Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 03:14 PM EST

PDB ID	:	3Q0A
Title	:	X-ray crystal structure of the transcription initiation complex of the N4 mini-vRNAP with P2 promoter: Mismatch complex
Authors	:	Murakami, K.S.
Deposited on	:	2010-12-15
Resolution	:	2.69 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 (i) 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 (i)) were used in the production of this report:

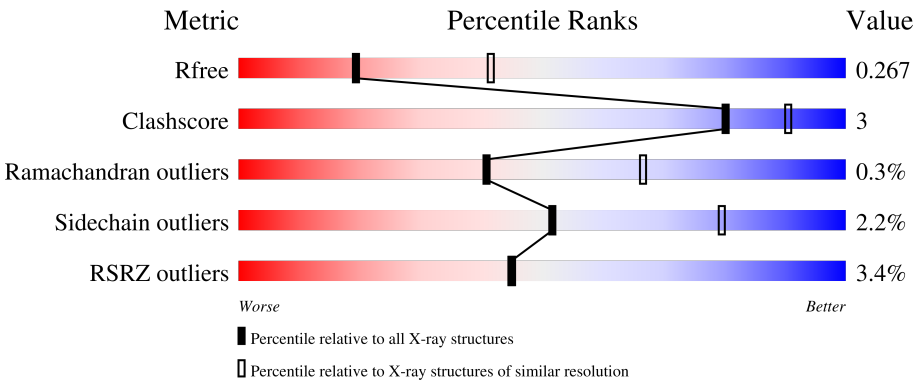
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	3% 91% 6% • •
1	B	1118	3% 89% 8% • •
2	C	36	6% 53% • 44%
2	D	36	3% 53% • 44%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18029 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
			Total	C	N	O	S			
1	A	1095	8454	5306	1435	1672	41	0	0	0
1	B	1094	8443	5299	1432	1671	41	0	0	0

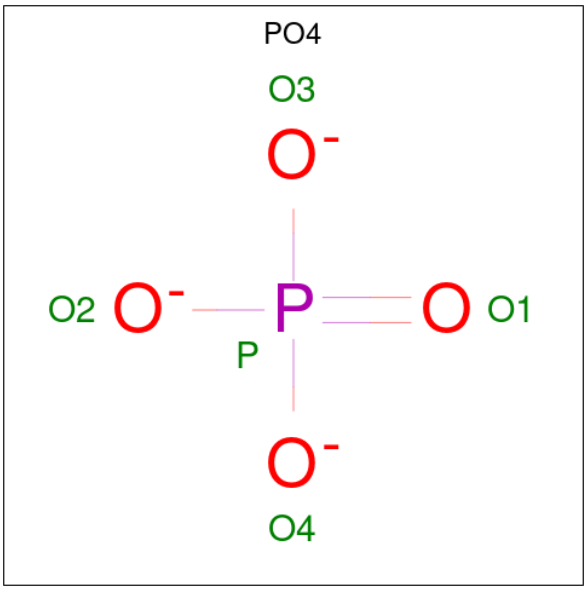
There are 24 discrepancies between the modelled and reference sequences:

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*A*GP*TP*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
			Total	C	N	O	P			
2	C	20	412	196	83	114	19	0	0	0
2	D	20	412	196	83	114	19	0	0	0

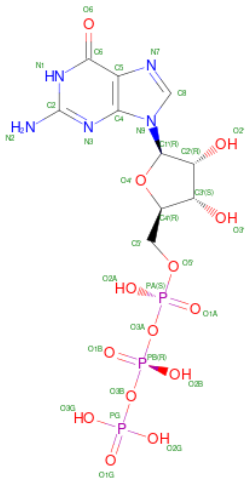
- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

GTP



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

- Molecule 5 is water.

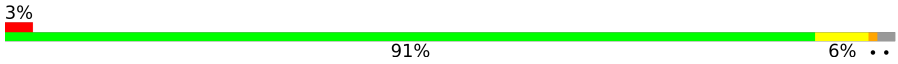
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	130	130	130	0	0
			Total	O		
5	C	9	9	9	0	0
			Total	O		
5	B	93	93	93	0	0
			Total	O		
5	D	2	2	2	0	0

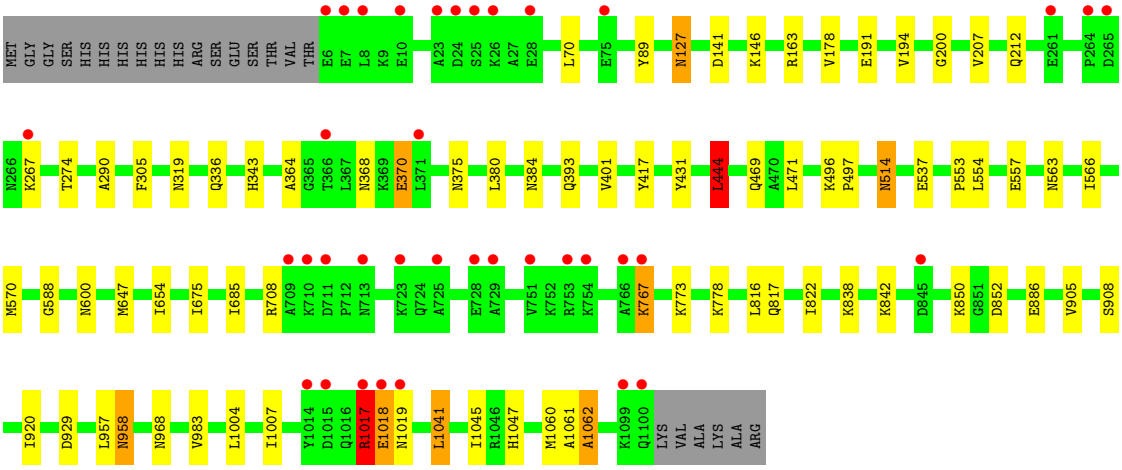
3 Residue-property plots (i)

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: Virion RNA polymerase

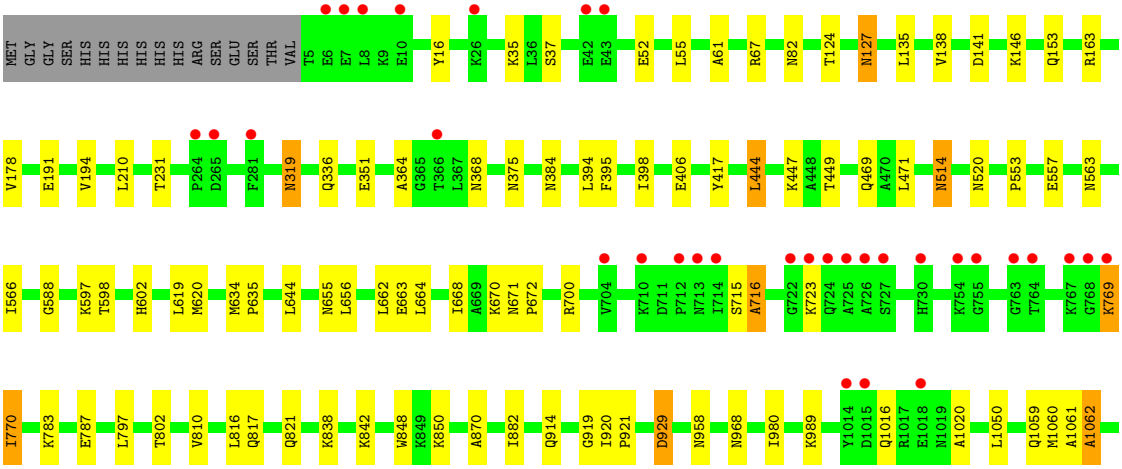
Chain A:

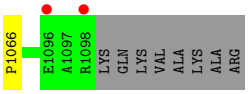




• Molecule 1: Virion RNA polymerase

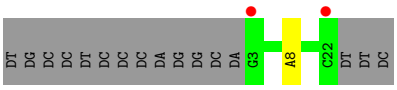
Chain B:





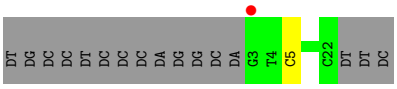
• Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*A*GP*TP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.35Å 111.38Å 275.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 49.39 – 2.69	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-2.69) 96.8 (49.39-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.19 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.276 0.212 , 0.267	Depositor DCC
R_{free} test set	3440 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18029	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, PO4

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	0.32	0/8583	0.47	1/11609 (0.0%)
1	B	0.32	0/8572	0.47	0/11596
2	C	0.62	0/464	1.15	0/715
2	D	0.63	0/464	1.13	0/715
All	All	0.34	0/18083	0.53	1/24635 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	444	LEU	CA-CB-CG	5.13	127.11	115.30

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	44	0
1	B	8443	0	8465	50	0
2	C	412	0	225	1	0
2	D	412	0	225	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	32	0	12	0	0
4	D	32	0	12	1	0
5	A	130	0	0	0	0
5	B	93	0	0	0	0
5	C	9	0	0	0	0
5	D	2	0	0	0	0
All	All	18029	0	17418	95	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 3.

All (95) 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:336:GLN:HE21	1:A:417:TYR:H	1.10	0.99
1:A:469:GLN:HE22	1:A:557:GLU:H	1.19	0.88
1:B:769:LYS:HG3	1:B:770:ILE:H	1.40	0.86
1:B:469:GLN:HE22	1:B:557:GLU:H	1.25	0.85
1:B:364:ALA:H	1:B:384:ASN:HD21	1.39	0.70
1:B:364:ALA:H	1:B:384:ASN:ND2	1.90	0.69
1:B:769:LYS:HG3	1:B:770:ILE:N	2.07	0.68
1:B:336:GLN:HE21	1:B:417:TYR:H	1.40	0.67
1:B:700:ARG:HE	1:B:723:LYS:HE3	1.59	0.67
1:B:191:GLU:HG3	1:B:375:ASN:HB3	1.78	0.65
1:B:816:LEU:HD23	1:B:980:ILE:HD13	1.79	0.64
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.81	0.63
1:A:127:ASN:HD22	1:A:127:ASN:H	1.47	0.61
1:A:968:ASN:HD21	1:A:1060:MET:H	1.49	0.61
1:A:514:ASN:HD22	1:A:514:ASN:H	1.49	0.59
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.06	0.56
1:B:514:ASN:HD22	1:B:514:ASN:H	1.54	0.56
1:B:351:GLU:HG3	1:B:395:PHE:CE2	2.41	0.55
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.71	0.55
1:A:336:GLN:HE21	1:A:417:TYR:N	1.93	0.55
1:A:958:ASN:H	1:A:958:ASN:HD22	1.55	0.55
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.72	0.55
1:A:496:LYS:HB3	1:A:497:PRO:HD3	1.89	0.54
1:A:336:GLN:NE2	1:A:417:TYR:H	1.94	0.54
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.89	0.54
1:B:351:GLU:HG3	1:B:395:PHE:HE2	1.73	0.53
1:A:554:LEU:HD23	1:A:957:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ILE:HD11	1:A:685:ILE:HG12	1.91	0.52
1:B:444:LEU:HG	1:B:553:PRO:HB2	1.91	0.52
1:B:449:THR:H	1:B:958:ASN:HD21	1.55	0.52
1:B:619:LEU:HD22	1:B:797:LEU:HD13	1.91	0.51
1:A:570:MET:O	1:A:1047:HIS:HE1	1.94	0.50
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.94	0.50
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.42	0.49
1:B:37:SER:HB3	1:B:231:THR:HG22	1.94	0.49
1:B:715:SER:O	1:B:716:ALA:HB3	2.11	0.49
1:A:191:GLU:HB3	1:A:375:ASN:HD22	1.79	0.48
1:A:767:LYS:HE3	1:A:767:LYS:HA	1.94	0.48
1:A:554:LEU:O	1:A:957:LEU:HG	2.13	0.48
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.14	0.48
1:A:127:ASN:HD22	1:A:127:ASN:N	2.10	0.48
1:B:968:ASN:HD21	1:B:1060:MET:H	1.62	0.47
1:B:566:ILE:HG13	1:B:588:GLY:HA3	1.94	0.47
1:B:55:LEU:HD12	1:B:153:GLN:HG2	1.94	0.47
1:B:882:ILE:HD13	1:B:919:GLY:HA2	1.97	0.46
1:B:135:LEU:O	1:B:138:VAL:HG22	2.16	0.46
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.97	0.46
1:A:838:LYS:O	1:A:842:LYS:HG2	2.15	0.46
1:B:127:ASN:HD22	1:B:127:ASN:H	1.62	0.46
1:A:200:GLY:HA2	1:A:274:THR:HG22	1.97	0.46
1:A:822:ILE:HG12	1:A:1007:ILE:HG23	1.97	0.46
1:A:968:ASN:ND2	1:A:1060:MET:H	2.11	0.46
1:B:655:ASN:HB2	1:B:663:GLU:HB3	1.98	0.45
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.57	0.45
1:A:305:PHE:HE1	1:A:401:VAL:HG22	1.82	0.45
1:A:647:MET:HB3	1:A:654:ILE:HG13	1.99	0.45
1:A:1018:GLU:HG3	1:A:1019:ASN:H	1.82	0.45
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.64	0.44
1:B:671:ASN:HB3	1:B:672:PRO:HD3	2.00	0.44
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.17	0.44
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.52	0.44
1:B:848:TRP:CH2	1:B:850:LYS:HA	2.53	0.44
1:A:370:GLU:HA	1:A:773:LYS:HE2	2.00	0.44
1:A:393:GLN:HG2	1:A:431:TYR:HB2	2.00	0.44
1:A:817:GLN:HB2	1:A:920:ILE:HD11	2.00	0.44
1:B:384:ASN:HD22	1:B:384:ASN:HA	1.61	0.44
1:A:141:ASP:HB2	1:A:146:LYS:HE3	1.99	0.43
1:B:802:THR:HG23	1:B:810:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:GLN:HE22	1:B:914:GLN:HE21	1.65	0.43
1:B:620:MET:HG3	1:B:664:LEU:HD12	2.00	0.43
1:B:783:LYS:O	1:B:787:GLU:HG2	2.18	0.43
1:B:1016:GLN:O	1:B:1020:ALA:HB2	2.19	0.42
1:A:343:HIS:HE1	1:A:537:GLU:OE2	2.03	0.42
1:A:364:ALA:H	1:A:384:ASN:HD21	1.66	0.42
1:B:141:ASP:HB2	1:B:146:LYS:HG2	2.02	0.42
1:B:598:THR:HG22	1:B:1066:PRO:HD3	2.02	0.42
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.55	0.42
1:A:566:ILE:HG13	1:A:588:GLY:HA3	2.02	0.41
1:B:563:ASN:HA	1:B:1059:GLN:HE22	1.85	0.41
1:B:920:ILE:HB	1:B:921:PRO:CD	2.50	0.41
1:A:886:GLU:HG3	1:A:908:SER:HB3	2.02	0.41
1:A:886:GLU:O	2:C:8:DA:H4'	2.20	0.41
1:A:1017:ARG:O	1:A:1019:ASN:N	2.54	0.41
1:B:668:ILE:H	1:B:668:ILE:HG13	1.73	0.41
1:B:634:MET:N	1:B:635:PRO:HD2	2.36	0.41
2:D:5:DC:N3	4:D:26:GTP:N1	2.60	0.41
1:B:61:ALA:HA	1:B:67:ARG:HB3	2.02	0.41
1:A:600:ASN:H	1:A:600:ASN:ND2	2.18	0.41
1:B:394:LEU:O	1:B:398:ILE:HG12	2.20	0.41
1:B:16:TYR:O	1:B:35:LYS:HE3	2.21	0.41
1:B:870:ALA:HB2	1:B:989:LYS:HD3	2.04	0.40
1:B:715:SER:O	1:B:716:ALA:CB	2.69	0.40
1:A:364:ALA:HB2	1:A:380:LEU:HD22	2.03	0.40
1:B:597:LYS:HE2	1:B:602:HIS:HB2	2.02	0.40
1:B:644:LEU:HD22	1:B:662:LEU:HD21	2.04	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	1093/1118 (98%)	1068 (98%)	22 (2%)	3 (0%)	41	66
1	B	1092/1118 (98%)	1064 (97%)	24 (2%)	4 (0%)	34	60
All	All	2185/2236 (98%)	2132 (98%)	46 (2%)	7 (0%)	41	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	A	1062	ALA
1	B	1062	ALA
1	A	1017	ARG
1	B	716	ALA
1	B	769	LYS
1	B	770	ILE

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%)	896 (98%)	20 (2%)	52	79
1	B	915/935 (98%)	895 (98%)	20 (2%)	52	79
All	All	1831/1870 (98%)	1791 (98%)	40 (2%)	52	79

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	127	ASN
1	A	163	ARG
1	A	212	GLN
1	A	267	LYS
1	A	319	ASN
1	A	368	ASN
1	A	370	GLU
1	A	444	LEU

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Mol	Chain	Res	Type
1	A	471	LEU
1	A	514	ASN
1	A	708	ARG
1	A	767	LYS
1	A	778	LYS
1	A	850	LYS
1	A	852	ASP
1	A	958	ASN
1	A	1004	LEU
1	A	1017	ARG
1	A	1041	LEU
1	B	52	GLU
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	163	ARG
1	B	210	LEU
1	B	319	ASN
1	B	368	ASN
1	B	406	GLU
1	B	444	LEU
1	B	447	LYS
1	B	471	LEU
1	B	514	ASN
1	B	520	ASN
1	B	656	LEU
1	B	670	LYS
1	B	817	GLN
1	B	838	LYS
1	B	929	ASP
1	B	1050	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) 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	212	GLN
1	A	225	ASN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	368	ASN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN
1	A	414	HIS
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	613	GLN
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	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	1035	ASN
1	A	1047	HIS
1	A	1059	GLN
1	B	82	ASN
1	B	127	ASN
1	B	140	GLN
1	B	150	GLN
1	B	186	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

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Mol	Chain	Res	Type
1	B	368	ASN
1	B	375	ASN
1	B	384	ASN
1	B	414	HIS
1	B	454	ASN
1	B	469	GLN
1	B	514	ASN
1	B	520	ASN
1	B	602	HIS
1	B	629	ASN
1	B	639	GLN
1	B	786	GLN
1	B	803	GLN
1	B	815	GLN
1	B	817	GLN
1	B	833	GLN
1	B	878	GLN
1	B	892	ASN
1	B	893	GLN
1	B	914	GLN
1	B	954	ASN
1	B	958	ASN
1	B	968	ASN
1	B	1035	ASN
1	B	1047	HIS
1	B	1059	GLN

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)

4 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	PO4	A	1107	-	4,4,4	0.91	0	6,6,6	0.45	0
4	GTP	C	26	-	26,34,34	1.09	2 (7%)	32,54,54	1.53	7 (21%)
3	PO4	B	1107	-	4,4,4	0.88	0	6,6,6	0.44	0
4	GTP	D	26	-	26,34,34	1.10	2 (7%)	32,54,54	1.49	7 (21%)

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	C	26	-	-	5/18/38/38	0/3/3/3
4	GTP	D	26	-	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	26	GTP	C5-C6	-3.85	1.39	1.47
4	C	26	GTP	C5-C6	-3.79	1.39	1.47
4	C	26	GTP	C2-N3	2.26	1.38	1.33
4	D	26	GTP	C2-N3	2.25	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	26	GTP	C5-C6-N1	3.19	119.59	113.95
4	D	26	GTP	PB-O3B-PG	-3.16	121.97	132.83
4	C	26	GTP	PB-O3B-PG	-3.06	122.34	132.83
4	C	26	GTP	C5-C6-N1	3.04	119.32	113.95
4	D	26	GTP	PA-O3A-PB	-2.96	122.67	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	26	GTP	C8-N7-C5	2.95	108.61	102.99
4	C	26	GTP	C3'-C2'-C1'	2.91	105.35	100.98
4	D	26	GTP	C8-N7-C5	2.90	108.51	102.99
4	C	26	GTP	PA-O3A-PB	-2.82	123.16	132.83
4	D	26	GTP	C2-N1-C6	-2.81	119.92	125.10
4	C	26	GTP	C2-N1-C6	-2.70	120.13	125.10
4	D	26	GTP	C3'-C2'-C1'	2.28	104.40	100.98
4	C	26	GTP	O6-C6-C5	-2.17	120.14	124.37
4	D	26	GTP	O6-C6-C5	-2.08	120.30	124.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	26	GTP	C5'-O5'-PA-O1A
4	C	26	GTP	PB-O3A-PA-O5'
4	C	26	GTP	C5'-O5'-PA-O3A
4	C	26	GTP	O4'-C4'-C5'-O5'
4	C	26	GTP	C5'-O5'-PA-O2A
4	D	26	GTP	PG-O3B-PB-O2B
4	D	26	GTP	C5'-O5'-PA-O1A

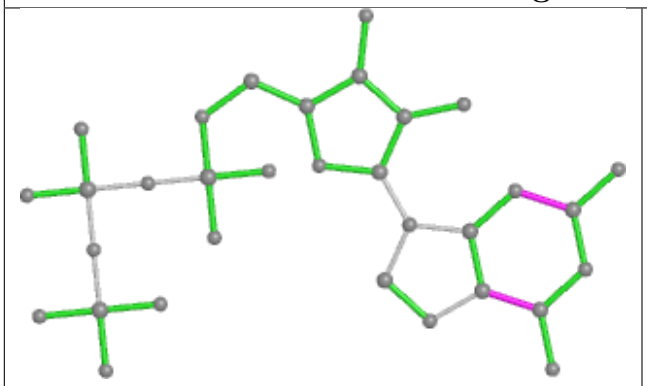
There are no ring outliers.

1 monomer is involved in 1 short contact:

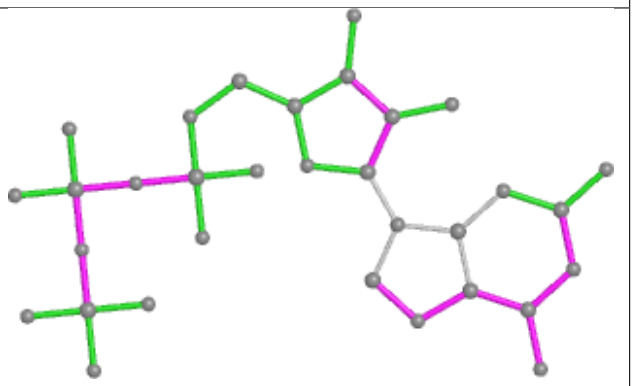
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	26	GTP	1	0

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 then 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.

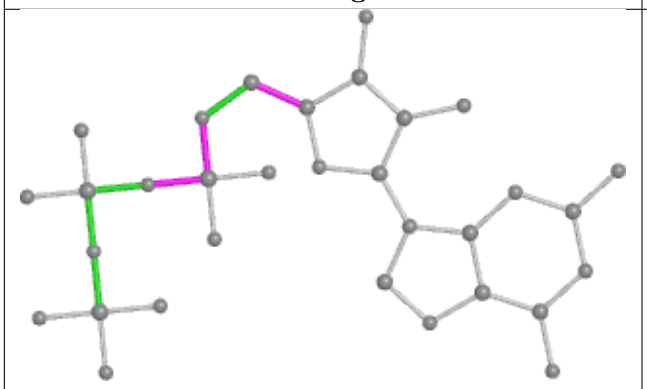
Ligand GTP C 26



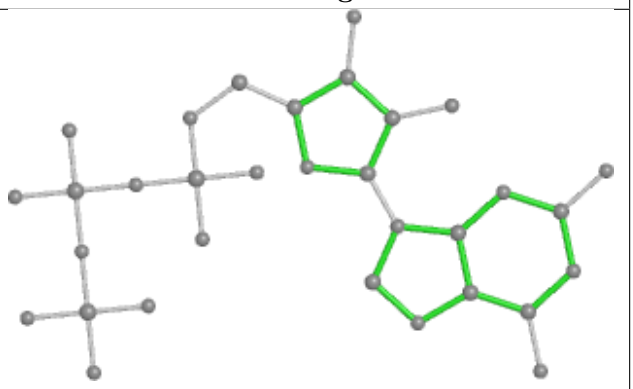
Bond lengths



Bond angles

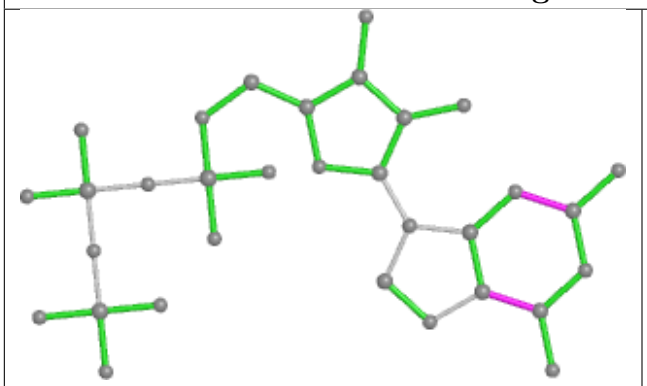


Torsions

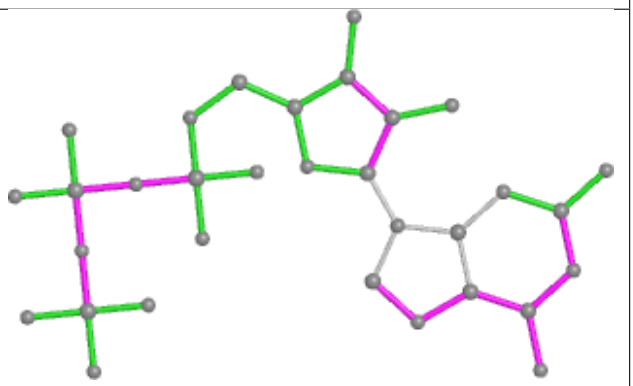


Rings

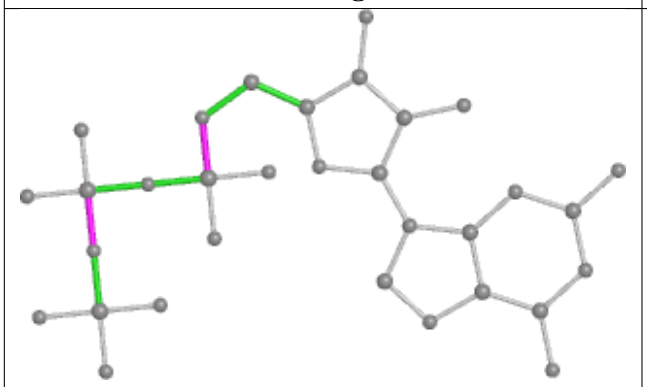
Ligand GTP D 26



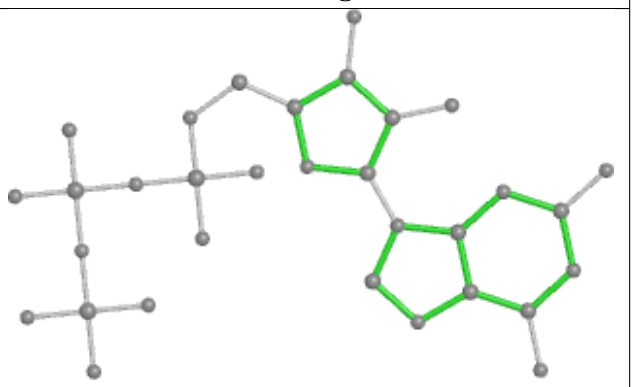
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	1095/1118 (97%)	0.03	37 (3%)	45	45	12, 26, 49, 60	0
1	B	1094/1118 (97%)	0.05	35 (3%)	47	48	11, 26, 46, 64	0
2	C	20/36 (55%)	0.03	2 (10%)	7	5	24, 34, 52, 54	0
2	D	20/36 (55%)	-0.11	1 (5%)	28	27	17, 30, 47, 56	0
All	All	2229/2308 (96%)	0.04	75 (3%)	45	45	11, 26, 48, 64	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1018	GLU	5.6
1	A	10	GLU	4.8
1	A	7	GLU	4.7
1	A	28	GLU	4.4
1	A	1015	ASP	3.7
1	B	726	ALA	3.7
1	B	725	ALA	3.6
1	A	8	LEU	3.6
1	B	6	GLU	3.5
1	B	7	GLU	3.4
1	B	1018	GLU	3.4
1	B	264	PRO	3.4
1	A	1100	GLN	3.3
1	A	725	ALA	3.3
1	A	1014	TYR	3.3
1	A	713	ASN	3.2
1	B	1096	GLU	3.2
1	B	10	GLU	3.2
1	B	1015	ASP	3.2
1	A	754	LYS	3.2
1	A	1019	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	3.1
1	A	265	ASP	3.1
1	B	265	ASP	3.0
1	B	1014	TYR	3.0
1	B	769	LYS	3.0
1	B	1098	ARG	3.0
1	B	714	ILE	2.9
1	B	366	THR	2.9
1	A	261	GLU	2.8
2	D	3	DG	2.8
1	B	281	PHE	2.8
1	B	727	SER	2.7
1	A	26	LYS	2.7
1	A	766	ALA	2.7
1	A	845	ASP	2.7
1	B	713	ASN	2.7
1	B	730	HIS	2.7
1	B	723	LYS	2.7
1	A	729	ALA	2.6
1	A	24	ASP	2.6
1	A	753	ARG	2.6
1	A	264	PRO	2.5
1	B	710	LYS	2.4
1	B	767	LYS	2.4
1	A	267	LYS	2.4
1	A	767	LYS	2.4
1	B	42	GLU	2.4
1	B	43	GLU	2.4
1	A	1017	ARG	2.3
1	B	755	GLY	2.3
1	B	712	PRO	2.3
1	B	763	GLY	2.3
1	A	366	THR	2.3
1	A	728	GLU	2.3
1	B	26	LYS	2.3
1	A	711	ASP	2.2
1	B	722	GLY	2.2
1	A	751	VAL	2.2
1	A	6	GLU	2.2
2	C	22	DC	2.2
1	A	25	SER	2.2
1	A	723	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	754	LYS	2.2
1	B	764	THR	2.2
1	A	371	LEU	2.1
1	A	709	ALA	2.1
2	C	3	DG	2.1
1	A	710	LYS	2.1
1	B	768	GLY	2.1
1	B	704	VAL	2.1
1	A	1099	LYS	2.0
1	A	75	GLU	2.0
1	B	724	GLN	2.0
1	A	23	ALA	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)

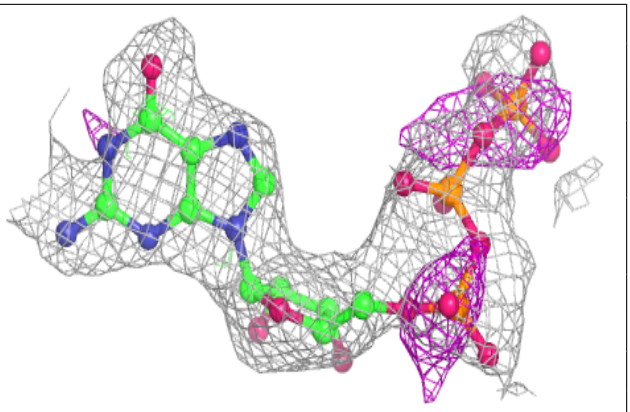
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

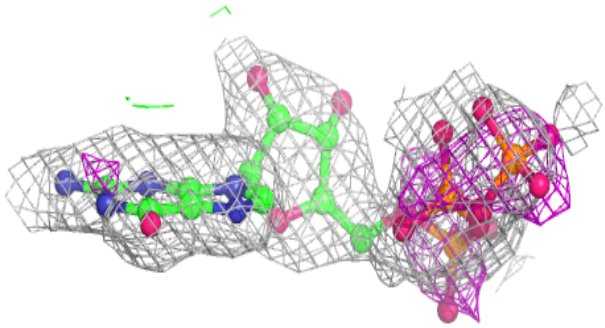
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GTP	C	26	32/32	0.79	0.25	43,47,58,58	0
4	GTP	D	26	32/32	0.80	0.28	54,58,68,68	0
3	PO4	B	1107	5/5	0.91	0.23	57,57,57,57	0
3	PO4	A	1107	5/5	0.96	0.20	38,38,38,38	0

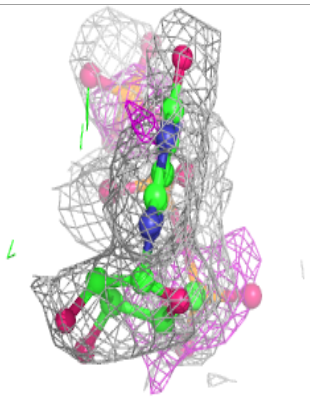
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP C 26:

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

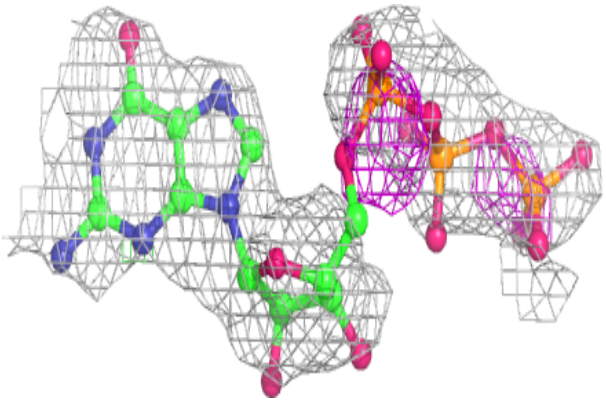


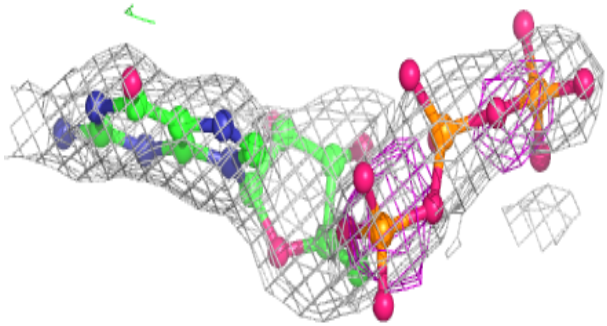


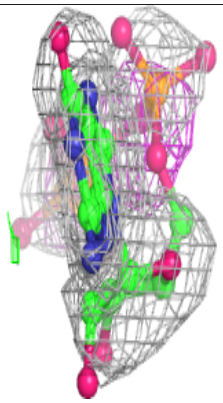


Electron density around GTP D 26:

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







6.5 Other polymers (i)

There are no such residues in this entry.