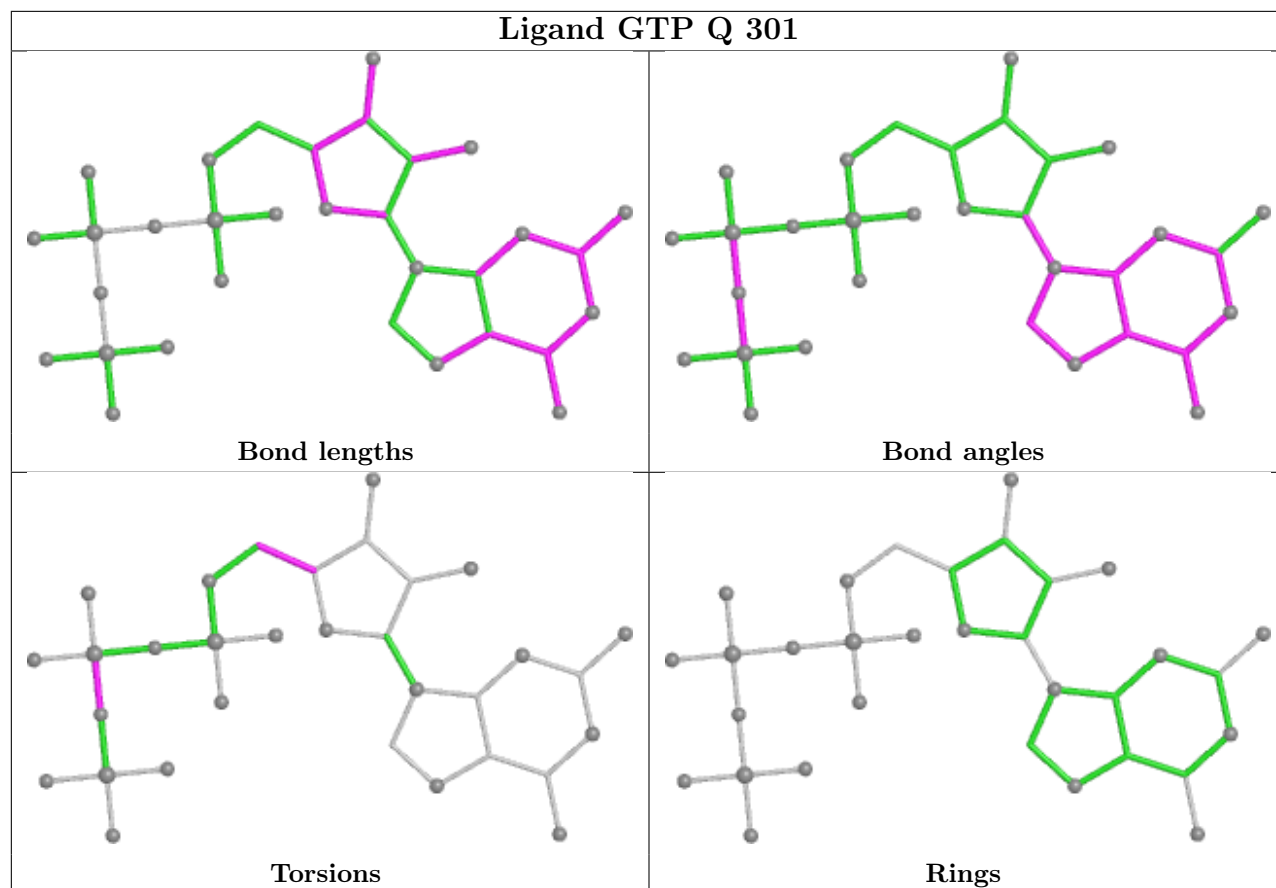


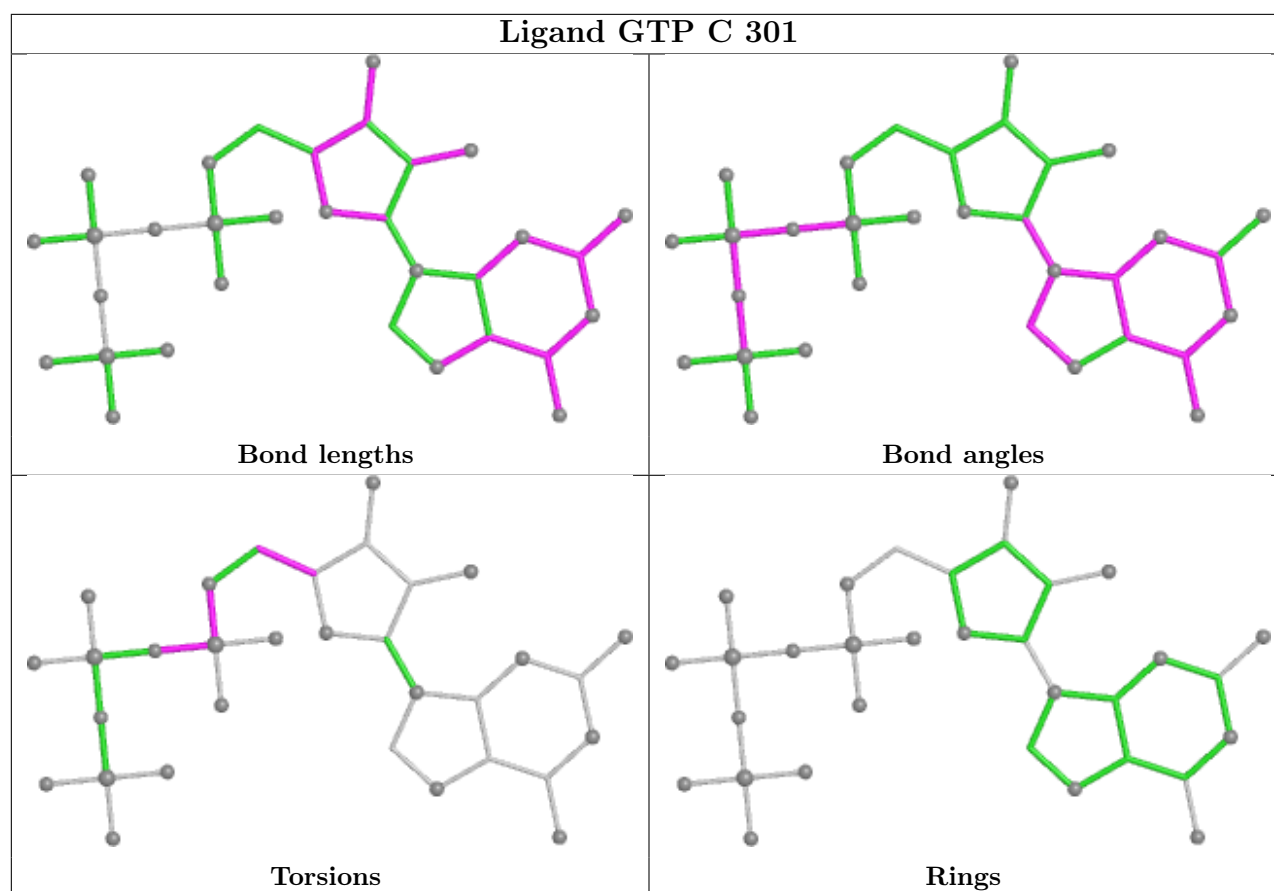
Ligand GTP J 301



Ligand GTP E 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	239/248 (96%)	-2.00	0 100 100	17, 35, 77, 141	0
1	B	239/248 (96%)	-2.00	0 100 100	15, 31, 76, 106	0
1	C	239/248 (96%)	-1.98	0 100 100	16, 34, 83, 146	0
1	D	237/248 (95%)	-2.01	0 100 100	16, 32, 74, 104	0
1	E	236/248 (95%)	-2.02	0 100 100	17, 31, 76, 103	0
1	F	237/248 (95%)	-2.02	0 100 100	16, 31, 64, 106	0
1	G	239/248 (96%)	-1.98	0 100 100	16, 36, 77, 122	0
1	H	239/248 (96%)	-1.93	0 100 100	19, 42, 106, 131	0
1	I	238/248 (95%)	-1.94	0 100 100	17, 41, 88, 125	0
1	J	236/248 (95%)	-2.02	0 100 100	17, 34, 71, 125	0
1	K	236/248 (95%)	-1.98	0 100 100	20, 40, 73, 108	0
1	L	237/248 (95%)	-2.01	0 100 100	15, 31, 78, 101	0
1	M	236/248 (95%)	-1.95	0 100 100	18, 46, 99, 119	0
1	N	237/248 (95%)	-1.94	0 100 100	17, 44, 99, 147	0
1	O	237/248 (95%)	-1.92	0 100 100	17, 44, 96, 135	0
1	P	237/248 (95%)	-1.95	0 100 100	15, 38, 85, 160	0
1	Q	237/248 (95%)	-1.93	0 100 100	19, 46, 100, 117	0
1	R	237/248 (95%)	-1.92	0 100 100	20, 48, 99, 129	0
All	All	4273/4464 (95%)	-1.97	0 100 100	15, 38, 89, 160	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

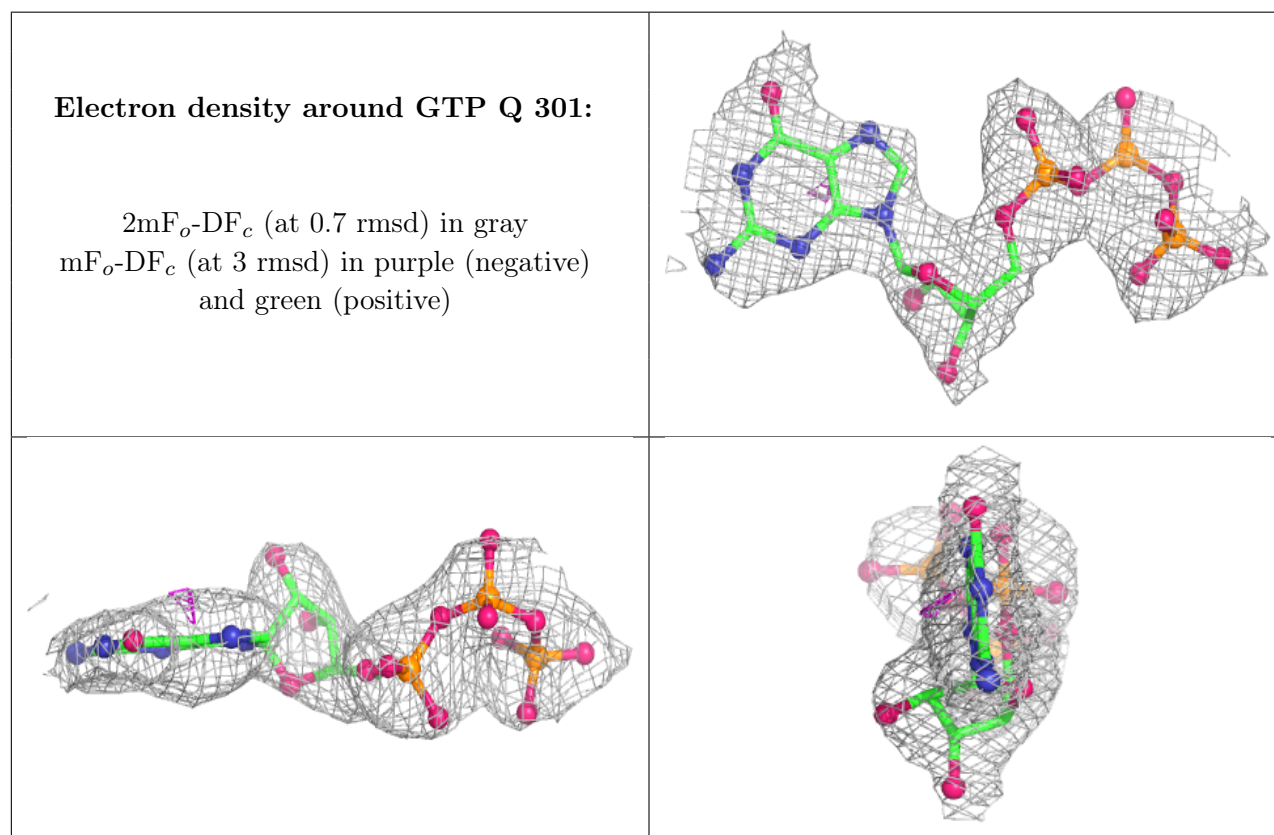
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GTP	Q	301	32/32	0.99	0.02	41,56,80,81	0
2	GTP	R	301	32/32	0.99	0.02	43,55,86,87	0
3	GOL	C	302	6/6	0.99	0.02	34,39,41,43	0
3	GOL	A	302	6/6	0.99	0.03	28,31,33,33	0
3	GOL	A	303	6/6	0.99	0.04	47,49,49,50	0
3	GOL	A	304	6/6	0.99	0.02	51,54,55,56	0
3	GOL	D	302	6/6	0.99	0.03	35,38,42,44	0
3	GOL	E	304	6/6	0.99	0.02	45,48,49,50	0
3	GOL	E	305	6/6	0.99	0.03	44,48,51,51	0
3	GOL	G	302	6/6	0.99	0.03	35,35,37,38	0
3	GOL	H	302	6/6	0.99	0.03	54,56,57,59	0
3	GOL	J	302	6/6	0.99	0.02	42,46,48,50	0
3	GOL	J	303	6/6	0.99	0.04	39,40,41,42	0
3	GOL	K	302	6/6	0.99	0.03	48,50,51,52	0
3	GOL	L	302	6/6	0.99	0.02	30,38,42,44	0
3	GOL	L	303	6/6	0.99	0.03	34,42,45,46	0
3	GOL	L	304	6/6	0.99	0.03	47,48,48,48	0
3	GOL	O	302	6/6	0.99	0.02	48,52,53,54	0
3	GOL	P	302	6/6	0.99	0.03	45,47,48,50	0
3	GOL	P	303	6/6	0.99	0.03	47,47,48,49	0
3	GOL	Q	302	6/6	0.99	0.03	38,41,43,44	0
2	GTP	E	301	32/32	1.00	0.02	35,44,68,69	0
2	GTP	F	301	32/32	1.00	0.01	28,45,71,72	0
2	GTP	G	301	32/32	1.00	0.01	34,55,77,77	0
3	GOL	D	303	6/6	1.00	0.02	28,35,37,37	0
3	GOL	E	302	6/6	1.00	0.02	23,29,30,33	0
3	GOL	E	303	6/6	1.00	0.03	25,27,35,39	0
2	GTP	H	301	32/32	1.00	0.02	38,50,82,83	0
2	GTP	I	301	32/32	1.00	0.02	34,52,76,77	0
3	GOL	F	302	6/6	1.00	0.03	31,33,34,34	0
3	GOL	F	303	6/6	1.00	0.02	35,40,40,43	0
2	GTP	J	301	32/32	1.00	0.02	31,48,69,70	0

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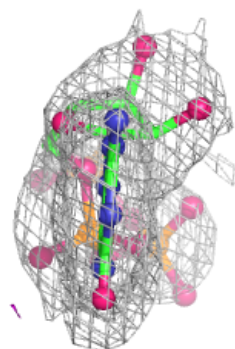
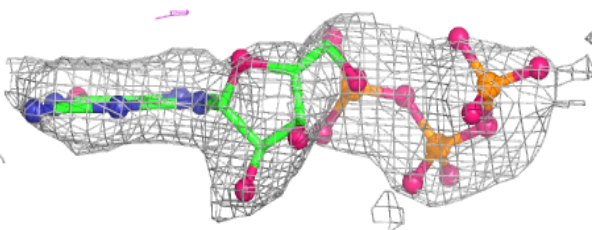
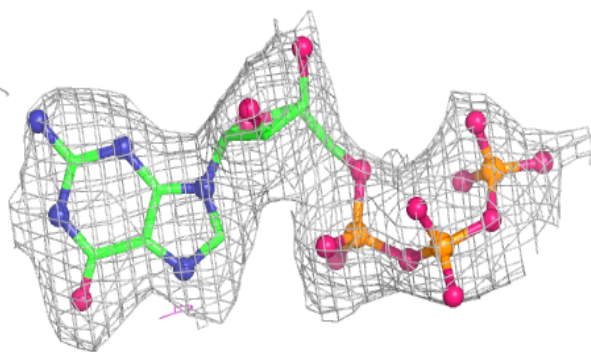
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GTP	K	301	32/32	1.00	0.02	41,52,83,84	0
2	GTP	L	301	32/32	1.00	0.02	28,40,68,69	0
2	GTP	M	301	32/32	1.00	0.02	39,56,83,84	0
2	GTP	N	301	32/32	1.00	0.02	36,58,86,87	0
2	GTP	O	301	32/32	1.00	0.02	41,56,80,81	0
2	GTP	P	301	32/32	1.00	0.02	41,53,79,79	0
2	GTP	C	301	32/32	1.00	0.02	38,49,79,80	0
2	GTP	A	301	32/32	1.00	0.02	35,55,81,82	0
2	GTP	B	301	32/32	1.00	0.02	31,45,80,80	0
3	GOL	C	303	6/6	1.00	0.02	49,50,52,52	0
2	GTP	D	301	32/32	1.00	0.01	30,49,70,71	0
3	GOL	Q	303	6/6	1.00	0.03	50,52,54,55	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.

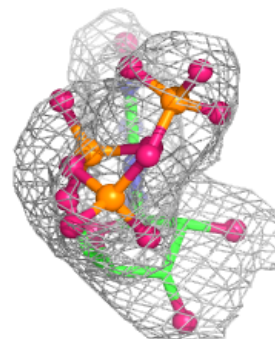
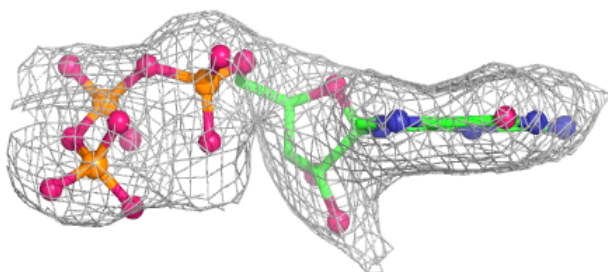
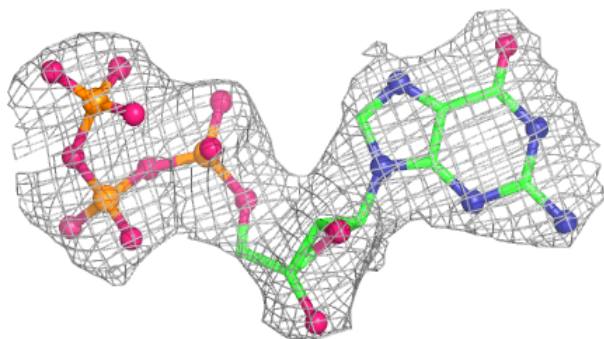


Electron density around GTP R 301:

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

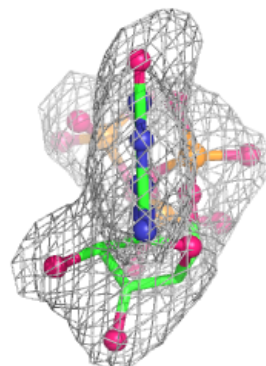
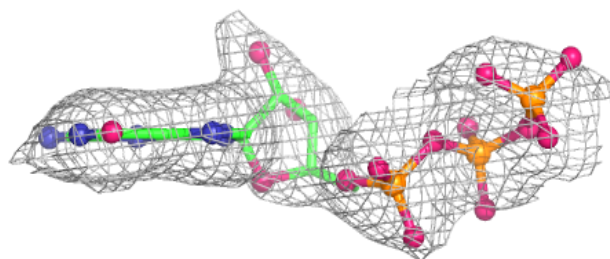
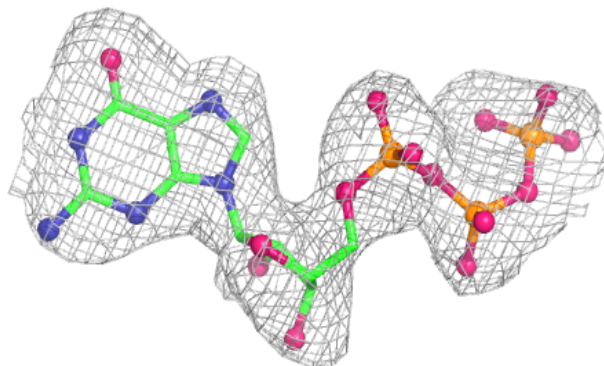
**Electron density around GTP E 301:**

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

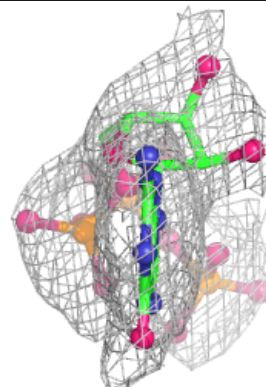
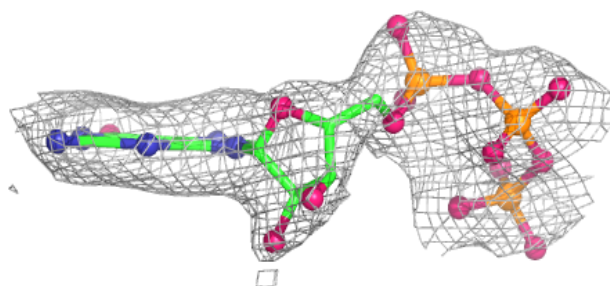
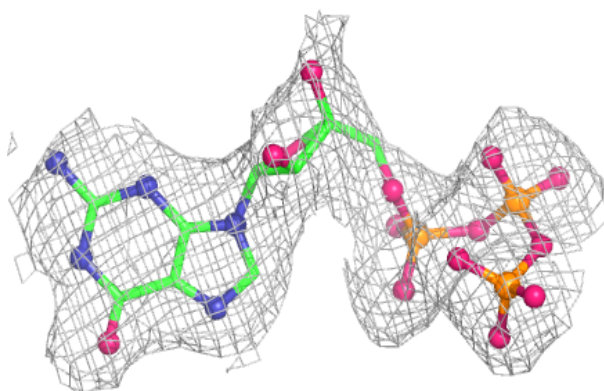


Electron density around GTP F 301:

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

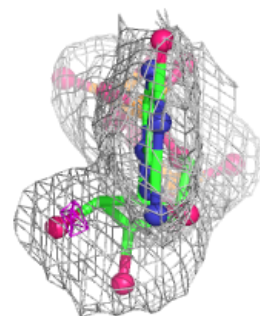
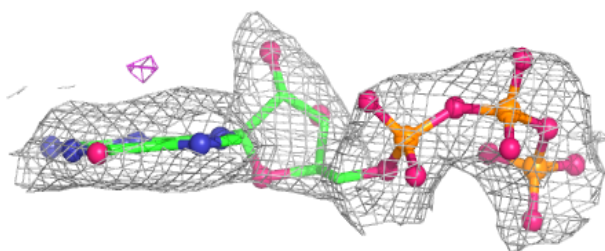
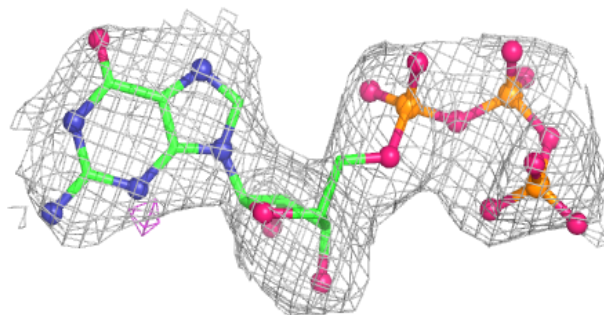
**Electron density around GTP G 301:**

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and green (positive)

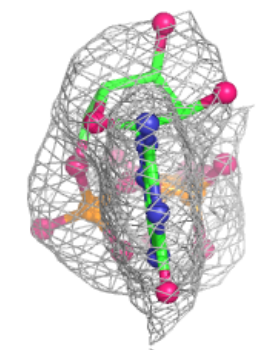
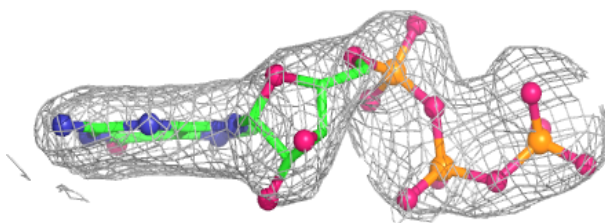
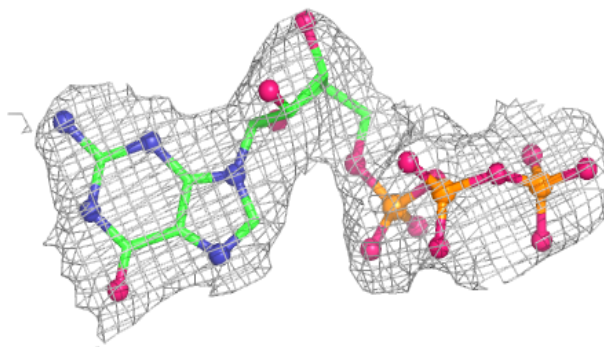


Electron density around GTP H 301:

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

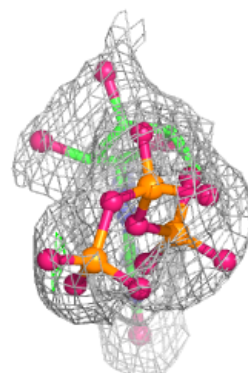
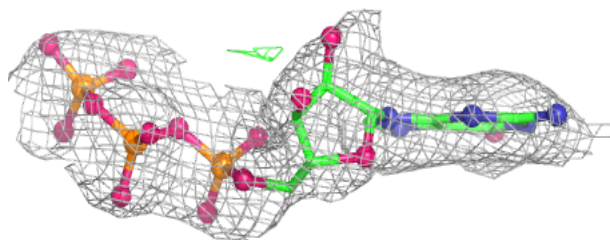
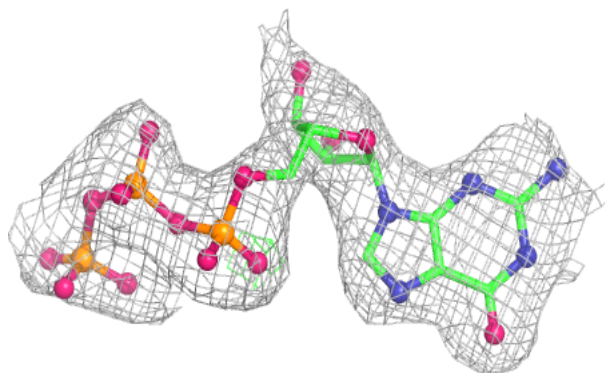
**Electron density around GTP I 301:**

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

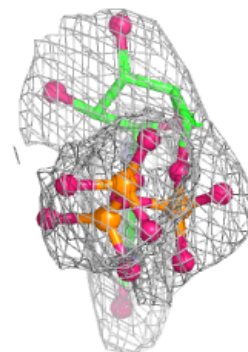
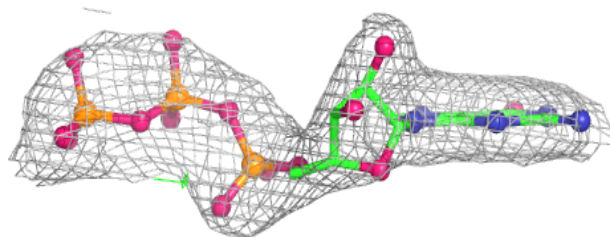
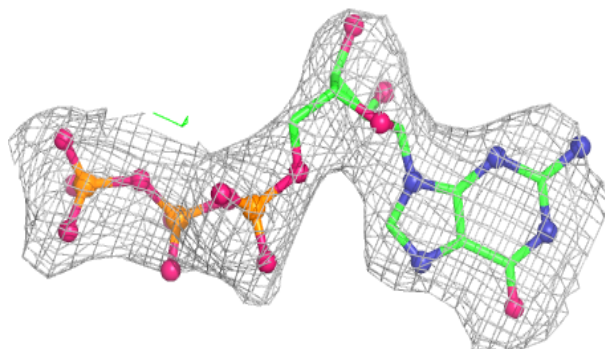


Electron density around GTP J 301:

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

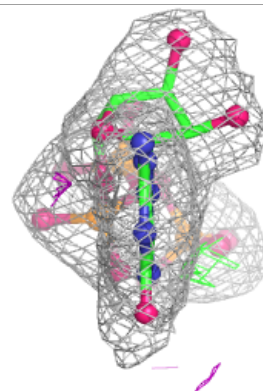
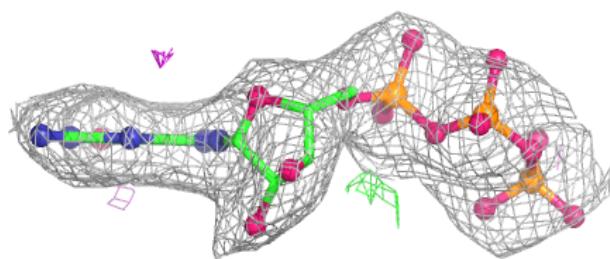
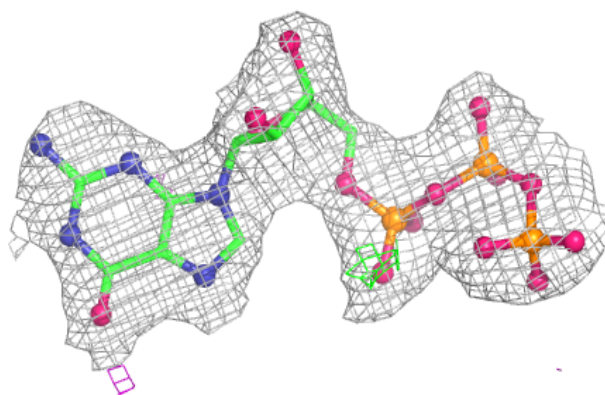
**Electron density around GTP K 301:**

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

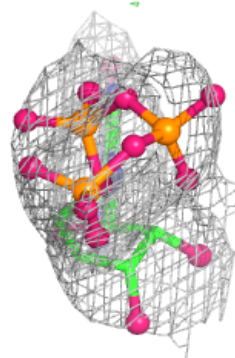
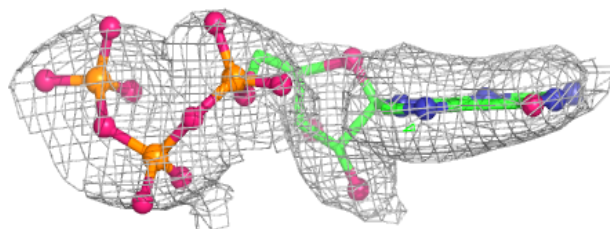
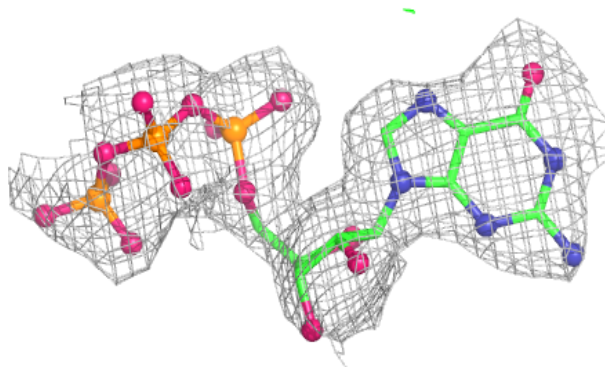


Electron density around GTP L 301:

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

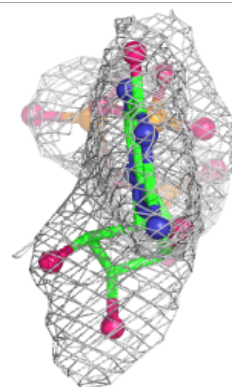
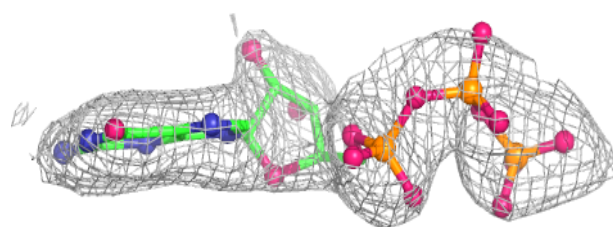
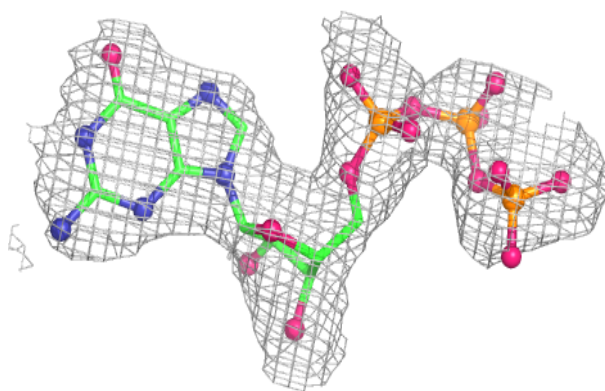
**Electron density around GTP M 301:**

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

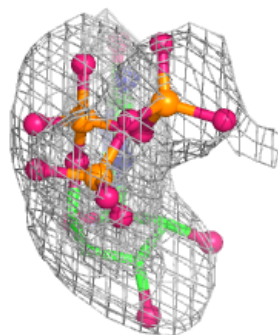
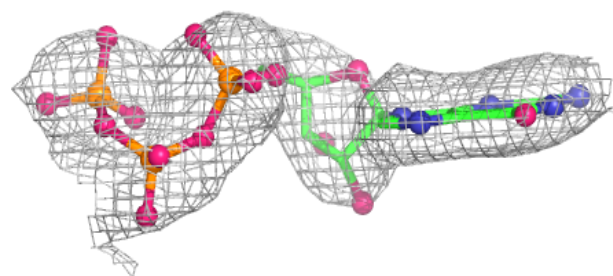
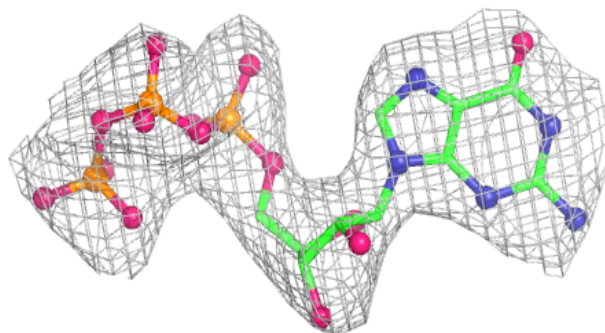


Electron density around GTP N 301:

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

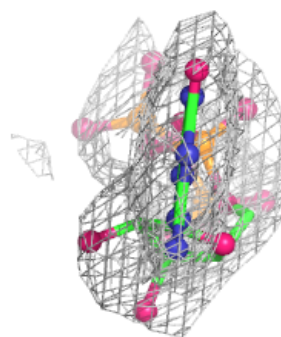
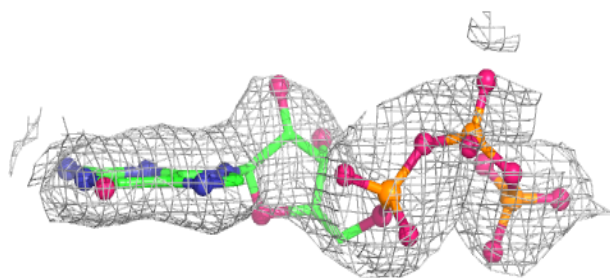
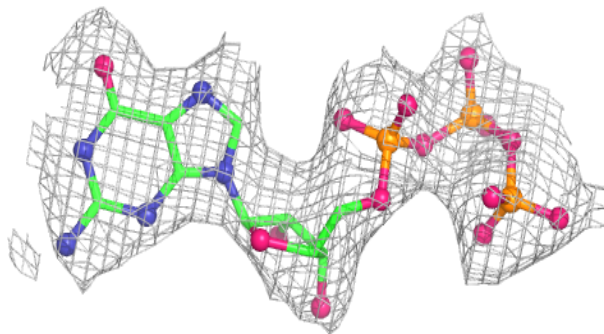
**Electron density around GTP O 301:**

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

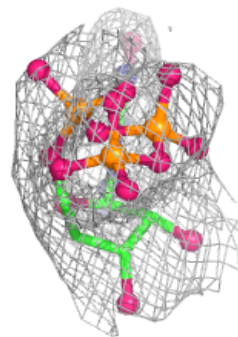
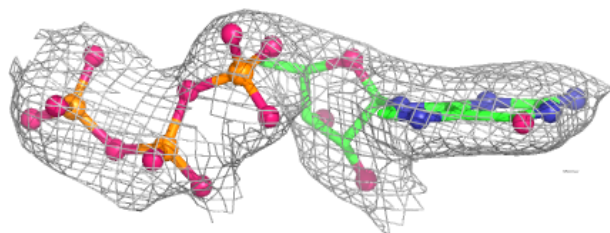
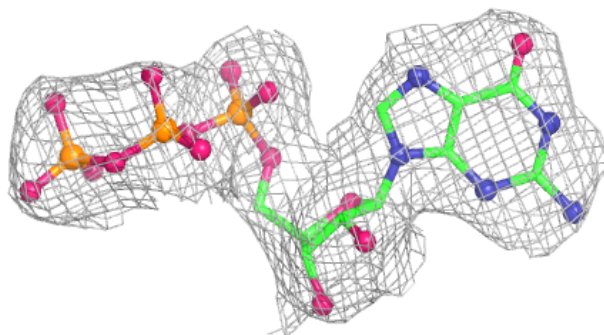


Electron density around GTP P 301:

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

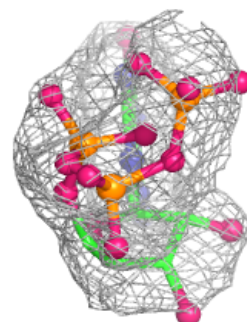
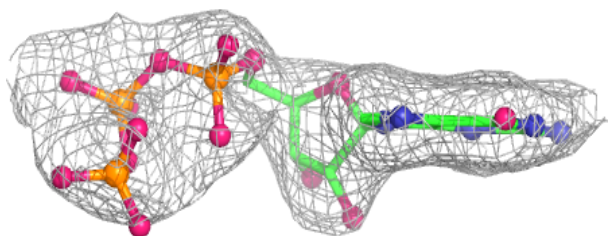
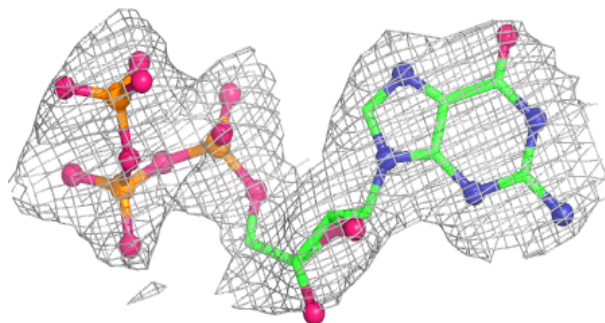
**Electron density around GTP C 301:**

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

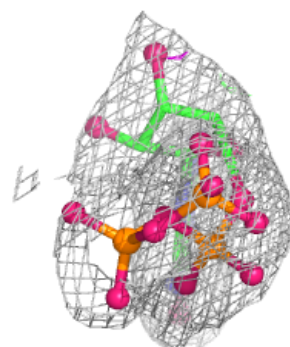
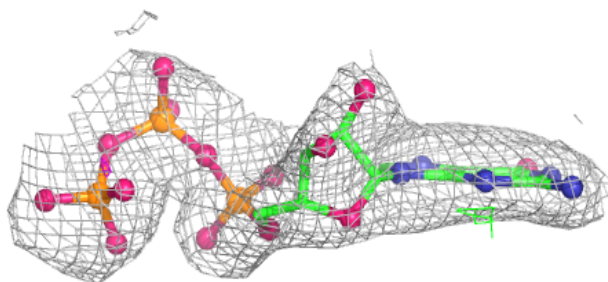
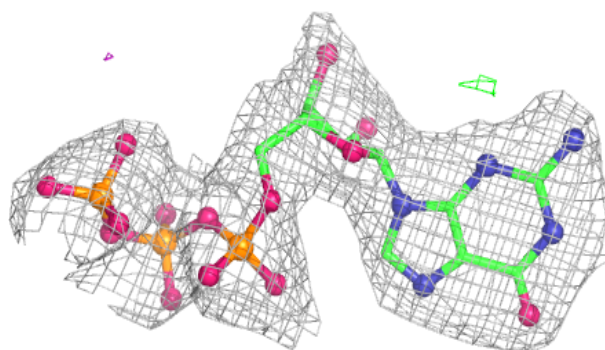


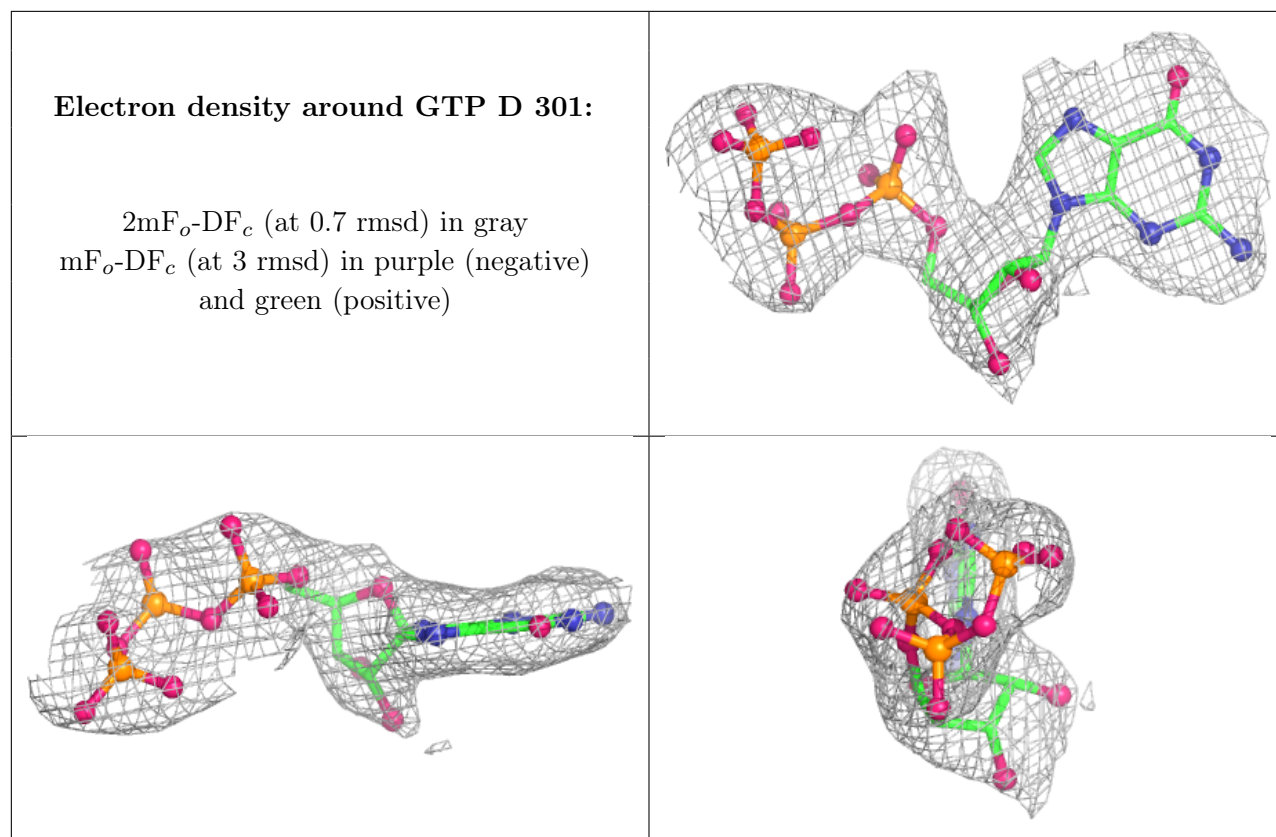
Electron density around GTP A 301:

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

**Electron density around GTP B 301:**

$2mF_o-DF_c$ (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.