



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 03:32 pm GMT

PDB ID : 6SVS
Title : Crystal Structure of U:A-U-rich RNA triple helix with 11 consecutive base triples
Authors : Ruszkowska, A.; Ruszkowski, M.; Hulewicz, J.P.; Dauter, Z.; Brown, J.A.
Deposited on : 2019-09-18
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

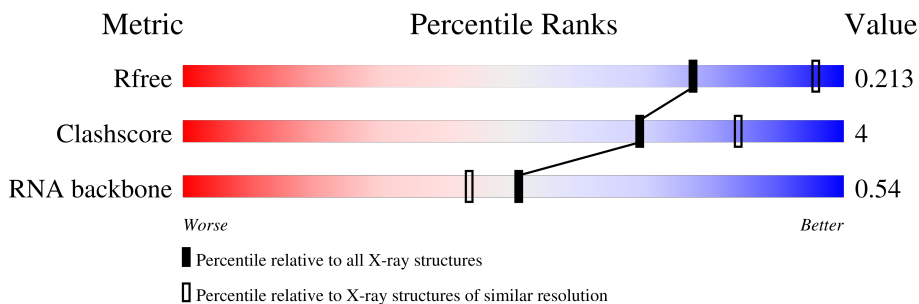
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	77	<div> <div style="width: 74%; background-color: green;"></div> <div style="width: 26%; background-color: yellow;"></div> </div> <div>74% 26%</div>
1	B	77	<div> <div style="width: 70%; background-color: green;"></div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> </div> <div>70% 27% .</div>

2 Entry composition [i](#)

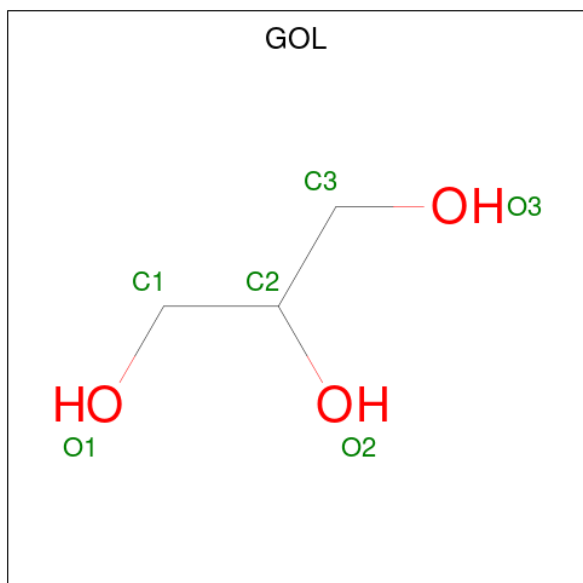
There are 6 unique types of molecules in this entry. The entry contains 3397 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA chain called RNA (79-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	77	Total	C	N	O	P	0	0	0
			1629	731	278	543	77			
1	B	77	Total	C	N	O	P	0	0	0
			1629	731	278	543	77			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

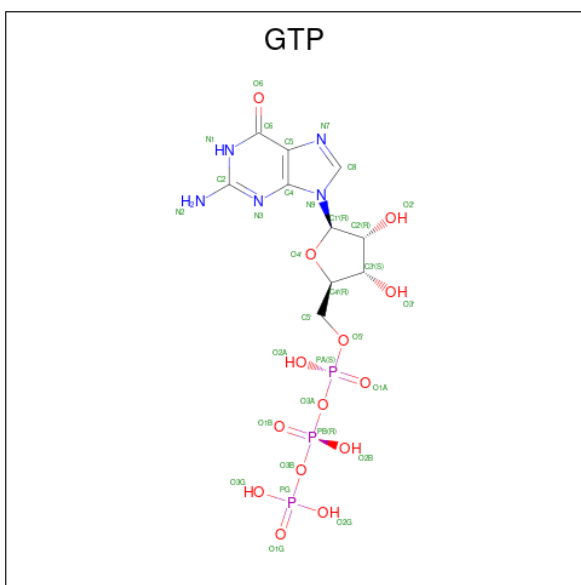


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

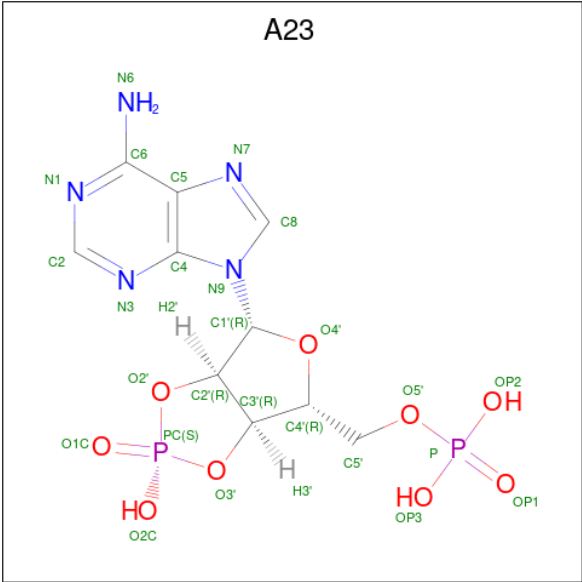
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Ca 4 4	0	0
3	B	4	Total Ca 4 4	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

- Molecule 5 is ADENOSINE-5'-PHOSPHATE-2',3'-CYCLIC PHOSPHATE (three-letter code: A23) (formula: $\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_9\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	10	5	8	2		
5	B	1	Total	C	N	O	P	0	0
			25	10	5	8	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	1	Total	O	0	0
			1	1		

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA (79-mer)

Chain A:  74% 26%



- Molecule 1: RNA (79-mer)

Chain B:  70% 27% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.72Å 78.11Å 84.02Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	40.70 – 2.50 40.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	54.3 (40.70-2.50) 54.3 (40.73-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.167 , 0.213 0.167 , 0.213	Depositor DCC
R_{free} test set	633 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A23, GTP, GOL, CA

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	0.48	0/1820	0.93	0/2830
1	B	0.38	0/1820	0.91	0/2830
All	All	0.44	0/3640	0.92	0/5660

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

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	1629	0	818	6	0
1	B	1629	0	818	12	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	32	0	11	0	0
4	B	32	0	11	0	0
5	A	25	0	10	0	0
5	B	25	0	10	0	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
All	All	3397	0	1694	18	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 (18) 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:B:16:U:H1'	1:B:77:A:H5''	1.71	0.73
1:B:13:U:H2'	1:B:14:U:O4'	2.09	0.52
1:B:32:U:H2'	1:B:33:C:C6	2.46	0.51
1:A:50:U:O2'	1:A:52:G:OP2	2.26	0.50
1:B:39:G:H2'	1:B:40:U:C5	2.48	0.48
1:B:45:C:H2'	1:B:46:U:C6	2.49	0.47
1:A:18:C:H42	1:A:39:G:H1	1.64	0.46
1:B:39:G:H2'	1:B:40:U:C6	2.52	0.45
1:A:39:G:H2'	1:A:40:U:C6	2.52	0.45
1:B:30:A:C5	1:B:31:G:H1'	2.52	0.44
1:B:6:G:H1	1:B:53:C:H42	1.66	0.43
1:B:30:A:N7	1:B:31:G:H1'	2.34	0.43
1:B:57:U:C4	1:B:58:C:C4	3.06	0.43
1:A:30:A:C5	1:A:31:G:H1'	2.54	0.42
1:A:32:U:H2'	1:A:33:C:C6	2.55	0.42
1:A:28:A:H2'	1:A:29:A:C8	2.56	0.41
1:B:45:C:H2'	1:B:46:U:H6	1.87	0.40
1:B:28:A:H2'	1:B:29:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	76/77 (98%)	9 (11%)	0
1	B	76/77 (98%)	7 (9%)	0
All	All	152/154 (98%)	16 (10%)	0

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	C
1	A	23	A
1	A	36	C
1	A	53	C
1	A	57	U
1	A	62	A
1	A	68	A
1	A	69	A
1	A	72	A
1	B	28	A
1	B	40	U
1	B	59	U
1	B	68	A
1	B	69	A
1	B	70	A
1	B	76	A

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	101	-	5,5,5	0.96	0	5,5,5	0.93	0
4	GTP	B	106	1,3	26,34,34	2.30	7 (26%)	33,54,54	2.01	5 (15%)
4	GTP	A	106	1,3	26,34,34	2.02	6 (23%)	33,54,54	2.13	6 (18%)
5	A23	A	107	1	19,28,29	0.94	1 (5%)	19,43,46	1.07	1 (5%)
2	GOL	A	101	-	5,5,5	1.02	0	5,5,5	0.98	0
5	A23	B	107	1	19,28,29	0.89	0	19,43,46	1.07	1 (5%)

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	GOL	B	101	-	-	3/4/4/4	-
4	GTP	B	106	1,3	-	6/18/38/38	0/3/3/3
4	GTP	A	106	1,3	-	4/18/38/38	0/3/3/3
5	A23	A	107	1	-	2/3/35/36	0/4/4/4
2	GOL	A	101	-	-	0/4/4/4	-
5	A23	B	107	1	-	3/3/35/36	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	106	GTP	PA-O5'	6.41	1.85	1.59
4	B	106	GTP	C6-N1	6.12	1.43	1.33
4	A	106	GTP	C6-N1	5.82	1.43	1.33
4	A	106	GTP	PA-O5'	4.98	1.79	1.59
4	A	106	GTP	O3'-C3'	-3.37	1.35	1.43
4	B	106	GTP	C2-N1	3.31	1.41	1.35
4	B	106	GTP	C2'-C1'	3.29	1.58	1.53
4	B	106	GTP	C5'-C4'	3.18	1.61	1.51
4	A	106	GTP	O5'-C5'	-3.06	1.33	1.44
4	B	106	GTP	C2-N2	2.69	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	106	GTP	O5'-C5'	-2.61	1.34	1.44
4	A	106	GTP	C2-N1	2.48	1.39	1.35
4	A	106	GTP	C2-N2	2.38	1.38	1.33
5	A	107	A23	C4-N3	2.06	1.38	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	106	GTP	C5-C6-N1	-8.37	111.98	123.43
4	B	106	GTP	C5-C6-N1	-8.19	112.23	123.43
4	B	106	GTP	O5'-PA-O1A	-3.67	94.72	109.07
4	A	106	GTP	C2-N1-C6	3.56	121.59	115.93
4	A	106	GTP	C2-N3-C4	-3.47	111.40	115.36
4	B	106	GTP	C2-N1-C6	3.18	120.97	115.93
4	A	106	GTP	O5'-PA-O1A	-2.89	97.76	109.07
4	B	106	GTP	C2-N3-C4	-2.84	112.12	115.36
4	A	106	GTP	C1'-N9-C4	-2.48	122.28	126.64
5	B	107	A23	O2C-PC-O1C	2.30	117.33	109.89
5	A	107	A23	O2C-PC-O1C	2.26	117.20	109.89
4	B	106	GTP	O2A-PA-O5'	-2.22	97.42	107.75
4	A	106	GTP	C4-C5-N7	2.05	111.54	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	106	GTP	O4'-C4'-C5'-O5'
4	B	106	GTP	PB-O3B-PG-O2G
4	B	106	GTP	C5'-O5'-PA-O1A
4	B	106	GTP	C5'-O5'-PA-O2A
5	A	107	A23	O4'-C4'-C5'-O5'
5	B	107	A23	O4'-C4'-C5'-O5'
5	B	107	A23	C3'-C4'-C5'-O5'
4	A	106	GTP	C3'-C4'-C5'-O5'
5	A	107	A23	C3'-C4'-C5'-O5'
2	B	101	GOL	O1-C1-C2-C3
2	B	101	GOL	C1-C2-C3-O3
2	B	101	GOL	O1-C1-C2-O2
4	B	106	GTP	PB-O3A-PA-O5'
4	B	106	GTP	C5'-O5'-PA-O3A
5	B	107	A23	C4'-C5'-O5'-P
4	A	106	GTP	PG-O3B-PB-O3A

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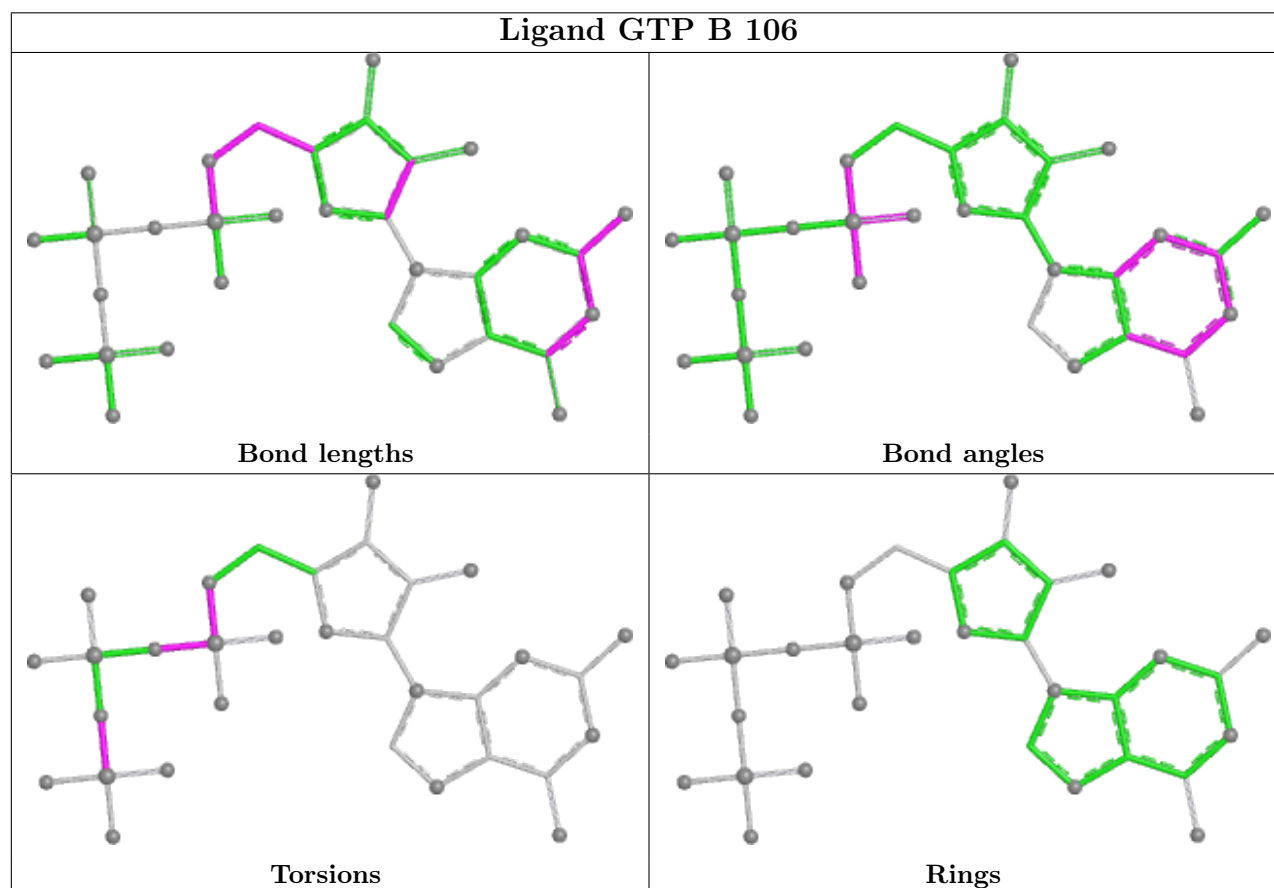
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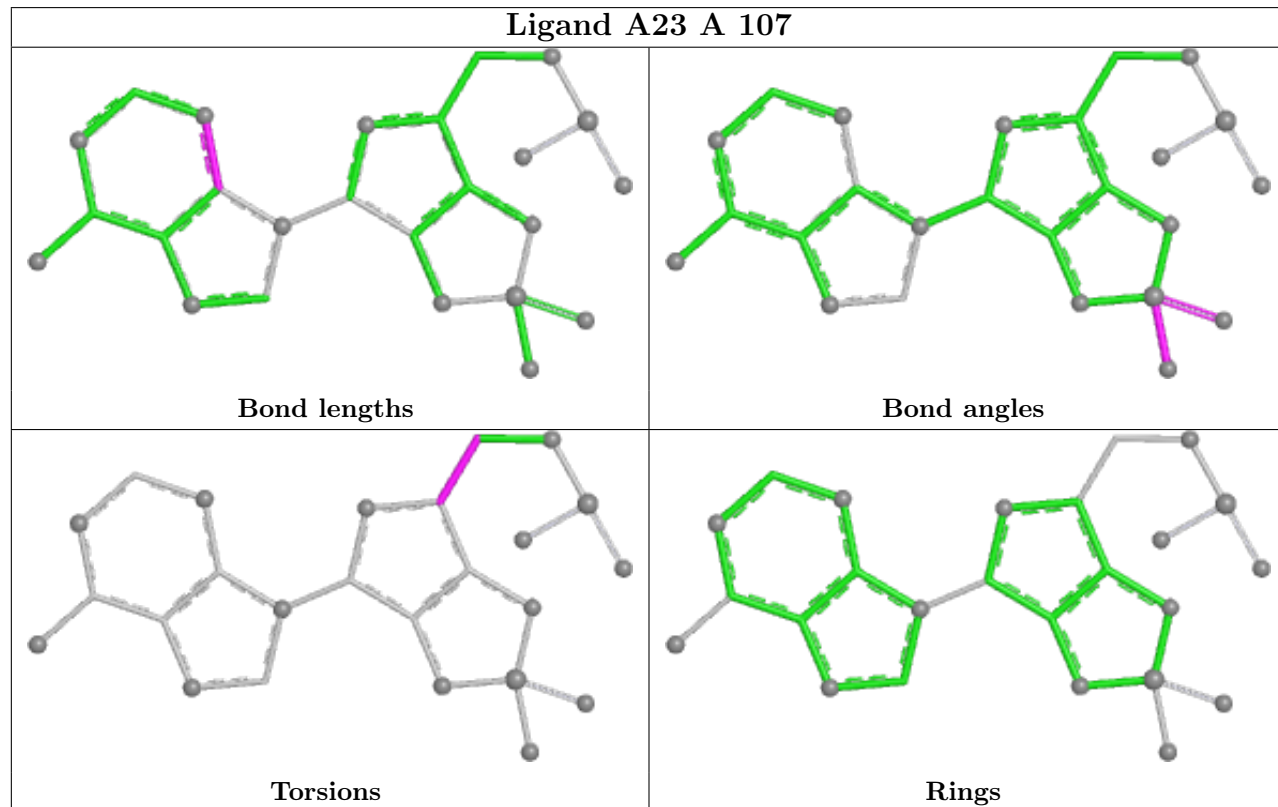
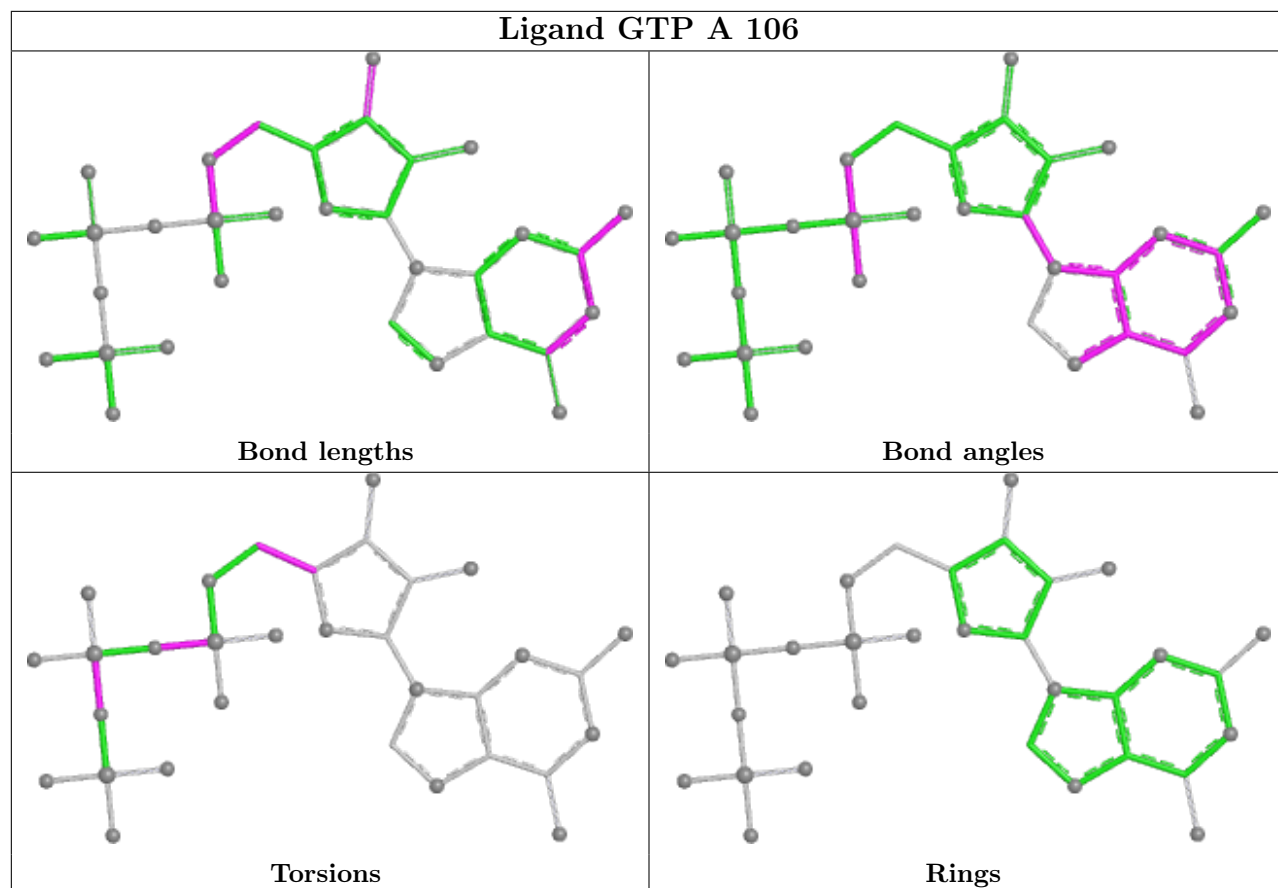
Mol	Chain	Res	Type	Atoms
4	A	106	GTP	PB-O3A-PA-O1A
4	B	106	GTP	PB-O3A-PA-O2A

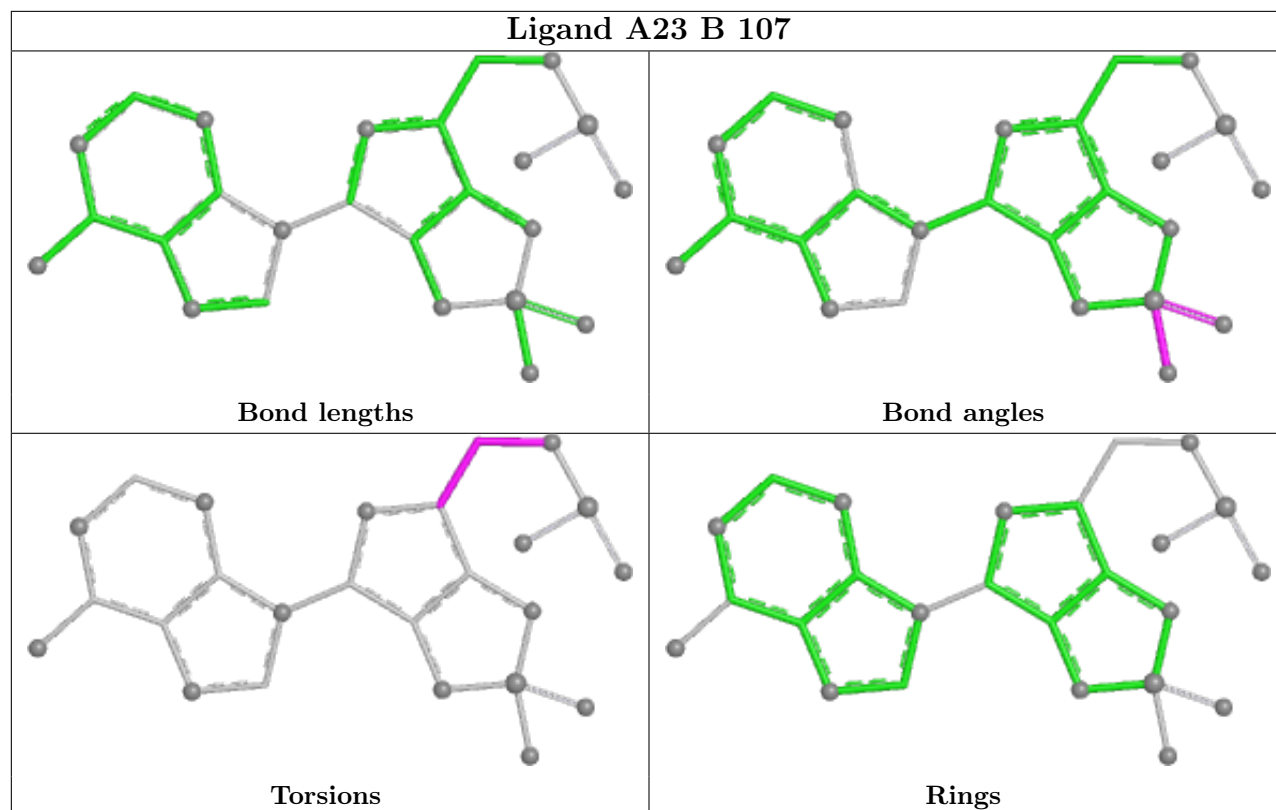
There are no ring outliers.

No monomer is involved in short contacts.

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.







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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

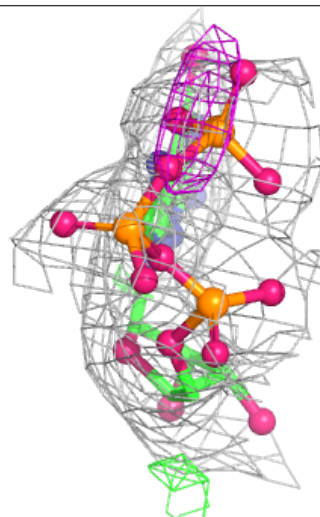
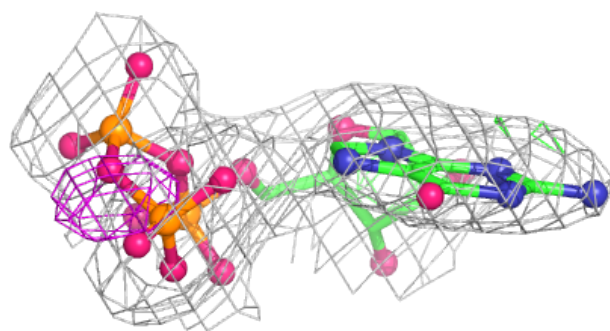
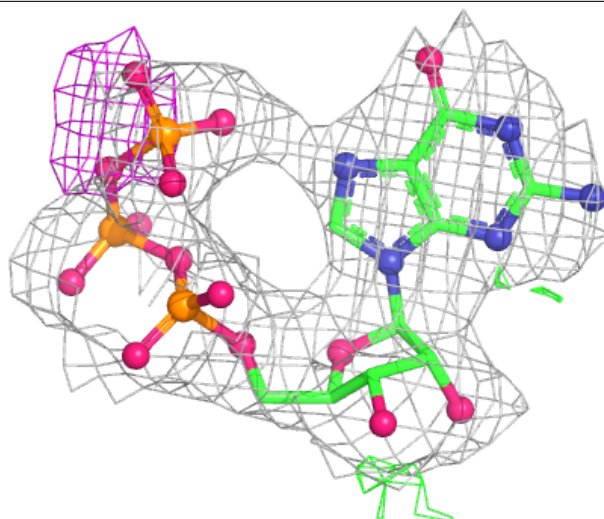
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

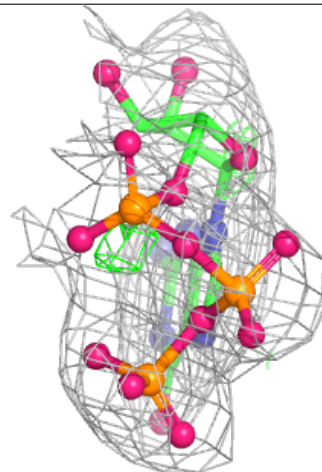
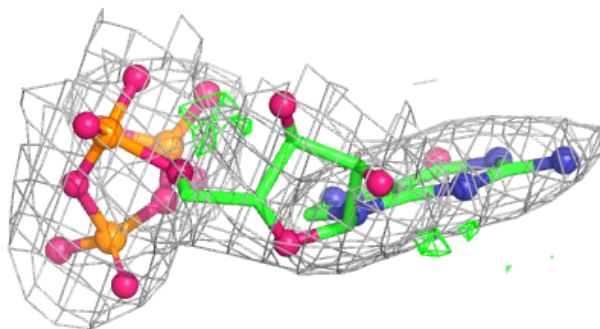
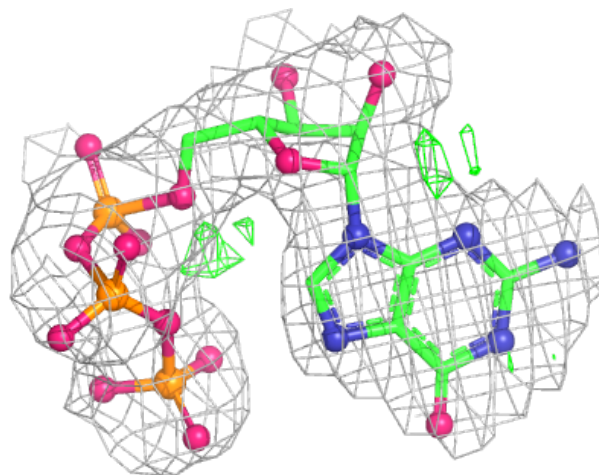
Electron density around GTP A 106:

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



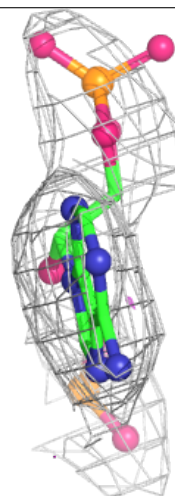
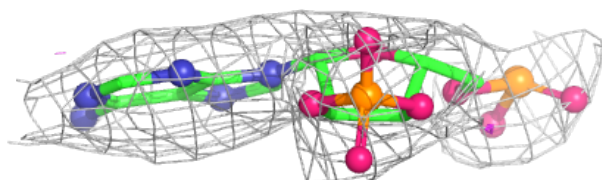
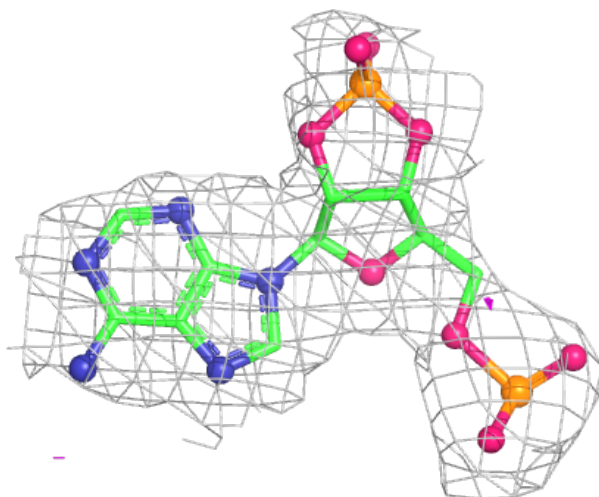
Electron density around GTP B 106:

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



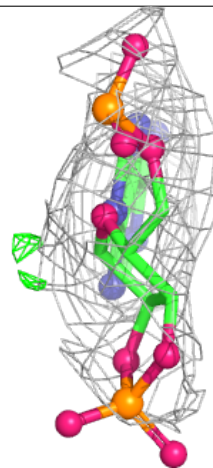
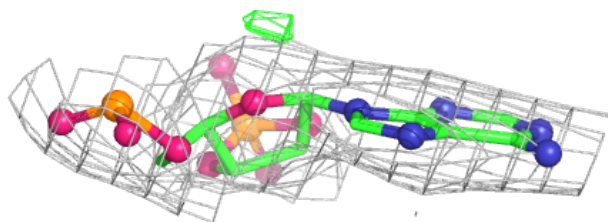
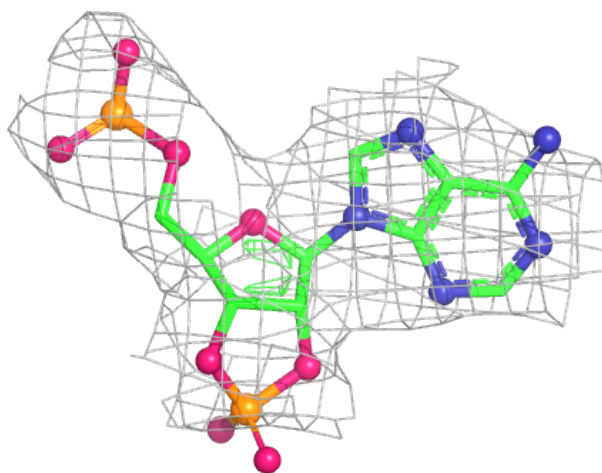
Electron density around A23 A 107:

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



Electron density around A23 B 107:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.