



# Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2022 – 07:31 pm GMT

Deposition ID : D\_1292121132

**This wwPDB validation report is NOT for manuscript review**

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
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)	:	2.26

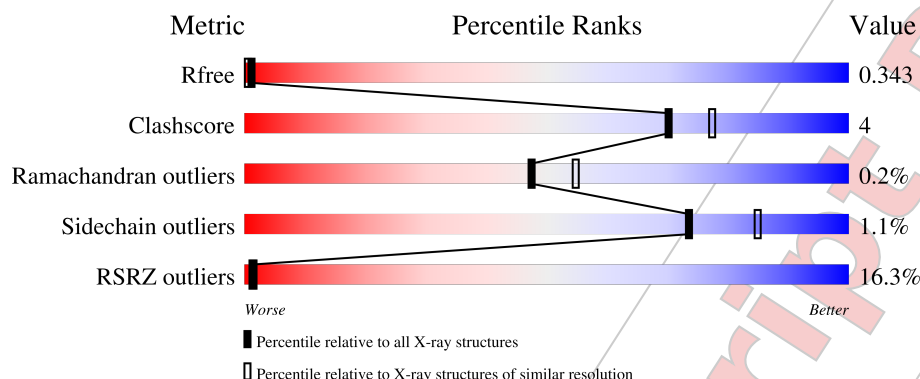
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	437	<div> <div>11%</div> <div>93%</div> <div>6%</div> </div>
2	B	426	<div> <div>24%</div> <div>88%</div> <div>12%</div> </div>
3	F	155	<div> <div>11%</div> <div>90%</div> <div>10%</div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8352 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3444	2183	584	653	24	4	8	0

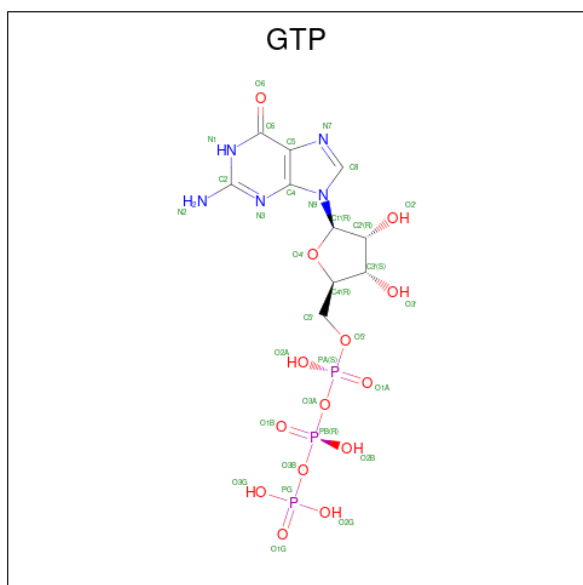
- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3347	2105	568	647	27	5	3	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	155	1154	727	198	226	3	0	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

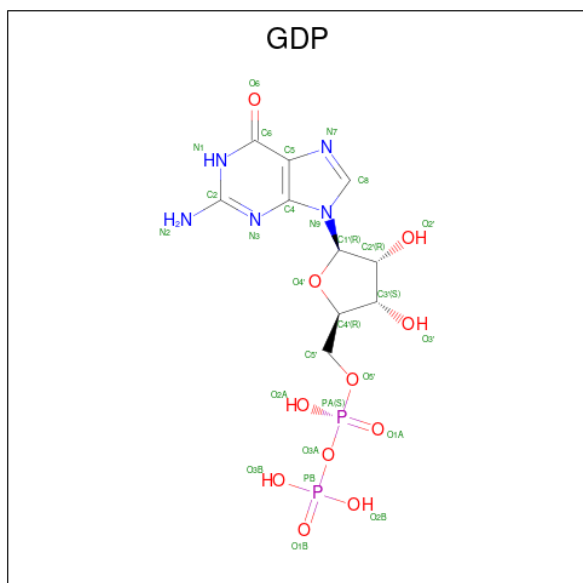


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is a ligand with the chemical component id XXX but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for XXX. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			23	16	2	5		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		

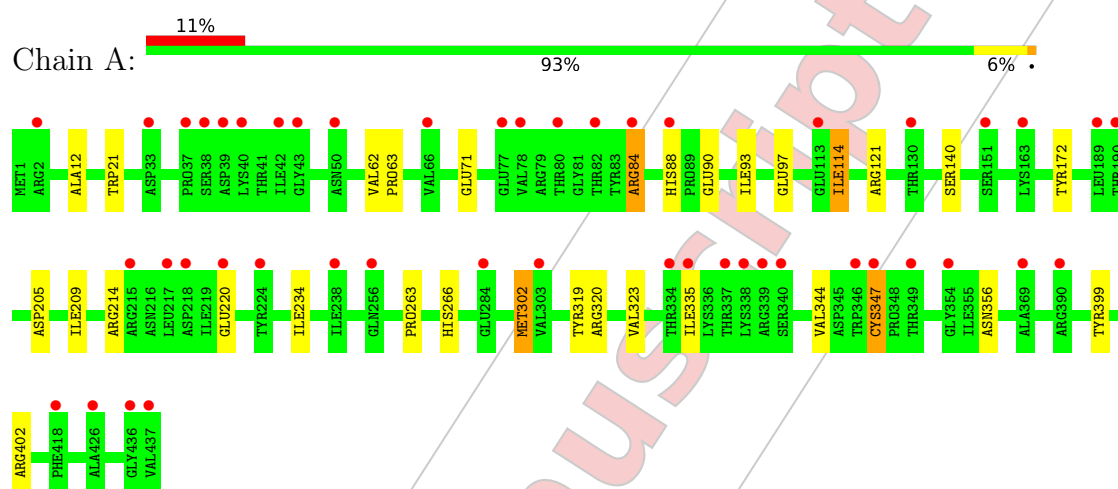
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	322	Total	O	0	0
			322	322		

### 3 Residue-property plots

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

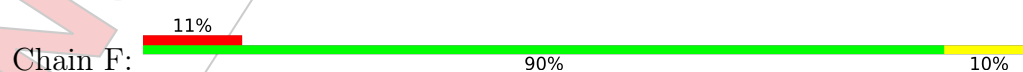
#### • Molecule 1:



#### • Molecule 2:



#### • Molecule 3:



ASP13	+	LYS17	+	ALA22	+	ASP28	+	ILE32	+	LEU33	+	ASN36	+	ASP39	+	VAL40	+	ASN41	+	ALA42	+	TYR57	+	GLU61	+	VAL65	+	LEU66	+	ILE80	+	LEU93	+	LYS101	+	ALA104	+	ALA120	+	ALA121	+	VAL131	+	LEU132	+	LEU133	+	LYS134	+	THR148	+	ALA149	+	PHE150	+	ASP151	+	ILE152	+	GLY157	+	LEU161	+	ALA162	+	GLU163	+	ILE164	+	LEU165	+	GLN166	+	LYS167	+
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.53Å 92.58Å 83.99Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	9.49 – 2.20 9.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (9.49-2.20) 93.7 (9.49-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 2.21Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.311 , 0.343 0.311 , 0.343	Depositor DCC
$R_{free}$ test set	1858 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GDP, CA, XXX, MG

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	0.24	0/3546	0.46	0/4816
2	B	0.24	0/3429	0.45	0/4644
3	F	0.23	0/1170	0.40	0/1590
All	All	0.24	0/8145	0.44	0/11050

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	3444	0	3368	19	0
2	B	3347	0	3226	30	0
3	F	1154	0	1156	9	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
6	B	28	0	12	1	0
7	B	23	0	1	0	0
8	C	1	0	0	0	0
9	S	322	0	0	8	0
All	All	8352	0	7775	56	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 (56) 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)
2:B:161:ASP:O	2:B:251:ARG:NH2	2.24	0.70
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.73	0.69
2:B:201:CYS:SG	9:S:311:HOH:O	2.53	0.67
2:B:145:SER:HG	2:B:188:SER:HG	1.43	0.62
1:A:263:PRO:O	1:A:266:HIS:ND1	2.27	0.61
2:B:145:SER:OG	2:B:188:SER:OG	2.18	0.60
1:A:320:ARG:NH2	9:S:305:HOH:O	2.34	0.59
3:F:101:LYS:NZ	9:S:263:HOH:O	2.36	0.58
2:B:363:MET:SD	9:S:284:HOH:O	2.57	0.57
2:B:135:LEU:HB3	2:B:166:THR:HG22	1.86	0.56
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.88	0.56
2:B:1:MET:N	2:B:249:ASP:HB3	2.21	0.55
2:B:209:ASP:HB3	2:B:213:ARG:HH21	1.72	0.54
1:A:209:ILE:HD11	1:A:302[B]:MET:HG3	1.88	0.54
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.89	0.53
2:B:211:CYS:HA	2:B:215:LEU:HB2	1.92	0.52
1:A:90:GLU:O	1:A:121:ARG:NH1	2.44	0.51
2:B:11:GLN:NE2	9:S:306:HOH:O	2.44	0.50
2:B:307:HIS:ND1	2:B:376:GLU:OE2	2.39	0.50
3:F:36:ASN:ND2	9:S:296:HOH:O	2.44	0.50
3:F:133:LEU:HD11	3:F:165:LEU:HD23	1.93	0.50
2:B:23:VAL:HG21	2:B:230:SER:HB2	1.95	0.49
2:B:31:ASP:OD1	2:B:35:SER:N	2.45	0.49
2:B:170:MET:HB2	2:B:203:ASP:HA	1.93	0.48
2:B:178:THR:HG22	2:B:180:VAL:HG22	1.96	0.48
2:B:61:PRO:HD3	2:B:84:ILE:HG13	1.94	0.48
1:A:84:ARG:NH2	9:S:241:HOH:O	2.39	0.48
1:A:93:ILE:HG22	1:A:114:ILE:HD11	1.96	0.47
3:F:40:VAL:HG13	3:F:66:LEU:HD22	1.96	0.47
2:B:396:HIS:NE2	3:F:57:TYR:OH	2.38	0.46
2:B:52:ASN:OD1	2:B:62:ARG:NH2	2.49	0.46
2:B:1:MET:H1	2:B:249:ASP:HB3	1.81	0.46
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.51	0.46
1:A:84:ARG:NH1	9:S:299:HOH:O	2.48	0.46
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.51	0.45
2:B:67:ASP:OD1	2:B:68:LEU:N	2.50	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.52	0.44
3:F:17:LYS:HG2	3:F:33:LEU:HD11	1.99	0.43
1:A:209:ILE:HD11	1:A:302[A]:MET:HG3	1.99	0.43
1:A:97:GLU:HG3	2:B:1:MET:SD	2.59	0.42
2:B:117:LEU:HD11	2:B:154:LYS:HB3	2.01	0.42
2:B:121:ARG:HG3	2:B:158:GLU:OE2	2.19	0.42
2:B:45:GLU:HG2	2:B:243:PRO:HG3	2.02	0.42
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.00	0.42
1:A:214:ARG:NH1	1:A:220:GLU:O	2.53	0.42
2:B:211:CYS:HB3	2:B:217:LEU:HD12	2.02	0.42
2:B:178:THR:HB	2:B:181:GLU:HG3	2.02	0.41
3:F:39:ASP:HB3	3:F:42:ALA:HB2	2.01	0.41
3:F:93:LEU:HD11	3:F:131:VAL:HG21	2.03	0.41
1:A:234:ILE:HD13	1:A:302[A]:MET:SD	2.61	0.40
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.03	0.40
2:B:165:ASN:HD22	2:B:198:GLU:HG3	1.86	0.40
1:A:320:ARG:HA	1:A:356:ASN:O	2.21	0.40
1:A:319:TYR:HB3	1:A:323:VAL:HG21	2.03	0.40
1:A:399:TYR:O	1:A:402:ARG:NH1	2.50	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/437 (101%)	430 (97%)	12 (3%)	1 (0%)	47	55
2	B	425/426 (100%)	413 (97%)	11 (3%)	1 (0%)	47	55
3	F	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
All	All	1021/1018 (100%)	993 (97%)	26 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ILE
2	B	2	ARG

### 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	373/368 (101%)	367 (98%)	6 (2%)	62	76
2	B	367/368 (100%)	363 (99%)	4 (1%)	73	85
3	F	120/120 (100%)	120 (100%)	0	100	100
All	All	860/856 (100%)	850 (99%)	10 (1%)	73	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	84	ARG
1	A	302[A]	MET
1	A	302[B]	MET
1	A	335	ILE
1	A	347	CYS
2	B	2	ARG
2	B	39	ASP
2	B	44	LEU
2	B	137	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	GLN
2	B	165	ASN
3	F	36	ASN
3	F	102	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic and 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 2 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
4	GTP	A	501	5	26,34,34	0.98	1 (3%)	33,54,54	1.83	7 (21%)
6	GDP	B	501	-	24,30,30	1.17	2 (8%)	31,47,47	1.96	8 (25%)

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
4	GTP	A	501	5	-	7/18/38/38	0/3/3/3
6	GDP	B	501	-	-	3/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	GDP	C5-C6	4.15	1.48	1.41
4	A	501	GTP	C6-N1	3.13	1.38	1.33
6	B	501	GDP	C5-C4	2.45	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	N3-C2-N1	-5.37	120.06	127.22
6	B	501	GDP	C2-N3-C4	4.93	120.99	115.36
4	A	501	GTP	C2-N3-C4	4.26	120.23	115.36
6	B	501	GDP	C2-N1-C6	4.03	122.34	115.93
6	B	501	GDP	C5-C6-N1	-3.92	118.07	123.43
6	B	501	GDP	C4-C5-C6	-3.90	117.07	120.80
6	B	501	GDP	N3-C2-N1	-3.34	122.76	127.22
4	A	501	GTP	PB-O3B-PG	-3.17	121.93	132.83
4	A	501	GTP	PA-O3A-PB	-3.16	121.99	132.83
6	B	501	GDP	PA-O3A-PB	-2.90	122.88	132.83
4	A	501	GTP	C5-C6-N1	-2.88	119.50	123.43
6	B	501	GDP	C3'-C2'-C1'	2.79	105.19	100.98
4	A	501	GTP	C3'-C2'-C1'	2.77	105.16	100.98
6	B	501	GDP	C4-C5-N7	-2.68	106.61	109.40
4	A	501	GTP	C2-N1-C6	2.59	120.05	115.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C3'-C4'-C5'-O5'
4	A	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	O4'-C4'-C5'-O5'
6	B	501	GDP	C5'-O5'-PA-O3A

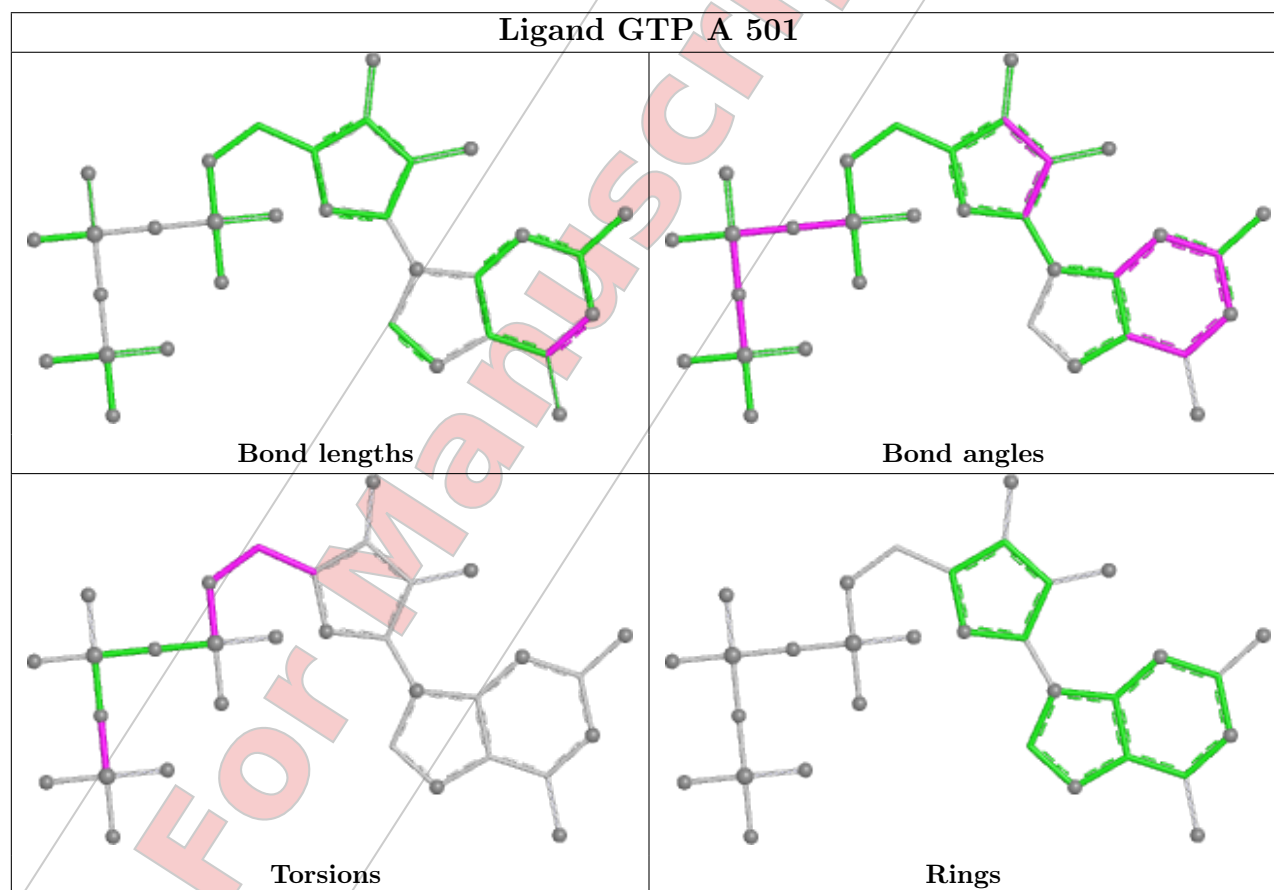
There are no ring outliers.

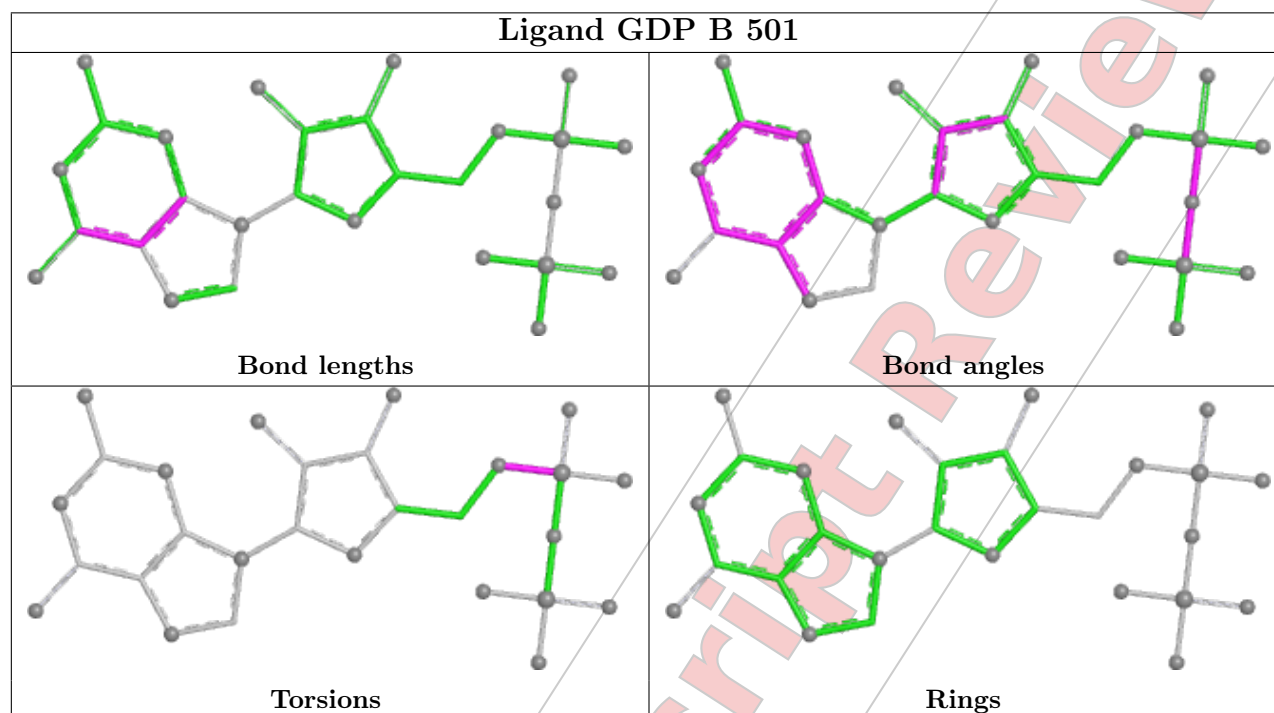
1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GDP	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	278:SER	C	284:LEU	N	12.02



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/437 (100%)	0.92	47 (10%) <b>5</b> <b>5</b>	18, 28, 44, 65	0
2	B	426/426 (100%)	1.43	102 (23%) <b>0</b> <b>0</b>	22, 37, 58, 71	0
3	F	155/155 (100%)	0.96	17 (10%) <b>5</b> <b>4</b>	22, 28, 41, 53	0
All	All	1018/1018 (100%)	1.14	166 (16%) <b>1</b> <b>1</b>	18, 30, 54, 71	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	73	MET	7.2
2	B	277	GLY	6.9
2	B	246	LEU	6.8
2	B	41	ASP	6.7
2	B	95	SER	6.1
2	B	278	SER	6.0
2	B	93	GLY	5.8
2	B	335	ASN	5.7
1	A	339	ARG	5.6
2	B	1	MET	5.6
2	B	431	ASP	5.6
2	B	332	ASN	5.3
1	A	436	GLY	5.2
1	A	437	VAL	5.2
2	B	79	GLY	4.8
2	B	109	GLY	4.5
2	B	117	LEU	4.5
2	B	430	ALA	4.5
2	B	36	TYR	4.4
3	F	167	LYS	4.4
1	A	349	THR	4.3
2	B	83	GLN	4.2
1	A	37	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	82	GLY	3.9
1	A	337	THR	3.9
2	B	323	MET	3.8
2	B	331	LEU	3.8
2	B	42	LEU	3.7
1	A	369	ALA	3.7
1	A	50	ASN	3.6
2	B	130	LEU	3.6
1	A	82	THR	3.6
1	A	2	ARG	3.5
1	A	347	CYS	3.5
2	B	231	ALA	3.5
2	B	291	GLN	3.4
2	B	57	ASN	3.4
2	B	337	ASN	3.3
2	B	322	SER	3.3
1	A	217	LEU	3.3
3	F	13	ASP	3.3
2	B	92	PHE	3.2
2	B	218	THR	3.2
2	B	333	VAL	3.2
2	B	107	THR	3.2
2	B	71	GLY	3.1
1	A	113	GLU	3.0
2	B	126	SER	3.0
1	A	43	GLY	3.0
2	B	40	SER	3.0
2	B	127	CYS	3.0
2	B	155	ILE	3.0
1	A	220	GLU	3.0
1	A	335	ILE	3.0
2	B	77	ARG	2.9
2	B	113	VAL	2.9
2	B	320	ARG	2.9
2	B	373	ALA	2.9
2	B	84	ILE	2.9
1	A	130	THR	2.9
1	A	426	ALA	2.9
2	B	324	LYS	2.9
1	A	77	GLU	2.9
2	B	394	PHE	2.9
1	A	78	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	284	GLU	2.9
1	A	42	ILE	2.8
2	B	76	VAL	2.8
2	B	409	THR	2.8
1	A	38	SER	2.8
1	A	84	ARG	2.8
1	A	238	ILE	2.8
1	A	340	SER	2.8
1	A	33	ASP	2.7
2	B	87	PRO	2.7
2	B	287	PRO	2.7
2	B	145	SER	2.7
2	B	111	GLU	2.7
2	B	303	CYS	2.7
3	F	61	GLU	2.7
2	B	39	ASP	2.7
1	A	334	THR	2.7
2	B	358	PRO	2.7
3	F	163	GLU	2.7
2	B	29	GLY	2.7
2	B	215	LEU	2.6
2	B	115	SER	2.6
2	B	360	GLY	2.6
1	A	224	TYR	2.6
2	B	88	ASP	2.6
2	B	38	GLY	2.6
3	F	148	THR	2.5
2	B	158	GLU	2.5
1	A	80	THR	2.5
2	B	248	ALA	2.5
2	B	276	ARG	2.5
1	A	346	TRP	2.5
2	B	89	ASN	2.5
2	B	396	HIS	2.5
3	F	120	ALA	2.4
2	B	397	TRP	2.4
2	B	59	TYR	2.4
2	B	31	ASP	2.4
3	F	22	ALA	2.4
1	A	215	ARG	2.4
2	B	90	PHE	2.4
2	B	286	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	88	HIS	2.4
2	B	80	PRO	2.4
2	B	385	PHE	2.4
3	F	157	GLY	2.3
2	B	206	ALA	2.3
2	B	315	ALA	2.3
2	B	176	SER	2.3
1	A	338	LYS	2.3
3	F	33	LEU	2.3
2	B	328	GLU	2.3
2	B	78	SER	2.3
2	B	10	GLY	2.3
1	A	151	SER	2.3
2	B	75	SER	2.3
2	B	364	SER	2.3
2	B	334	GLN	2.3
1	A	218	ASP	2.3
2	B	245	GLN	2.3
2	B	37	HIS	2.2
1	A	40	LYS	2.2
1	A	163	LYS	2.2
1	A	66	VAL	2.2
2	B	401	GLU	2.2
3	F	150	PHE	2.2
2	B	35	SER	2.2
1	A	190	THR	2.2
2	B	72	THR	2.2
2	B	319	GLY	2.2
1	A	390	ARG	2.2
2	B	199	THR	2.2
2	B	70	PRO	2.2
3	F	65	VAL	2.1
2	B	284	LEU	2.1
2	B	326	VAL	2.1
2	B	212	PHE	2.1
3	F	134	LYS	2.1
1	A	256[A]	GLN	2.1
2	B	47	ILE	2.1
3	F	152	ILE	2.1
3	F	104	ALA	2.1
2	B	34	GLY	2.1
2	B	227	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	129	CYS	2.1
3	F	32	ILE	2.1
2	B	389	PHE	2.1
1	A	189	LEU	2.1
3	F	28	ASP	2.1
1	A	354	GLY	2.0
2	B	329	GLN	2.0
2	B	2	ARG	2.0
2	B	144	GLY	2.0
2	B	221	THR	2.0
1	A	303	VAL	2.0
1	A	418	PHE	2.0
2	B	106	TYR	2.0
2	B	201	CYS	2.0
3	F	90	ILE	2.0
1	A	39	ASP	2.0
2	B	26	ASP	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](#)

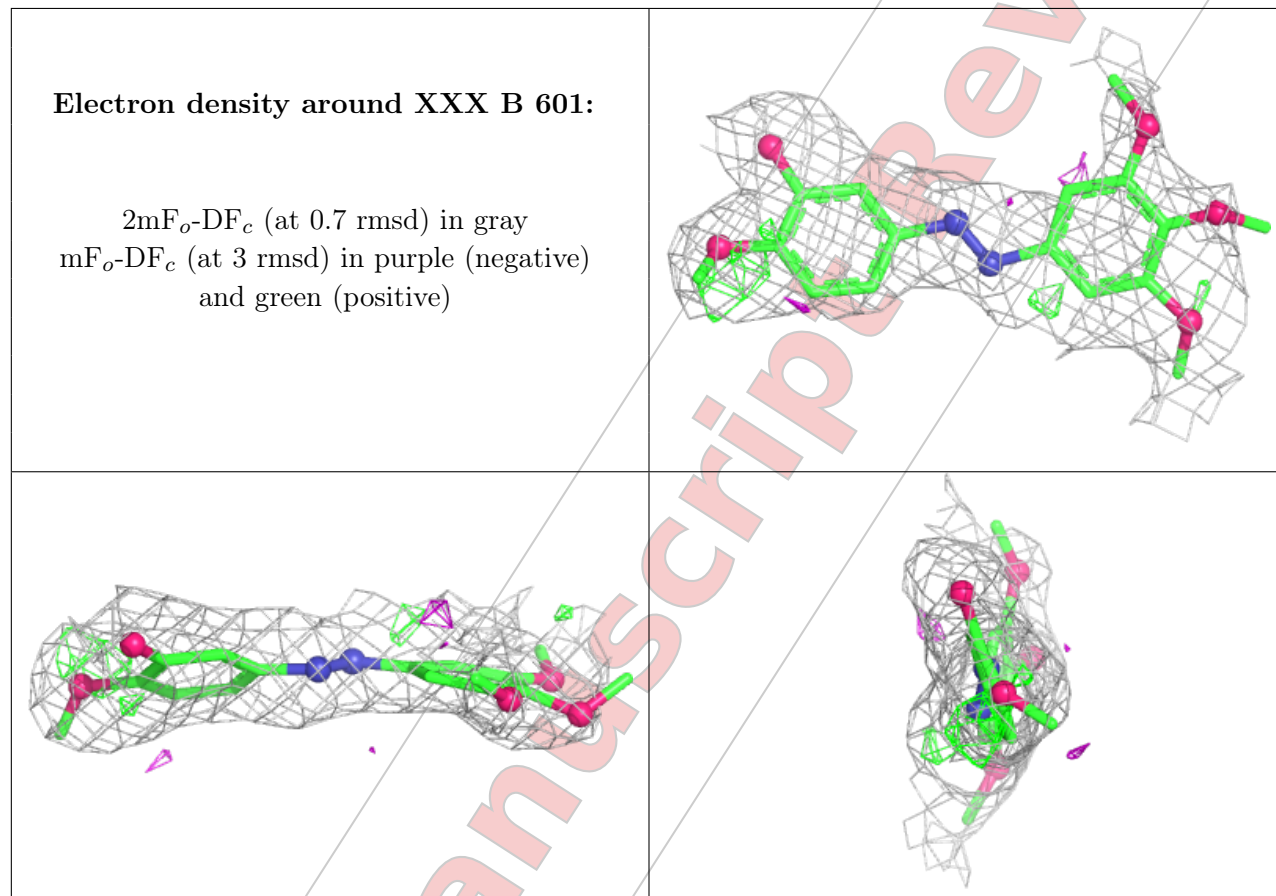
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	XXX	B	601	23/?	0.79	0.24	24,34,41,45	0
5	MG	A	502	1/?	0.83	0.17	28,28,28,28	0
8	CA	C	1	1/?	0.87	0.08	35,35,35,35	0
6	GDP	B	501	28/?	0.90	0.17	28,30,35,39	0
4	GTP	A	501	32/?	0.91	0.16	17,21,23,25	0

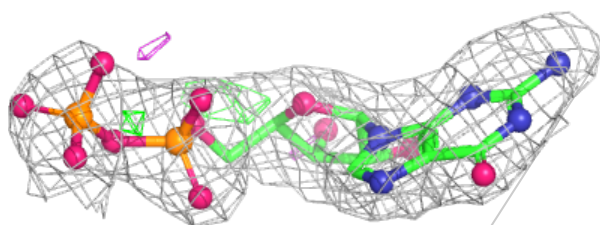
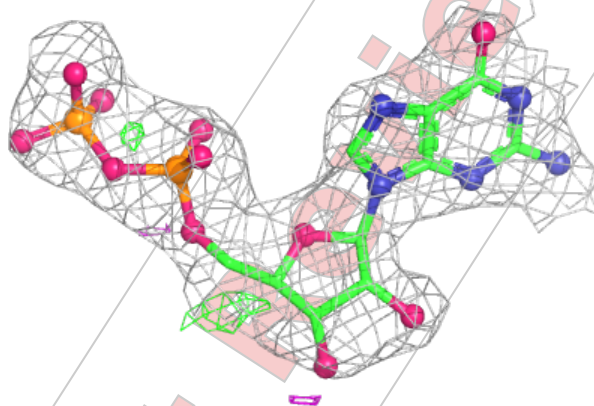
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





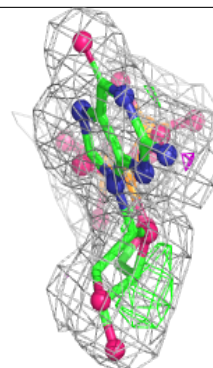
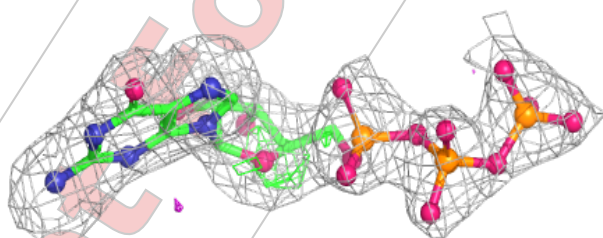
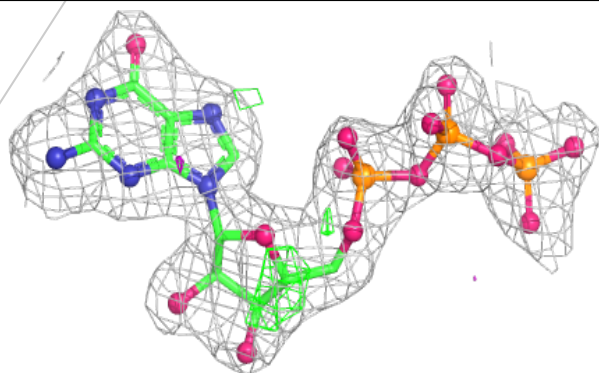
**Electron density around GDP B 501:**

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



**Electron density around GTP 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.

Not For Manuscript Review