



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2019 – 03:45 AM EDT

PDB ID : 3Q22  
Title : X-ray crystal structure of the N4 mini-VRNAP and P2\_7a promoter transcription initiation complex with GTP and Magnesium: substrate complex I  
Authors : Gleghorn, M.L.; Murakami, K.S.  
Deposited on : 2010-12-19  
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

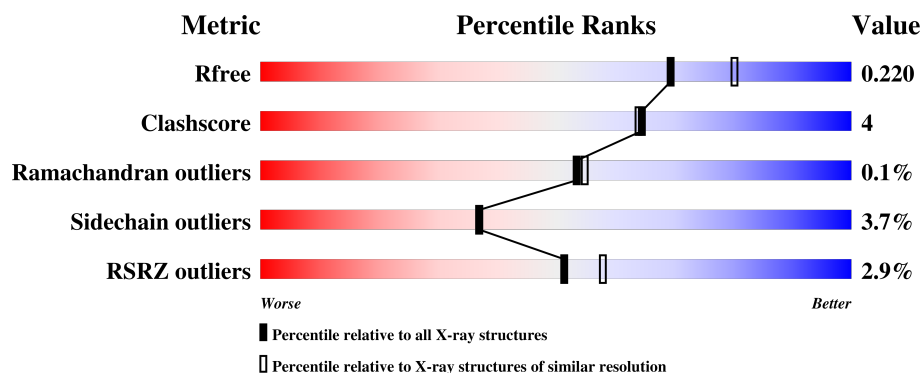
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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))
$R_{free}$	111664	5449 (2.14-2.10)
Clashscore	122126	5972 (2.14-2.10)
Ramachandran outliers	120053	5914 (2.14-2.10)
Sidechain outliers	120020	5915 (2.14-2.10)
RSRZ outliers	108989	5321 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1118	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	1118	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
2	C	36	<div> <div>3%</div> <div>47%</div> <div>8%</div> <div>44%</div> </div>
2	D	36	<div> <div>3%</div> <div>50%</div> <div>8%</div> <div>42%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19285 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1094	Total	C	N	O	S	0	0	0
			8443	5299	1432	1671	41			

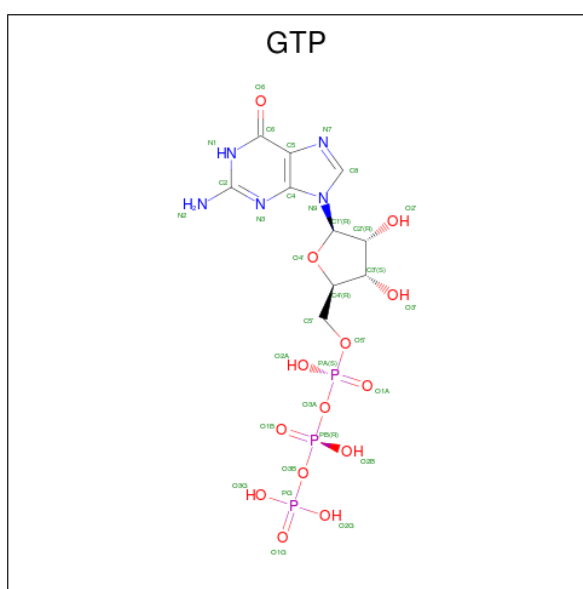
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q859P9
A	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-8	SER	-	EXPRESSION TAG	UNP Q859P9
A	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
A	0	SER	-	EXPRESSION TAG	UNP Q859P9
B	-11	MET	-	EXPRESSION TAG	UNP Q859P9
B	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-8	SER	-	EXPRESSION TAG	UNP Q859P9
B	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
B	0	SER	-	EXPRESSION TAG	UNP Q859P9

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*GP\*CP\*CP\*TP\*CP\*CP\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*AP\*AP\*GP\*AP\*AP\*GP\*CP\*GP\*GP\*AP\*GP\*CP\*TP\*TP\*CP\*TP\*TP\*C)-3').

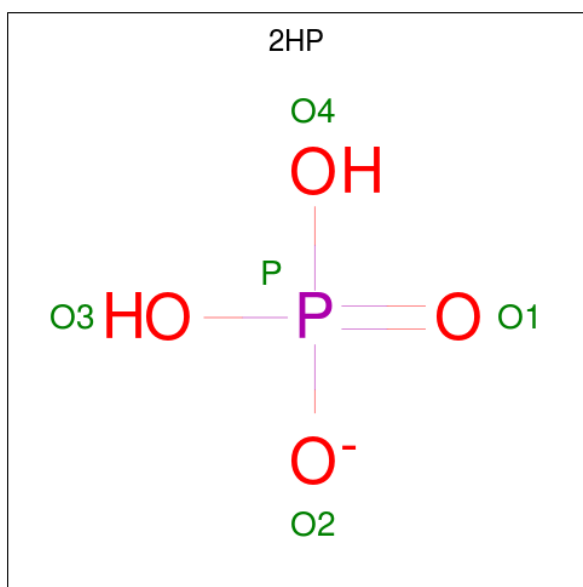
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			396	185	79	112	20			
2	D	21	Total	C	N	O	P	0	0	0
			432	205	83	123	21			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 4 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula:  $H_2O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

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

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

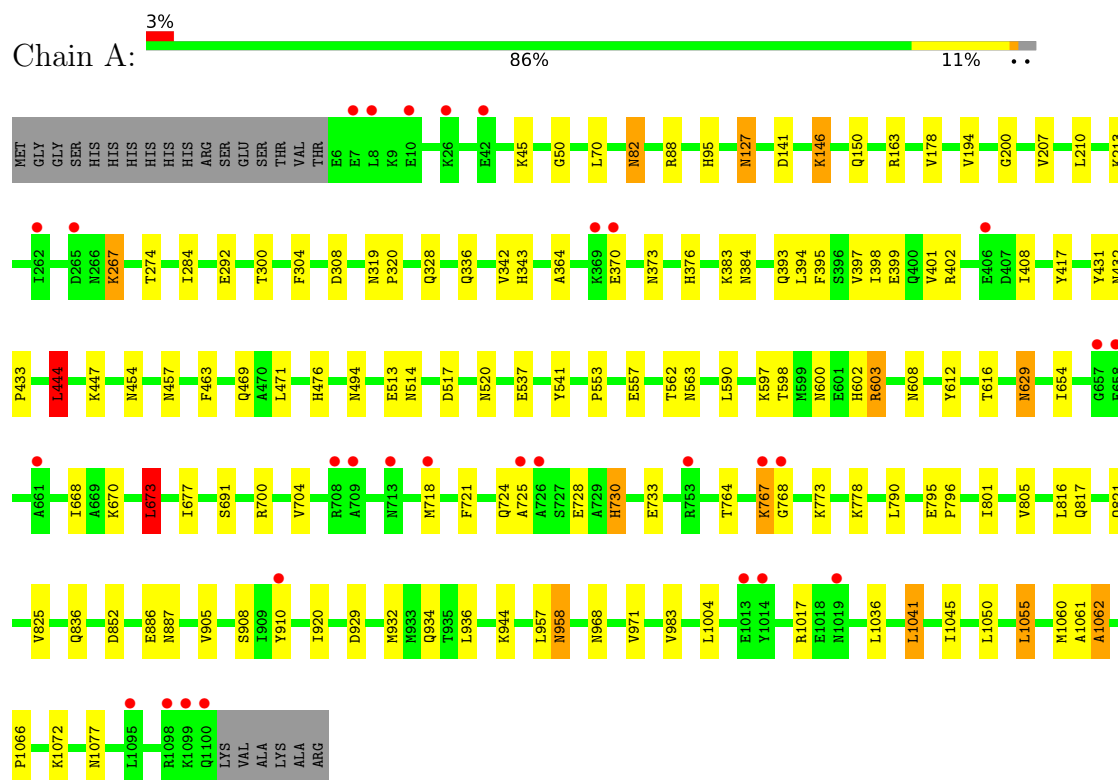
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	610	Total	O	0	0
			610	610		
6	C	50	Total	O	0	0
			50	50		
6	B	692	Total	O	0	0
			692	692		
6	D	68	Total	O	0	0
			68	68		

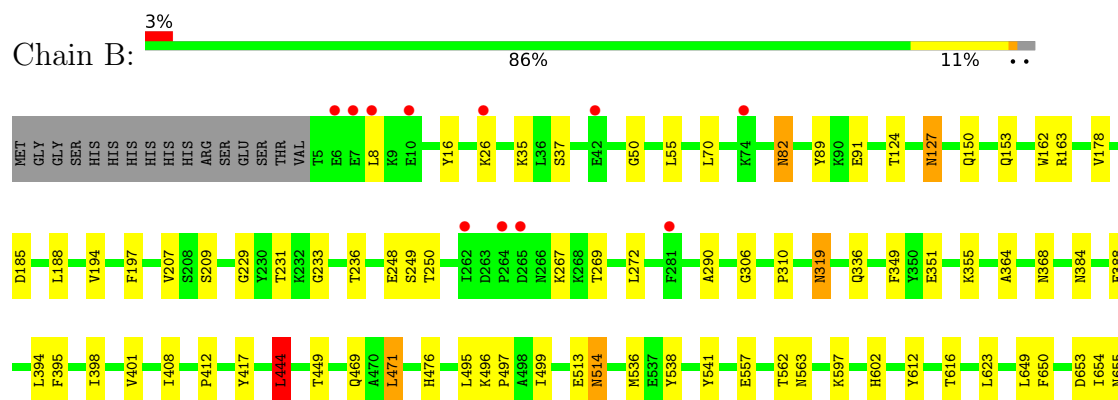
### 3 Residue-property plots

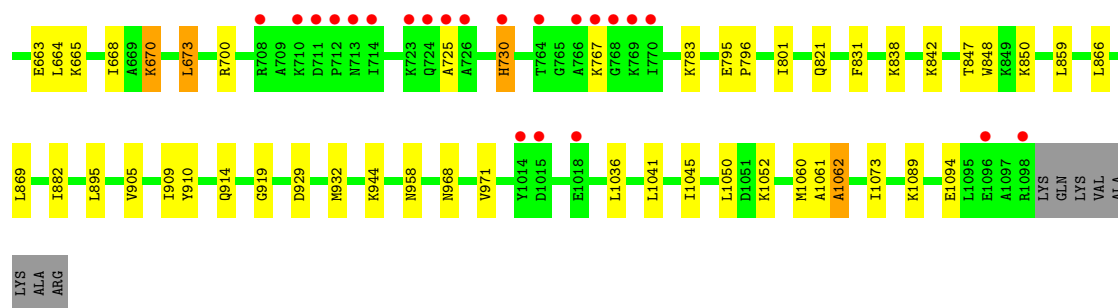
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

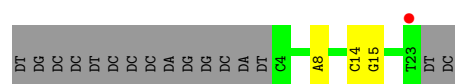


#### • Molecule 1: Virion RNA polymerase

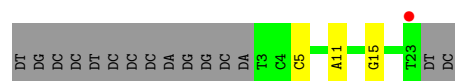




- Molecule 2: DNA (5'-D(\*TP\*GP\*CP\*CP\*TP\*CP\*CP\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*AP\*AP\*GP\*AP\*AP\*GP\*CP\*GP\*GP\*AP\*GP\*CP\*TP\*TP\*CP\*TP\*TP\*C)-3')



- Molecule 2: DNA (5'-D(\*TP\*GP\*CP\*CP\*TP\*CP\*CP\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*CP\*CP\*AP\*AP\*AP\*AP\*GP\*AP\*AP\*GP\*CP\*GP\*GP\*AP\*GP\*CP\*TP\*TP\*CP\*TP\*TP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.30Å 111.79Å 276.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.11 47.81 – 2.11	Depositor EDS
% Data completeness (in resolution range)	89.1 (50.00-2.11) 89.1 (47.81-2.11)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, $R_{free}$	0.208 , 0.219 0.208 , 0.220	Depositor DCC
$R_{free}$ test set	6713 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 2HP, 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	0.40	0/8583	0.55	2/11609 (0.0%)
1	B	0.40	0/8572	0.54	1/11596 (0.0%)
2	C	0.66	0/445	1.23	2/685 (0.3%)
2	D	0.66	0/485	1.21	2/746 (0.3%)
All	All	0.42	0/18085	0.60	7/24636 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	LEU	CA-CB-CG	7.95	133.57	115.30
1	B	444	LEU	CA-CB-CG	7.82	133.29	115.30
1	A	673	LEU	CA-CB-CG	5.86	128.78	115.30
2	C	14	DC	O4'-C1'-N1	5.50	111.85	108.00
2	C	15	DG	P-O3'-C3'	5.24	125.99	119.70
2	D	5	DC	O4'-C4'-C3'	-5.17	102.43	104.50
2	D	15	DG	P-O3'-C3'	5.01	125.72	119.70

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	8454	0	8479	81	0
1	B	8443	0	8465	77	0
2	C	396	0	211	1	0
2	D	432	0	236	1	0
3	A	64	0	24	2	0
3	B	32	0	12	0	0
3	D	32	0	12	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	610	0	0	7	0
6	B	692	0	0	6	1
6	C	50	0	0	0	0
6	D	68	0	0	0	1
All	All	19285	0	17439	157	1

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 (157) 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:A:469:GLN:HE22	1:A:557:GLU:H	1.12	0.91
1:B:469:GLN:HE22	1:B:557:GLU:H	1.14	0.91
1:A:336:GLN:HE21	1:A:417:TYR:H	1.21	0.88
1:B:336:GLN:HE21	1:B:417:TYR:H	1.16	0.87
1:B:850:LYS:O	6:B:2046:HOH:O	1.96	0.82
1:B:932:MET:CE	1:B:971:VAL:HG22	2.12	0.80
1:B:673:LEU:HD13	1:B:801:ILE:HG23	1.65	0.77
1:A:932:MET:CE	6:A:1630:HOH:O	2.33	0.77
1:A:932:MET:HE2	6:A:1630:HOH:O	1.86	0.74
1:B:932:MET:SD	6:B:1714:HOH:O	2.45	0.74
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.23	0.72
1:A:127:ASN:H	1:A:127:ASN:HD22	1.37	0.72
1:A:958:ASN:HD22	1:A:958:ASN:H	1.37	0.71
1:B:932:MET:HE3	6:B:2048:HOH:O	1.90	0.71
1:A:364:ALA:H	1:A:384:ASN:HD21	1.38	0.71
1:B:449:THR:H	1:B:958:ASN:HD21	1.38	0.70
1:B:650:PHE:HE2	1:B:700:ARG:HG3	1.57	0.70
1:B:932:MET:HE1	1:B:971:VAL:HG22	1.76	0.68
1:A:852:ASP:O	6:A:1632:HOH:O	2.11	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:932:MET:HE2	1:B:971:VAL:HG22	1.76	0.67
1:A:141:ASP:HB2	1:A:146:LYS:HG2	1.75	0.67
1:A:469:GLN:NE2	1:A:557:GLU:H	1.90	0.67
1:B:364:ALA:H	1:B:384:ASN:ND2	1.93	0.67
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.76	0.66
1:A:968:ASN:HD21	1:A:1060:MET:H	1.44	0.66
1:A:469:GLN:HE22	1:A:557:GLU:N	1.92	0.64
1:A:364:ALA:H	1:A:384:ASN:ND2	1.95	0.64
1:B:469:GLN:HE22	1:B:557:GLU:N	1.92	0.64
1:B:932:MET:CE	6:B:2048:HOH:O	2.44	0.64
1:B:469:GLN:NE2	1:B:557:GLU:H	1.92	0.63
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.80	0.63
1:A:654:ILE:HD11	1:A:668:ILE:HG21	1.81	0.63
1:A:767:LYS:HE3	1:A:768:GLY:H	1.64	0.62
1:A:597:LYS:NZ	1:A:602:HIS:HD2	1.97	0.62
1:A:82:ASN:HD22	1:A:82:ASN:C	2.05	0.60
1:B:882:ILE:HD13	1:B:919:GLY:HA2	1.85	0.59
1:B:616:THR:HG23	1:B:664:LEU:HB2	1.84	0.58
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.38	0.58
1:B:351:GLU:HG3	1:B:395:PHE:CE2	2.39	0.57
1:B:91:GLU:HG3	6:B:1574:HOH:O	2.03	0.57
1:A:821:GLN:O	1:A:825:VAL:HG23	2.05	0.57
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.87	0.57
1:B:1045:ILE:HD12	1:B:1094:GLU:HG3	1.87	0.57
1:B:127:ASN:H	1:B:127:ASN:HD22	1.52	0.56
1:B:16:TYR:O	1:B:35:LYS:HE3	2.05	0.56
1:B:162:TRP:HE1	1:B:209:SER:HB2	1.71	0.56
1:A:1077:ASN:HB3	6:A:1426:HOH:O	2.06	0.55
1:B:654:ILE:HD11	1:B:668:ILE:HG21	1.87	0.55
1:A:932:MET:HE3	6:A:1630:HOH:O	2.02	0.55
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.88	0.55
1:B:932:MET:HE1	1:B:971:VAL:CG2	2.36	0.55
1:A:397:VAL:O	1:A:401:VAL:HG23	2.06	0.55
1:B:82:ASN:C	1:B:82:ASN:HD22	2.09	0.54
1:B:364:ALA:H	1:B:384:ASN:HD21	1.54	0.54
1:B:655:ASN:HB2	1:B:663:GLU:HB3	1.90	0.54
1:A:886:GLU:O	2:C:8:DA:H4'	2.07	0.54
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.73	0.54
1:A:342:VAL:HG11	1:A:408:ILE:HD12	1.91	0.53
1:B:185:ASP:HB3	1:B:188:LEU:HD12	1.91	0.53
1:B:50:GLY:H	1:B:150:GLN:HE22	1.55	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLU:HB2	1:A:796:PRO:HD3	1.90	0.53
1:A:1072:LYS:HA	1:A:1072:LYS:HE2	1.91	0.53
1:A:213:LYS:HE3	1:A:292:GLU:OE1	2.10	0.53
1:A:968:ASN:ND2	1:A:1060:MET:H	2.06	0.52
3:A:1107:GTP:H5'	3:A:1107:GTP:PB	2.50	0.52
1:A:721:PHE:HA	1:A:724:GLN:HE21	1.73	0.52
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.91	0.52
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.93	0.51
1:B:612:TYR:CD1	1:B:670:LYS:HG2	2.45	0.51
1:A:513:GLU:HB3	1:B:513:GLU:OE2	2.11	0.51
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.93	0.51
1:B:229:GLY:O	1:B:233:GLY:HA3	2.11	0.51
1:B:650:PHE:CE2	1:B:700:ARG:HG3	2.41	0.51
1:A:395:PHE:O	1:A:399:GLU:HG2	2.11	0.51
1:B:968:ASN:HD21	1:B:1060:MET:H	1.57	0.50
1:B:37:SER:HB3	1:B:231:THR:HG22	1.93	0.50
1:B:336:GLN:NE2	1:B:417:TYR:H	1.98	0.49
1:A:127:ASN:N	1:A:127:ASN:HD22	2.08	0.49
1:A:45:LYS:HE3	6:A:1377:HOH:O	2.12	0.49
1:B:249:SER:O	1:B:250:THR:HB	2.11	0.49
1:A:320:PRO:HD2	1:A:910:TYR:CE2	2.48	0.49
1:B:449:THR:H	1:B:958:ASN:ND2	2.08	0.48
1:B:267:LYS:HE2	1:B:267:LYS:HA	1.94	0.48
1:B:50:GLY:H	1:B:150:GLN:NE2	2.12	0.48
1:A:958:ASN:ND2	1:A:958:ASN:H	2.10	0.48
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.95	0.48
1:A:932:MET:CE	1:A:971:VAL:HG22	2.44	0.48
1:B:26:LYS:HG2	1:B:847:THR:HG21	1.96	0.47
1:A:95:HIS:HA	1:B:248:GLU:O	2.15	0.47
1:B:401:VAL:HG12	1:B:408:ILE:HG13	1.95	0.47
1:B:821:GLN:HE22	1:B:914:GLN:HE21	1.63	0.47
1:B:236:THR:HG21	1:B:895:LEU:HD23	1.96	0.47
1:A:670:LYS:NZ	3:A:1108:GTP:O3A	2.48	0.46
1:A:677:ILE:HD11	1:A:805:VAL:HG11	1.97	0.46
1:B:616:THR:CG2	1:B:664:LEU:HB2	2.45	0.46
1:B:514:ASN:H	1:B:514:ASN:HD22	1.63	0.46
1:B:653:ASP:HA	1:B:665:LYS:HD2	1.96	0.46
1:B:310:PRO:HG2	1:B:336:GLN:HB3	1.98	0.46
1:B:471:LEU:HG	1:B:495:LEU:HD11	1.97	0.46
1:B:496:LYS:HB3	1:B:497:PRO:HD3	1.98	0.46
1:A:393:GLN:HG2	1:A:431:TYR:CB	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:GLU:HB3	1:B:796:PRO:HD3	1.98	0.46
1:B:16:TYR:O	1:B:35:LYS:CE	2.64	0.46
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.17	0.45
1:A:370:GLU:HA	1:A:773:LYS:HE2	1.98	0.45
1:B:499:ILE:HD12	1:B:538:TYR:HD2	1.82	0.45
1:A:200:GLY:HA2	1:A:274:THR:HG22	1.99	0.45
1:A:373:ASN:HD22	1:A:376:HIS:H	1.63	0.45
1:B:394:LEU:O	1:B:398:ILE:HG12	2.17	0.45
1:B:725:ALA:HB1	1:B:730:HIS:HB3	1.97	0.45
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.17	0.45
1:A:600:ASN:H	1:A:600:ASN:ND2	2.14	0.45
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.82	0.45
1:B:55:LEU:HD12	1:B:153:GLN:HG2	1.99	0.44
1:B:269:THR:O	2:D:11:DA:H5'	2.17	0.44
1:A:454:ASN:HB3	1:A:457:ASN:ND2	2.32	0.44
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.99	0.44
1:A:328:GLN:HG2	1:A:934:GLN:OE1	2.16	0.44
1:A:304:PHE:HB3	1:A:308:ASP:O	2.17	0.44
1:A:50:GLY:H	1:A:150:GLN:NE2	2.16	0.44
1:B:319:ASN:HD22	1:B:910:TYR:HE1	1.64	0.44
1:B:444:LEU:HB3	6:B:1423:HOH:O	2.18	0.44
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.18	0.43
1:A:700:ARG:O	1:A:704:VAL:HG23	2.19	0.43
1:A:673:LEU:HD22	1:A:801:ILE:HG23	2.00	0.43
1:B:127:ASN:N	1:B:127:ASN:HD22	2.16	0.43
1:B:476:HIS:ND1	4:B:1108:2HP:O2	2.32	0.43
1:A:432:ASN:HB2	1:A:433:PRO:HD2	2.01	0.43
1:A:677:ILE:O	1:A:920:ILE:HG21	2.18	0.43
1:A:790:LEU:O	1:A:795:GLU:HG2	2.19	0.43
1:A:447:LYS:HE3	6:A:1345:HOH:O	2.18	0.43
1:A:725:ALA:HB1	1:A:730:HIS:HB3	2.01	0.42
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.55	0.42
1:A:598:THR:HG22	1:A:1066:PRO:HD3	2.02	0.42
1:A:562:THR:HG22	1:A:612:TYR:CE1	2.54	0.42
1:A:718:MET:HG2	1:A:728:GLU:HG3	2.00	0.42
1:A:394:LEU:O	1:A:398:ILE:HG12	2.19	0.42
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.65	0.42
1:A:597:LYS:HZ1	1:A:602:HIS:HD2	1.68	0.42
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.47	0.42
1:B:197:PHE:CD1	1:B:272:LEU:HD21	2.55	0.42
1:A:590:LEU:HD11	1:A:1055:LEU:HG	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:HIS:O	1:A:733:GLU:HG2	2.21	0.41
1:A:932:MET:HE2	1:A:971:VAL:HG22	2.00	0.41
1:A:463:PHE:HA	1:A:957:LEU:HD13	2.03	0.41
1:B:1052:LYS:HB3	1:B:1073:ILE:HD12	2.02	0.41
1:A:343:HIS:HE1	1:A:537:GLU:OE2	2.04	0.41
1:A:629:ASN:HD22	1:A:629:ASN:N	2.18	0.41
1:A:476:HIS:ND1	4:A:1109:2HP:O2	2.35	0.41
1:A:616:THR:HG23	1:A:668:ILE:HD11	2.02	0.41
1:B:306:GLY:HA2	1:B:412:PRO:HG2	2.03	0.41
1:B:831:PHE:HD2	1:B:866:LEU:HD11	1.85	0.41
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.56	0.41
1:B:597:LYS:NZ	1:B:602:HIS:HD2	2.18	0.41
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.73	0.41
1:A:82:ASN:ND2	1:A:82:ASN:C	2.70	0.41
1:B:349:PHE:HB2	1:B:536:MET:CE	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1460:HOH:O	6:D:93:HOH:O[4_527]	1.81	0.39

## 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	1093/1118 (98%)	1068 (98%)	24 (2%)	1 (0%)	53	55
1	B	1092/1118 (98%)	1067 (98%)	24 (2%)	1 (0%)	53	55
All	All	2185/2236 (98%)	2135 (98%)	48 (2%)	2 (0%)	53	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1062	ALA
1	B	1062	ALA

### 5.3.2 Protein sidechains [i](#)

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	916/935 (98%)	876 (96%)	40 (4%)	31	29
1	B	915/935 (98%)	887 (97%)	28 (3%)	43	45
All	All	1831/1870 (98%)	1763 (96%)	68 (4%)	37	37

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	82	ASN
1	A	88	ARG
1	A	127	ASN
1	A	146	LYS
1	A	163	ARG
1	A	210	LEU
1	A	267	LYS
1	A	284	ILE
1	A	300	THR
1	A	319	ASN
1	A	383	LYS
1	A	444	LEU
1	A	471	LEU
1	A	494	ASN
1	A	514	ASN
1	A	517	ASP
1	A	520	ASN
1	A	541	TYR
1	A	603	ARG
1	A	629	ASN
1	A	673	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	691	SER
1	A	730	HIS
1	A	764	THR
1	A	767	LYS
1	A	778	LYS
1	A	817	GLN
1	A	836	GLN
1	A	887	ASN
1	A	908	SER
1	A	936	LEU
1	A	944	LYS
1	A	958	ASN
1	A	1004	LEU
1	A	1017	ARG
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1055	LEU
1	B	8	LEU
1	B	70	LEU
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	163	ARG
1	B	319	ASN
1	B	368	ASN
1	B	444	LEU
1	B	471	LEU
1	B	514	ASN
1	B	541	TYR
1	B	623	LEU
1	B	649	LEU
1	B	670	LYS
1	B	673	LEU
1	B	730	HIS
1	B	767	LYS
1	B	783	LYS
1	B	838	LYS
1	B	859	LEU
1	B	869	LEU
1	B	909	ILE
1	B	944	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU
1	B	1089	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	169	ASN
1	A	186	GLN
1	A	212	GLN
1	A	316	GLN
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN
1	A	414	HIS
1	A	457	ASN
1	A	469	GLN
1	A	506	ASN
1	A	514	ASN
1	A	563	ASN
1	A	600	ASN
1	A	602	HIS
1	A	629	ASN
1	A	639	GLN
1	A	724	GLN
1	A	781	GLN
1	A	815	GLN
1	A	817	GLN
1	A	823	GLN
1	A	833	GLN
1	A	863	GLN
1	A	893	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	1035	ASN
1	A	1038	ASN
1	A	1047	HIS
1	A	1059	GLN
1	B	82	ASN
1	B	122	GLN
1	B	127	ASN
1	B	150	GLN
1	B	196	GLN
1	B	255	ASN
1	B	314	ASN
1	B	316	GLN
1	B	319	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	368	ASN
1	B	376	HIS
1	B	384	ASN
1	B	414	HIS
1	B	469	GLN
1	B	506	ASN
1	B	514	ASN
1	B	520	ASN
1	B	563	ASN
1	B	602	HIS
1	B	629	ASN
1	B	639	GLN
1	B	724	GLN
1	B	815	GLN
1	B	817	GLN
1	B	892	ASN
1	B	893	GLN
1	B	914	GLN
1	B	958	ASN
1	B	968	ASN
1	B	1035	ASN
1	B	1047	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1059	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 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$
3	GTP	A	1107	-	26,34,34	0.96	1 (3%)	29,54,54	1.87	7 (24%)
3	GTP	A	1108	5	26,34,34	1.00	1 (3%)	29,54,54	1.86	7 (24%)
4	2HP	A	1109	-	4,4,4	5.55	2 (50%)	6,6,6	0.99	0
3	GTP	B	1107	5	26,34,34	1.00	2 (7%)	29,54,54	1.80	6 (20%)
4	2HP	B	1108	-	4,4,4	5.70	2 (50%)	6,6,6	0.95	0
3	GTP	D	26	-	26,34,34	1.00	1 (3%)	29,54,54	1.92	7 (24%)

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	A	1107	-	-	6/18/38/38	0/3/3/3
3	GTP	A	1108	5	-	5/18/38/38	0/3/3/3
3	GTP	B	1107	5	-	3/18/38/38	0/3/3/3
3	GTP	D	26	-	-	6/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1108	2HP	P-O4	8.06	1.79	1.54
4	B	1108	2HP	P-O3	8.00	1.78	1.54
4	A	1109	2HP	P-O3	7.83	1.78	1.54
4	A	1109	2HP	P-O4	7.78	1.78	1.54
3	D	26	GTP	C6-N1	3.38	1.38	1.33
3	A	1108	GTP	C6-N1	3.36	1.38	1.33
3	B	1107	GTP	C6-N1	3.32	1.38	1.33
3	A	1107	GTP	C6-N1	3.07	1.38	1.33
3	B	1107	GTP	C2-N1	2.17	1.39	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1108	GTP	N3-C2-N1	-5.73	119.50	127.25
3	B	1107	GTP	N3-C2-N1	-5.41	119.93	127.25
3	A	1107	GTP	N3-C2-N1	-5.38	119.98	127.25
3	D	26	GTP	N3-C2-N1	-5.36	120.00	127.25
3	D	26	GTP	C2-N3-C4	4.92	120.98	115.36
3	B	1107	GTP	C2-N3-C4	4.43	120.42	115.36
3	A	1108	GTP	C2-N3-C4	4.15	120.10	115.36
3	A	1107	GTP	PB-O3B-PG	-4.15	119.38	132.57
3	A	1107	GTP	C2-N3-C4	4.06	120.00	115.36
3	D	26	GTP	PB-O3B-PG	-3.57	121.24	132.57
3	A	1108	GTP	C6-N1-C2	3.28	120.72	116.06
3	A	1107	GTP	C5-C6-N1	-3.09	119.17	123.47
3	A	1107	GTP	C6-N1-C2	3.08	120.45	116.06
3	D	26	GTP	PA-O3A-PB	-3.07	122.83	132.57
3	B	1107	GTP	C5-C6-N1	-2.94	119.38	123.47
3	A	1108	GTP	C5-C6-N1	-2.93	119.40	123.47
3	B	1107	GTP	C6-N1-C2	2.84	120.11	116.06
3	D	26	GTP	C5-C6-N1	-2.75	119.65	123.47
3	D	26	GTP	C6-N1-C2	2.61	119.78	116.06
3	A	1108	GTP	N2-C2-N1	2.51	121.18	117.25
3	B	1107	GTP	PB-O3B-PG	-2.50	124.63	132.57

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1107	GTP	N2-C2-N1	2.37	120.96	117.25
3	D	26	GTP	N2-C2-N1	2.20	120.69	117.25
3	A	1108	GTP	C6-C5-C4	-2.20	118.67	120.79
3	A	1107	GTP	PA-O3A-PB	-2.11	125.88	132.57
3	A	1107	GTP	N2-C2-N1	2.08	120.50	117.25
3	A	1108	GTP	C1'-N9-C4	-2.07	123.05	126.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	26	GTP	C5'-O5'-PA-O3A
3	D	26	GTP	C5'-O5'-PA-O1A
3	D	26	GTP	C5'-O5'-PA-O2A
3	A	1107	GTP	C5'-O5'-PA-O1A
3	D	26	GTP	O4'-C4'-C5'-O5'
3	D	26	GTP	C3'-C4'-C5'-O5'
3	A	1107	GTP	O4'-C4'-C5'-O5'
3	A	1108	GTP	PA-O3A-PB-O2B
3	A	1108	GTP	PB-O3B-PG-O1G
3	A	1107	GTP	C3'-C4'-C5'-O5'
3	D	26	GTP	PB-O3A-PA-O1A
3	A	1107	GTP	PA-O3A-PB-O2B
3	B	1107	GTP	PB-O3B-PG-O1G
3	B	1107	GTP	PA-O3A-PB-O2B
3	A	1108	GTP	PB-O3B-PG-O2G
3	A	1107	GTP	PB-O3B-PG-O2G
3	A	1107	GTP	PB-O3B-PG-O3G
3	A	1108	GTP	PA-O3A-PB-O1B
3	A	1108	GTP	PB-O3B-PG-O3G
3	B	1107	GTP	PB-O3B-PG-O2G

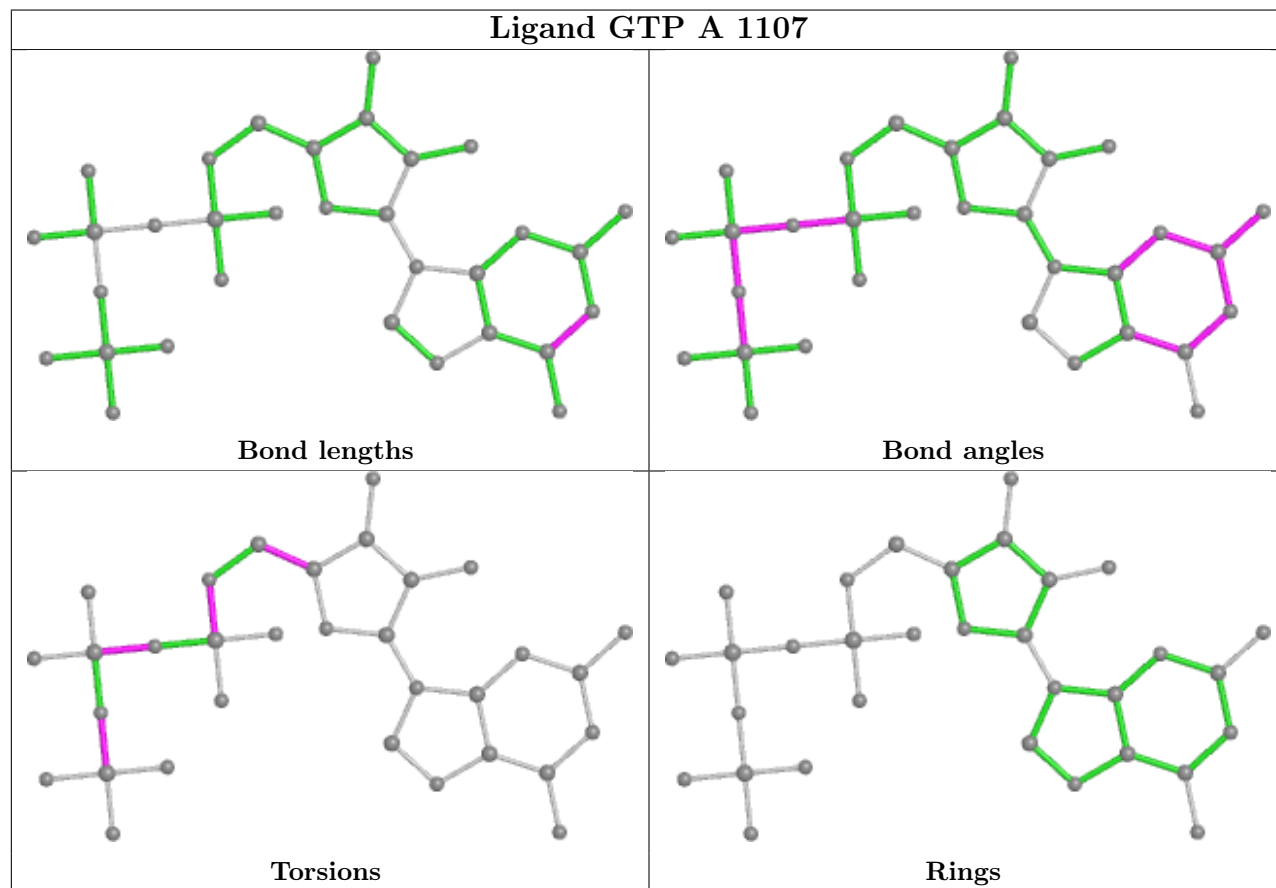
There are no ring outliers.

2 monomers are involved in 2 short contacts:

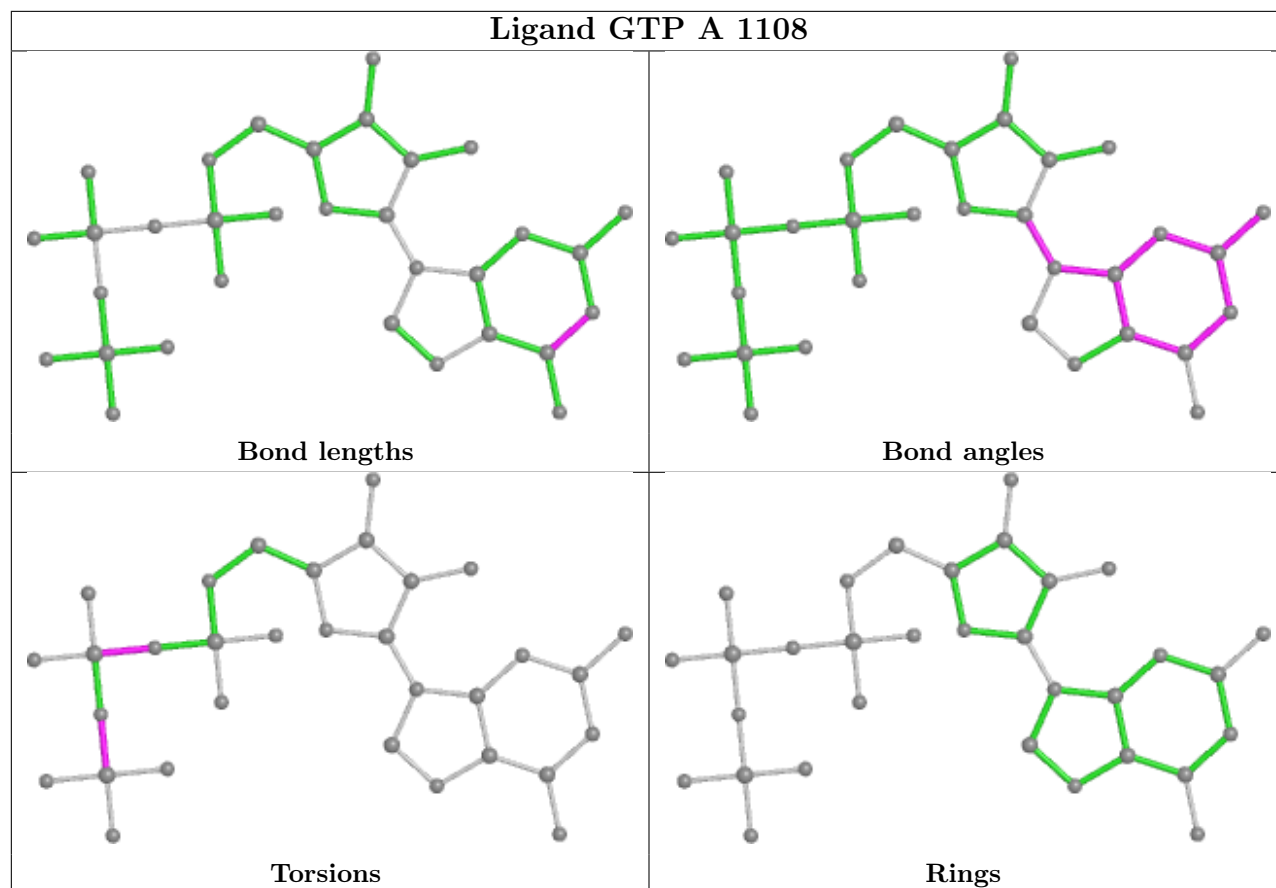
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1107	GTP	1	0
3	A	1108	GTP	1	0

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

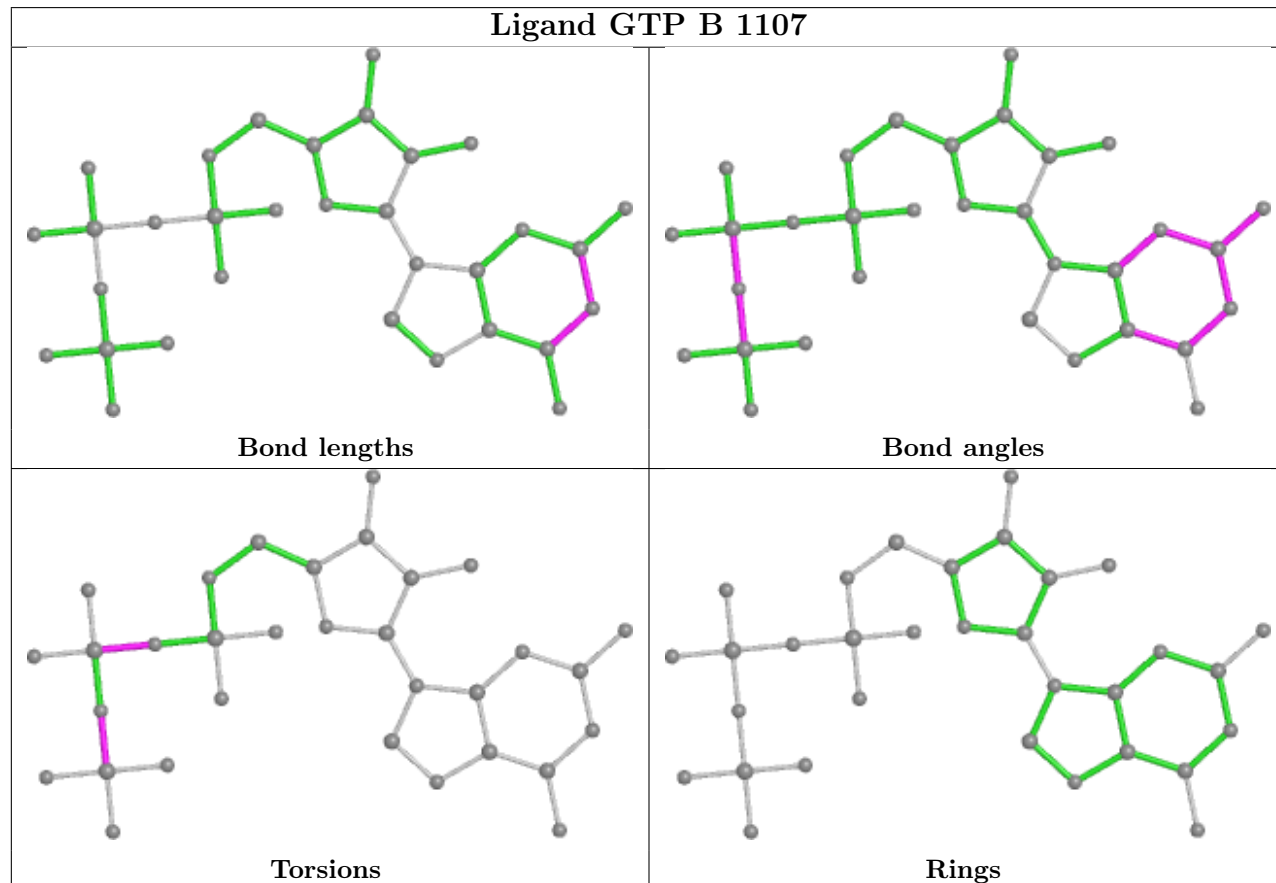
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

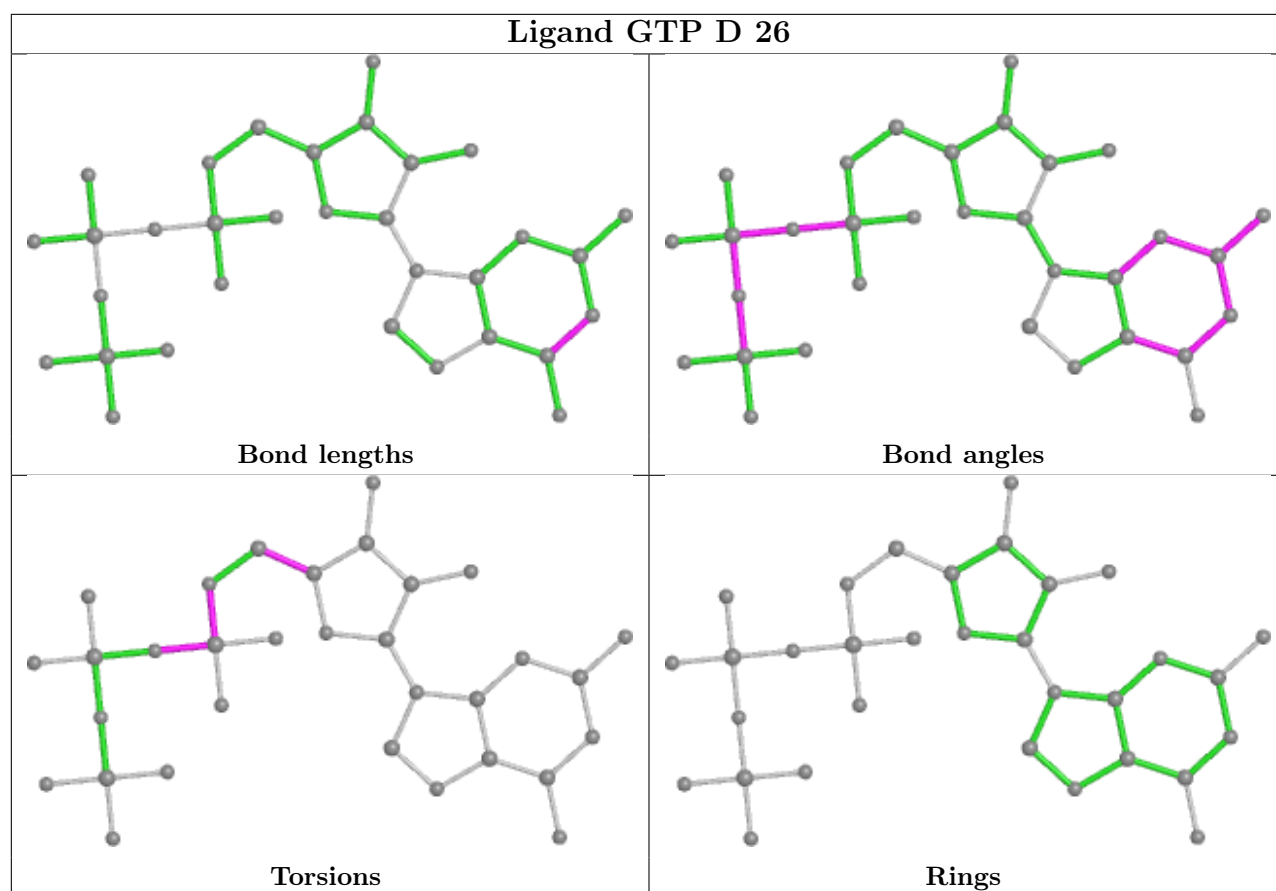


## Ligand GTP A 1108



## Ligand GTP B 1107





## 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, 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	1095/1118 (97%)	-0.03	30 (2%) 54 60	15, 29, 53, 69	0
1	B	1094/1118 (97%)	0.01	33 (3%) 50 57	15, 27, 48, 78	0
2	C	20/36 (55%)	-0.45	1 (5%) 29 35	22, 33, 53, 60	0
2	D	21/36 (58%)	-0.41	1 (4%) 30 36	23, 27, 46, 67	0
All	All	2230/2308 (96%)	-0.02	65 (2%) 51 58	15, 28, 51, 78	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	725	ALA	6.4
1	B	713	ASN	6.4
1	B	723	LYS	5.9
1	A	8	LEU	5.5
1	A	1014	TYR	4.5
1	B	264	PRO	4.5
1	B	724	GLN	4.5
1	A	7	GLU	4.4
1	A	1019	ASN	4.3
1	A	1098	ARG	4.3
1	B	726	ALA	4.2
1	B	764	THR	4.1
1	B	1098	ARG	3.4
1	A	369	LYS	3.3
1	B	730	HIS	3.3
1	B	710	LYS	3.3
1	A	910	TYR	3.2
1	A	767	LYS	3.1
1	B	42	GLU	3.1
1	B	265	ASP	3.0
1	A	658	GLU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	1014	TYR	2.9
1	A	10	GLU	2.9
1	B	769	LYS	2.9
1	A	1100	GLN	2.9
1	B	768	GLY	2.8
1	A	768	GLY	2.7
1	A	725	ALA	2.7
1	A	713	ASN	2.6
1	B	1015	ASP	2.6
1	B	262	ILE	2.6
1	A	1099	LYS	2.6
1	B	767	LYS	2.6
1	B	712	PRO	2.6
1	B	7	GLU	2.6
1	A	726	ALA	2.6
1	B	708	ARG	2.5
2	C	23	DT	2.5
1	B	766	ALA	2.5
1	A	262	ILE	2.4
1	B	281	PHE	2.4
1	B	770	ILE	2.4
1	A	265	ASP	2.4
1	B	8	LEU	2.4
1	A	42	GLU	2.4
1	B	1096	GLU	2.4
1	B	74	LYS	2.3
1	B	1018	GLU	2.3
1	B	6	GLU	2.3
1	B	714	ILE	2.3
1	A	718	MET	2.2
1	A	370	GLU	2.2
1	A	661	ALA	2.2
1	A	1095	LEU	2.2
1	B	10	GLU	2.2
1	A	657	GLY	2.2
1	A	708	ARG	2.2
1	A	753	ARG	2.2
1	B	26	LYS	2.1
1	A	1013	GLU	2.1
1	A	406	GLU	2.1
1	A	709	ALA	2.1
2	D	23	DT	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	26	LYS	2.0
1	B	711	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

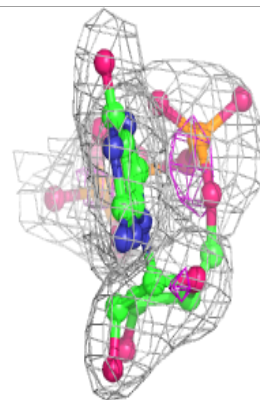
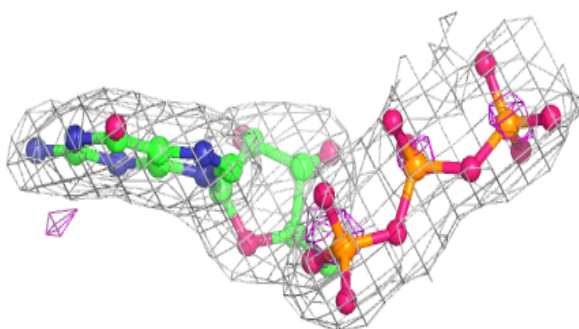
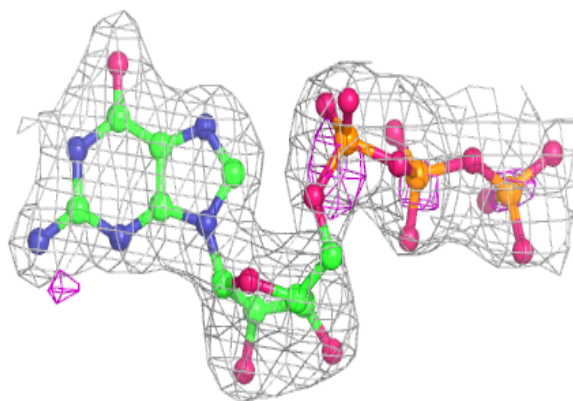
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GTP	D	26	32/32	0.84	0.15	37,44,70,70	0
3	GTP	A	1107	32/32	0.90	0.13	25,33,60,60	0
5	MG	B	1109	1/1	0.94	0.07	27,27,27,27	0
5	MG	A	1110	1/1	0.95	0.09	22,22,22,22	0
4	2HP	B	1108	5/5	0.95	0.12	44,44,44,44	0
4	2HP	A	1109	5/5	0.96	0.16	45,45,45,46	0
3	GTP	A	1108	32/32	0.97	0.10	18,21,27,28	0
3	GTP	B	1107	32/32	0.97	0.09	23,26,34,35	0

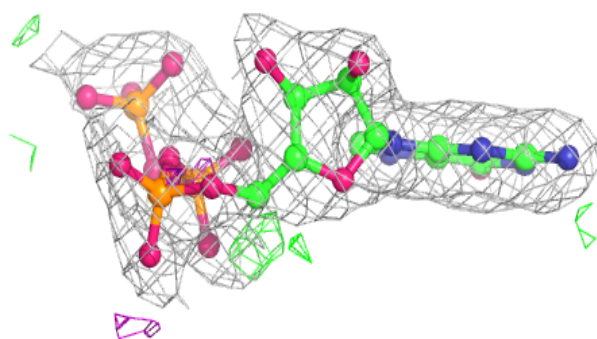
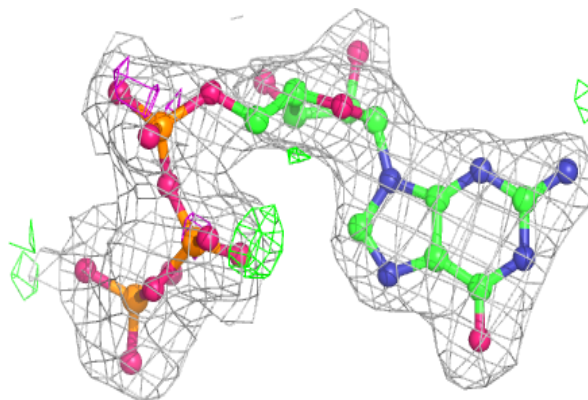
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GTP D 26:**

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

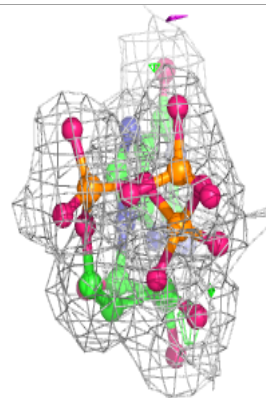
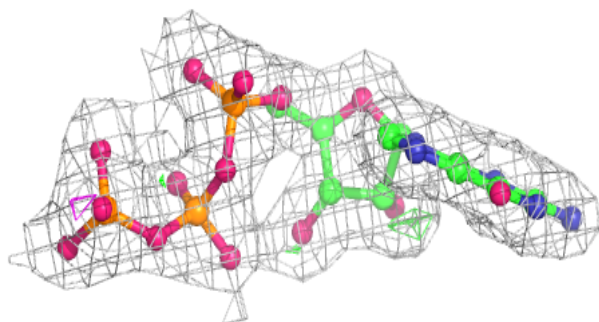
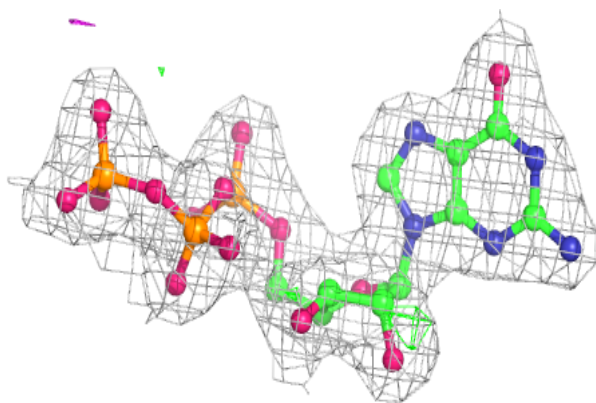
**Electron density around GTP A 1107:**

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

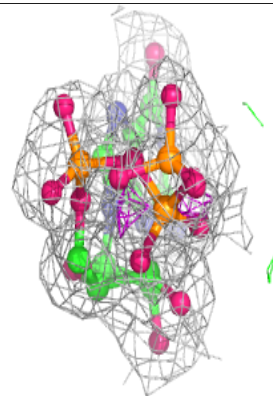
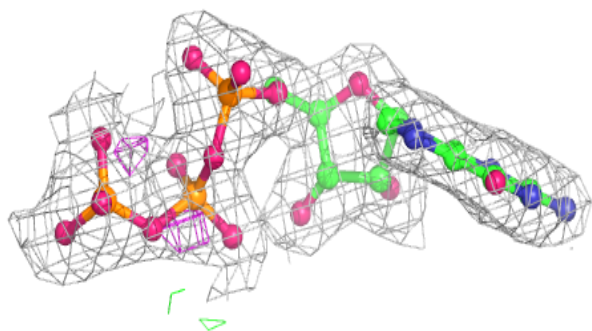
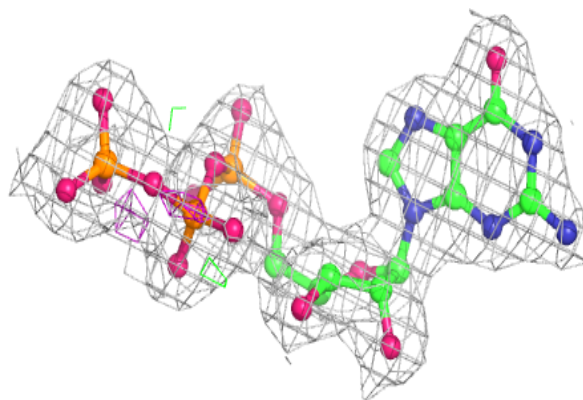


**Electron density around GTP A 1108:**

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

**Electron density around GTP B 1107:**

$2mF_o-DF_c$  (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.