



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 07:24 pm BST

PDB ID : 9HG3 / pdb_00009hg3
Title : Crystal structure of M. smegmatis GMP reductase in complex with GMP and GTP.
Authors : Dolezal, M.; Pichova, I.
Deposited on : 2024-11-18
Resolution : 2.30 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

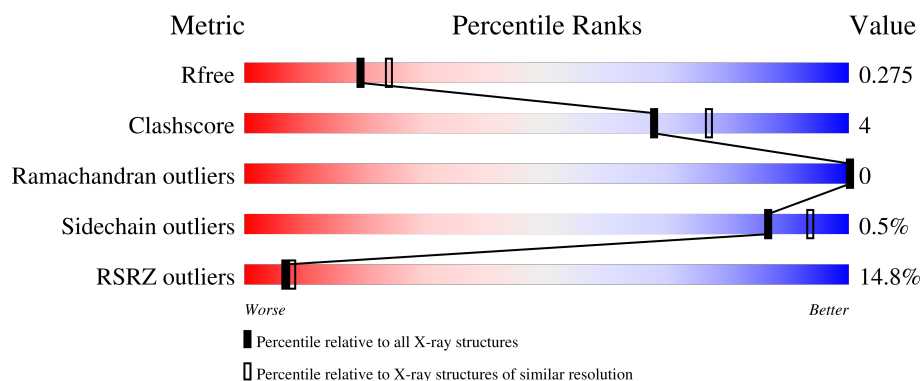
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	496	<div> <div>5%</div> <div>85%</div> <div>7%</div> <div>7%</div> </div>
1	B	496	<div> <div>6%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	C	496	<div> <div>6%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	D	496	<div> <div>4%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	E	496	<div> <div>25%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	496	<div><div></div><div>32%</div><div></div><div>78%</div><div>14%</div><div>7%</div></div>
1	G	496	<div><div></div><div>20%</div><div></div><div>85%</div><div>8%</div><div>7%</div></div>
1	H	496	<div><div></div><div>13%</div><div></div><div>84%</div><div>8%</div><div>7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27456 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 GMP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	B	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	C	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	D	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	E	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	F	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	G	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			
1	H	460	Total	C	N	O	S	0	0	0
			3344	2086	597	647	14			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP A0QYE8
A	480	THR	-	expression tag	UNP A0QYE8
A	481	ALA	-	expression tag	UNP A0QYE8
A	482	ALA	-	expression tag	UNP A0QYE8
A	483	ALA	-	expression tag	UNP A0QYE8
A	484	LYS	-	expression tag	UNP A0QYE8
A	485	GLU	-	expression tag	UNP A0QYE8
A	486	ASP	-	expression tag	UNP A0QYE8
A	487	LEU	-	expression tag	UNP A0QYE8
A	488	GLU	-	expression tag	UNP A0QYE8
A	489	HIS	-	expression tag	UNP A0QYE8
A	490	HIS	-	expression tag	UNP A0QYE8
A	491	HIS	-	expression tag	UNP A0QYE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	HIS	-	expression tag	UNP A0QYE8
A	493	HIS	-	expression tag	UNP A0QYE8
A	494	HIS	-	expression tag	UNP A0QYE8
A	495	HIS	-	expression tag	UNP A0QYE8
A	496	HIS	-	expression tag	UNP A0QYE8
B	2	VAL	-	insertion	UNP A0QYE8
B	480	THR	-	expression tag	UNP A0QYE8
B	481	ALA	-	expression tag	UNP A0QYE8
B	482	ALA	-	expression tag	UNP A0QYE8
B	483	ALA	-	expression tag	UNP A0QYE8
B	484	LYS	-	expression tag	UNP A0QYE8
B	485	GLU	-	expression tag	UNP A0QYE8
B	486	ASP	-	expression tag	UNP A0QYE8
B	487	LEU	-	expression tag	UNP A0QYE8
B	488	GLU	-	expression tag	UNP A0QYE8
B	489	HIS	-	expression tag	UNP A0QYE8
B	490	HIS	-	expression tag	UNP A0QYE8
B	491	HIS	-	expression tag	UNP A0QYE8
B	492	HIS	-	expression tag	UNP A0QYE8
B	493	HIS	-	expression tag	UNP A0QYE8
B	494	HIS	-	expression tag	UNP A0QYE8
B	495	HIS	-	expression tag	UNP A0QYE8
B	496	HIS	-	expression tag	UNP A0QYE8
C	2	VAL	-	insertion	UNP A0QYE8
C	480	THR	-	expression tag	UNP A0QYE8
C	481	ALA	-	expression tag	UNP A0QYE8
C	482	ALA	-	expression tag	UNP A0QYE8
C	483	ALA	-	expression tag	UNP A0QYE8
C	484	LYS	-	expression tag	UNP A0QYE8
C	485	GLU	-	expression tag	UNP A0QYE8
C	486	ASP	-	expression tag	UNP A0QYE8
C	487	LEU	-	expression tag	UNP A0QYE8
C	488	GLU	-	expression tag	UNP A0QYE8
C	489	HIS	-	expression tag	UNP A0QYE8
C	490	HIS	-	expression tag	UNP A0QYE8
C	491	HIS	-	expression tag	UNP A0QYE8
C	492	HIS	-	expression tag	UNP A0QYE8
C	493	HIS	-	expression tag	UNP A0QYE8
C	494	HIS	-	expression tag	UNP A0QYE8
C	495	HIS	-	expression tag	UNP A0QYE8
C	496	HIS	-	expression tag	UNP A0QYE8
D	2	VAL	-	insertion	UNP A0QYE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	480	THR	-	expression tag	UNP A0QYE8
D	481	ALA	-	expression tag	UNP A0QYE8
D	482	ALA	-	expression tag	UNP A0QYE8
D	483	ALA	-	expression tag	UNP A0QYE8
D	484	LYS	-	expression tag	UNP A0QYE8
D	485	GLU	-	expression tag	UNP A0QYE8
D	486	ASP	-	expression tag	UNP A0QYE8
D	487	LEU	-	expression tag	UNP A0QYE8
D	488	GLU	-	expression tag	UNP A0QYE8
D	489	HIS	-	expression tag	UNP A0QYE8
D	490	HIS	-	expression tag	UNP A0QYE8
D	491	HIS	-	expression tag	UNP A0QYE8
D	492	HIS	-	expression tag	UNP A0QYE8
D	493	HIS	-	expression tag	UNP A0QYE8
D	494	HIS	-	expression tag	UNP A0QYE8
D	495	HIS	-	expression tag	UNP A0QYE8
D	496	HIS	-	expression tag	UNP A0QYE8
E	2	VAL	-	insertion	UNP A0QYE8
E	480	THR	-	expression tag	UNP A0QYE8
E	481	ALA	-	expression tag	UNP A0QYE8
E	482	ALA	-	expression tag	UNP A0QYE8
E	483	ALA	-	expression tag	UNP A0QYE8
E	484	LYS	-	expression tag	UNP A0QYE8
E	485	GLU	-	expression tag	UNP A0QYE8
E	486	ASP	-	expression tag	UNP A0QYE8
E	487	LEU	-	expression tag	UNP A0QYE8
E	488	GLU	-	expression tag	UNP A0QYE8
E	489	HIS	-	expression tag	UNP A0QYE8
E	490	HIS	-	expression tag	UNP A0QYE8
E	491	HIS	-	expression tag	UNP A0QYE8
E	492	HIS	-	expression tag	UNP A0QYE8
E	493	HIS	-	expression tag	UNP A0QYE8
E	494	HIS	-	expression tag	UNP A0QYE8
E	495	HIS	-	expression tag	UNP A0QYE8
E	496	HIS	-	expression tag	UNP A0QYE8
F	2	VAL	-	insertion	UNP A0QYE8
F	480	THR	-	expression tag	UNP A0QYE8
F	481	ALA	-	expression tag	UNP A0QYE8
F	482	ALA	-	expression tag	UNP A0QYE8
F	483	ALA	-	expression tag	UNP A0QYE8
F	484	LYS	-	expression tag	UNP A0QYE8
F	485	GLU	-	expression tag	UNP A0QYE8

Continued on next page...

Continued from previous page...

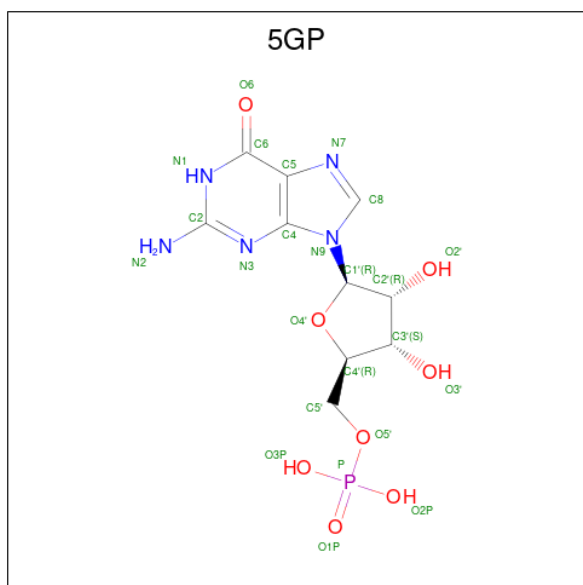
Chain	Residue	Modelled	Actual	Comment	Reference
F	486	ASP	-	expression tag	UNP A0QYE8
F	487	LEU	-	expression tag	UNP A0QYE8
F	488	GLU	-	expression tag	UNP A0QYE8
F	489	HIS	-	expression tag	UNP A0QYE8
F	490	HIS	-	expression tag	UNP A0QYE8
F	491	HIS	-	expression tag	UNP A0QYE8
F	492	HIS	-	expression tag	UNP A0QYE8
F	493	HIS	-	expression tag	UNP A0QYE8
F	494	HIS	-	expression tag	UNP A0QYE8
F	495	HIS	-	expression tag	UNP A0QYE8
F	496	HIS	-	expression tag	UNP A0QYE8
G	2	VAL	-	insertion	UNP A0QYE8
G	480	THR	-	expression tag	UNP A0QYE8
G	481	ALA	-	expression tag	UNP A0QYE8
G	482	ALA	-	expression tag	UNP A0QYE8
G	483	ALA	-	expression tag	UNP A0QYE8
G	484	LYS	-	expression tag	UNP A0QYE8
G	485	GLU	-	expression tag	UNP A0QYE8
G	486	ASP	-	expression tag	UNP A0QYE8
G	487	LEU	-	expression tag	UNP A0QYE8
G	488	GLU	-	expression tag	UNP A0QYE8
G	489	HIS	-	expression tag	UNP A0QYE8
G	490	HIS	-	expression tag	UNP A0QYE8
G	491	HIS	-	expression tag	UNP A0QYE8
G	492	HIS	-	expression tag	UNP A0QYE8
G	493	HIS	-	expression tag	UNP A0QYE8
G	494	HIS	-	expression tag	UNP A0QYE8
G	495	HIS	-	expression tag	UNP A0QYE8
G	496	HIS	-	expression tag	UNP A0QYE8
H	2	VAL	-	insertion	UNP A0QYE8
H	480	THR	-	expression tag	UNP A0QYE8
H	481	ALA	-	expression tag	UNP A0QYE8
H	482	ALA	-	expression tag	UNP A0QYE8
H	483	ALA	-	expression tag	UNP A0QYE8
H	484	LYS	-	expression tag	UNP A0QYE8
H	485	GLU	-	expression tag	UNP A0QYE8
H	486	ASP	-	expression tag	UNP A0QYE8
H	487	LEU	-	expression tag	UNP A0QYE8
H	488	GLU	-	expression tag	UNP A0QYE8
H	489	HIS	-	expression tag	UNP A0QYE8
H	490	HIS	-	expression tag	UNP A0QYE8
H	491	HIS	-	expression tag	UNP A0QYE8

Continued on next page...

Continued from previous page...

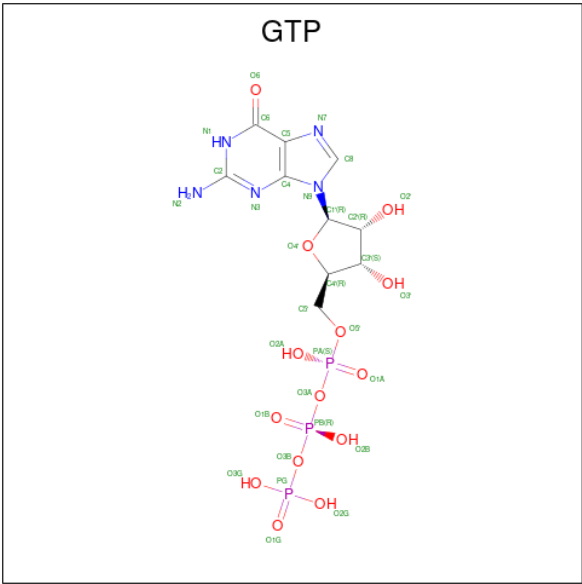
Chain	Residue	Modelled	Actual	Comment	Reference
H	492	HIS	-	expression tag	UNP A0QYE8
H	493	HIS	-	expression tag	UNP A0QYE8
H	494	HIS	-	expression tag	UNP A0QYE8
H	495	HIS	-	expression tag	UNP A0QYE8
H	496	HIS	-	expression tag	UNP A0QYE8

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	F	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	G	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	H	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

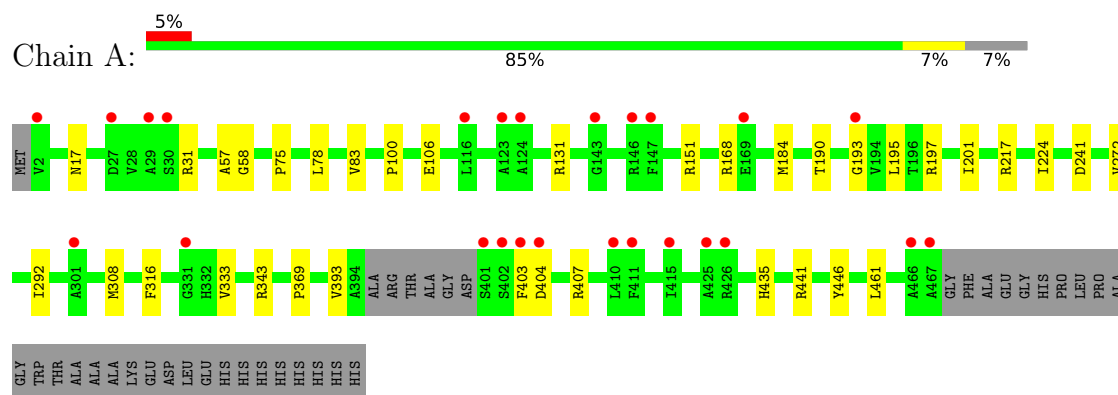


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	B	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	C	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	D	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	E	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	F	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	G	1	Total	C	N	O	P	0	1
			64	20	10	28	6		
3	H	1	Total	C	N	O	P	0	1
			64	20	10	28	6		

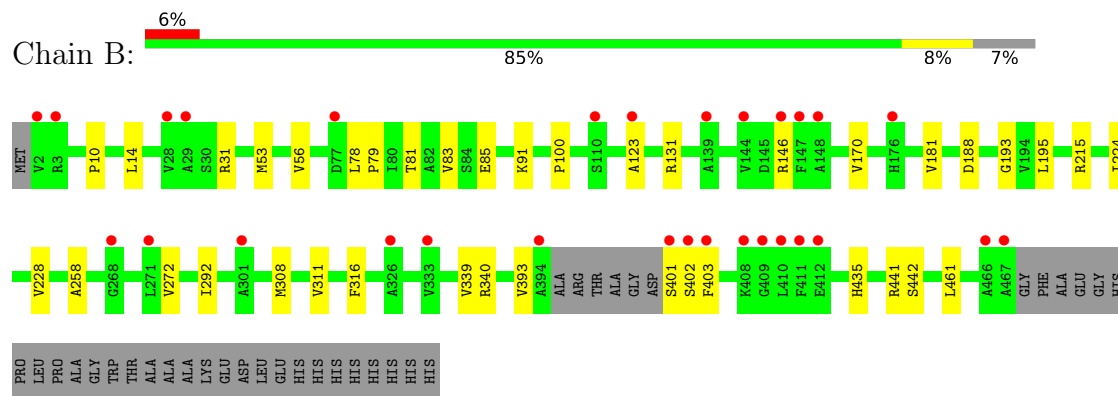
3 Residue-property plots [i](#)

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

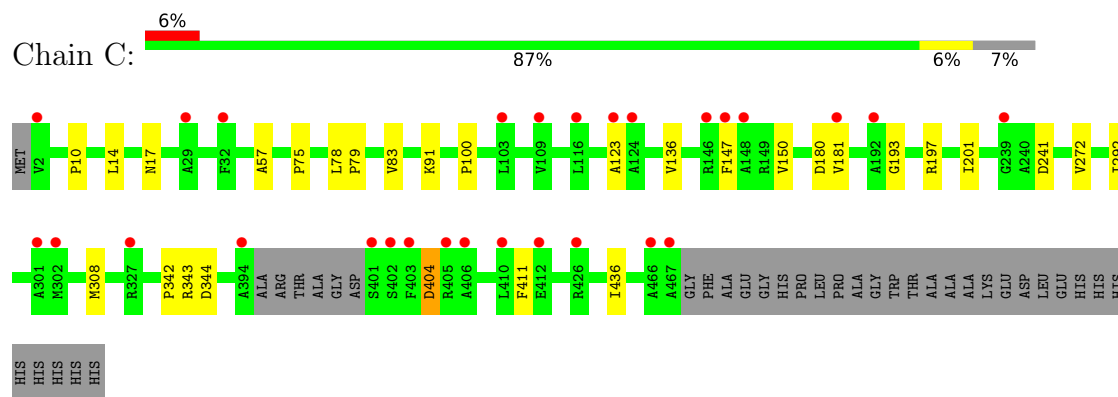
• Molecule 1: GMP reductase



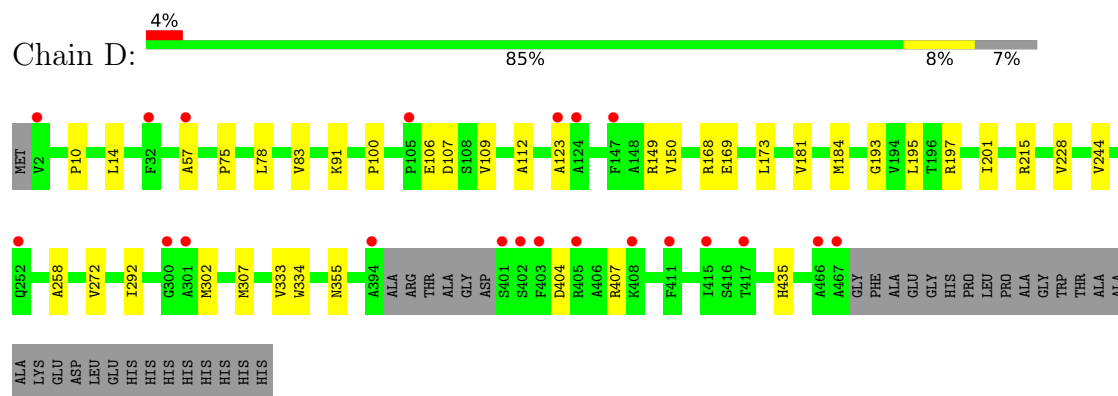
• Molecule 1: GMP reductase



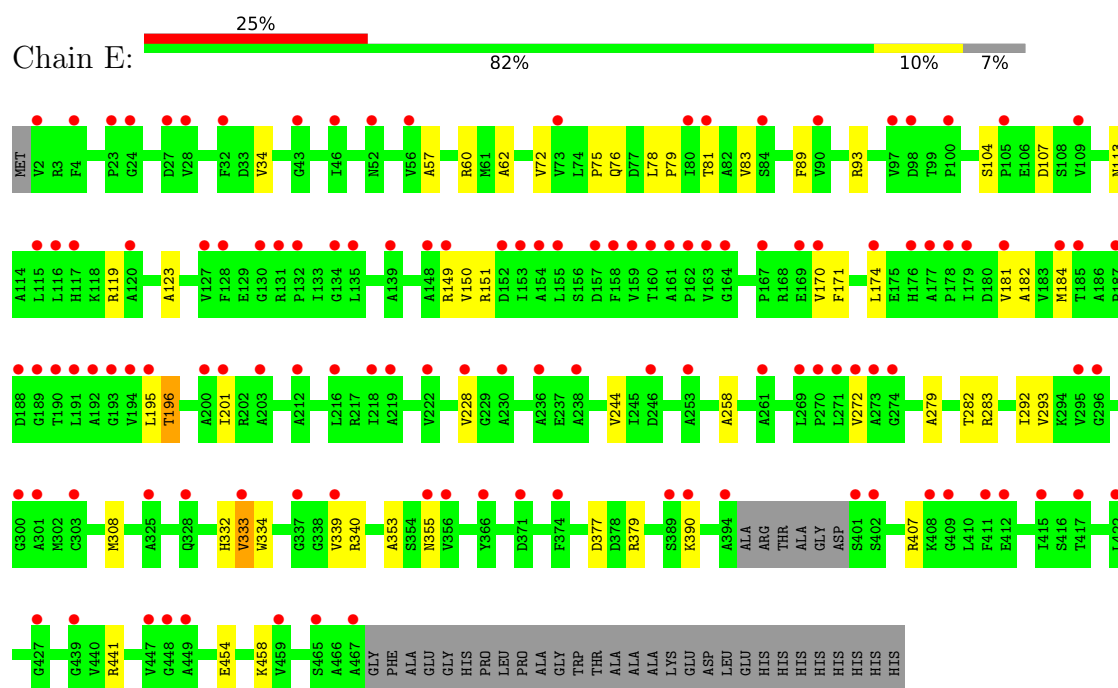
• Molecule 1: GMP reductase



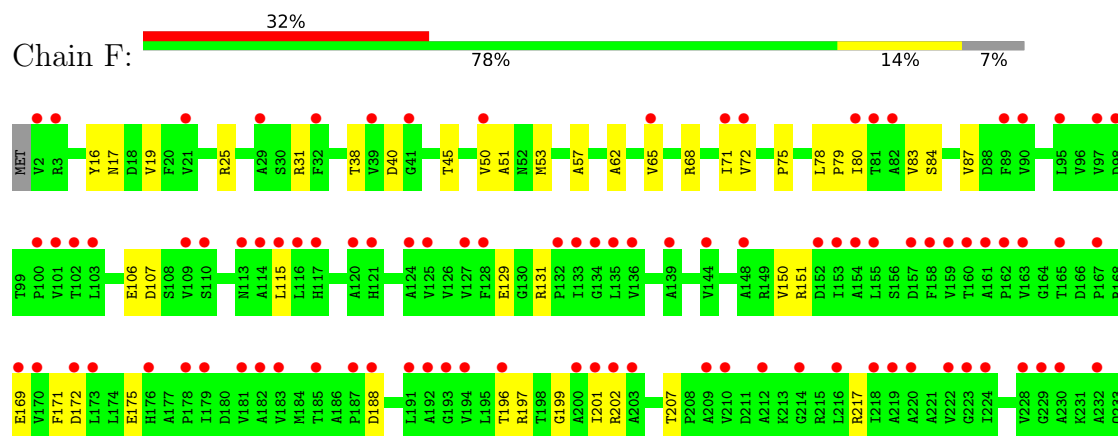
- Molecule 1: GMP reductase

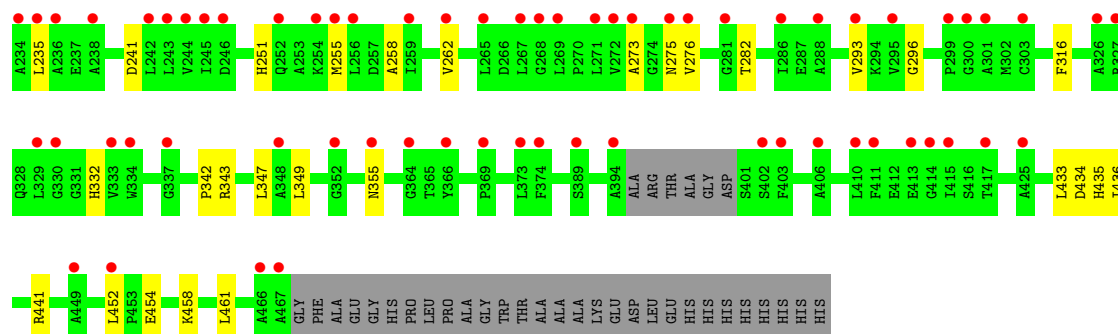


- Molecule 1: GMP reductase

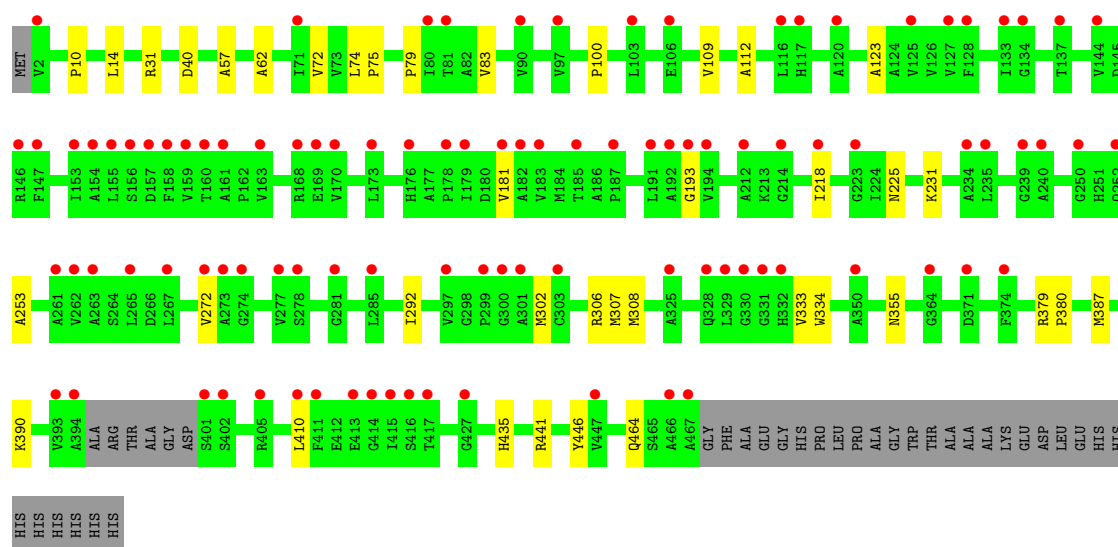
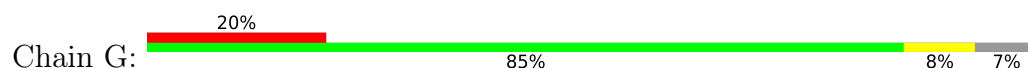


- Molecule 1: GMP reductase

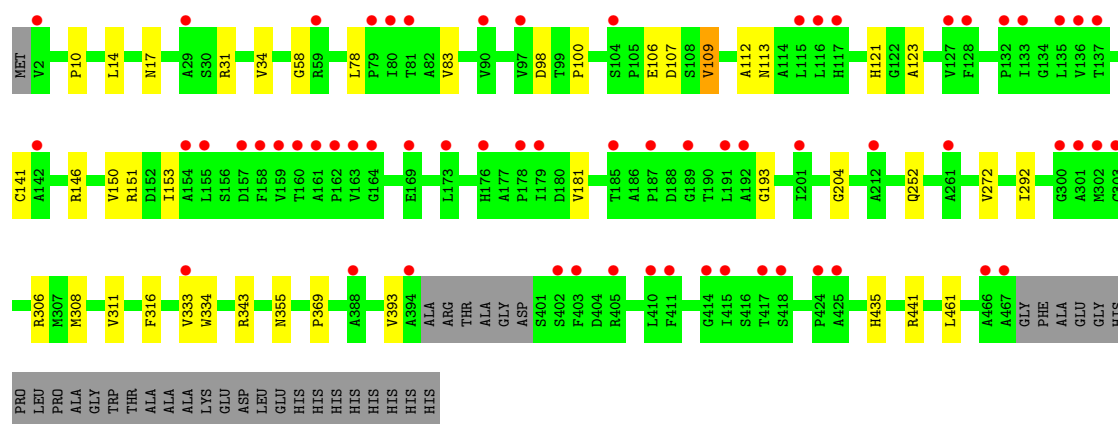
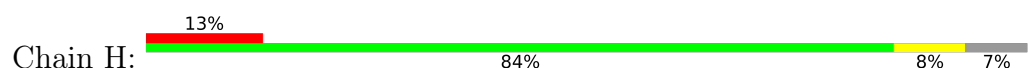




• Molecule 1: GMP reductase



• Molecule 1: GMP reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.08Å 145.93Å 146.32Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	112.48 – 2.30 112.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (112.48-2.30) 99.5 (112.48-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21_5204	Depositor
R, R_{free}	0.250 , 0.274 0.251 , 0.275	Depositor DCC
R_{free} test set	10407 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27456	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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 43.20 % 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 1.8267e-04. 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, 5GP

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	0.08	0/3397	0.22	0/4625
1	B	0.08	0/3397	0.23	0/4625
1	C	0.07	0/3397	0.21	0/4625
1	D	0.08	0/3397	0.22	0/4625
1	E	0.09	0/3397	0.23	0/4625
1	F	0.12	0/3397	0.26	0/4625
1	G	0.08	0/3397	0.22	0/4625
1	H	0.08	0/3397	0.22	0/4625
All	All	0.09	0/27176	0.23	0/37000

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	3344	0	3343	22	0
1	B	3344	0	3343	24	0
1	C	3344	0	3343	20	0
1	D	3344	0	3343	22	0
1	E	3344	0	3343	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3344	0	3343	47	0
1	G	3344	0	3343	25	0
1	H	3344	0	3343	22	0
2	A	24	0	12	0	0
2	B	24	0	12	0	0
2	C	24	0	12	0	0
2	D	24	0	12	0	0
2	E	24	0	12	0	0
2	F	24	0	12	0	0
2	G	24	0	12	0	0
2	H	24	0	12	0	0
3	A	64	0	24	0	0
3	B	64	0	24	0	0
3	C	64	0	24	0	0
3	D	64	0	24	0	0
3	E	64	0	24	0	0
3	F	64	0	24	2	0
3	G	64	0	24	0	0
3	H	64	0	24	0	0
All	All	27456	0	27032	193	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 4.

All (193) 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:F:342:PRO:HB3	1:F:436:ILE:HA	1.73	0.70
1:F:17:ASN:OD1	1:F:343:ARG:NH2	2.27	0.67
1:H:17:ASN:OD1	1:H:343:ARG:NH2	2.28	0.66
1:F:45:THR:HG21	1:F:207:THR:HB	1.78	0.65
1:A:404:ASP:HA	1:A:407:ARG:HD3	1.79	0.64
1:F:106:GLU:OE2	1:F:151:ARG:NH2	2.22	0.64
1:H:106:GLU:OE2	1:H:151:ARG:NH1	2.28	0.64
1:F:275:ASN:ND2	1:F:296:GLY:O	2.30	0.63
1:H:141:CYS:O	1:H:146:ARG:NH2	2.31	0.63
1:B:146:ARG:HA	1:B:146:ARG:HE	1.64	0.63
1:C:17:ASN:OD1	1:C:343:ARG:NH2	2.32	0.62
1:F:78:LEU:HD12	1:F:79:PRO:HD2	1.82	0.61
1:C:272:VAL:HG22	1:C:292:ILE:HB	1.82	0.61
1:F:196:THR:HG23	1:F:199:GLY:H	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:VAL:HG22	1:E:292:ILE:HB	1.83	0.61
1:F:282:THR:HG23	1:F:293:VAL:HG21	1.83	0.60
1:H:272:VAL:HG22	1:H:292:ILE:HB	1.83	0.60
1:B:123:ALA:HB3	1:B:181:VAL:HG21	1.84	0.60
1:C:78:LEU:HD12	1:C:79:PRO:HD2	1.85	0.59
1:B:31:ARG:NH1	1:B:442:SER:OG	2.35	0.59
1:C:342:PRO:HB3	1:C:436:ILE:HA	1.84	0.59
1:F:454:GLU:HB3	1:F:458:LYS:HE3	1.84	0.58
1:G:272:VAL:HG22	1:G:292:ILE:HB	1.86	0.57
1:E:78:LEU:HD12	1:E:79:PRO:HD2	1.86	0.57
1:E:244:VAL:HG22	1:E:272:VAL:HB	1.87	0.57
1:D:272:VAL:HG22	1:D:292:ILE:HB	1.87	0.56
1:B:131:ARG:NH1	1:B:188:ASP:O	2.38	0.56
1:F:217:ARG:HH11	1:F:241:ASP:HB3	1.71	0.55
1:H:100:PRO:HD3	1:H:193:GLY:HA2	1.88	0.55
1:C:123:ALA:HB3	1:C:181:VAL:HG21	1.89	0.55
1:B:272:VAL:HG22	1:B:292:ILE:HB	1.89	0.55
1:G:464:GLN:OE1	1:H:306:ARG:NH1	2.36	0.55
1:A:17:ASN:OD1	1:A:343:ARG:NH2	2.38	0.55
1:H:316:PHE:HZ	1:H:461:LEU:HD13	1.72	0.55
1:G:334:TRP:CD1	1:G:355:ASN:HB2	2.42	0.54
1:E:407:ARG:NH2	1:H:204:GLY:O	2.40	0.54
1:F:171:PHE:CE2	1:F:201:ILE:HD11	2.43	0.54
1:A:435:HIS:NE2	1:B:308:MET:SD	2.81	0.54
1:B:339:VAL:O	1:B:340:ARG:NH1	2.39	0.54
1:F:171:PHE:HE2	1:F:201:ILE:HD11	1.74	0.53
1:F:25:ARG:HH21	1:G:253:ALA:HB2	1.74	0.53
1:H:252:GLN:HE22	1:H:393:VAL:HG11	1.73	0.53
1:F:19:VAL:HG23	1:F:347:LEU:HD13	1.90	0.53
1:G:225:ASN:O	1:G:231:LYS:NZ	2.42	0.53
1:F:71:ILE:HD12	1:F:217:ARG:HB3	1.92	0.52
1:C:100:PRO:HD3	1:C:193:GLY:HA2	1.92	0.52
1:C:343:ARG:NH1	1:C:344:ASP:OD1	2.43	0.52
1:E:123:ALA:HB3	1:E:181:VAL:HG21	1.92	0.52
1:A:272:VAL:HG22	1:A:292:ILE:HB	1.91	0.52
1:F:342:PRO:HG2	1:G:308:MET:HA	1.91	0.51
1:E:170:VAL:HG21	1:E:184:MET:HE1	1.92	0.51
1:A:184:MET:HE3	1:A:195:LEU:HB3	1.93	0.51
1:F:251:HIS:HB2	1:F:276:VAL:HG12	1.91	0.51
1:B:31:ARG:NH2	1:C:411:PHE:O	2.44	0.51
1:F:258:ALA:O	1:F:262:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ARG:NH2	1:G:253:ALA:HB2	2.27	0.50
1:G:435:HIS:NE2	1:H:308:MET:SD	2.85	0.50
1:A:316:PHE:HZ	1:A:461:LEU:HD13	1.77	0.50
1:G:302:MET:HA	1:G:307:MET:HE3	1.93	0.50
1:D:106:GLU:O	1:D:149:ARG:HD3	2.12	0.50
1:F:31:ARG:HB3	1:F:441:ARG:HB3	1.93	0.49
1:D:302:MET:HA	1:D:307:MET:HE3	1.95	0.49
1:E:333:VAL:HG12	1:E:353:ALA:HA	1.94	0.49
1:F:435:HIS:NE2	1:G:308:MET:SD	2.85	0.49
1:D:100:PRO:HD3	1:D:193:GLY:HA2	1.95	0.49
1:E:282:THR:HG23	1:E:293:VAL:HG21	1.95	0.48
1:H:31:ARG:HB3	1:H:441:ARG:HB3	1.94	0.48
1:F:255:MET:HE1	1:F:273:ALA:HB1	1.94	0.48
1:A:106:GLU:OE2	1:A:151:ARG:NH2	2.46	0.48
1:B:316:PHE:HZ	1:B:461:LEU:HD13	1.78	0.48
1:C:147:PHE:HB3	3:F:502[B]:GTP:H4'	1.95	0.48
1:E:228:VAL:HG11	1:E:258:ALA:HB1	1.94	0.48
1:F:202:ARG:NH2	1:F:434:ASP:OD2	2.42	0.48
1:F:175:GLU:HA	1:F:197:ARG:NH1	2.28	0.48
1:H:123:ALA:HB3	1:H:181:VAL:HG21	1.96	0.48
1:A:308:MET:SD	1:D:435:HIS:NE2	2.86	0.48
1:D:107:ASP:O	1:D:150:VAL:HG13	2.13	0.48
1:F:83:VAL:O	1:F:87:VAL:HG23	2.14	0.47
1:E:454:GLU:HB3	1:E:458:LYS:HD2	1.96	0.47
1:A:100:PRO:HD3	1:A:193:GLY:HA2	1.97	0.47
1:E:308:MET:SD	1:H:435:HIS:NE2	2.88	0.47
1:E:334:TRP:CD1	1:E:355:ASN:HB2	2.50	0.47
1:F:78:LEU:HD23	1:F:83:VAL:HG22	1.97	0.47
1:G:100:PRO:HD3	1:G:193:GLY:HA2	1.97	0.46
1:F:80:ILE:O	1:F:84:SER:OG	2.28	0.46
1:B:91:LYS:HB3	1:B:215:ARG:HD2	1.98	0.46
1:B:100:PRO:HD3	1:B:193:GLY:HA2	1.98	0.46
1:E:292:ILE:HD12	1:E:332:HIS:HB2	1.98	0.46
1:F:129:GLU:O	1:F:131:ARG:NH1	2.44	0.46
1:E:171:PHE:CE1	1:E:201:ILE:HD11	2.50	0.46
1:D:404:ASP:HA	1:D:407:ARG:HD3	1.97	0.46
1:G:379:ARG:HE	1:G:380:PRO:HD2	1.80	0.46
1:E:89:PHE:O	1:E:93:ARG:HG2	2.16	0.46
1:A:403:PHE:HB2	1:D:168:ARG:CZ	2.46	0.46
1:C:404:ASP:N	1:C:404:ASP:OD1	2.46	0.46
1:B:78:LEU:HD23	1:B:83:VAL:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:HD23	1:C:83:VAL:HG22	1.98	0.45
1:D:78:LEU:HD23	1:D:83:VAL:HG22	1.98	0.45
1:E:34:VAL:O	1:E:441:ARG:NH1	2.47	0.45
1:F:40:ASP:HA	1:F:332:HIS:CD2	2.51	0.45
1:F:50:VAL:HB	1:F:72:VAL:HA	1.98	0.45
1:G:40:ASP:OD2	1:G:355:ASN:ND2	2.49	0.45
1:A:224:ILE:HD11	1:A:393:VAL:HG22	1.98	0.45
1:D:109:VAL:HA	1:D:112:ALA:HB3	1.97	0.45
1:H:98:ASP:OD2	1:H:121:HIS:HE1	1.99	0.45
1:A:78:LEU:HD23	1:A:83:VAL:HG22	1.99	0.45
1:F:68:ARG:HH21	1:F:202:ARG:HB2	1.82	0.45
1:G:74:LEU:HD21	1:G:218:ILE:HD11	1.99	0.45
1:H:58:GLY:HA3	1:H:369:PRO:HG3	1.98	0.45
1:B:31:ARG:HB3	1:B:441:ARG:HB3	1.98	0.45
1:F:434:ASP:OD2	1:G:410:LEU:HD11	2.17	0.45
1:G:109:VAL:HA	1:G:112:ALA:HB3	1.98	0.45
1:H:34:VAL:O	1:H:441:ARG:NH1	2.50	0.44
1:F:38:THR:HG21	1:F:355:ASN:HD21	1.83	0.44
1:F:171:PHE:C	1:F:171:PHE:CD1	2.96	0.44
1:G:123:ALA:HB3	1:G:181:VAL:HG21	1.99	0.44
1:E:279:ALA:O	1:E:283:ARG:HG2	2.17	0.44
1:A:197:ARG:O	1:A:201:ILE:HG12	2.18	0.44
1:A:403:PHE:CE1	1:D:201:ILE:HD13	2.52	0.44
1:D:91:LYS:HB3	1:D:215:ARG:HD2	1.99	0.44
1:D:184:MET:HE3	1:D:195:LEU:HB3	2.00	0.44
1:G:446:TYR:CG	1:H:311:VAL:HG11	2.53	0.44
1:F:349:LEU:HD13	1:F:452:LEU:HD22	1.99	0.44
1:G:31:ARG:HB3	1:G:441:ARG:HB3	2.00	0.44
1:C:91:LYS:NZ	1:C:241:ASP:OD2	2.41	0.43
1:F:51:ALA:HB3	1:F:53:MET:HE2	1.99	0.43
1:A:58:GLY:HA3	1:A:369:PRO:HG3	1.99	0.43
1:F:107:ASP:O	1:F:150:VAL:HG23	2.18	0.43
1:D:10:PRO:HG3	1:D:14:LEU:HD21	1.99	0.43
1:E:57:ALA:HB3	1:E:75:PRO:HD3	2.00	0.43
1:B:53:MET:HB2	1:B:56:VAL:HG12	1.99	0.43
1:C:10:PRO:HG3	1:C:14:LEU:HD21	2.01	0.43
1:C:147:PHE:HB3	3:F:502[A]:GTP:H4'	1.99	0.43
1:F:65:VAL:HG23	1:F:433:LEU:HD11	2.00	0.43
1:H:10:PRO:HG3	1:H:14:LEU:HD21	2.00	0.43
1:E:104:SER:N	1:E:107:ASP:OD2	2.46	0.43
1:B:401:SER:OG	1:B:402:SER:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:HIS:NE2	1:C:308:MET:SD	2.92	0.43
1:F:169:GLU:HA	1:F:172:ASP:OD2	2.18	0.43
1:F:62:ALA:HA	1:F:72:VAL:HG21	2.01	0.43
1:B:10:PRO:HG3	1:B:14:LEU:HD21	2.01	0.43
1:A:217:ARG:HA	1:A:241:ASP:OD2	2.19	0.42
1:A:403:PHE:CD2	1:A:407:ARG:HD2	2.53	0.42
1:C:197:ARG:O	1:C:201:ILE:HG12	2.19	0.42
1:D:123:ALA:HB3	1:D:181:VAL:HG21	2.02	0.42
1:E:78:LEU:HD23	1:E:83:VAL:HG22	1.99	0.42
1:E:334:TRP:NE1	1:E:355:ASN:HB2	2.34	0.42
1:D:168:ARG:HA	1:D:168:ARG:HD2	1.92	0.42
1:H:78:LEU:HD23	1:H:83:VAL:HG22	2.01	0.42
1:E:377:ASP:HB2	1:E:379:ARG:HG3	2.00	0.42
1:F:171:PHE:C	1:F:171:PHE:HD1	2.27	0.42
1:G:10:PRO:HG3	1:G:14:LEU:HD21	2.02	0.42
1:G:387:MET:HB3	1:G:390:LYS:HB2	2.02	0.42
1:H:334:TRP:CD1	1:H:355:ASN:HB2	2.54	0.42
1:B:224:ILE:HD11	1:B:393:VAL:HG22	2.01	0.42
1:D:334:TRP:CD1	1:D:355:ASN:HB2	2.55	0.42
1:E:60:ARG:HG2	1:E:119:ARG:HH11	1.84	0.42
1:E:62:ALA:HA	1:E:72:VAL:HG21	2.02	0.42
1:E:149:ARG:HB2	1:E:151:ARG:HG2	2.01	0.42
1:H:109:VAL:HA	1:H:112:ALA:HB3	2.01	0.42
1:D:57:ALA:HB3	1:D:75:PRO:HD3	2.02	0.42
1:E:174:LEU:HD11	1:E:182:ALA:HB2	2.02	0.42
1:G:62:ALA:HA	1:G:72:VAL:HG21	2.01	0.42
1:C:147:PHE:CZ	1:F:115:LEU:HG	2.55	0.41
1:E:339:VAL:O	1:E:340:ARG:NH1	2.49	0.41
1:D:244:VAL:HG22	1:D:272:VAL:HB	2.02	0.41
1:B:81:THR:O	1:B:85:GLU:HG3	2.21	0.41
1:D:169:GLU:O	1:D:173:LEU:HG	2.19	0.41
1:B:228:VAL:HG11	1:B:258:ALA:HB1	2.02	0.41
1:E:76:GLN:NE2	1:E:390:LYS:O	2.51	0.41
1:C:136:VAL:HG21	1:C:150:VAL:HG13	2.03	0.41
1:E:60:ARG:HG2	1:E:119:ARG:NH1	2.36	0.41
1:C:57:ALA:HB3	1:C:75:PRO:HD3	2.01	0.41
1:A:131:ARG:HG2	1:A:190:THR:HA	2.03	0.41
1:E:107:ASP:O	1:E:150:VAL:HG23	2.20	0.41
1:A:31:ARG:HB3	1:A:441:ARG:HB3	2.02	0.41
1:B:170:VAL:HG11	1:B:195:LEU:HD23	2.03	0.41
1:F:188:ASP:OD1	1:F:188:ASP:N	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:VAL:HG11	1:D:258:ALA:HB1	2.03	0.41
1:F:57:ALA:HB3	1:F:75:PRO:HD3	2.02	0.41
1:A:57:ALA:HB3	1:A:75:PRO:HD3	2.02	0.40
1:A:168:ARG:CZ	1:B:403:PHE:HB2	2.51	0.40
1:A:446:TYR:CG	1:B:311:VAL:HG11	2.56	0.40
1:C:180:ASP:OD2	1:C:197:ARG:HD3	2.21	0.40
1:B:78:LEU:HD12	1:B:79:PRO:HD2	2.04	0.40
1:D:197:ARG:O	1:D:201:ILE:HG12	2.21	0.40
1:E:195:LEU:HD13	1:E:196:THR:O	2.21	0.40
1:F:16:TYR:HB3	1:F:343:ARG:HH12	1.87	0.40
1:F:343:ARG:HD3	1:G:306:ARG:O	2.22	0.40
1:G:57:ALA:HB3	1:G:75:PRO:HD3	2.03	0.40
1:H:107:ASP:O	1:H:150:VAL:HG23	2.21	0.40
1:F:316:PHE:HZ	1:F:461:LEU:HD13	1.85	0.40
1:G:79:PRO:O	1:G:83:VAL:HG23	2.22	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	456/496 (92%)	442 (97%)	14 (3%)	0	100	100
1	B	456/496 (92%)	443 (97%)	13 (3%)	0	100	100
1	C	456/496 (92%)	442 (97%)	14 (3%)	0	100	100
1	D	456/496 (92%)	442 (97%)	14 (3%)	0	100	100
1	E	456/496 (92%)	439 (96%)	17 (4%)	0	100	100
1	F	456/496 (92%)	440 (96%)	16 (4%)	0	100	100
1	G	456/496 (92%)	439 (96%)	17 (4%)	0	100	100
1	H	456/496 (92%)	439 (96%)	17 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3648/3968 (92%)	3526 (97%)	122 (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	345/372 (93%)	344 (100%)	1 (0%)	91	96
1	B	345/372 (93%)	345 (100%)	0	100	100
1	C	345/372 (93%)	344 (100%)	1 (0%)	91	96
1	D	345/372 (93%)	344 (100%)	1 (0%)	91	96
1	E	345/372 (93%)	341 (99%)	4 (1%)	67	81
1	F	345/372 (93%)	344 (100%)	1 (0%)	91	96
1	G	345/372 (93%)	344 (100%)	1 (0%)	91	96
1	H	345/372 (93%)	341 (99%)	4 (1%)	67	81
All	All	2760/2976 (93%)	2747 (100%)	13 (0%)	86	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	C	404	ASP
1	D	333	VAL
1	E	81	THR
1	E	113	ASN
1	E	196	THR
1	E	333	VAL
1	F	235	LEU
1	G	333	VAL
1	H	109	VAL
1	H	113	ASN
1	H	153	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	A	341	HIS
1	B	113	ASN
1	B	117	HIS
1	B	341	HIS
1	C	176	HIS
1	C	341	HIS
1	D	117	HIS
1	D	332	HIS
1	D	464	GLN
1	E	328	GLN
1	E	341	HIS
1	F	252	GLN
1	F	341	HIS
1	G	332	HIS
1	H	121	HIS
1	H	252	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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	$\# Z > 2$
3	GTP	G	502[A]	-	26,34,34	0.66	0	32,54,54	0.60	0
3	GTP	F	502[A]	-	26,34,34	0.65	0	32,54,54	0.61	0
3	GTP	E	502[B]	-	26,34,34	0.65	0	32,54,54	0.60	0
3	GTP	H	502[A]	-	26,34,34	0.66	0	32,54,54	0.59	0
3	GTP	C	502[B]	-	26,34,34	0.67	0	32,54,54	0.58	0
2	5GP	F	501	-	22,26,26	0.54	0	26,40,40	0.72	0
3	GTP	D	502[A]	-	26,34,34	0.66	0	32,54,54	0.59	0
3	GTP	A	502[A]	-	26,34,34	0.66	0	32,54,54	0.59	0
2	5GP	H	501	-	22,26,26	0.53	0	26,40,40	0.73	0
2	5GP	E	501	-	22,26,26	0.55	0	26,40,40	0.72	0
3	GTP	F	502[B]	-	26,34,34	0.65	0	32,54,54	0.59	0
2	5GP	G	501	-	22,26,26	0.53	0	26,40,40	0.71	0
3	GTP	G	502[B]	-	26,34,34	0.66	0	32,54,54	0.59	0
2	5GP	D	501	-	22,26,26	0.53	0	26,40,40	0.71	0
3	GTP	H	502[B]	-	26,34,34	0.66	0	32,54,54	0.60	0
3	GTP	D	502[B]	-	26,34,34	0.66	0	32,54,54	0.59	0
2	5GP	C	501	-	22,26,26	0.54	0	26,40,40	0.72	0
3	GTP	B	502[A]	-	26,34,34	0.66	0	32,54,54	0.59	0
3	GTP	A	502[B]	-	26,34,34	0.66	0	32,54,54	0.59	0
2	5GP	B	501	-	22,26,26	0.53	0	26,40,40	0.72	0
3	GTP	B	502[B]	-	26,34,34	0.67	0	32,54,54	0.59	0
3	GTP	C	502[A]	-	26,34,34	0.66	0	32,54,54	0.59	0
3	GTP	E	502[A]	-	26,34,34	0.66	0	32,54,54	0.59	0
2	5GP	A	501	-	22,26,26	0.53	0	26,40,40	0.71	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
3	GTP	G	502[A]	-	-	4/18/38/38	0/3/3/3
3	GTP	F	502[A]	-	-	4/18/38/38	0/3/3/3
3	GTP	E	502[B]	-	-	2/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	H	502[A]	-	-	2/18/38/38	0/3/3/3
3	GTP	C	502[B]	-	-	5/18/38/38	0/3/3/3
2	5GP	F	501	-	-	0/6/26/26	0/3/3/3
3	GTP	D	502[A]	-	-	3/18/38/38	0/3/3/3
3	GTP	A	502[A]	-	-	4/18/38/38	0/3/3/3
2	5GP	H	501	-	-	0/6/26/26	0/3/3/3
2	5GP	E	501	-	-	0/6/26/26	0/3/3/3
3	GTP	F	502[B]	-	-	3/18/38/38	0/3/3/3
2	5GP	G	501	-	-	0/6/26/26	0/3/3/3
3	GTP	G	502[B]	-	-	1/18/38/38	0/3/3/3
2	5GP	D	501	-	-	0/6/26/26	0/3/3/3
3	GTP	H	502[B]	-	-	1/18/38/38	0/3/3/3
3	GTP	D	502[B]	-	-	1/18/38/38	0/3/3/3
2	5GP	C	501	-	-	0/6/26/26	0/3/3/3
3	GTP	B	502[A]	-	-	2/18/38/38	0/3/3/3
3	GTP	A	502[B]	-	-	2/18/38/38	0/3/3/3
2	5GP	B	501	-	-	0/6/26/26	0/3/3/3
3	GTP	B	502[B]	-	-	3/18/38/38	0/3/3/3
3	GTP	C	502[A]	-	-	7/18/38/38	0/3/3/3
3	GTP	E	502[A]	-	-	2/18/38/38	0/3/3/3
2	5GP	A	501	-	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[B]	GTP	C5'-O5'-PA-O3A
3	B	502[B]	GTP	PB-O3B-PG-O3G
3	C	502[A]	GTP	C5'-O5'-PA-O3A
3	C	502[A]	GTP	C5'-O5'-PA-O1A
3	C	502[A]	GTP	O4'-C4'-C5'-O5'
3	C	502[A]	GTP	C3'-C4'-C5'-O5'
3	C	502[B]	GTP	O4'-C4'-C5'-O5'
3	F	502[B]	GTP	PB-O3B-PG-O3G
3	C	502[B]	GTP	C3'-C4'-C5'-O5'
3	F	502[A]	GTP	O4'-C4'-C5'-O5'
3	F	502[A]	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

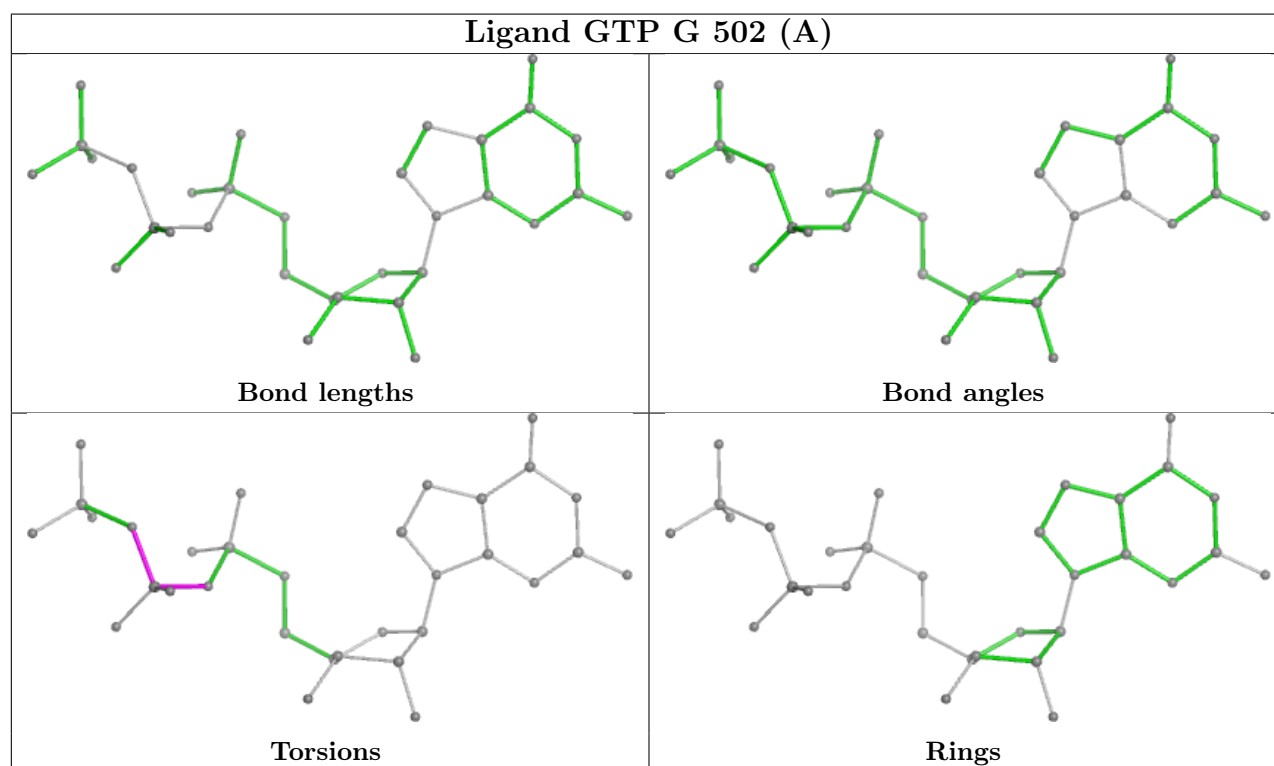
Mol	Chain	Res	Type	Atoms
3	E	502[B]	GTP	PB-O3B-PG-O1G
3	B	502[A]	GTP	PG-O3B-PB-O1B
3	D	502[A]	GTP	PA-O3A-PB-O1B
3	E	502[A]	GTP	PG-O3B-PB-O1B
3	F	502[A]	GTP	PG-O3B-PB-O1B
3	G	502[A]	GTP	PG-O3B-PB-O1B
3	H	502[A]	GTP	PG-O3B-PB-O1B
3	C	502[A]	GTP	PG-O3B-PB-O2B
3	C	502[B]	GTP	PB-O3A-PA-O2A
3	D	502[A]	GTP	PG-O3B-PB-O2B
3	A	502[B]	GTP	C5'-O5'-PA-O1A
3	C	502[A]	GTP	C5'-O5'-PA-O2A
3	B	502[A]	GTP	PG-O3B-PB-O2B
3	B	502[B]	GTP	PB-O3A-PA-O2A
3	C	502[A]	GTP	PG-O3B-PB-O1B
3	D	502[A]	GTP	PG-O3B-PB-O1B
3	E	502[B]	GTP	PB-O3A-PA-O2A
3	F	502[A]	GTP	PG-O3B-PB-O2B
3	G	502[A]	GTP	PG-O3B-PB-O2B
3	H	502[A]	GTP	PG-O3B-PB-O2B
3	B	502[B]	GTP	PB-O3B-PG-O1G
3	F	502[B]	GTP	PB-O3B-PG-O1G
3	H	502[B]	GTP	PB-O3B-PG-O1G
3	A	502[A]	GTP	PB-O3A-PA-O1A
3	E	502[A]	GTP	PG-O3B-PB-O2B
3	A	502[A]	GTP	PB-O3B-PG-O1G
3	C	502[B]	GTP	PB-O3B-PG-O1G
3	A	502[A]	GTP	PB-O3B-PG-O2G
3	A	502[A]	GTP	PB-O3A-PA-O2A
3	C	502[B]	GTP	PB-O3A-PA-O1A
3	D	502[B]	GTP	PB-O3A-PA-O2A
3	F	502[B]	GTP	PB-O3A-PA-O2A
3	G	502[A]	GTP	PA-O3A-PB-O1B
3	G	502[B]	GTP	PB-O3A-PA-O2A
3	G	502[A]	GTP	PA-O3A-PB-O3B

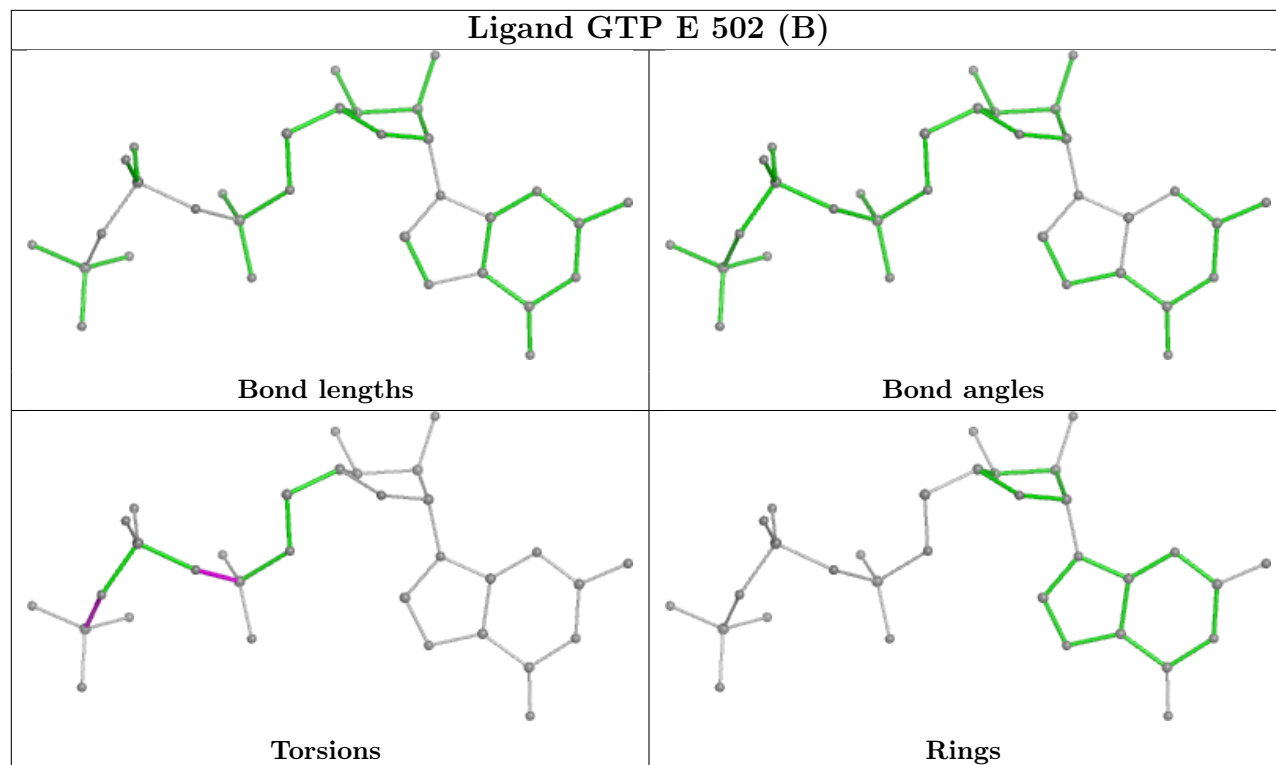
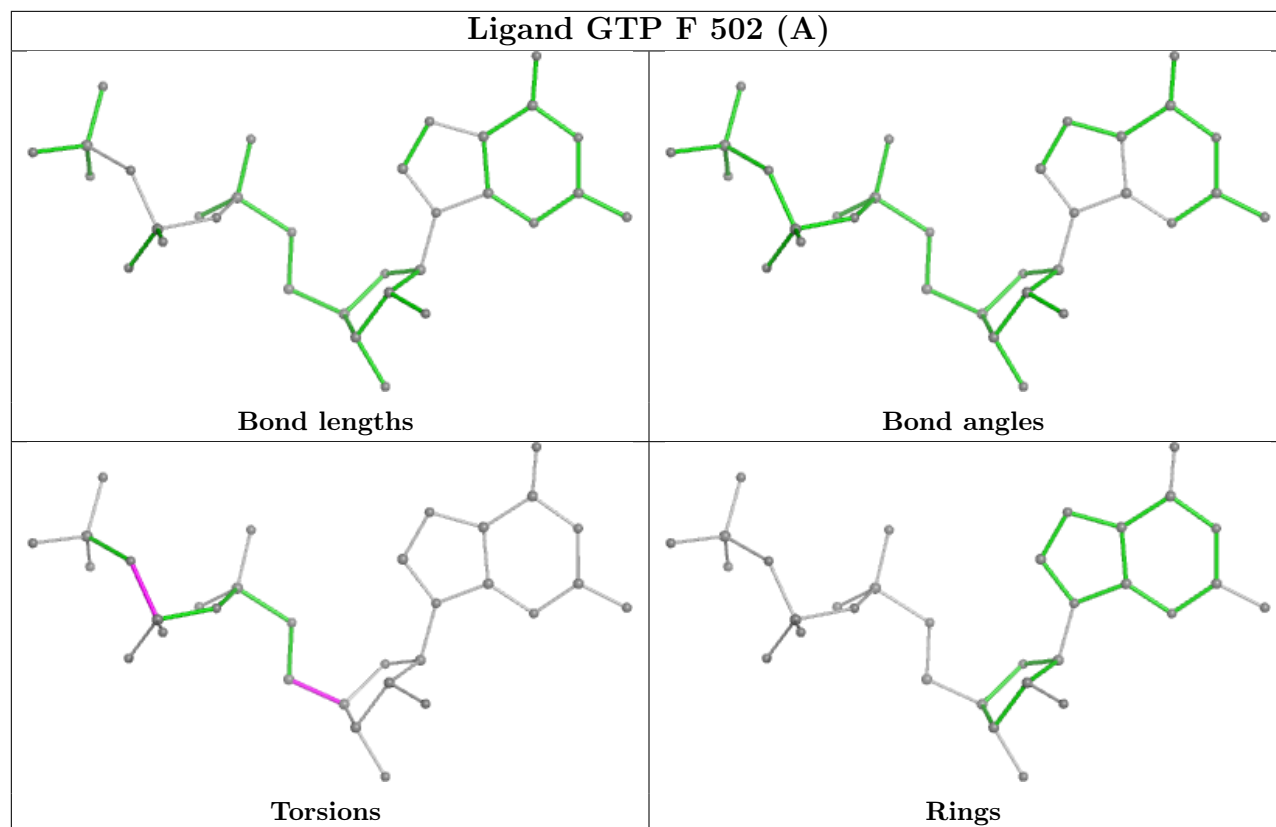
There are no ring outliers.

2 monomers are involved in 2 short contacts:

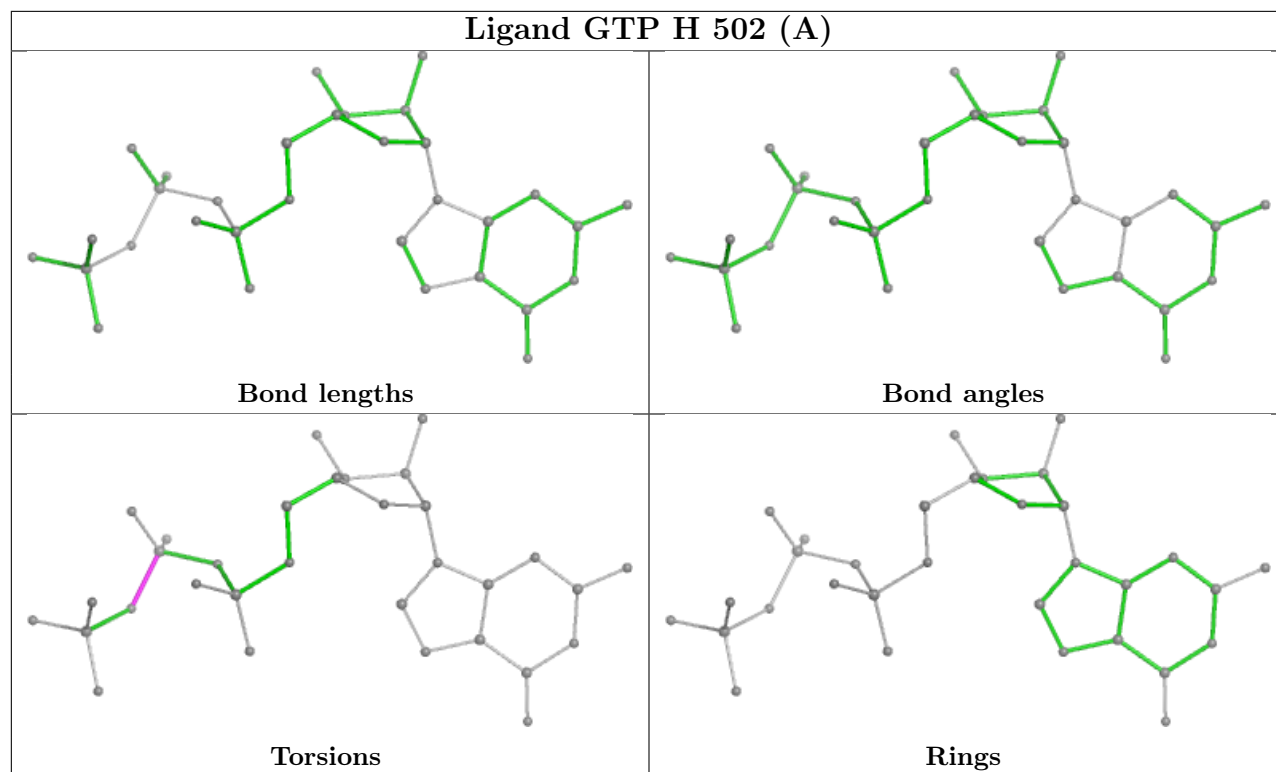
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502[A]	GTP	1	0
3	F	502[B]	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

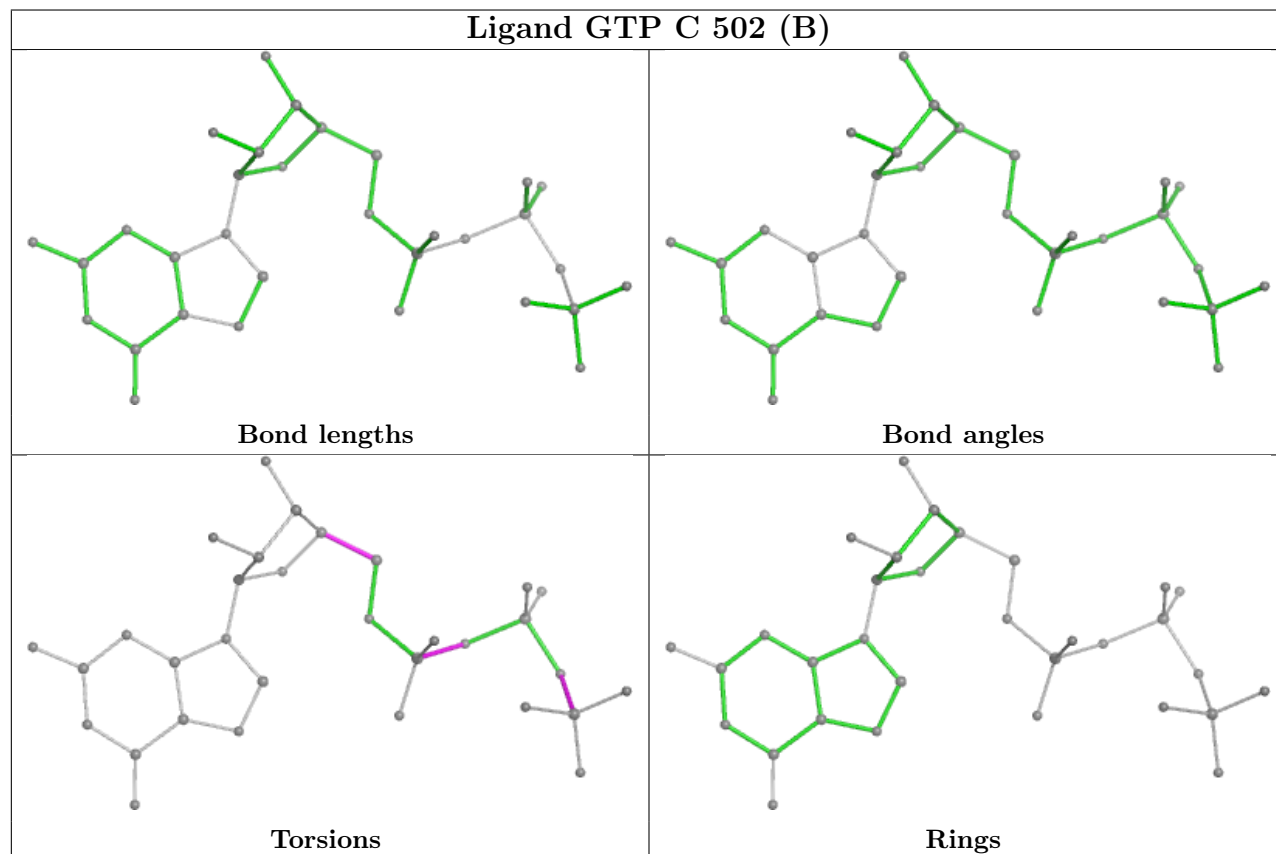




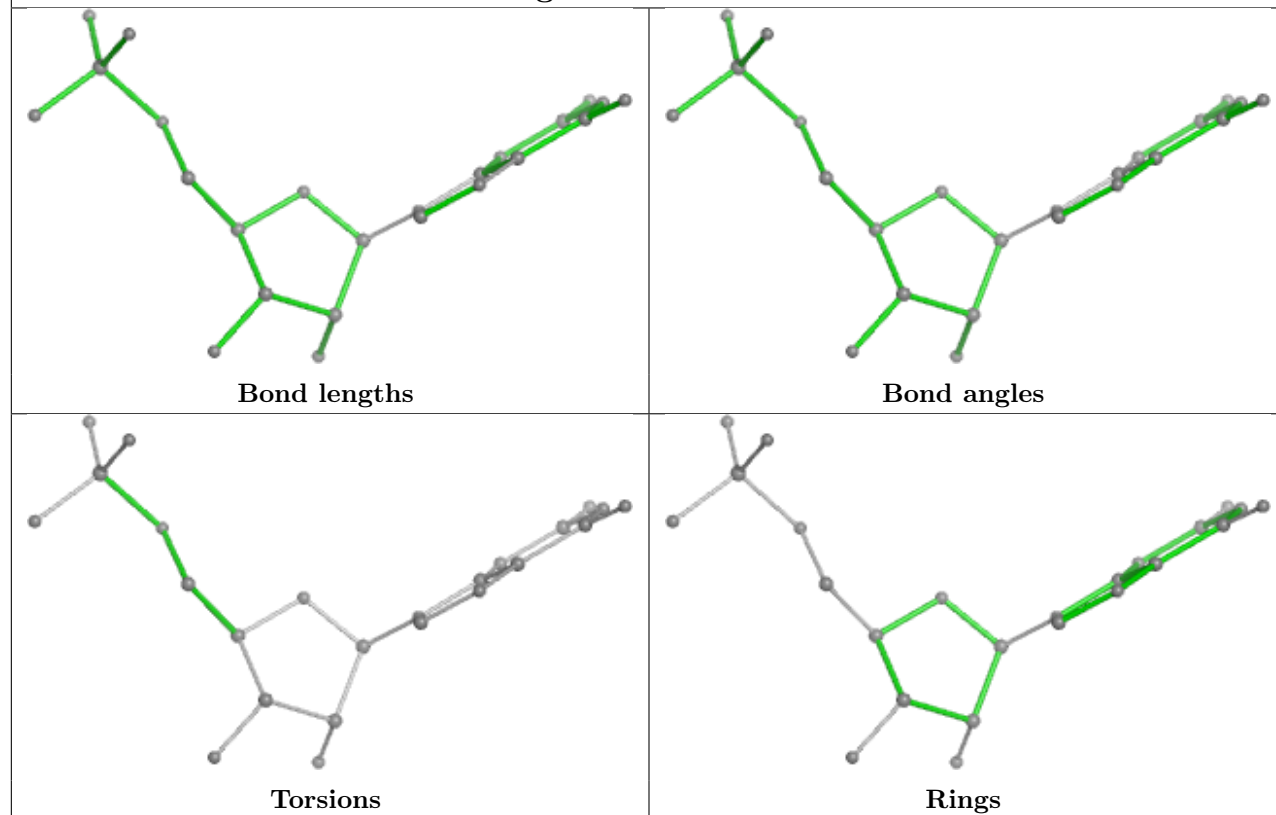
Ligand GTP H 502 (A)



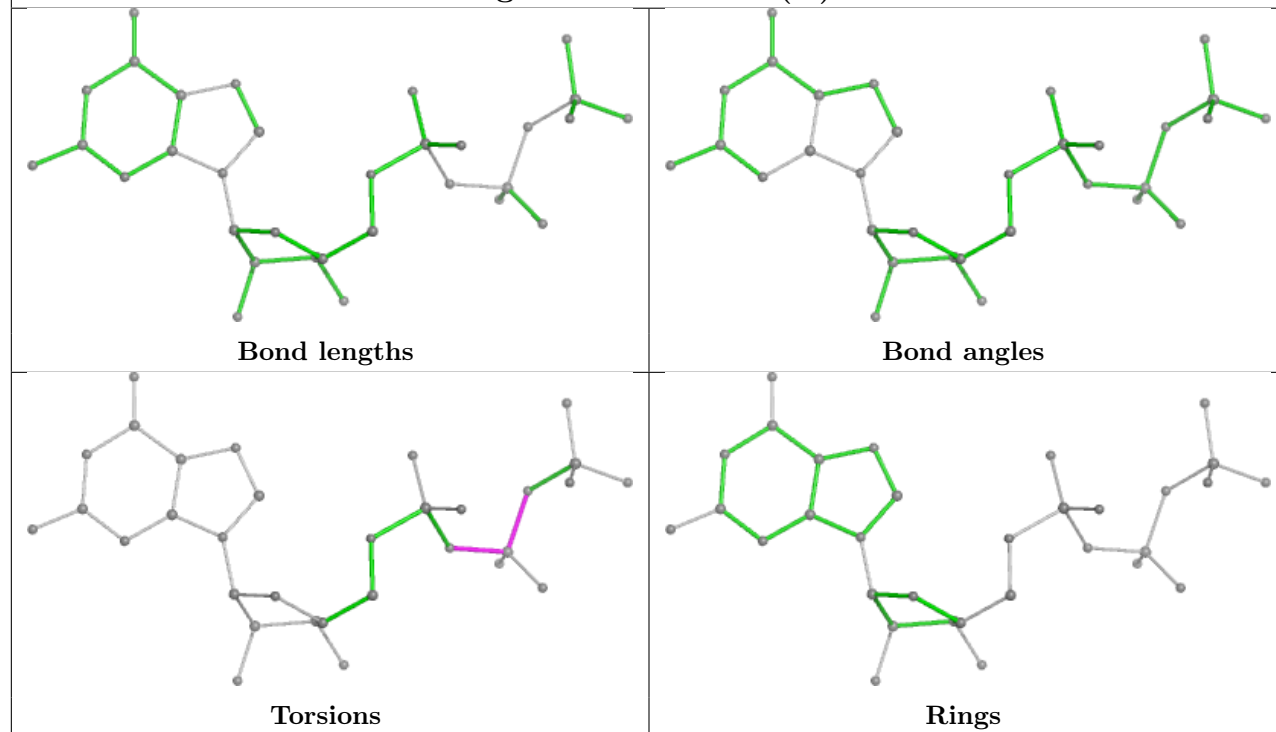
Ligand GTP C 502 (B)



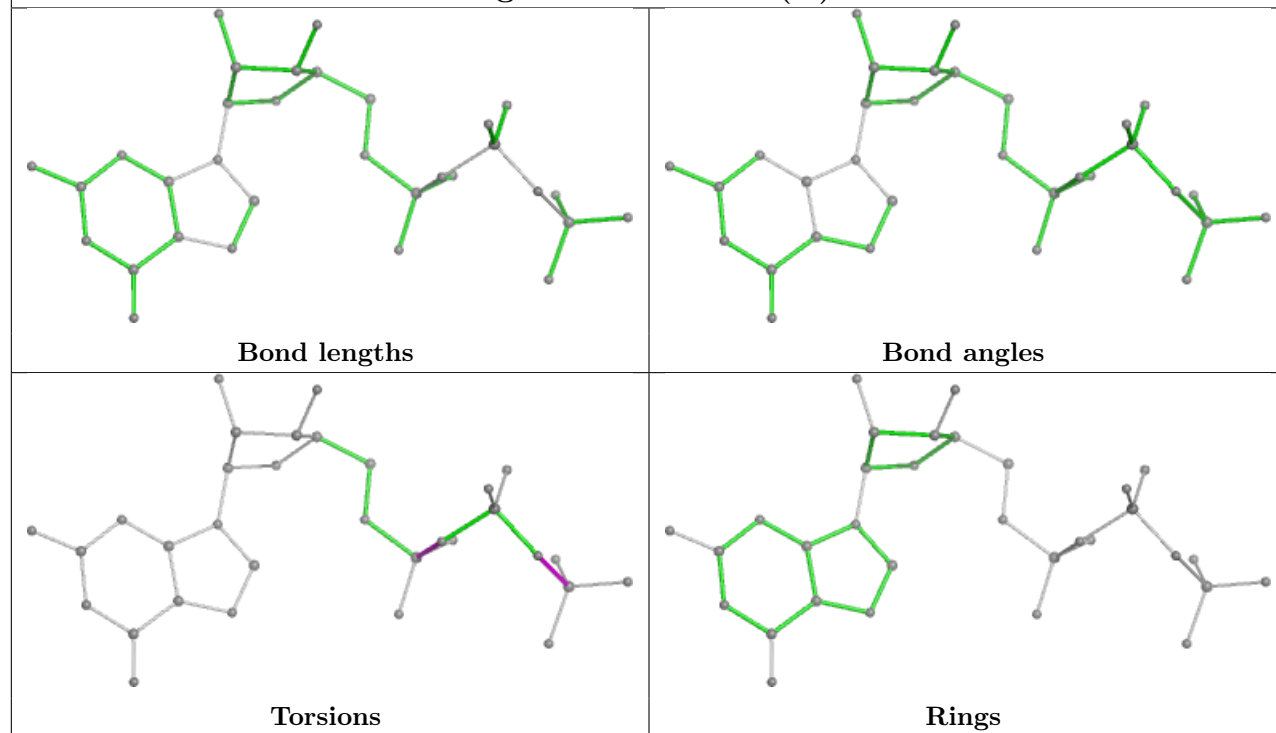
Ligand 5GP F 501



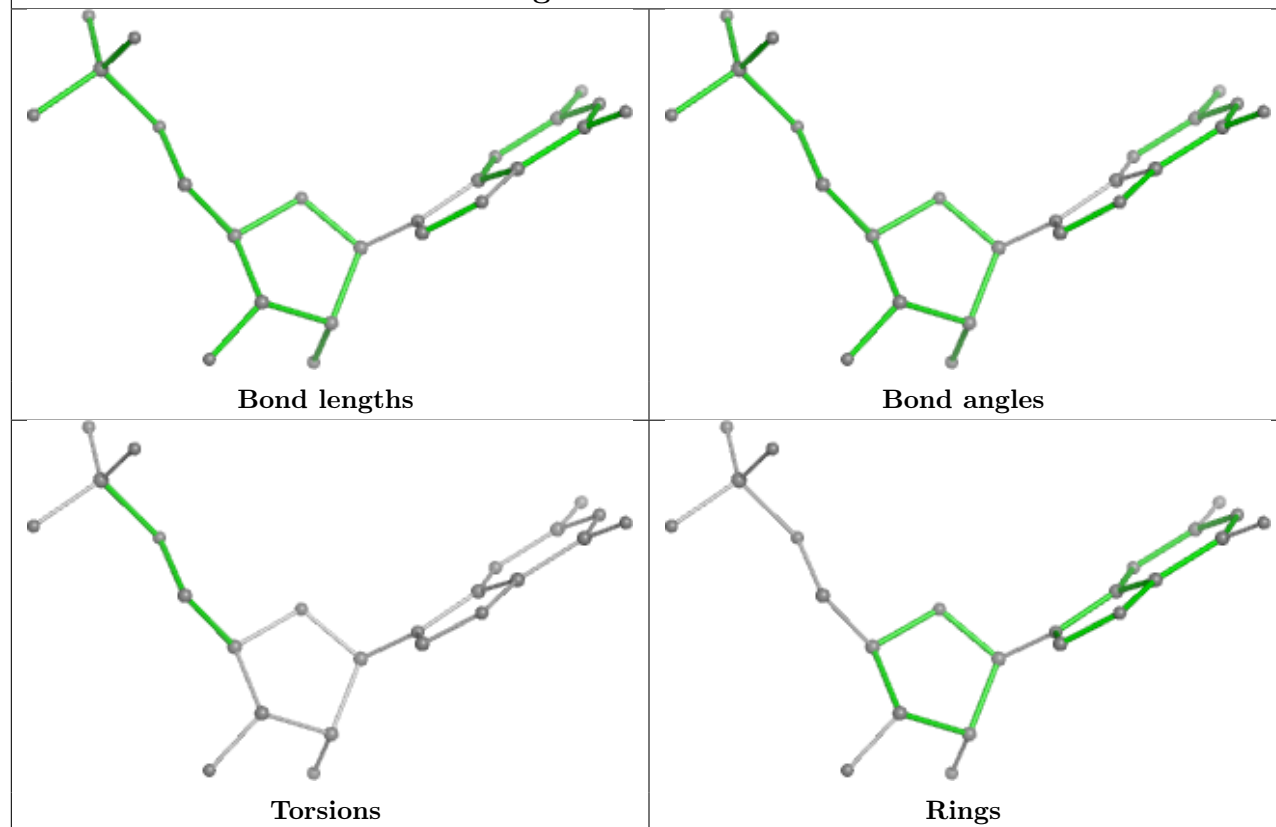
Ligand GTP D 502 (A)



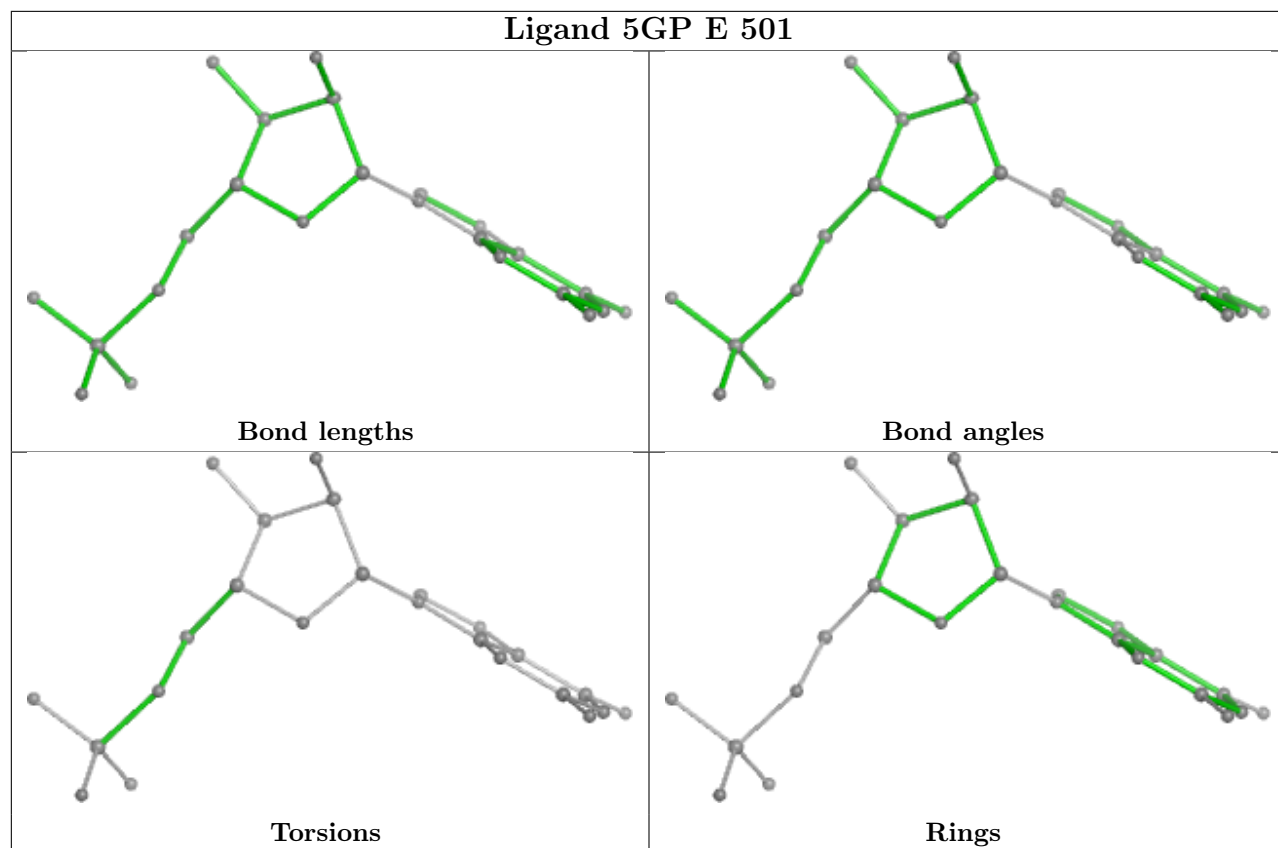
Ligand GTP A 502 (A)



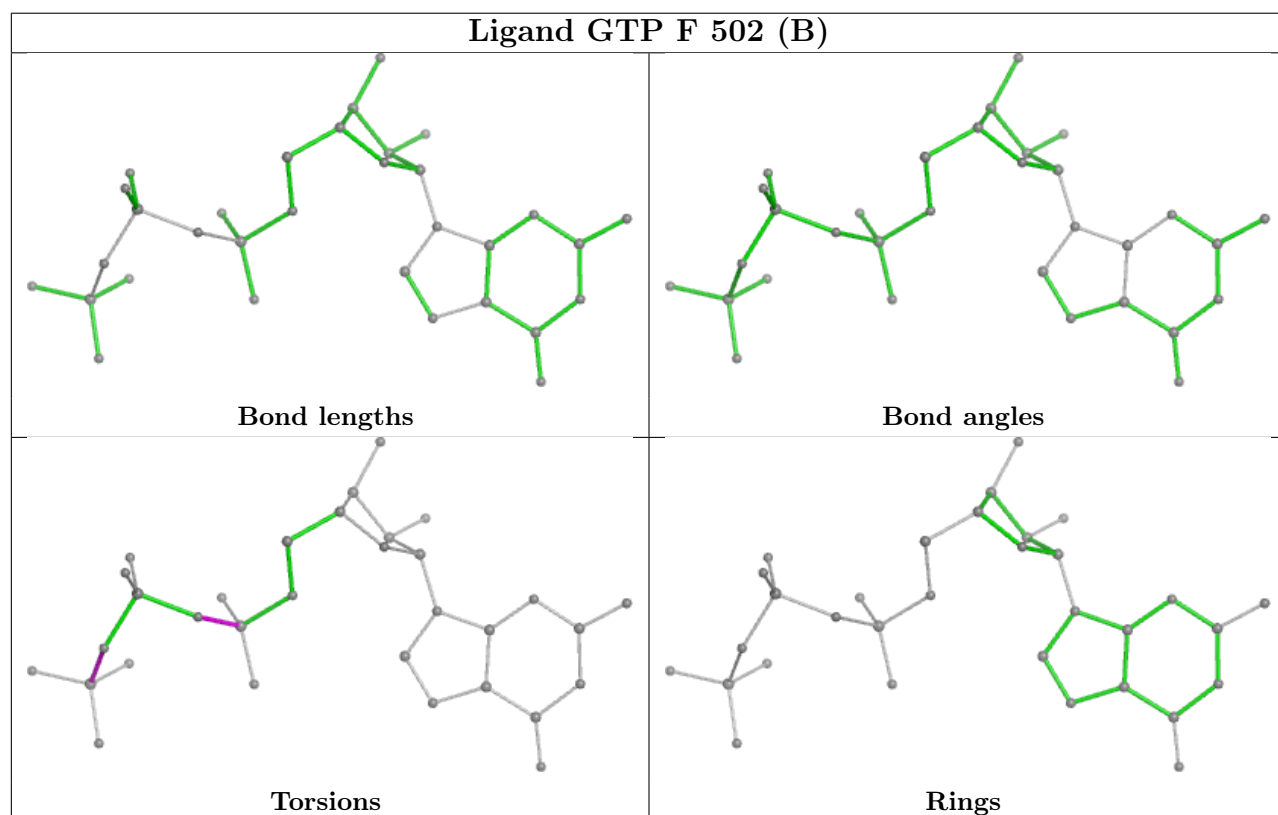
Ligand 5GP H 501



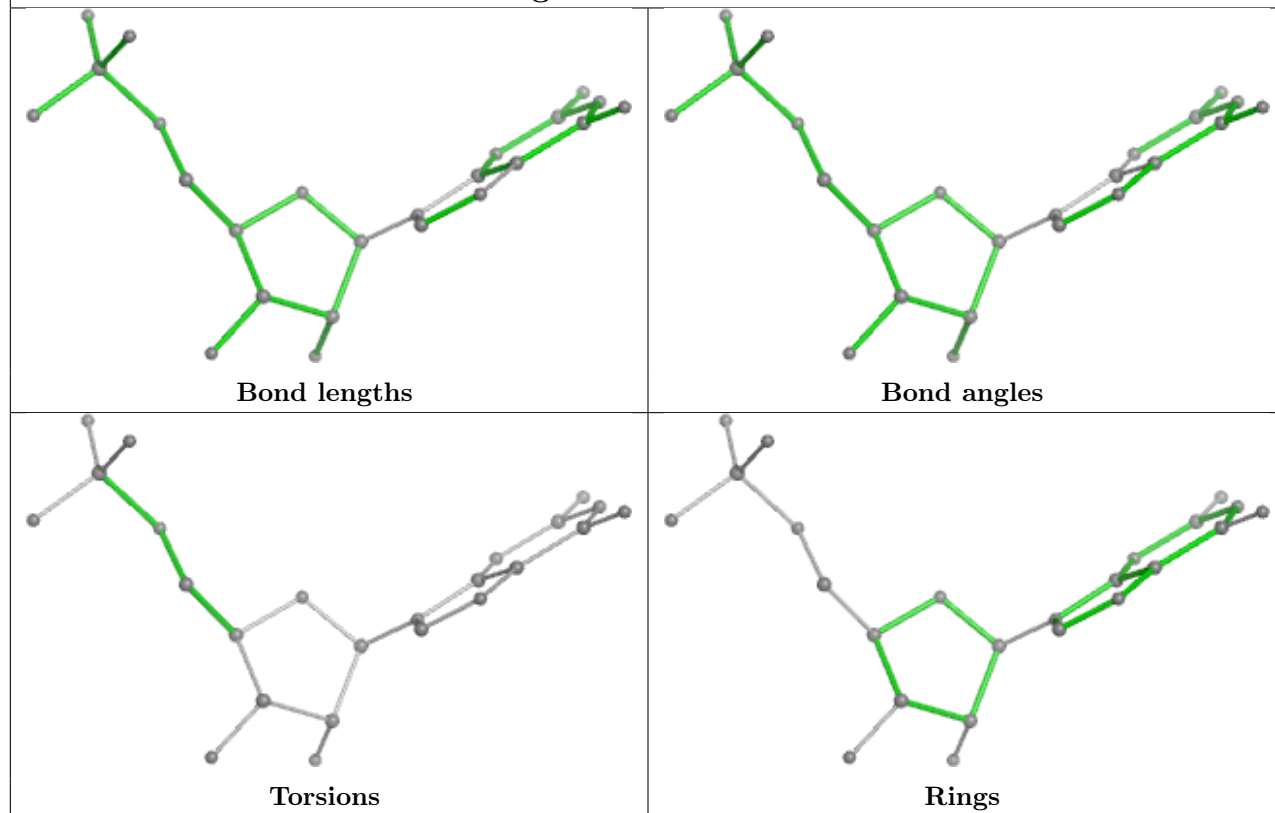
Ligand 5GP E 501



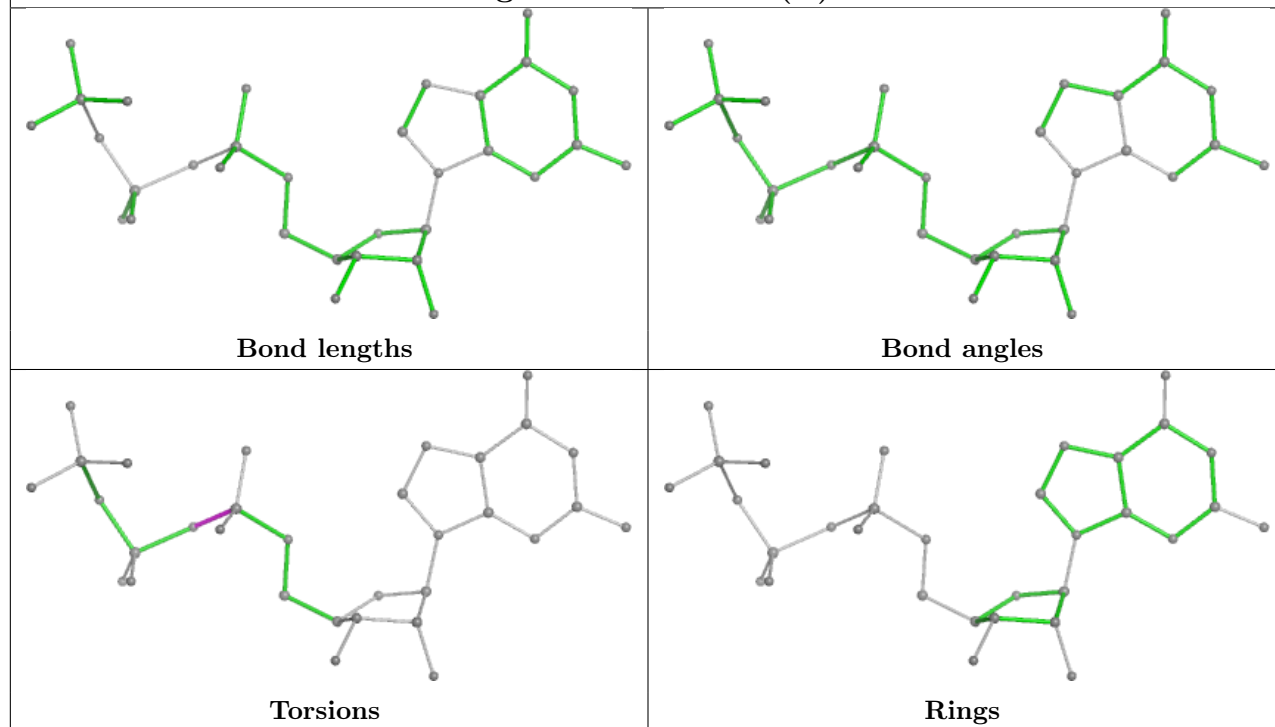
Ligand GTP F 502 (B)

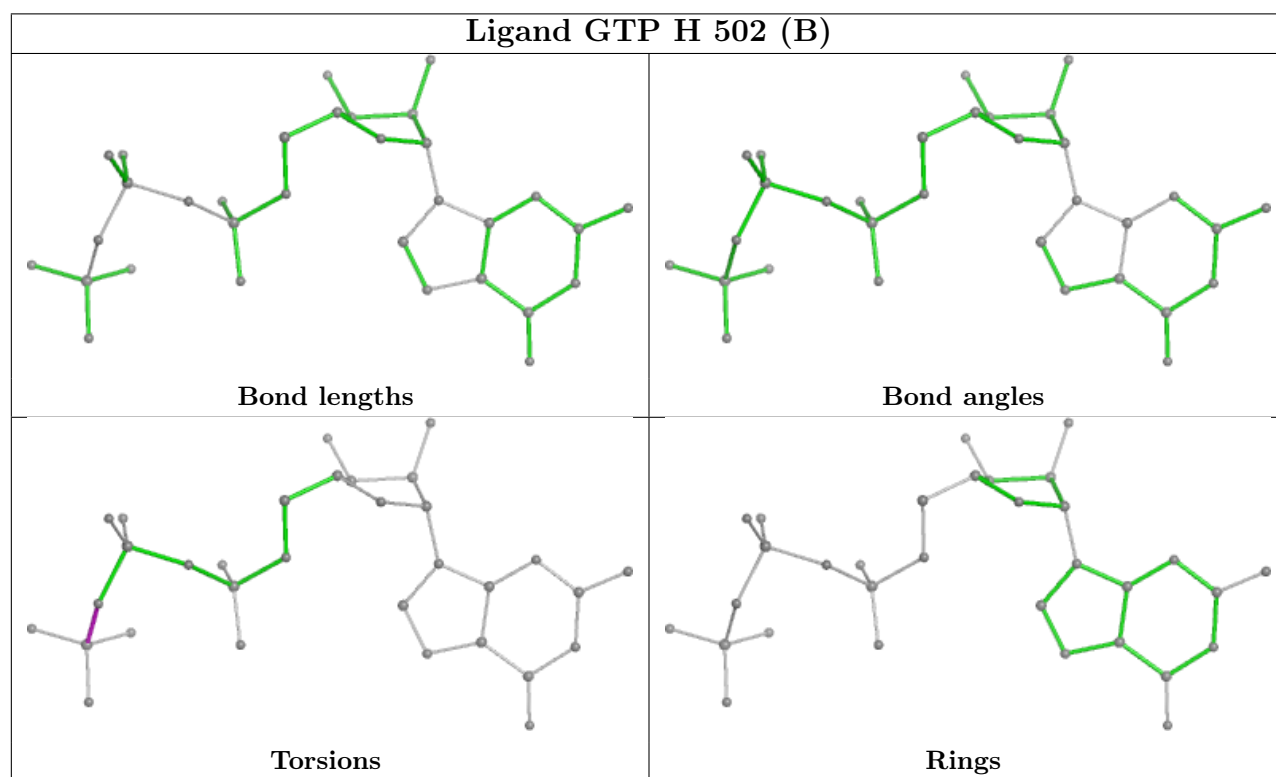
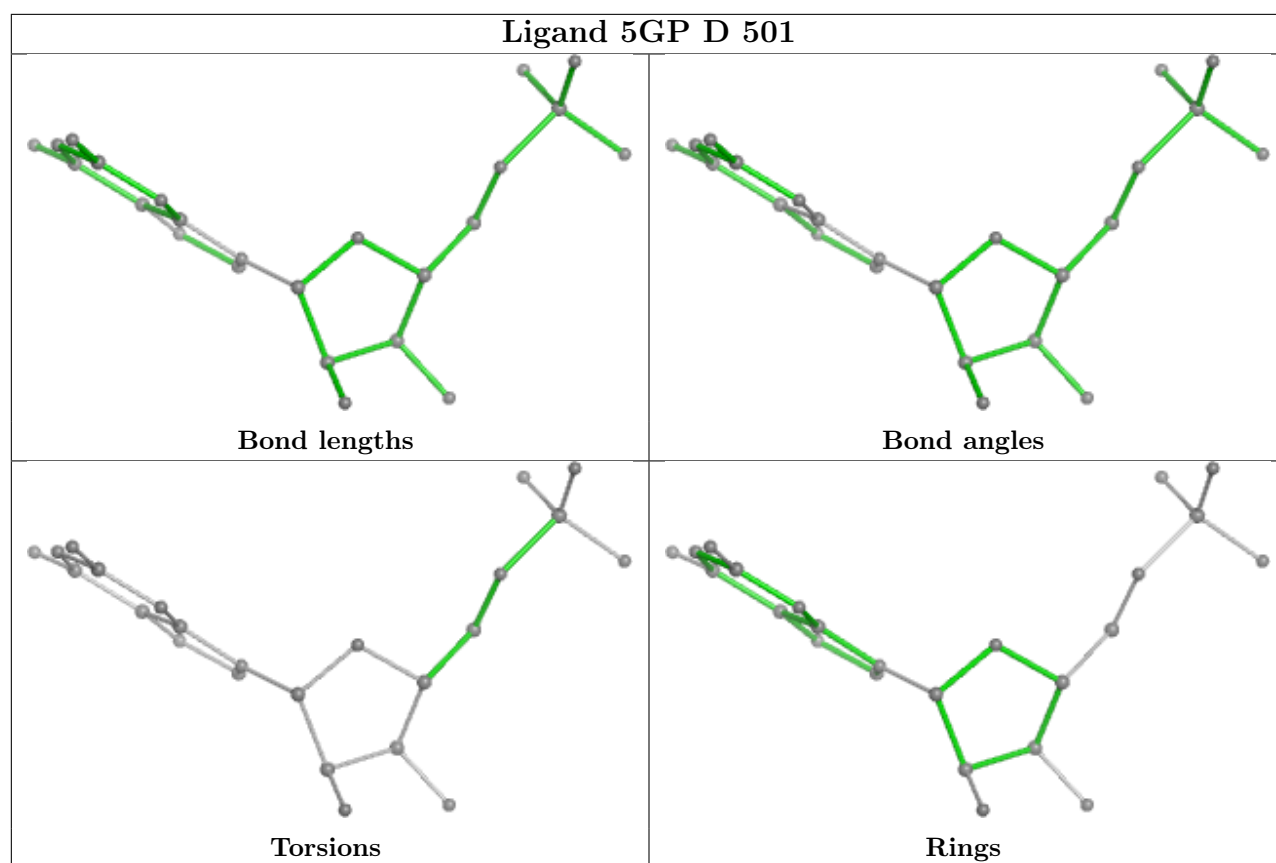


Ligand 5GP G 501

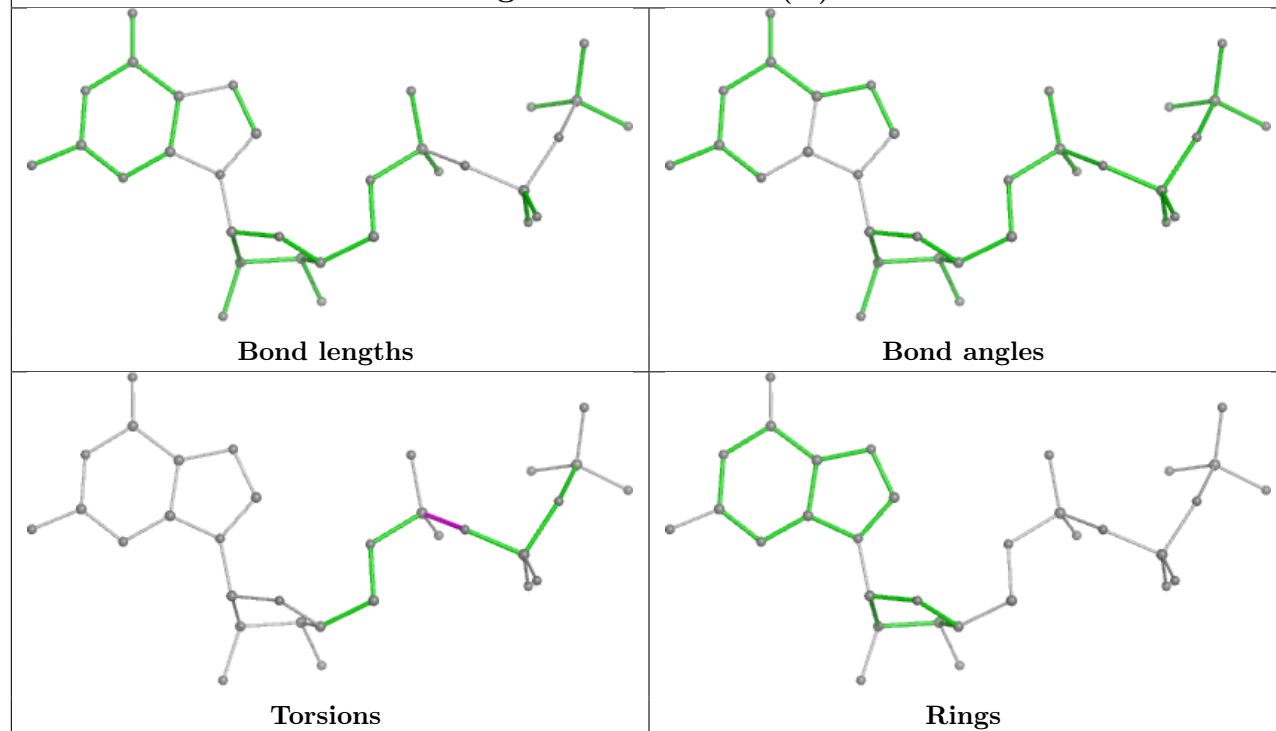


Ligand GTP G 502 (B)

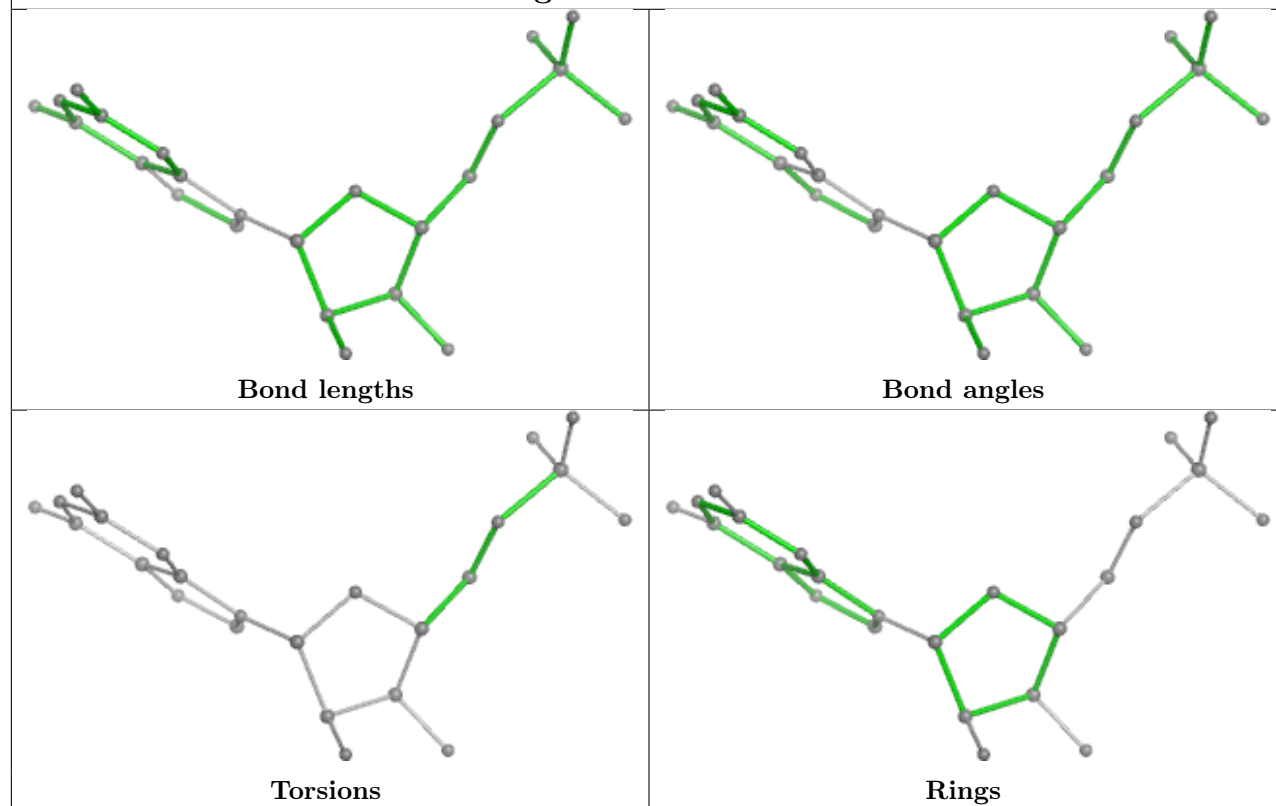




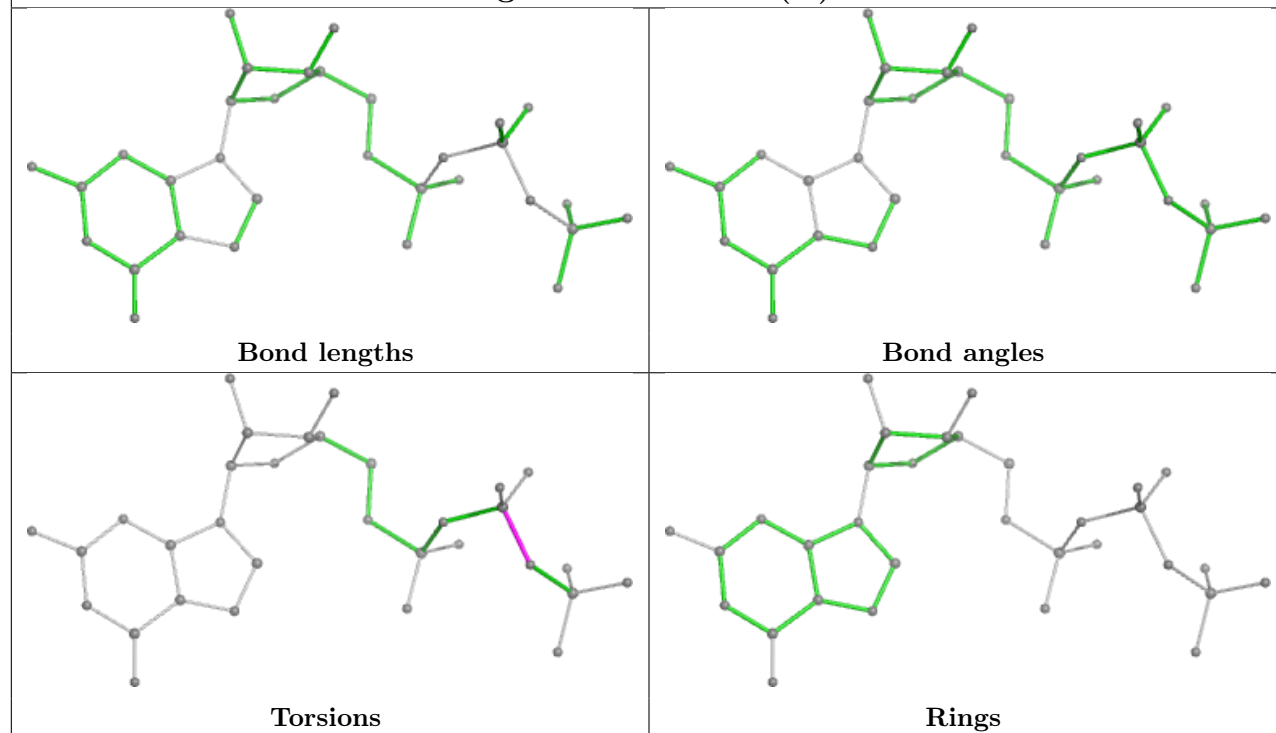
Ligand GTP D 502 (B)



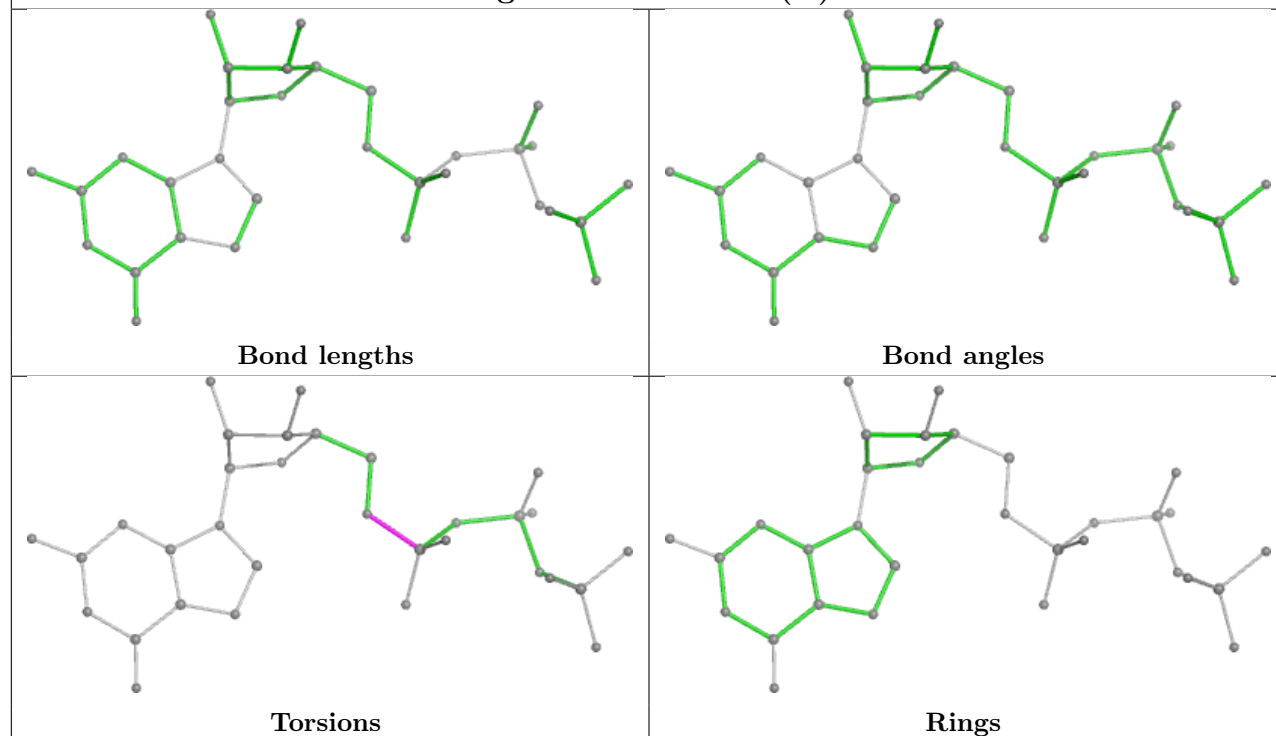
Ligand 5GP C 501



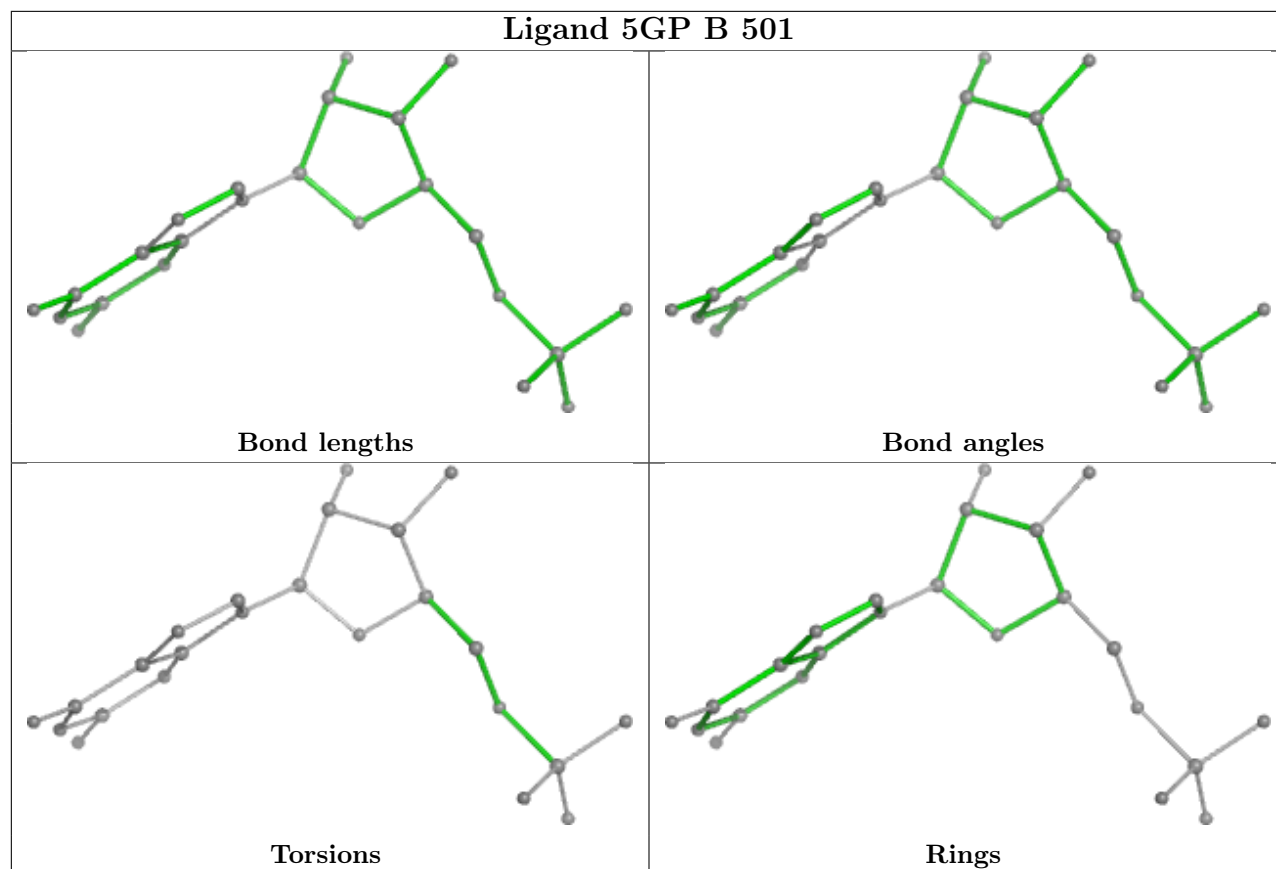
Ligand GTP B 502 (A)



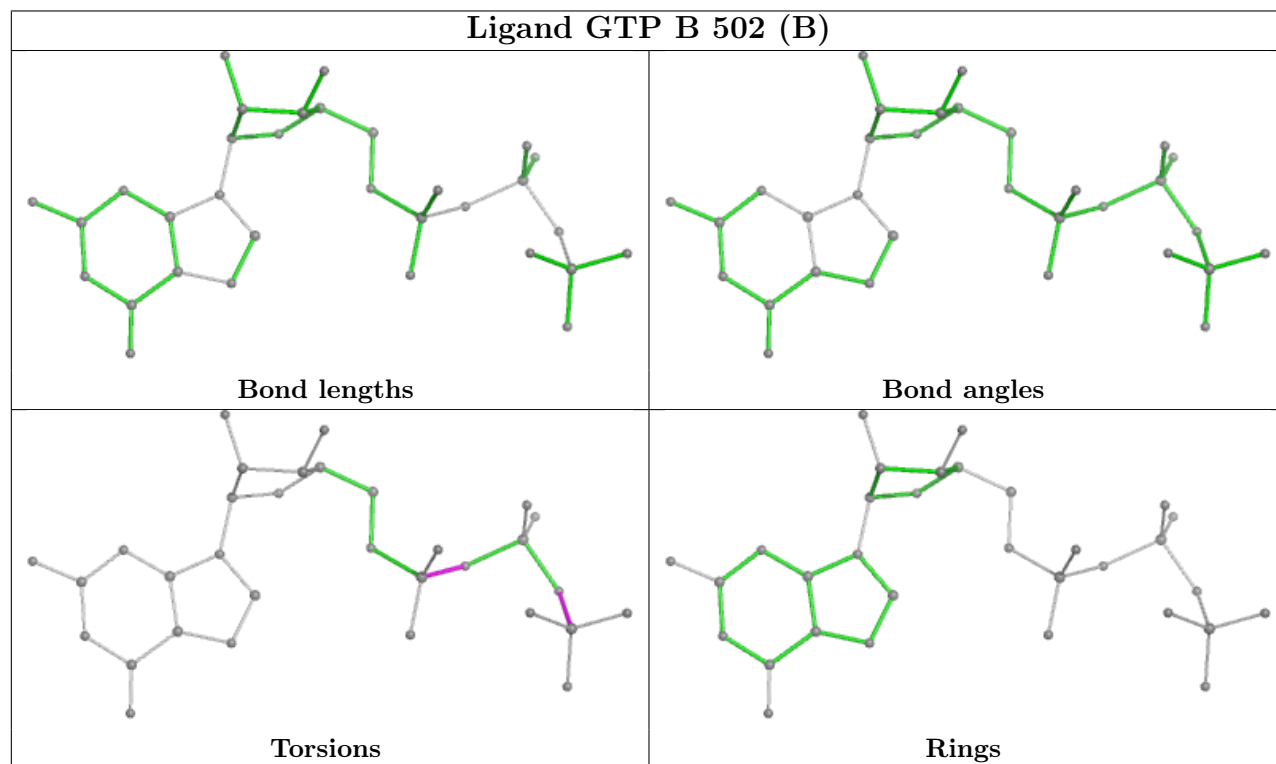
Ligand GTP A 502 (B)



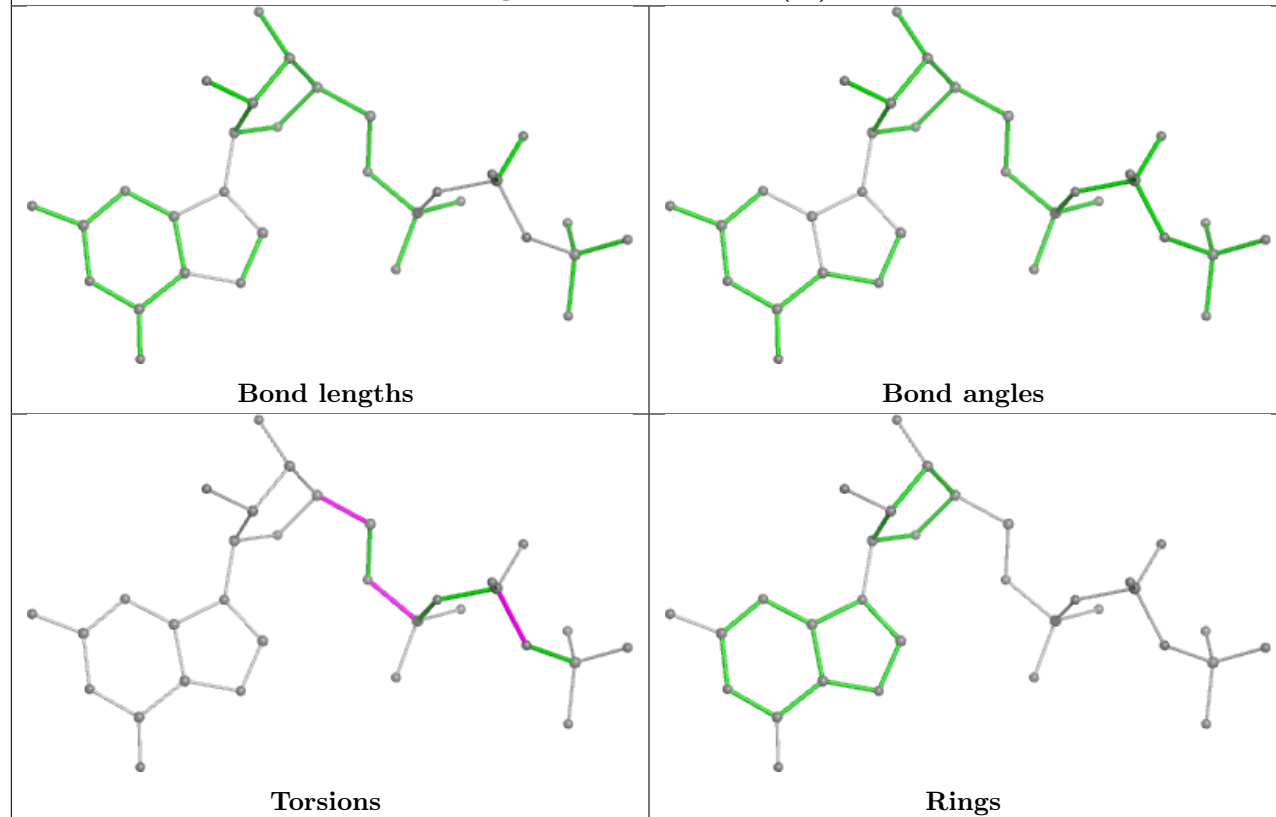
Ligand 5GP B 501



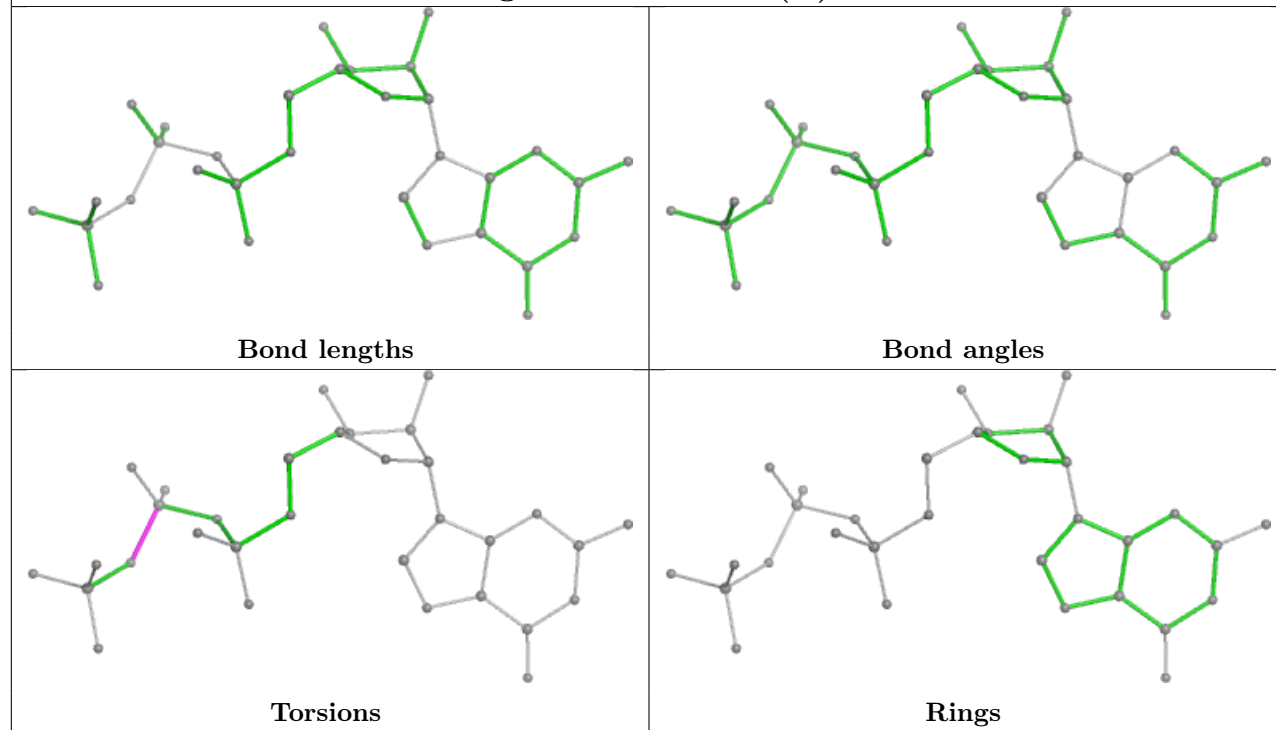
Ligand GTP B 502 (B)

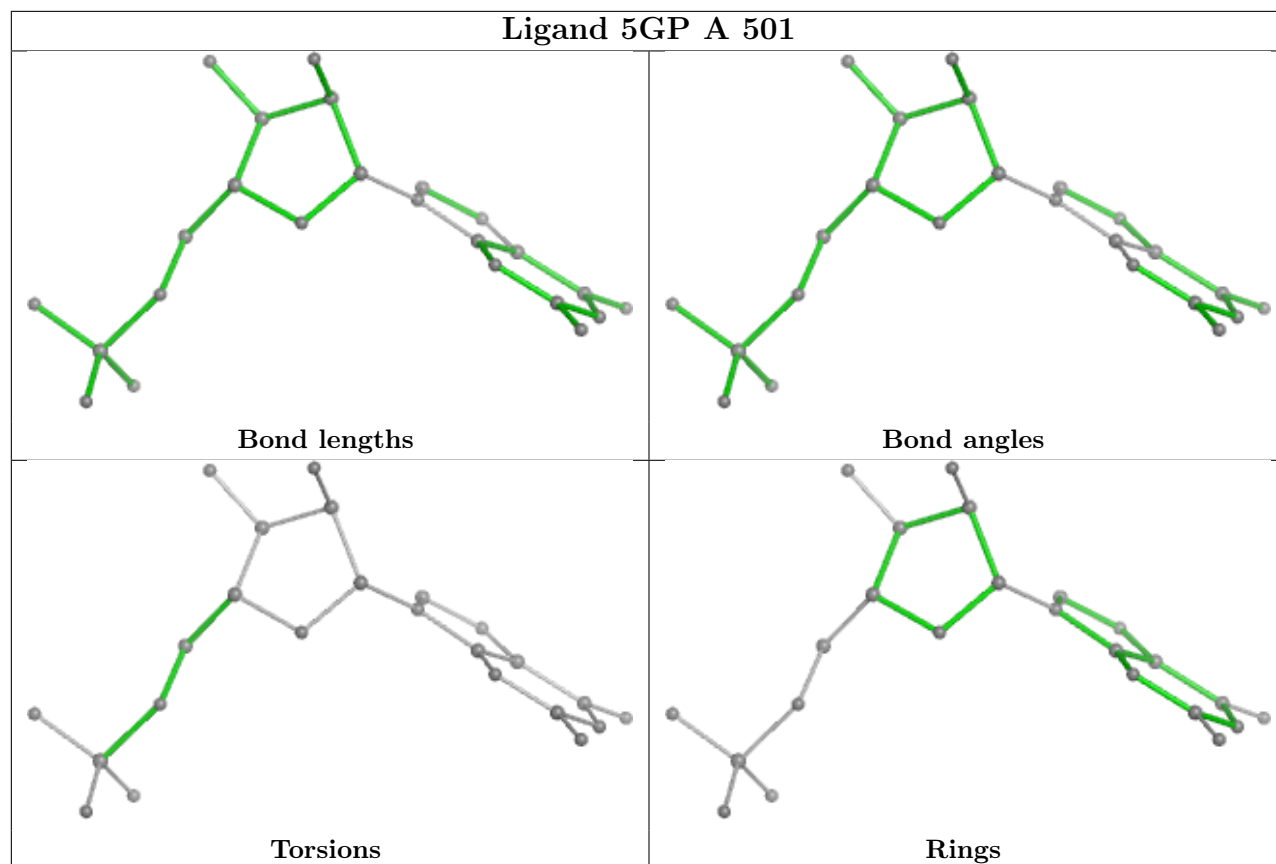


Ligand GTP C 502 (A)



Ligand GTP E 502 (A)





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	460/496 (92%)	0.37	25 (5%) 32 34	35, 49, 79, 102	0
1	B	460/496 (92%)	0.52	29 (6%) 27 29	38, 54, 81, 108	0
1	C	460/496 (92%)	0.67	28 (6%) 28 30	40, 59, 86, 108	0
1	D	460/496 (92%)	0.47	21 (4%) 38 39	36, 54, 81, 107	0
1	E	460/496 (92%)	1.52	123 (26%) 2 2	49, 75, 102, 126	0
1	F	460/496 (92%)	1.77	158 (34%) 1 1	60, 86, 110, 128	0
1	G	460/496 (92%)	1.40	99 (21%) 3 3	48, 72, 101, 128	0
1	H	460/496 (92%)	1.02	63 (13%) 8 9	44, 63, 94, 113	0
All	All	3680/3968 (92%)	0.97	546 (14%) 7 8	35, 63, 97, 128	0

All (546) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	163	VAL	5.5
1	B	403	PHE	5.5
1	A	403	PHE	5.4
1	E	128	PHE	5.0
1	E	193	GLY	4.9
1	H	414	GLY	4.7
1	C	124	ALA	4.7
1	E	163	VAL	4.6
1	F	80	ILE	4.6
1	C	403	PHE	4.6
1	E	155	LEU	4.5
1	E	191	LEU	4.5
1	H	155	LEU	4.5
1	F	194	VAL	4.4
1	G	194	VAL	4.3
1	E	187	PRO	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	178	PRO	4.2
1	F	158	PHE	4.2
1	F	103	LEU	4.2
1	F	191	LEU	4.2
1	C	123	ALA	4.1
1	E	158	PHE	4.1
1	F	120	ALA	4.1
1	G	467	ALA	4.1
1	F	117	HIS	4.1
1	E	116	LEU	4.0
1	C	109	VAL	4.0
1	G	281	GLY	4.0
1	F	415	ILE	4.0
1	E	339	VAL	3.9
1	G	117	HIS	3.9
1	H	187	PRO	3.9
1	G	2	VAL	3.9
1	F	394	ALA	3.9
1	G	411	PHE	3.9
1	H	128	PHE	3.9
1	F	223	GLY	3.9
1	F	179	ILE	3.8
1	F	155	LEU	3.8
1	F	300	GLY	3.8
1	E	411	PHE	3.8
1	F	222	VAL	3.8
1	C	302	MET	3.8
1	F	157	ASP	3.7
1	D	401	SER	3.7
1	E	161	ALA	3.7
1	F	374	PHE	3.7
1	D	300	GLY	3.7
1	D	394	ALA	3.7
1	H	467	ALA	3.7
1	G	155	LEU	3.7
1	F	271	LEU	3.6
1	G	325	ALA	3.6
1	F	364	GLY	3.6
1	F	411	PHE	3.6
1	H	411	PHE	3.6
1	H	185	THR	3.6
1	G	272	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	394	ALA	3.6
1	F	245	ILE	3.6
1	G	191	LEU	3.6
1	D	301	ALA	3.6
1	E	325	ALA	3.6
1	D	403	PHE	3.5
1	G	415	ILE	3.5
1	H	179	ILE	3.5
1	F	273	ALA	3.5
1	F	301	ALA	3.5
1	H	163	VAL	3.5
1	G	394	ALA	3.5
1	F	41	GLY	3.5
1	G	300	GLY	3.5
1	G	128	PHE	3.5
1	F	65	VAL	3.5
1	F	109	VAL	3.5
1	E	132	PRO	3.4
1	F	132	PRO	3.4
1	B	409	GLY	3.4
1	E	192	ALA	3.4
1	F	185	THR	3.4
1	F	187	PRO	3.4
1	H	117	HIS	3.4
1	F	334	TRP	3.4
1	E	194	VAL	3.4
1	F	128	PHE	3.4
1	H	303	CYS	3.4
1	E	273	ALA	3.4
1	F	127	VAL	3.3
1	G	116	LEU	3.3
1	E	394	ALA	3.3
1	H	466	ALA	3.3
1	G	187	PRO	3.3
1	F	148	ALA	3.3
1	F	160	THR	3.3
1	H	415	ILE	3.3
1	G	278	SER	3.3
1	E	447	VAL	3.3
1	F	116	LEU	3.3
1	A	467	ALA	3.3
1	C	394	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	158	PHE	3.2
1	H	158	PHE	3.2
1	F	72	VAL	3.2
1	F	272	VAL	3.2
1	G	159	VAL	3.2
1	B	326	ALA	3.2
1	F	218	ILE	3.2
1	H	178	PRO	3.2
1	H	191	LEU	3.2
1	C	148	ALA	3.2
1	E	169	GLU	3.2
1	E	179	ILE	3.2
1	F	242	LEU	3.2
1	G	103	LEU	3.2
1	E	296	GLY	3.2
1	F	170	VAL	3.2
1	B	467	ALA	3.2
1	F	303	CYS	3.2
1	G	267	LEU	3.2
1	G	331	GLY	3.2
1	E	467	ALA	3.1
1	F	192	ALA	3.1
1	F	153	ILE	3.1
1	C	239	GLY	3.1
1	C	405	ARG	3.1
1	G	134	GLY	3.1
1	H	403	PHE	3.1
1	E	117	HIS	3.1
1	G	273	ALA	3.1
1	E	184	MET	3.1
1	G	303	CYS	3.1
1	E	356	VAL	3.1
1	F	100	PRO	3.1
1	C	401	SER	3.1
1	F	134	GLY	3.1
1	E	97	VAL	3.1
1	F	232	ALA	3.1
1	F	183	VAL	3.0
1	E	154	ALA	3.0
1	G	160	THR	3.0
1	D	415	ILE	3.0
1	G	133	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	269	LEU	3.0
1	F	193	GLY	3.0
1	G	239	GLY	3.0
1	E	272	VAL	3.0
1	C	466	ALA	3.0
1	F	238	ALA	3.0
1	H	161	ALA	3.0
1	E	160	THR	3.0
1	F	176	HIS	3.0
1	G	176	HIS	3.0
1	G	179	ILE	3.0
1	F	173	LEU	3.0
1	F	243	LEU	3.0
1	F	295	VAL	3.0
1	H	159	VAL	3.0
1	H	157	ASP	3.0
1	A	29	ALA	3.0
1	A	466	ALA	3.0
1	B	29	ALA	3.0
1	E	120	ALA	3.0
1	F	115	LEU	3.0
1	F	235	LEU	3.0
1	E	159	VAL	3.0
1	F	114	ALA	3.0
1	F	161	ALA	3.0
1	F	178	PRO	3.0
1	E	185	THR	2.9
1	F	366	TYR	2.9
1	E	389	SER	2.9
1	F	2	VAL	2.9
1	F	121	HIS	2.9
1	F	467	ALA	2.9
1	H	2	VAL	2.9
1	F	167	PRO	2.9
1	D	57	ALA	2.9
1	H	160	THR	2.9
1	F	337	GLY	2.9
1	E	174	LEU	2.9
1	H	116	LEU	2.9
1	H	97	VAL	2.9
1	F	162	PRO	2.9
1	G	178	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	466	ALA	2.9
1	F	230	ALA	2.9
1	F	135	LEU	2.9
1	G	410	LEU	2.9
1	F	113	ASN	2.9
1	C	147	PHE	2.8
1	E	2	VAL	2.8
1	F	276	VAL	2.8
1	G	163	VAL	2.8
1	H	132	PRO	2.8
1	D	467	ALA	2.8
1	F	326	ALA	2.8
1	G	154	ALA	2.8
1	G	466	ALA	2.8
1	E	130	GLY	2.8
1	G	223	GLY	2.8
1	C	410	LEU	2.8
1	G	252	GLN	2.8
1	F	89	PHE	2.8
1	E	109	VAL	2.8
1	E	189	GLY	2.8
1	F	95	LEU	2.8
1	F	452	LEU	2.8
1	F	246	ASP	2.8
1	B	147	PHE	2.8
1	C	29	ALA	2.8
1	F	203	ALA	2.8
1	F	449	ALA	2.8
1	E	43	GLY	2.8
1	F	268	GLY	2.8
1	F	269	LEU	2.8
1	G	80	ILE	2.8
1	B	3	ARG	2.8
1	F	299	PRO	2.8
1	E	170	VAL	2.8
1	E	148	ALA	2.8
1	F	29	ALA	2.8
1	G	274	GLY	2.8
1	E	162	PRO	2.7
1	E	181	VAL	2.7
1	G	97	VAL	2.7
1	G	127	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	425	ALA	2.7
1	G	192	ALA	2.7
1	C	402	SER	2.7
1	G	402	SER	2.7
1	E	157	ASP	2.7
1	D	411	PHE	2.7
1	G	170	VAL	2.7
1	C	301	ALA	2.7
1	F	124	ALA	2.7
1	F	329	LEU	2.7
1	G	153	ILE	2.7
1	G	212	ALA	2.7
1	F	196	THR	2.7
1	G	137	THR	2.7
1	E	412	GLU	2.7
1	A	411	PHE	2.7
1	E	28	VAL	2.7
1	F	90	VAL	2.7
1	E	236	ALA	2.7
1	F	182	ALA	2.7
1	B	110	SER	2.6
1	E	371	ASP	2.6
1	B	2	VAL	2.6
1	E	32	PHE	2.6
1	F	159	VAL	2.6
1	E	219	ALA	2.6
1	F	220	ALA	2.6
1	G	120	ALA	2.6
1	F	165	THR	2.6
1	H	137	THR	2.6
1	D	2	VAL	2.6
1	E	222	VAL	2.6
1	E	333	VAL	2.6
1	E	459	VAL	2.6
1	F	50	VAL	2.6
1	C	467	ALA	2.6
1	G	250	GLY	2.6
1	G	330	GLY	2.6
1	C	116	LEU	2.6
1	E	422	LEU	2.6
1	F	133	ILE	2.6
1	B	408	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	176	HIS	2.6
1	D	405	ARG	2.6
1	D	147	PHE	2.6
1	A	123	ALA	2.6
1	B	333	VAL	2.6
1	E	301	ALA	2.6
1	F	209	ALA	2.6
1	F	236	ALA	2.6
1	F	262	VAL	2.6
1	F	330	GLY	2.6
1	F	333	VAL	2.6
1	B	401	SER	2.6
1	A	2	VAL	2.5
1	F	403	PHE	2.5
1	G	183	VAL	2.5
1	H	300	GLY	2.5
1	B	394	ALA	2.5
1	E	200	ALA	2.5
1	E	203	ALA	2.5
1	H	333	VAL	2.5
1	E	271	LEU	2.5
1	G	265	LEU	2.5
1	E	355	ASN	2.5
1	E	149	ARG	2.5
1	G	157	ASP	2.5
1	B	301	ALA	2.5
1	F	212	ALA	2.5
1	G	147	PHE	2.5
1	G	234	ALA	2.5
1	E	52	ASN	2.5
1	E	190	THR	2.5
1	D	252	GLN	2.5
1	G	218	ILE	2.5
1	G	405	ARG	2.5
1	B	402	SER	2.5
1	H	418	SER	2.5
1	F	98	ASP	2.5
1	B	411	PHE	2.5
1	C	2	VAL	2.5
1	D	466	ALA	2.5
1	E	127	VAL	2.5
1	F	244	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	374	PHE	2.5
1	C	146	ARG	2.5
1	E	100	PRO	2.5
1	E	409	GLY	2.5
1	G	181	VAL	2.5
1	F	216	LEU	2.5
1	E	23	PRO	2.5
1	F	201	ILE	2.4
1	A	143	GLY	2.4
1	E	274	GLY	2.4
1	B	139	ALA	2.4
1	G	125	VAL	2.4
1	G	161	ALA	2.4
1	E	4	PHE	2.4
1	F	81	THR	2.4
1	G	417	THR	2.4
1	G	299	PRO	2.4
1	A	401	SER	2.4
1	D	408	LYS	2.4
1	F	181	VAL	2.4
1	H	169	GLU	2.4
1	G	71	ILE	2.4
1	A	124	ALA	2.4
1	F	154	ALA	2.4
1	F	265	LEU	2.4
1	H	261	ALA	2.4
1	C	181	VAL	2.4
1	E	228	VAL	2.4
1	D	417	THR	2.4
1	C	412	GLU	2.4
1	A	30	SER	2.4
1	E	153	ILE	2.4
1	E	402	SER	2.4
1	E	176	HIS	2.4
1	G	146	ARG	2.4
1	G	193	GLY	2.4
1	H	164	GLY	2.4
1	A	425	ALA	2.4
1	B	148	ALA	2.4
1	E	135	LEU	2.4
1	E	195	LEU	2.4
1	E	212	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	295	VAL	2.3
1	E	374	PHE	2.3
1	G	393	VAL	2.3
1	G	447	VAL	2.3
1	G	81	THR	2.3
1	A	404	ASP	2.3
1	A	426	ARG	2.3
1	G	364	GLY	2.3
1	G	301	ALA	2.3
1	H	301	ALA	2.3
1	G	169	GLU	2.3
1	G	185	THR	2.3
1	E	465	SER	2.3
1	F	259	ILE	2.3
1	A	193	GLY	2.3
1	A	331	GLY	2.3
1	H	410	LEU	2.3
1	E	238	ALA	2.3
1	E	408	LYS	2.3
1	G	182	ALA	2.3
1	B	28	VAL	2.3
1	G	277	VAL	2.3
1	H	127	VAL	2.3
1	F	3	ARG	2.3
1	A	27	ASP	2.3
1	F	188	ASP	2.3
1	F	229	GLY	2.3
1	F	267	LEU	2.3
1	G	235	LEU	2.3
1	G	285	LEU	2.3
1	D	123	ALA	2.3
1	H	142	ALA	2.3
1	E	90	VAL	2.3
1	F	144	VAL	2.3
1	G	262	VAL	2.3
1	H	424	PRO	2.3
1	F	202	ARG	2.3
1	A	402	SER	2.3
1	E	84	SER	2.3
1	E	24	GLY	2.3
1	E	427	GLY	2.3
1	E	216	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	373	LEU	2.2
1	E	230	ALA	2.2
1	F	234	ALA	2.2
1	F	466	ALA	2.2
1	H	192	ALA	2.2
1	F	39	VAL	2.2
1	F	228	VAL	2.2
1	H	81	THR	2.2
1	F	152	ASP	2.2
1	F	286	ILE	2.2
1	G	401	SER	2.2
1	E	448	GLY	2.2
1	F	214	GLY	2.2
1	G	427	GLY	2.2
1	C	192	ALA	2.2
1	F	327	ARG	2.2
1	H	79	PRO	2.2
1	H	162	PRO	2.2
1	E	56	VAL	2.2
1	E	328	GLN	2.2
1	D	402	SER	2.2
1	E	152	ASP	2.2
1	E	201	ILE	2.2
1	E	218	ILE	2.2
1	A	169	GLU	2.2
1	G	106	GLU	2.2
1	B	146	ARG	2.2
1	F	410	LEU	2.2
1	H	405	ARG	2.2
1	E	366	TYR	2.2
1	A	301	ALA	2.2
1	C	406	ALA	2.2
1	E	105	PRO	2.2
1	E	270	PRO	2.2
1	F	200	ALA	2.2
1	F	288	ALA	2.2
1	G	261	ALA	2.2
1	H	425	ALA	2.2
1	E	81	THR	2.2
1	H	417	THR	2.2
1	G	90	VAL	2.2
1	E	246	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	303	CYS	2.2
1	E	439	GLY	2.2
1	G	214	GLY	2.2
1	H	133	ILE	2.2
1	C	103	LEU	2.2
1	H	135	LEU	2.2
1	H	173	LEU	2.2
1	B	176	HIS	2.2
1	E	167	PRO	2.2
1	E	253	ALA	2.2
1	H	29	ALA	2.2
1	F	210	VAL	2.2
1	H	136	VAL	2.2
1	C	32	PHE	2.2
1	E	27	ASP	2.2
1	E	401	SER	2.1
1	G	416	SER	2.1
1	E	46	ILE	2.1
1	A	410	LEU	2.1
1	G	173	LEU	2.1
1	G	328	GLN	2.1
1	G	350	ALA	2.1
1	H	154	ALA	2.1
1	F	417	THR	2.1
1	G	144	VAL	2.1
1	E	98	ASP	2.1
1	F	169	GLU	2.1
1	E	134	GLY	2.1
1	F	281	GLY	2.1
1	F	402	SER	2.1
1	G	156	SER	2.1
1	H	189	GLY	2.1
1	B	410	LEU	2.1
1	E	390	LYS	2.1
1	E	139	ALA	2.1
1	E	177	ALA	2.1
1	E	261	ALA	2.1
1	E	417	THR	2.1
1	F	102	THR	2.1
1	F	139	ALA	2.1
1	F	348	ALA	2.1
1	H	212	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	97	VAL	2.1
1	G	297	VAL	2.1
1	H	90	VAL	2.1
1	A	147	PHE	2.1
1	C	327	ARG	2.1
1	C	426	ARG	2.1
1	F	172	ASP	2.1
1	E	164	GLY	2.1
1	H	402	SER	2.1
1	A	415	ILE	2.1
1	E	80	ILE	2.1
1	F	71	ILE	2.1
1	H	201	ILE	2.1
1	B	271	LEU	2.1
1	G	240	ALA	2.1
1	H	388	ALA	2.1
1	F	21	VAL	2.1
1	F	101	VAL	2.1
1	F	125	VAL	2.1
1	F	293	VAL	2.1
1	D	32	PHE	2.1
1	E	131	ARG	2.1
1	B	77	ASP	2.1
1	E	188	ASP	2.1
1	G	371	ASP	2.1
1	E	337	GLY	2.1
1	E	415	ILE	2.1
1	F	254	LYS	2.1
1	F	252	GLN	2.1
1	F	355	ASN	2.1
1	G	329	LEU	2.1
1	F	82	ALA	2.1
1	F	255	MET	2.1
1	G	413	GLU	2.0
1	H	59	ARG	2.0
1	E	73	VAL	2.0
1	F	136	VAL	2.0
1	F	32	PHE	2.0
1	F	414	GLY	2.0
1	F	389	SER	2.0
1	H	104	SER	2.0
1	H	80	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	105	PRO	2.0
1	F	275	ASN	2.0
1	H	302	MET	2.0
1	A	146	ARG	2.0
1	B	123	ALA	2.0
1	B	412	GLU	2.0
1	D	124	ALA	2.0
1	E	449	ALA	2.0
1	F	219	ALA	2.0
1	F	406	ALA	2.0
1	F	413	GLU	2.0
1	G	168	ARG	2.0
1	G	263	ALA	2.0
1	B	144	VAL	2.0
1	B	268	GLY	2.0
1	E	300	GLY	2.0
1	F	352	GLY	2.0
1	G	414	GLY	2.0
1	G	332	HIS	2.0
1	F	110	SER	2.0
1	F	224	ILE	2.0
1	A	116	LEU	2.0
1	E	115	LEU	2.0
1	F	256	LEU	2.0
1	F	369	PRO	2.0
1	H	115	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

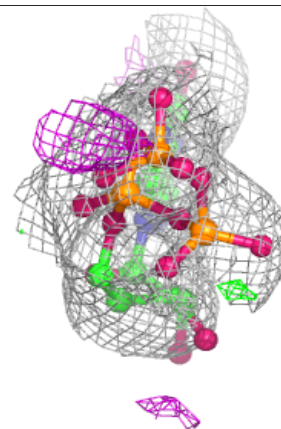
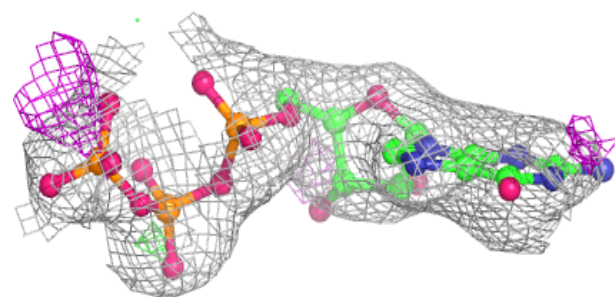
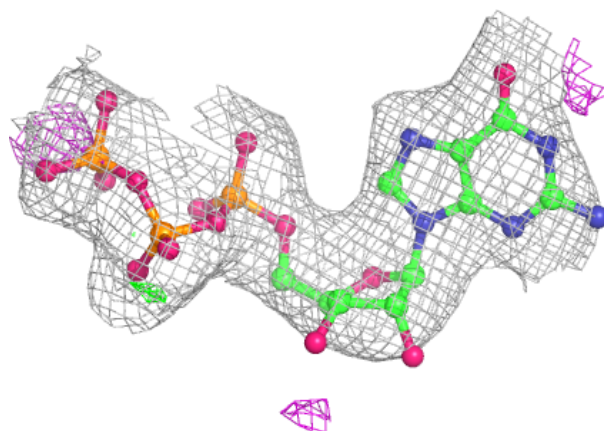
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GTP	E	502[A]	32/32	0.83	0.12	63,72,81,84	32
3	GTP	E	502[B]	32/32	0.83	0.12	64,73,80,84	32
3	GTP	G	502[A]	32/32	0.84	0.13	63,71,76,78	32
3	GTP	G	502[B]	32/32	0.84	0.13	63,71,75,78	32
3	GTP	F	502[A]	32/32	0.87	0.12	76,81,90,92	32
3	GTP	F	502[B]	32/32	0.87	0.12	76,82,89,91	32
3	GTP	H	502[A]	32/32	0.87	0.12	57,66,72,73	32
3	GTP	H	502[B]	32/32	0.87	0.12	59,66,72,75	32
3	GTP	C	502[A]	32/32	0.89	0.12	55,67,75,85	32
3	GTP	C	502[B]	32/32	0.89	0.12	53,66,75,85	32
3	GTP	D	502[A]	32/32	0.90	0.11	47,60,64,66	32
3	GTP	D	502[B]	32/32	0.90	0.11	53,61,64,65	32
2	5GP	F	501	24/24	0.91	0.09	58,69,83,89	0
2	5GP	G	501	24/24	0.91	0.10	46,59,70,73	0
3	GTP	A	502[A]	32/32	0.92	0.10	40,58,63,66	32
3	GTP	A	502[B]	32/32	0.92	0.10	42,58,65,66	32
3	GTP	B	502[A]	32/32	0.92	0.10	53,63,69,71	32
3	GTP	B	502[B]	32/32	0.92	0.10	55,63,69,75	32
2	5GP	C	501	24/24	0.93	0.09	38,50,57,62	0
2	5GP	E	501	24/24	0.94	0.08	50,59,69,72	0
2	5GP	A	501	24/24	0.95	0.07	33,39,47,50	0
2	5GP	H	501	24/24	0.95	0.07	38,48,55,64	0
2	5GP	B	501	24/24	0.96	0.06	30,44,51,56	0
2	5GP	D	501	24/24	0.96	0.07	36,46,57,61	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.

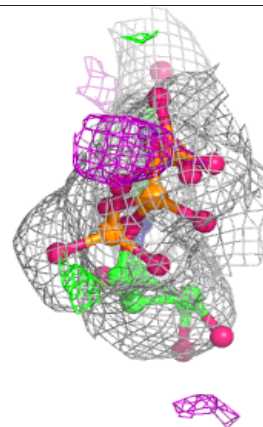
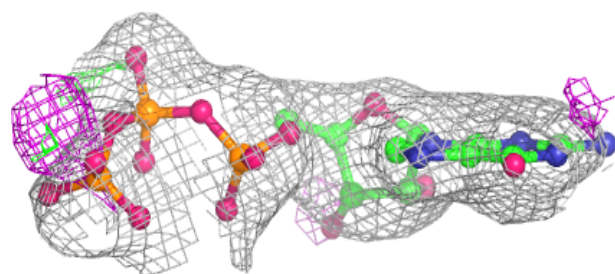
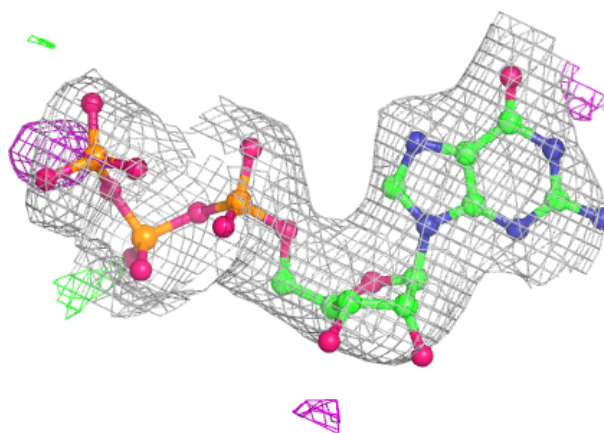
Electron density around GTP E 502 (A):

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

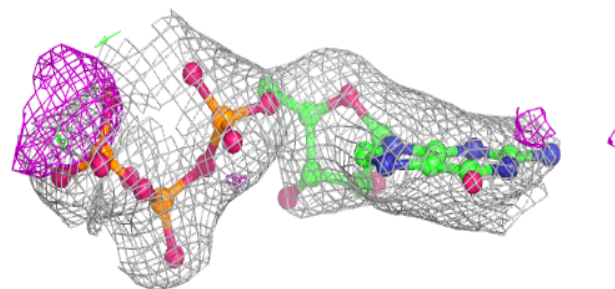
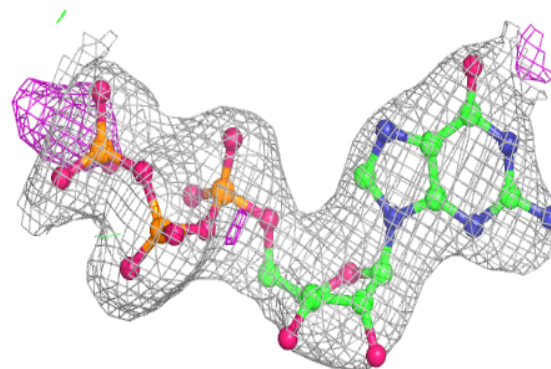


Electron density around GTP E 502 (B):

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

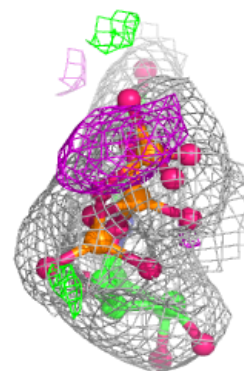
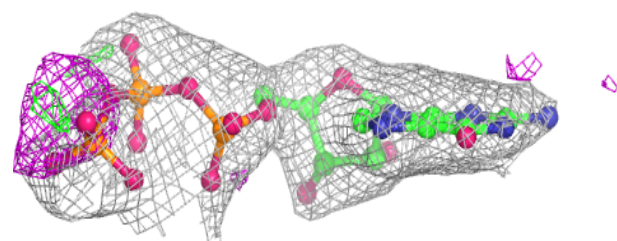
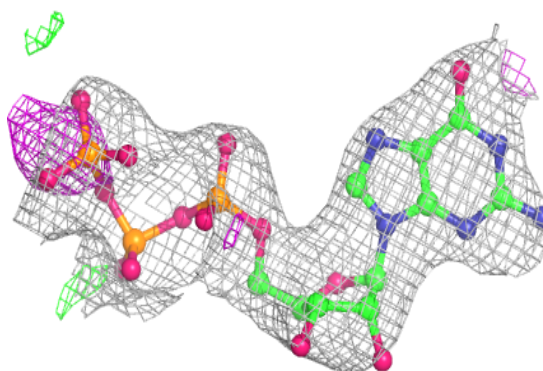
**Electron density around GTP G 502 (A):**

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

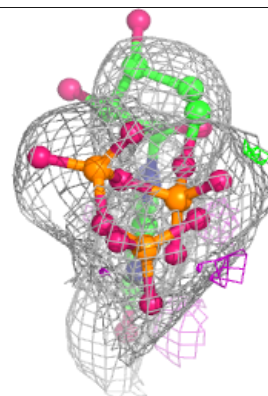
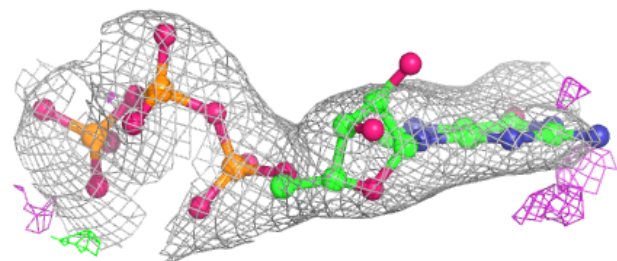
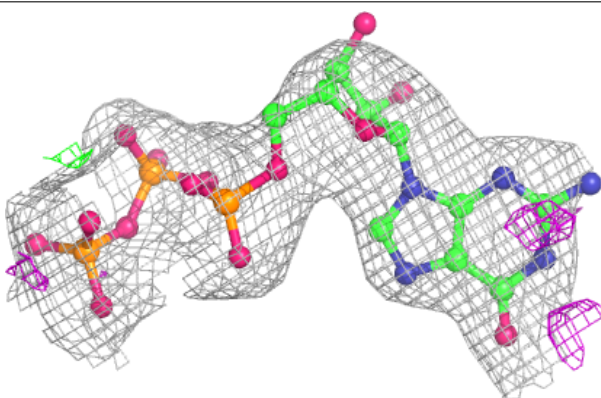


Electron density around GTP G 502 (B):

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

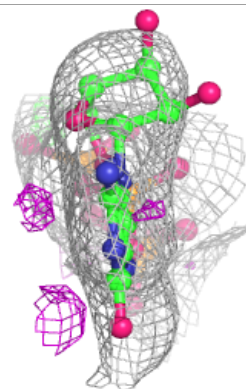
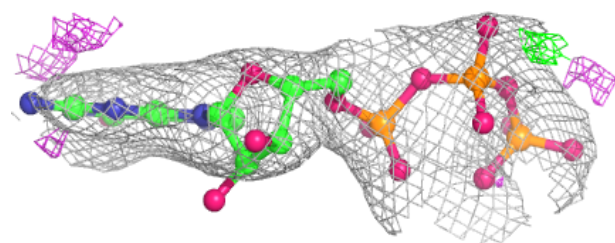
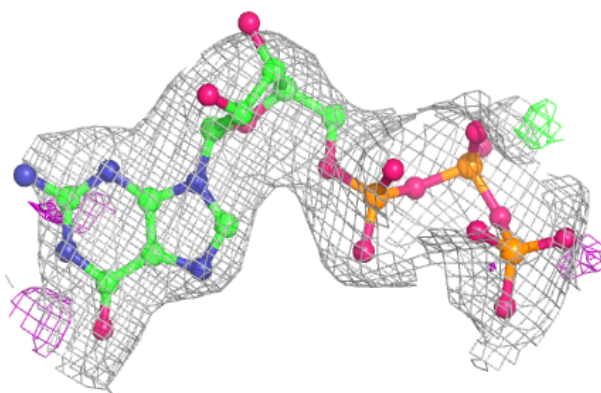
**Electron density around GTP F 502 (A):**

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

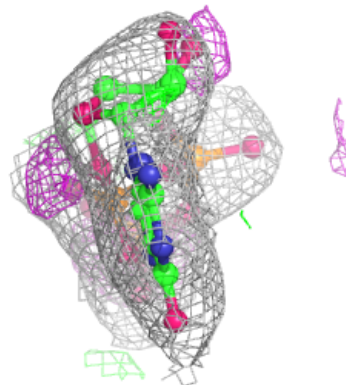
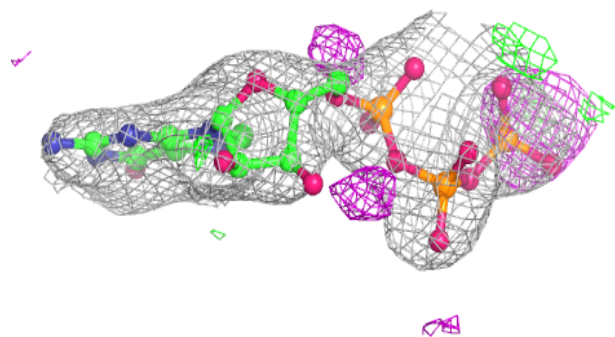
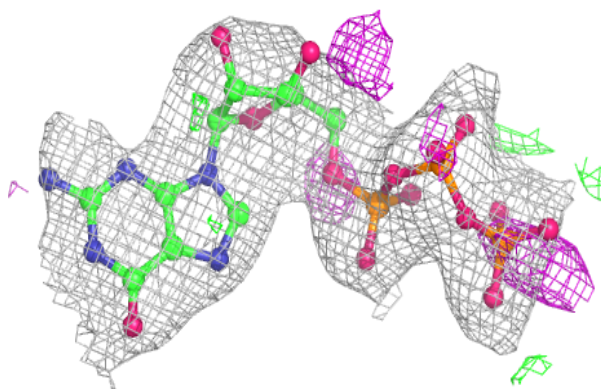


Electron density around GTP F 502 (B):

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

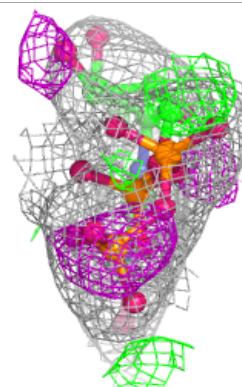
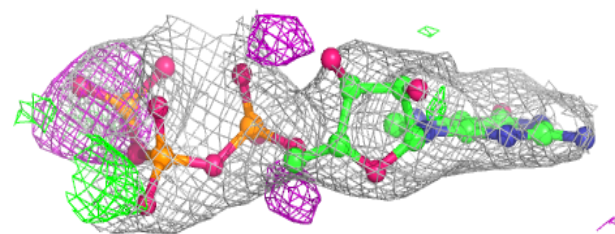
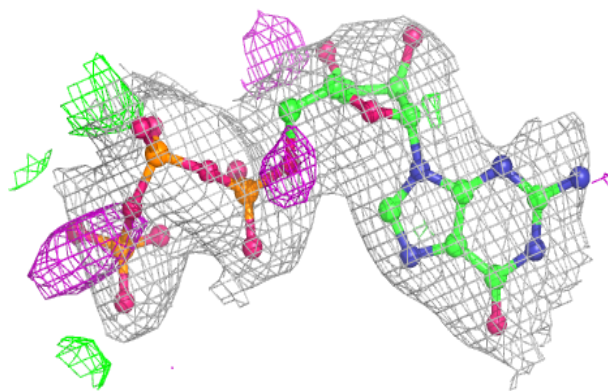
**Electron density around GTP H 502 (A):**

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

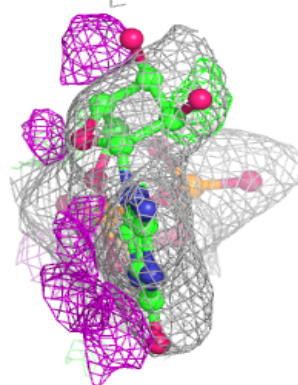
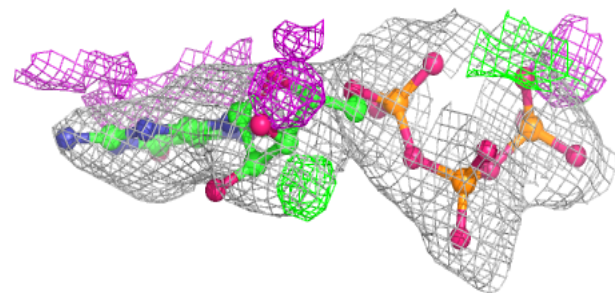
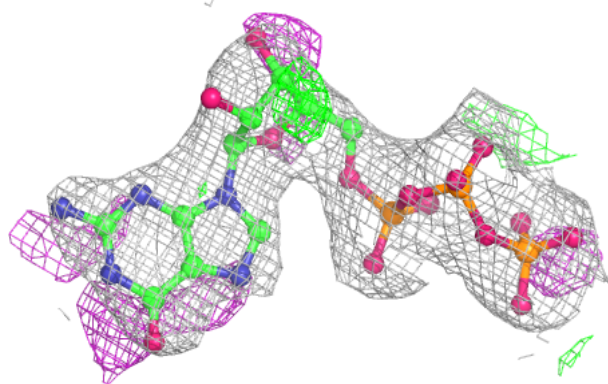


Electron density around GTP H 502 (B):

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

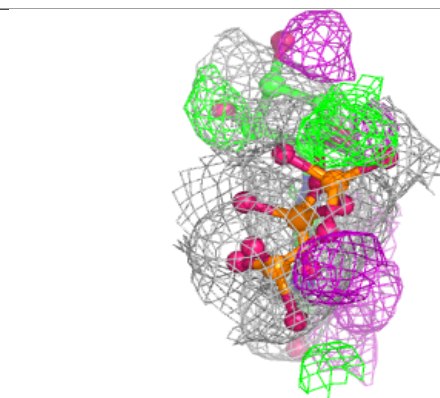
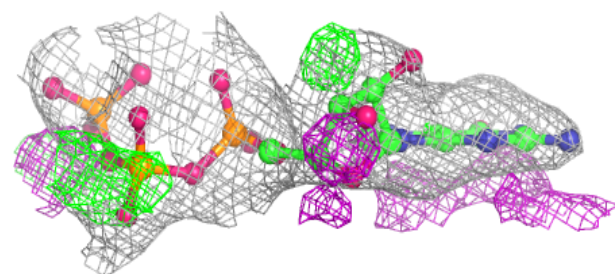
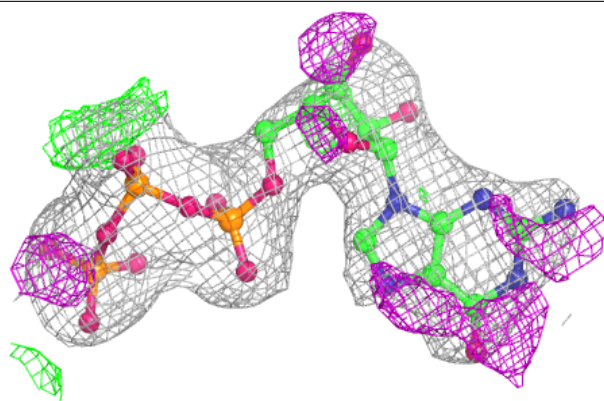
**Electron density around GTP C 502 (A):**

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

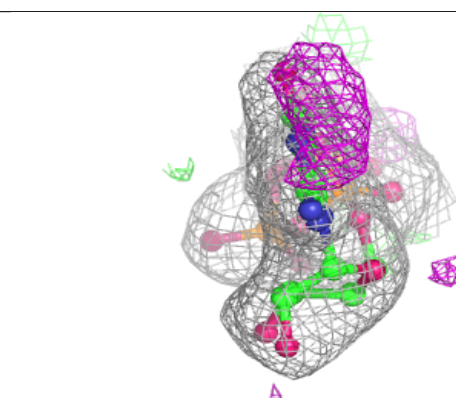
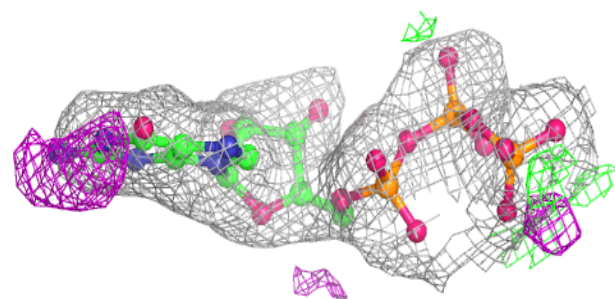
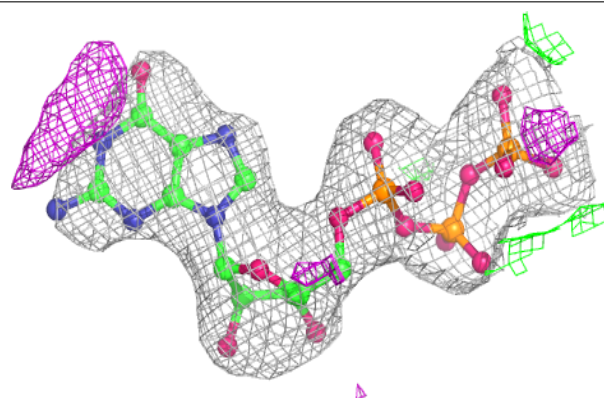


Electron density around GTP C 502 (B):

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

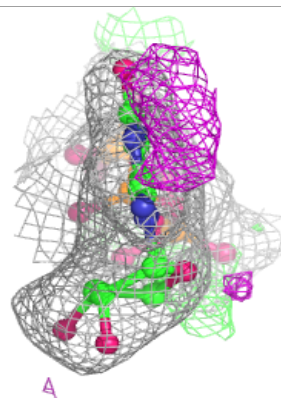
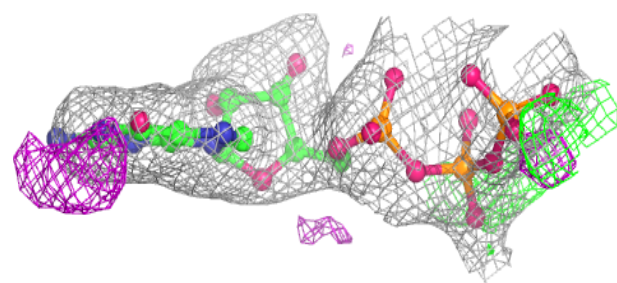
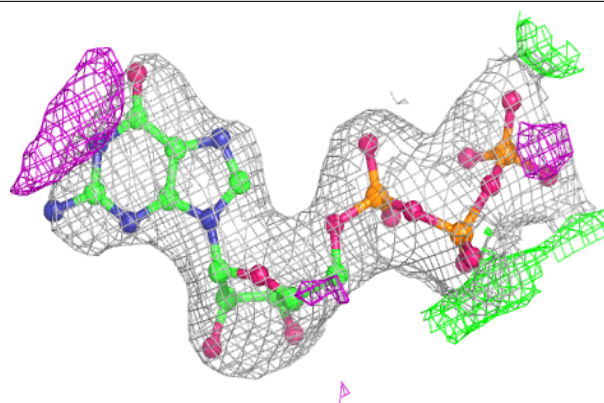
**Electron density around GTP D 502 (A):**

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

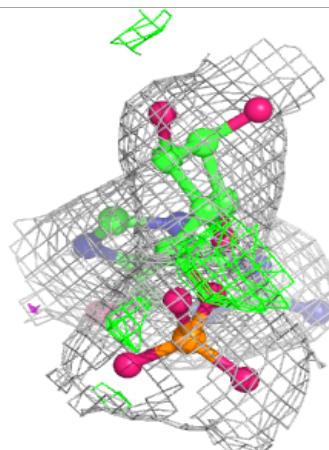
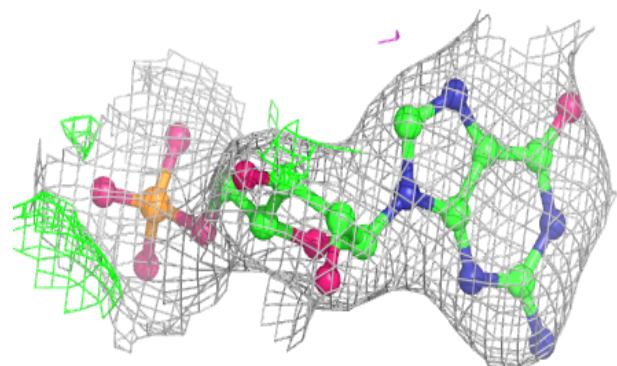
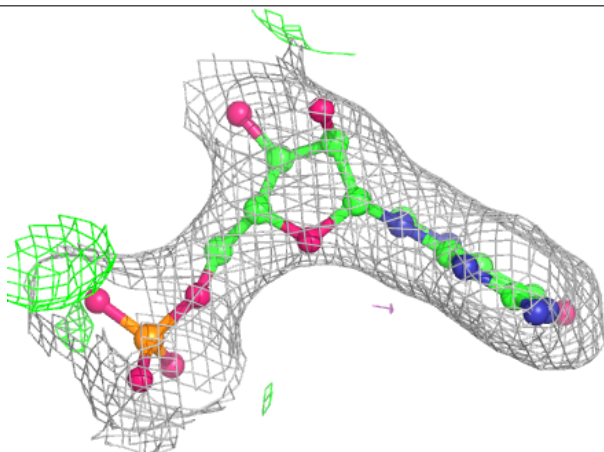


Electron density around GTP D 502 (B):

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

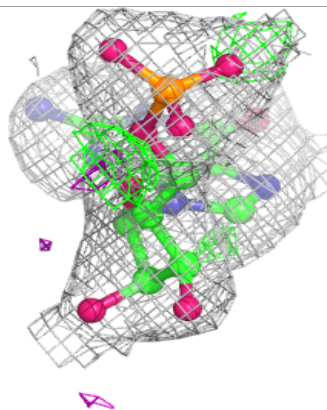
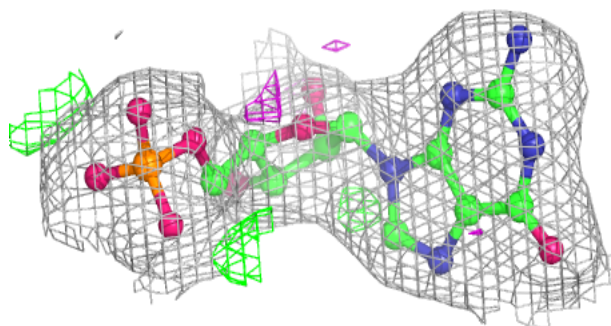
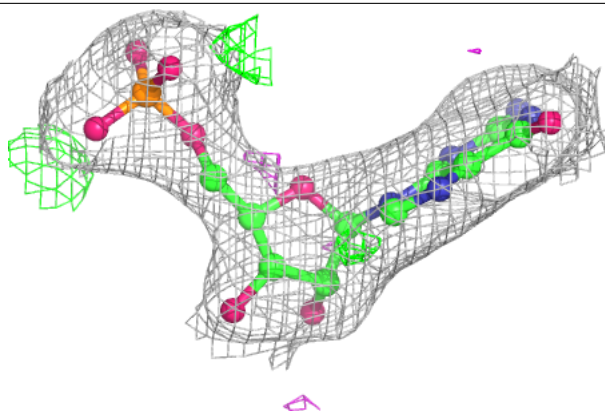
**Electron density around 5GP F 501:**

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

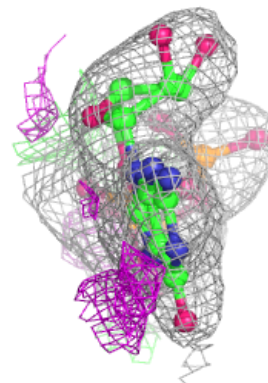
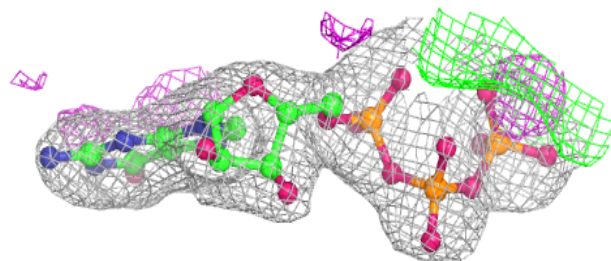
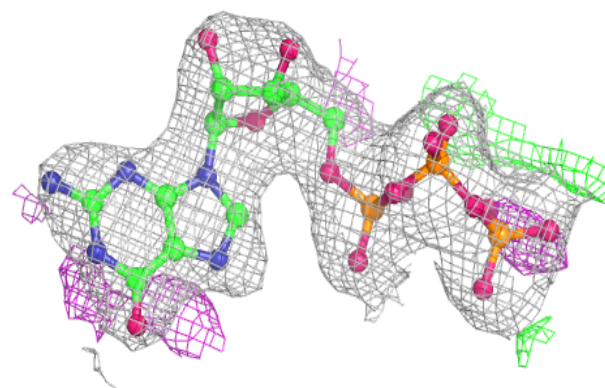


Electron density around 5GP G 501:

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

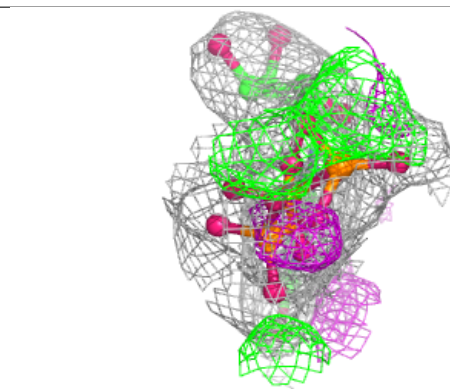
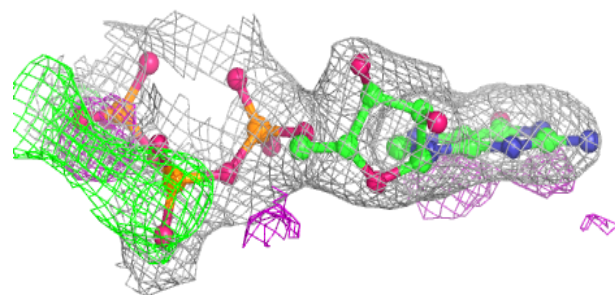
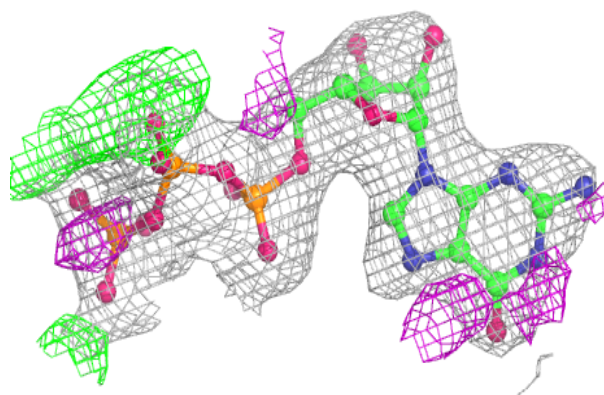
**Electron density around GTP A 502 (A):**

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

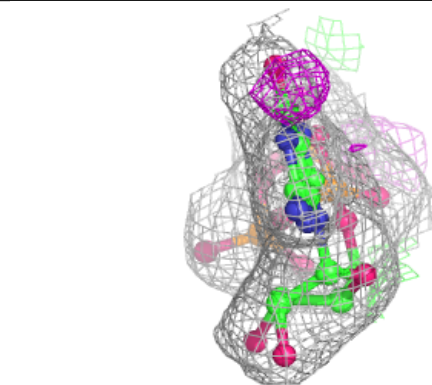
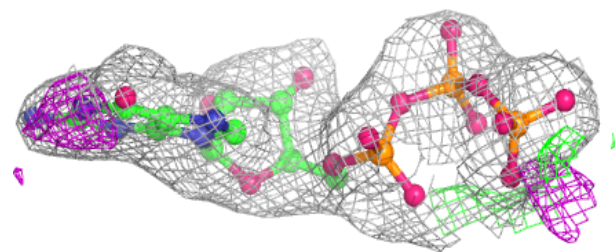
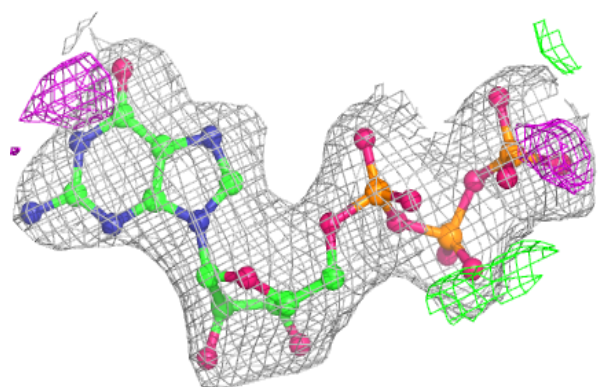


Electron density around GTP A 502 (B):

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

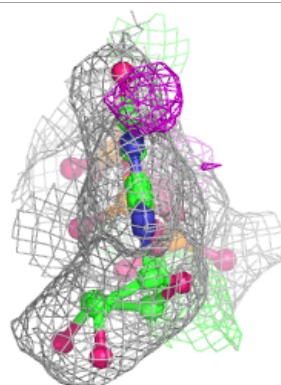
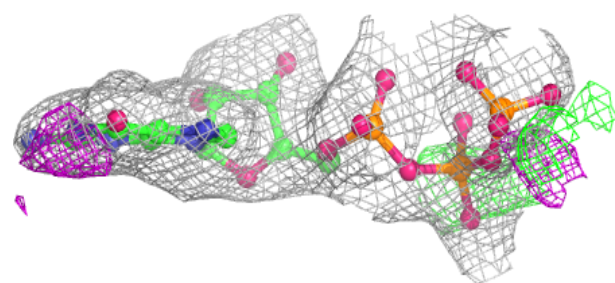
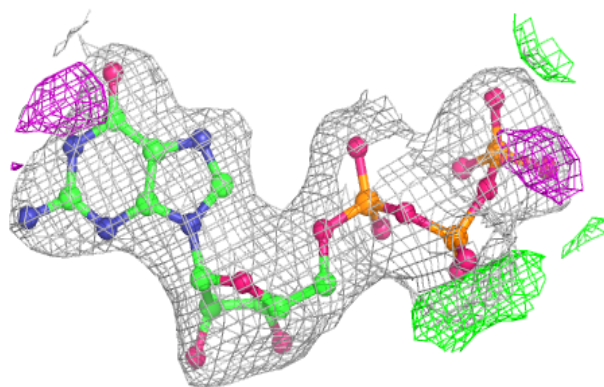
**Electron density around GTP B 502 (A):**

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

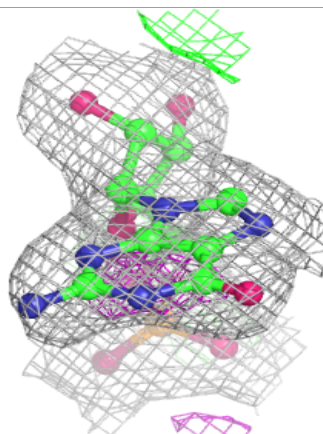
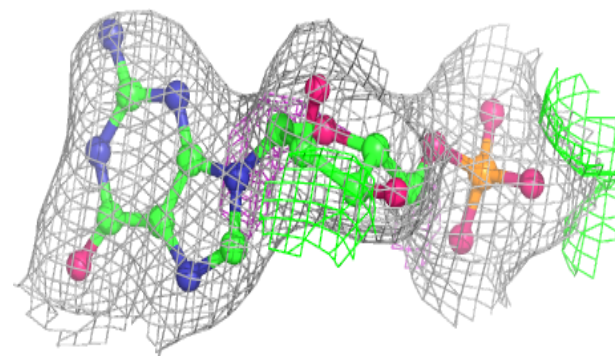
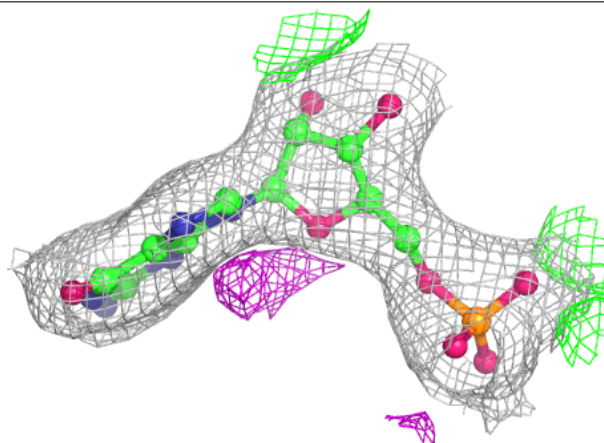


Electron density around GTP B 502 (B):

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

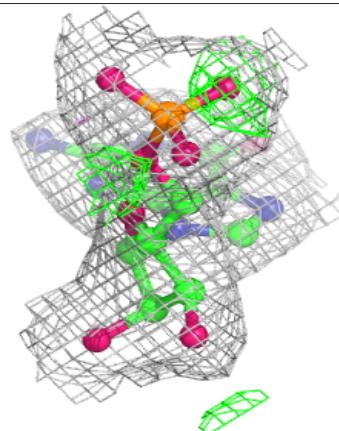
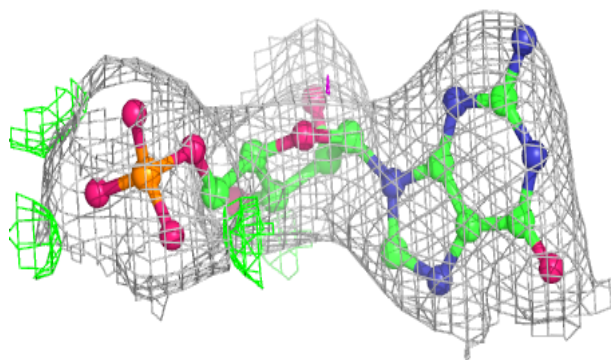
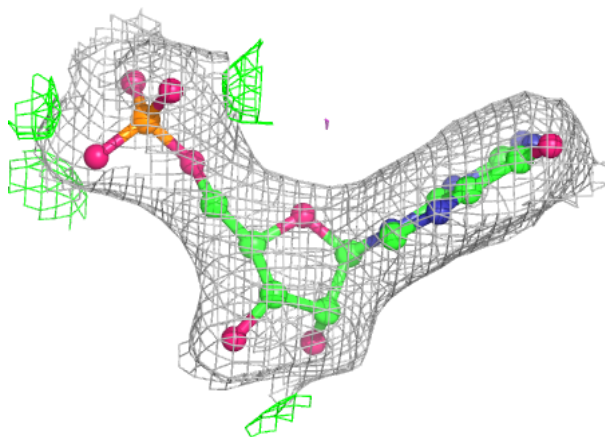
**Electron density around 5GP C 501:**

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



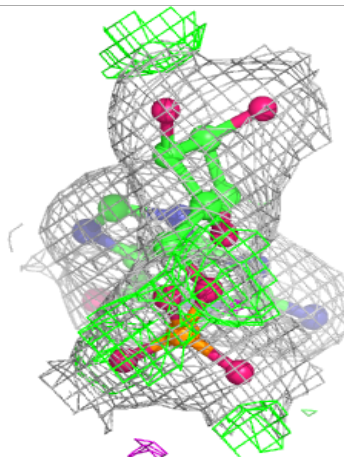
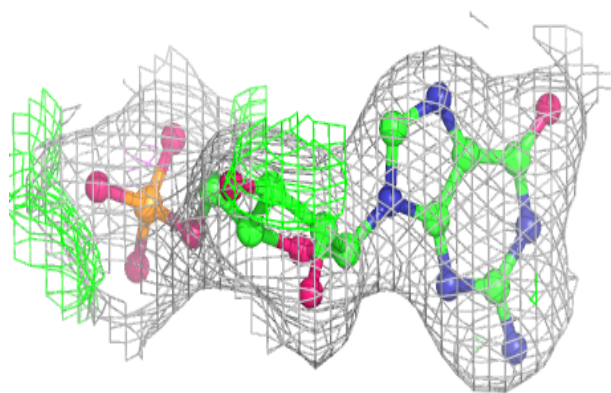
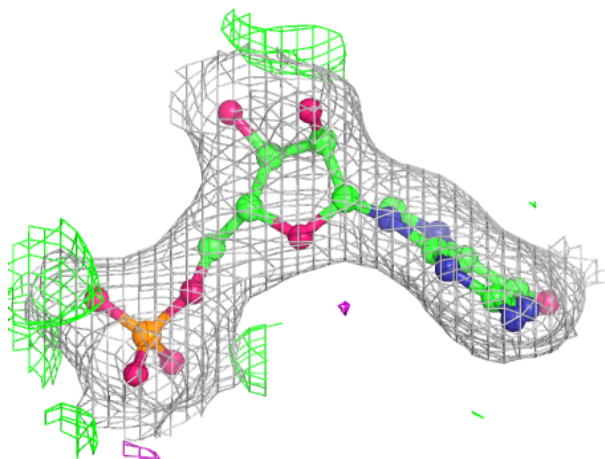
Electron density around 5GP E 501:

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



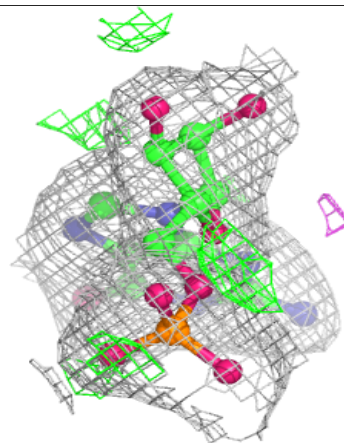
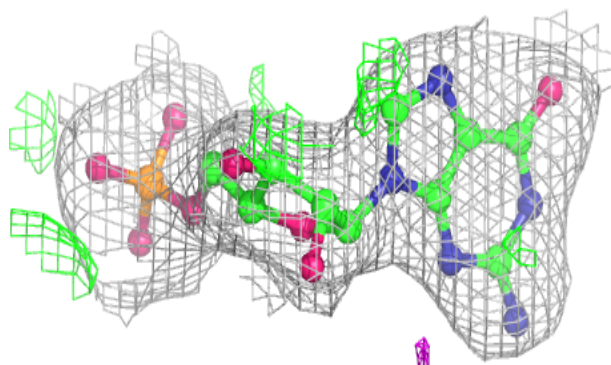
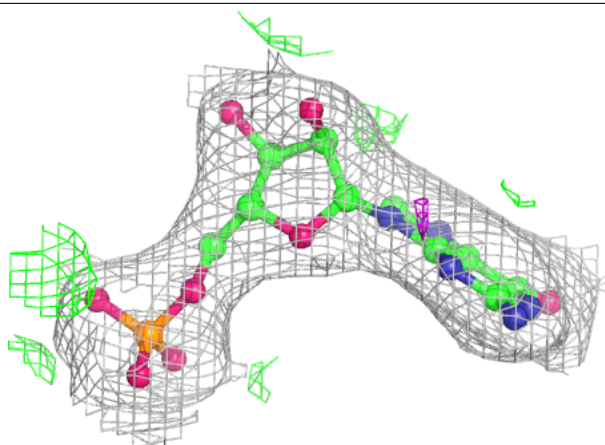
Electron density around 5GP A 501:

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



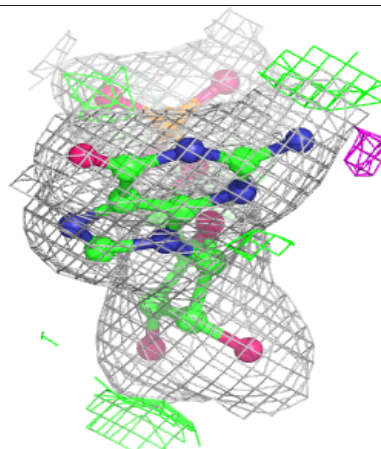
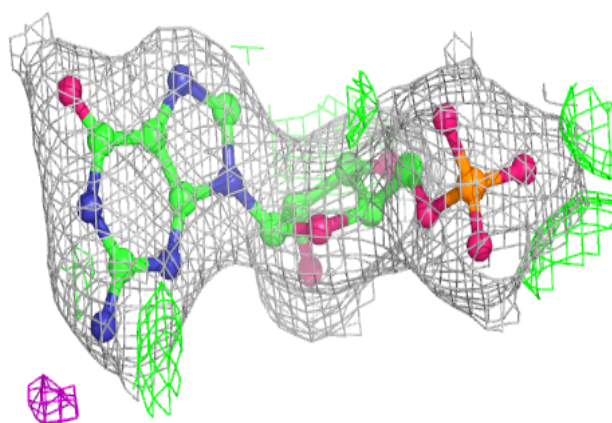
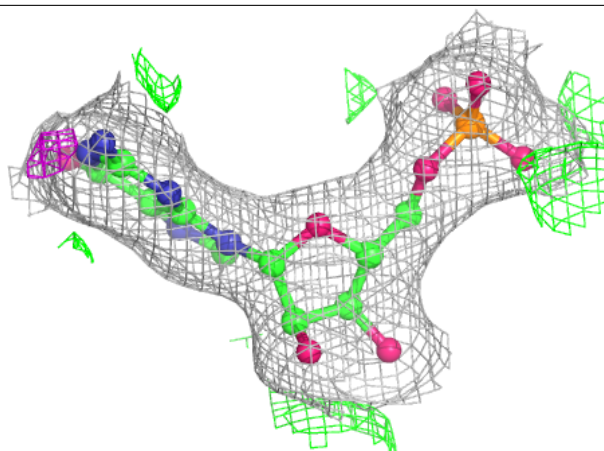
Electron density around 5GP H 501:

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



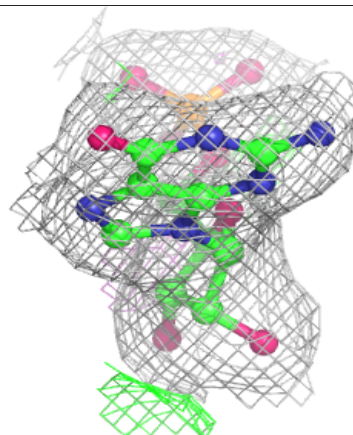
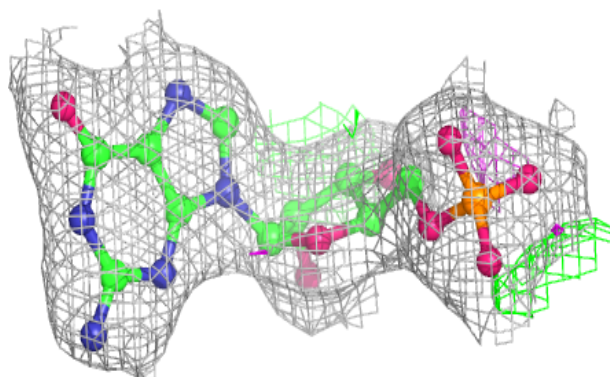
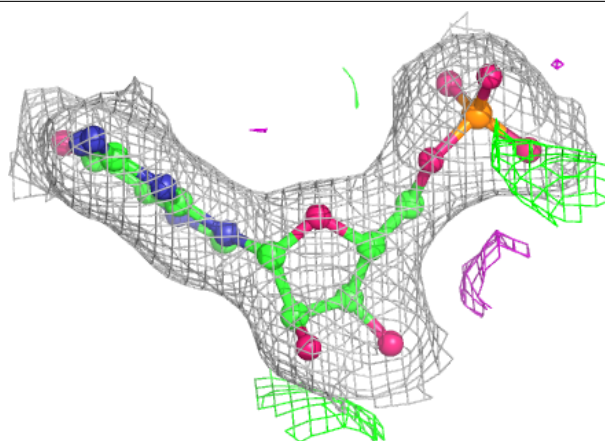
Electron density around 5GP B 501:

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



Electron density around 5GP D 501:

$2mF_o-DF_c$ (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.