



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 AM UTC

PDB ID : 4A8K / pdb_00004a8k
Title : Non-Catalytic Ions Direct the RNA-Dependent RNA Polymerase of Bacterial dsRNA virus phi6 from De Novo Initiation to Elongation
Authors : Wright, S.; Poranen, M.M.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2011-11-21
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

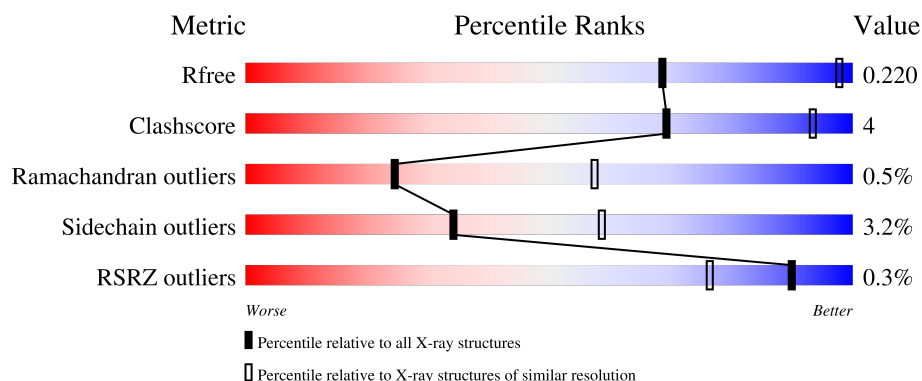
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	665	90% 9% .
1	B	665	87% 12% .
1	C	665	88% 11% .
2	E	4	75% 25% 75%
3	F	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16008 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			78	39	15	21	3			

- Molecule 3 is a DNA chain called 5'-D(*TP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	P	0	0	0
			36	19	5	11	1			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

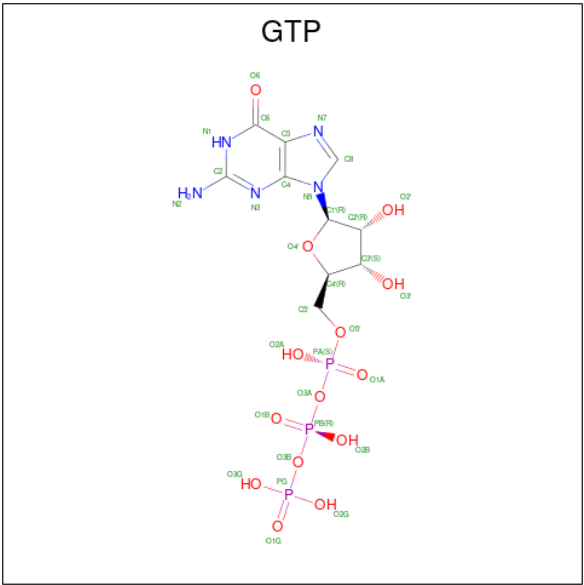
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

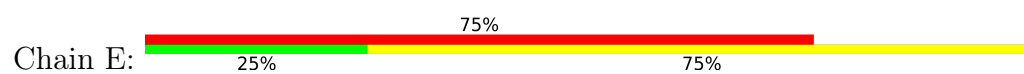
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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



● Molecule 3: 5'-D(*TP*CP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.53Å 93.03Å 140.86Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	46.51 – 3.50 46.51 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (46.51-3.50) 85.3 (46.51-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.276 , 0.307 0.215 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (5.86%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16008	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	0.70	0/5396	1.22	12/7297 (0.2%)
1	B	0.71	0/5396	1.30	16/7297 (0.2%)
1	C	0.71	0/5396	1.30	14/7297 (0.2%)
2	E	0.38	0/87	1.38	1/132 (0.8%)
3	F	0.52	0/39	1.74	1/58 (1.7%)
All	All	0.70	0/16314	1.28	44/22081 (0.2%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	DA	P-O3'-C3'	8.06	132.28	120.20
3	F	6	DT	P-O3'-C3'	7.53	131.50	120.20
1	C	302	PHE	N-CA-C	6.82	122.27	113.88
1	B	302	PHE	N-CA-C	6.70	122.11	113.88
1	A	302	PHE	N-CA-C	6.69	122.11	113.88
1	B	100	TRP	N-CA-C	-6.41	101.71	109.72
1	A	100	TRP	N-CA-C	-6.27	101.88	109.72
1	C	100	TRP	N-CA-C	-6.19	101.98	109.72
1	B	1	PRO	CA-C-N	6.15	133.29	121.54
1	B	1	PRO	C-N-CA	6.15	133.29	121.54
1	C	363	LEU	N-CA-C	6.03	117.30	109.64
1	B	229	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	363	LEU	N-CA-C	6.02	117.29	109.64
1	B	155	TYR	N-CA-C	6.01	119.80	112.23
1	C	229	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	229	ASP	CA-CB-CG	5.92	118.52	112.60
1	C	155	TYR	N-CA-C	5.72	119.44	112.23
1	A	363	LEU	N-CA-C	5.71	116.90	109.64
1	A	333	PRO	N-CA-C	5.64	119.74	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	PHE	N-CA-C	5.62	118.14	111.33
1	B	333	PRO	N-CA-C	5.60	119.68	110.55
1	C	333	PRO	N-CA-C	5.59	119.67	110.55
1	A	419	ALA	N-CA-C	5.45	118.50	109.79
1	B	277	PHE	N-CA-C	5.44	117.91	111.33
1	A	155	TYR	N-CA-C	5.44	119.08	112.23
1	B	437	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	277	PHE	N-CA-C	5.37	117.83	111.33
1	B	206	GLN	N-CA-C	-5.37	96.56	107.41
1	A	663	PRO	CA-C-N	5.31	131.26	121.70
1	A	663	PRO	C-N-CA	5.31	131.26	121.70
1	B	206	GLN	CA-C-N	5.29	128.11	120.38
1	B	206	GLN	C-N-CA	5.29	128.11	120.38
1	A	609	ALA	N-CA-C	5.19	117.68	111.71
1	B	609	ALA	N-CA-C	5.13	117.61	111.71
1	C	135	PHE	N-CA-C	5.13	119.18	113.02
1	B	78	ASN	CA-CB-CG	5.12	117.72	112.60
1	C	68	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	206	GLN	N-CA-C	-5.10	97.10	107.41
1	C	206	GLN	N-CA-C	-5.10	97.10	107.41
1	B	662	MET	N-CA-C	5.10	117.11	110.08
1	C	419	ALA	N-CA-C	5.09	119.09	110.02
1	C	206	GLN	CA-C-N	5.07	127.78	120.38
1	C	206	GLN	C-N-CA	5.07	127.78	120.38
1	C	70	ASP	CA-CB-CG	5.06	117.66	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5265	0	5165	34	0
1	B	5265	0	5164	44	0
1	C	5265	0	5165	38	0
2	E	78	0	47	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	36	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	2	0
5	B	32	0	11	3	0
5	C	32	0	12	4	0
All	All	16008	0	15601	111	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 (111) 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:C:270:ARG:HH22	5:C:1666:GTP:H5''	1.45	0.80
1:A:608:GLN:HE22	1:B:593:ARG:NH1	1.84	0.75
1:A:600:ARG:HH12	1:B:581:GLU:HG3	1.53	0.71
1:B:206:GLN:HG2	1:B:268:ARG:HD3	1.77	0.66
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.45	0.65
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.46	0.62
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.47	0.61
1:A:593:ARG:HG2	1:B:42:GLY:HA2	1.84	0.60
1:A:600:ARG:NH1	1:B:581:GLU:HG3	2.18	0.59
1:A:608:GLN:HE22	1:B:593:ARG:CZ	2.16	0.58
1:A:427:LYS:HE3	1:C:12:ILE:HG21	1.86	0.58
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.85	0.58
1:C:651:VAL:O	1:C:655:GLU:HB2	2.04	0.58
1:B:651:VAL:O	1:B:655:GLU:HB2	2.05	0.57
1:B:151:THR:HG22	1:B:163:LYS:HG3	1.87	0.56
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.71	0.55
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.70	0.55
1:A:651:VAL:O	1:A:655:GLU:HB2	2.06	0.55
1:B:328:HIS:C	1:B:328:HIS:CD2	2.84	0.55
1:C:151:THR:HG22	1:C:163:LYS:HG3	1.87	0.54
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.41	0.54
1:B:541:LYS:NZ	2:E:4:DA:H2''	2.23	0.54
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.42	0.54
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.72	0.54
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.44	0.51
1:A:534:SER:O	1:B:48:PRO:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:PRO:HG3	1:B:238:GLU:HG3	1.93	0.50
1:B:26:GLN:HB3	2:E:6:DT:C2	2.46	0.50
1:B:328:HIS:ND1	1:B:453:ASP:HB3	2.27	0.50
1:C:392:SER:O	1:C:398:THR:HG21	2.12	0.50
1:A:392:SER:O	1:A:398:THR:HG21	2.11	0.50
1:C:343:GLU:HA	1:C:343:GLU:OE1	2.12	0.49
1:A:407:SER:HA	1:A:448:GLN:HE22	1.77	0.49
1:B:392:SER:O	1:B:398:THR:HG21	2.12	0.49
5:B:1666:GTP:O2G	5:B:1666:GTP:O2B	2.30	0.49
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.13	0.49
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.95	0.49
1:B:130:ALA:HB2	1:B:408:ILE:HD11	1.95	0.49
1:B:270:ARG:NH1	5:B:1666:GTP:O2'	2.37	0.48
1:C:94:PRO:HB3	1:C:269:ARG:HG3	1.96	0.48
1:C:407:SER:HA	1:C:448:GLN:HE22	1.79	0.48
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.14	0.47
1:B:136:SER:OG	1:B:293:LYS:NZ	2.48	0.47
1:A:270:ARG:HH22	5:A:1666:GTP:C5'	2.26	0.47
1:B:70:ASP:OD2	1:B:74:ARG:HD2	2.14	0.47
1:C:70:ASP:OD2	1:C:74:ARG:HD2	2.14	0.47
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.97	0.47
1:B:417:HIS:CE1	1:B:474:MET:HE1	2.50	0.47
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.96	0.47
1:C:225:ARG:HG3	1:C:268:ARG:HG3	1.97	0.47
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.97	0.46
1:B:345:LEU:HG	1:B:354:VAL:HG11	1.97	0.46
1:B:407:SER:HA	1:B:448:GLN:HE22	1.81	0.46
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.16	0.46
1:C:270:ARG:NH2	5:C:1666:GTP:H5''	2.24	0.46
1:A:417:HIS:CE1	1:A:474:MET:HE1	2.51	0.46
1:C:270:ARG:HH12	5:C:1666:GTP:H3'	1.81	0.46
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.98	0.46
1:B:206:GLN:HB2	1:B:270:ARG:HD2	1.98	0.46
1:B:94:PRO:HB3	1:B:269:ARG:HG3	1.98	0.45
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.51	0.45
1:C:86:GLY:O	1:C:208:THR:HG22	2.16	0.45
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.52	0.45
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.99	0.45
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.52	0.45
1:A:475:LEU:HD21	1:A:482:PRO:HG3	1.99	0.44
1:C:151:THR:CG2	1:C:163:LYS:HG3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:HD22	1:C:398:THR:HG22	1.99	0.44
1:B:391:LEU:HD22	1:B:398:THR:HG22	1.98	0.44
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.83	0.44
1:C:301:THR:HG23	1:C:448:GLN:HG3	1.98	0.44
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.01	0.44
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.17	0.44
1:C:417:HIS:CE1	1:C:474:MET:HE1	2.52	0.44
1:B:286:VAL:O	1:B:289:PRO:HD2	2.18	0.44
1:A:301:THR:HG23	1:A:448:GLN:HG3	2.00	0.43
1:C:17:LEU:HA	1:C:190:TYR:OH	2.18	0.43
1:C:270:ARG:NH1	5:C:1666:GTP:H3'	2.33	0.43
1:B:89:HIS:CE1	1:B:211:ILE:HD11	2.54	0.43
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.99	0.43
1:A:392:SER:O	1:A:398:THR:CG2	2.66	0.43
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.82	0.43
1:B:392:SER:O	1:B:398:THR:CG2	2.67	0.43
1:C:54:LYS:NZ	1:C:91:ASN:HD21	2.17	0.43
1:C:130:ALA:HB2	1:C:408:ILE:HD11	2.01	0.43
1:C:163:LYS:HB2	1:C:163:LYS:HE3	1.81	0.43
1:A:270:ARG:HH22	5:A:1666:GTP:H5'	1.84	0.43
1:B:163:LYS:HE3	1:B:163:LYS:HB2	1.81	0.43
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.49	0.43
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.49	0.43
1:B:151:THR:CG2	1:B:163:LYS:HG3	2.49	0.42
1:A:391:LEU:HD22	1:A:398:THR:HG22	2.01	0.42
1:B:642:HIS:CE1	1:B:646:MET:HG3	2.54	0.42
1:A:151:THR:CG2	1:A:163:LYS:HG3	2.48	0.42
1:B:94:PRO:CB	1:B:269:ARG:HG3	2.50	0.42
1:C:392:SER:O	1:C:398:THR:CG2	2.67	0.42
1:C:85:PHE:O	1:C:211:ILE:HD12	2.19	0.42
1:B:132:ARG:NH1	1:B:343:GLU:OE2	2.53	0.42
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.85	0.42
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.16	0.41
1:C:72:TYR:CE2	1:C:476:LYS:HD3	2.54	0.41
1:A:217:THR:HG23	1:A:219:LYS:H	1.84	0.41
1:B:72:TYR:CE2	1:B:476:LYS:HD3	2.55	0.41
5:B:1666:GTP:O1B	5:B:1666:GTP:O1A	2.38	0.41
1:C:89:HIS:CE1	1:C:211:ILE:HD11	2.55	0.41
1:A:86:GLY:O	1:A:89:HIS:HD2	2.04	0.41
1:B:226:MET:HE1	1:B:244:ALA:HB2	2.03	0.41
1:C:131:VAL:HG11	1:C:343:GLU:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:ARG:HD3	1:C:664:ARG:H	1.86	0.41
1:B:78:ASN:ND2	1:B:80:VAL:H	2.19	0.41
1:C:153:ILE:HA	1:C:154:PRO:HA	1.84	0.41

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	662/665 (100%)	640 (97%)	20 (3%)	2 (0%)	36	67
1	B	662/665 (100%)	637 (96%)	22 (3%)	3 (0%)	24	57
1	C	662/665 (100%)	635 (96%)	23 (4%)	4 (1%)	21	54
All	All	1986/1995 (100%)	1912 (96%)	65 (3%)	9 (0%)	24	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ARG
1	B	2	ARG
1	B	607	ARG
1	C	607	ARG
1	C	136	SER
1	A	136	SER
1	C	2	ARG
1	C	368	GLY
1	B	368	GLY

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	557/558 (100%)	543 (98%)	14 (2%)	42	63
1	B	557/558 (100%)	537 (96%)	20 (4%)	31	57
1	C	557/558 (100%)	537 (96%)	20 (4%)	31	57
All	All	1671/1674 (100%)	1617 (97%)	54 (3%)	34	59

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	78	ASN
1	A	81	ARG
1	A	82	THR
1	A	102	LEU
1	A	163	LYS
1	A	269	ARG
1	A	362	LYS
1	A	391	LEU
1	A	404	LEU
1	A	418	THR
1	A	497	LEU
1	A	607	ARG
1	A	662	MET
1	B	30	ARG
1	B	41	GLU
1	B	63	ASP
1	B	78	ASN
1	B	82	THR
1	B	102	LEU
1	B	163	LYS
1	B	166	ILE
1	B	206	GLN
1	B	269	ARG
1	B	362	LYS
1	B	384	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	391	LEU
1	B	404	LEU
1	B	418	THR
1	B	450	SER
1	B	497	LEU
1	B	520	SER
1	B	596	LEU
1	B	662	MET
1	C	2	ARG
1	C	30	ARG
1	C	41	GLU
1	C	63	ASP
1	C	78	ASN
1	C	82	THR
1	C	102	LEU
1	C	163	LYS
1	C	269	ARG
1	C	270	ARG
1	C	362	LYS
1	C	384	ASN
1	C	391	LEU
1	C	404	LEU
1	C	418	THR
1	C	497	LEU
1	C	502	LEU
1	C	658	LEU
1	C	662	MET
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	255	GLN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	519	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	525	GLN
1	A	608	GLN
1	A	626	ASN
1	B	25	GLN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	191	GLN
1	B	255	GLN
1	B	309	ASN
1	B	448	GLN
1	B	519	ASN
1	B	525	GLN
1	B	626	ASN
1	C	26	GLN
1	C	78	ASN
1	C	91	ASN
1	C	255	GLN
1	C	309	ASN
1	C	448	GLN
1	C	519	ASN
1	C	525	GLN
1	C	626	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
5	GTP	A	1666	-	33,34,34	1.82	7 (21%)	50,54,54	2.07	13 (26%)
5	GTP	B	1666	-	33,34,34	1.12	3 (9%)	50,54,54	1.79	8 (16%)
5	GTP	C	1666	-	33,34,34	2.07	5 (15%)	50,54,54	1.72	8 (16%)

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
5	GTP	A	1666	-	-	3/22/38/38	0/3/3/3
5	GTP	B	1666	-	-	5/22/38/38	0/3/3/3
5	GTP	C	1666	-	-	5/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1666	GTP	PA-O3A	6.67	1.66	1.59
5	C	1666	GTP	PB-O3A	6.54	1.66	1.59
5	A	1666	GTP	PB-O3A	4.34	1.64	1.59
5	A	1666	GTP	PA-O3A	4.23	1.64	1.59
5	A	1666	GTP	PB-O3B	4.10	1.63	1.59
5	C	1666	GTP	PB-O3B	3.54	1.63	1.59
5	B	1666	GTP	C5-C4	3.12	1.47	1.38
5	A	1666	GTP	O4'-C1'	2.85	1.48	1.42
5	A	1666	GTP	C5-C4	2.34	1.45	1.38
5	C	1666	GTP	PG-O2G	2.31	1.63	1.54
5	A	1666	GTP	C2'-C3'	2.27	1.59	1.53
5	C	1666	GTP	O4'-C1'	2.23	1.47	1.42
5	A	1666	GTP	C4-N3	2.20	1.39	1.34
5	B	1666	GTP	C6-N1	-2.19	1.34	1.38
5	B	1666	GTP	C4-N9	-2.03	1.32	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1666	GTP	C5-C4-N3	-7.00	117.25	128.39
5	A	1666	GTP	N9-C4-N3	5.94	137.83	125.95
5	A	1666	GTP	C2-N3-C4	5.58	121.92	112.30
5	B	1666	GTP	C5-C4-N3	-5.45	119.72	128.39
5	C	1666	GTP	C2-N3-C4	5.31	121.45	112.30
5	C	1666	GTP	C5-C4-N3	-5.12	120.24	128.39
5	B	1666	GTP	C2-N3-C4	4.89	120.73	112.30
5	C	1666	GTP	N9-C4-N3	4.24	134.43	125.95
5	B	1666	GTP	N9-C4-N3	3.81	133.58	125.95
5	B	1666	GTP	C6-C5-N7	3.77	137.15	130.29
5	A	1666	GTP	O4'-C1'-C2'	-3.55	99.02	106.62
5	B	1666	GTP	C2'-C1'-N9	-3.44	103.67	113.25
5	A	1666	GTP	C8-N7-C5	3.18	109.93	104.26
5	C	1666	GTP	C8-N7-C5	2.99	109.59	104.26
5	B	1666	GTP	C4-C5-N7	-2.80	106.23	110.67
5	B	1666	GTP	C3'-C2'-C1'	2.67	106.51	101.46
5	A	1666	GTP	O5'-C5'-C4'	2.63	117.94	108.99
5	A	1666	GTP	O2'-C2'-C3'	2.49	119.81	111.82
5	B	1666	GTP	O4'-C1'-N9	2.45	113.92	108.36
5	C	1666	GTP	C6-C5-N7	2.37	134.61	130.29
5	C	1666	GTP	C2-N1-C6	-2.37	120.81	125.11
5	C	1666	GTP	O6-C6-C5	-2.36	120.29	126.53
5	A	1666	GTP	C2-N1-C6	-2.33	120.88	125.11
5	A	1666	GTP	C4-C5-N7	-2.25	107.10	110.67
5	A	1666	GTP	C3'-C2'-C1'	2.18	105.59	101.46
5	C	1666	GTP	C4-C5-N7	-2.18	107.22	110.67
5	A	1666	GTP	C1'-N9-C4	2.06	132.58	126.49
5	A	1666	GTP	O6-C6-C5	-2.05	121.13	126.53
5	A	1666	GTP	O4'-C1'-N9	2.01	112.91	108.36

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1666	GTP	C5'-O5'-PA-O3A
5	B	1666	GTP	C5'-O5'-PA-O1A
5	B	1666	GTP	C5'-O5'-PA-O2A
5	C	1666	GTP	C5'-O5'-PA-O3A
5	C	1666	GTP	C5'-O5'-PA-O1A
5	C	1666	GTP	O4'-C4'-C5'-O5'
5	C	1666	GTP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1666	GTP	O4'-C4'-C5'-O5'
5	A	1666	GTP	C3'-C4'-C5'-O5'
5	B	1666	GTP	O4'-C4'-C5'-O5'
5	A	1666	GTP	PB-O3B-PG-O3G
5	C	1666	GTP	C5'-O5'-PA-O2A
5	B	1666	GTP	C3'-C4'-C5'-O5'

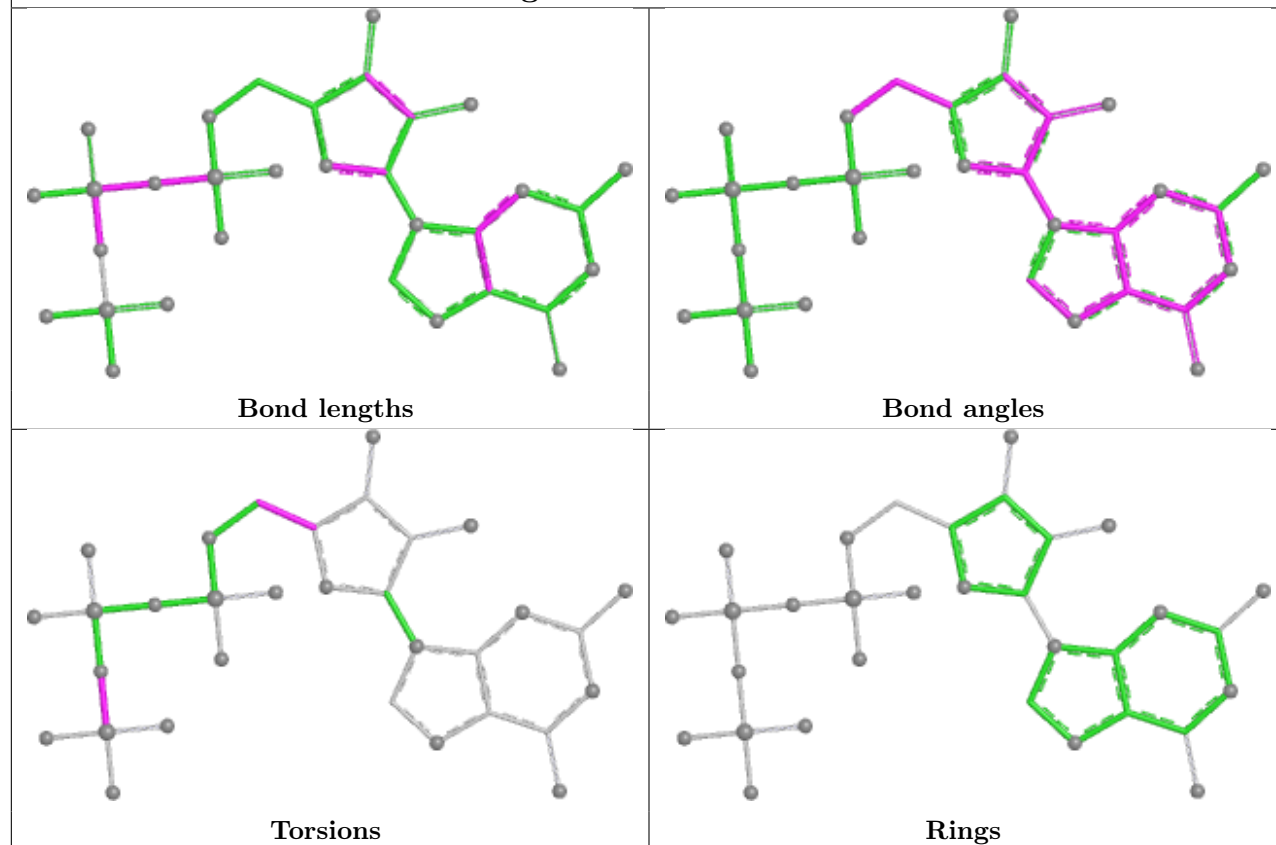
There are no ring outliers.

3 monomers are involved in 9 short contacts:

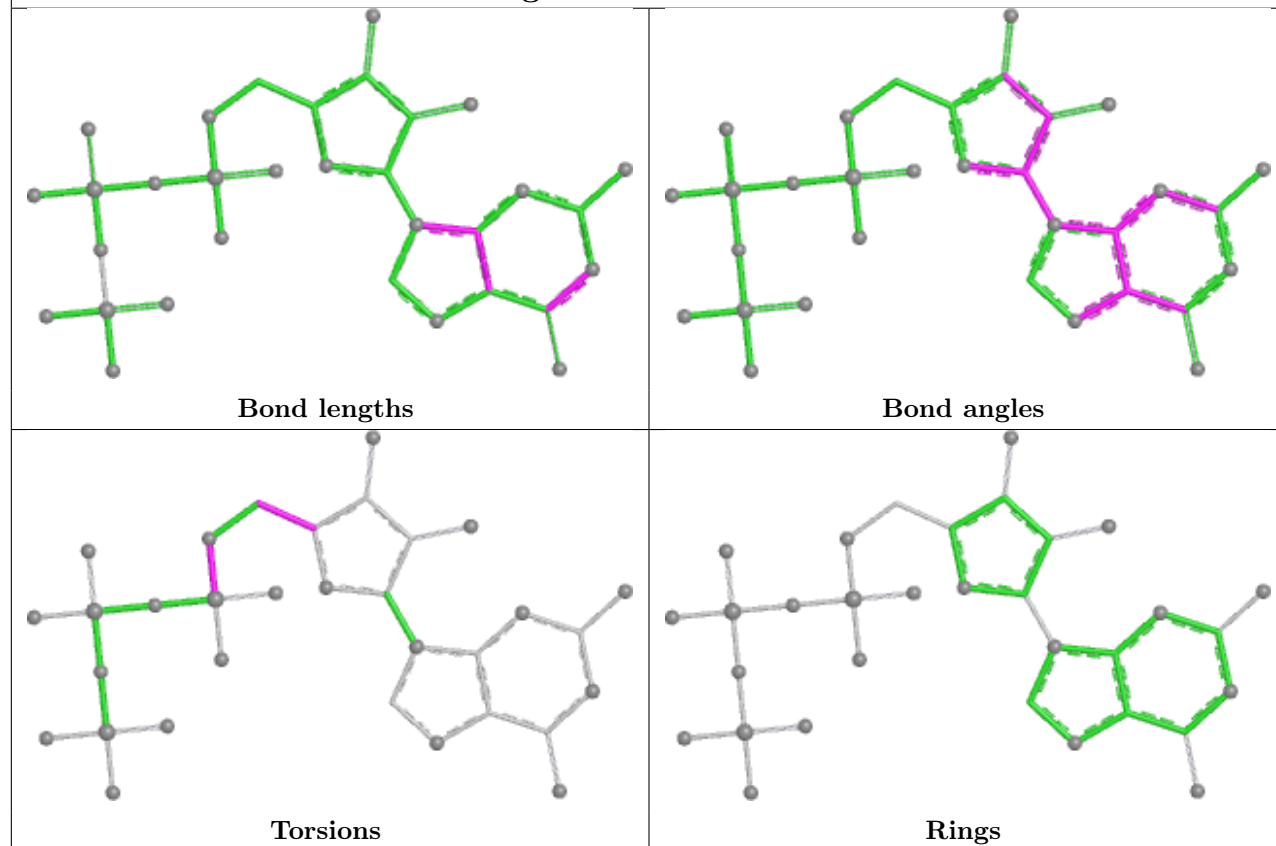
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1666	GTP	2	0
5	B	1666	GTP	3	0
5	C	1666	GTP	4	0

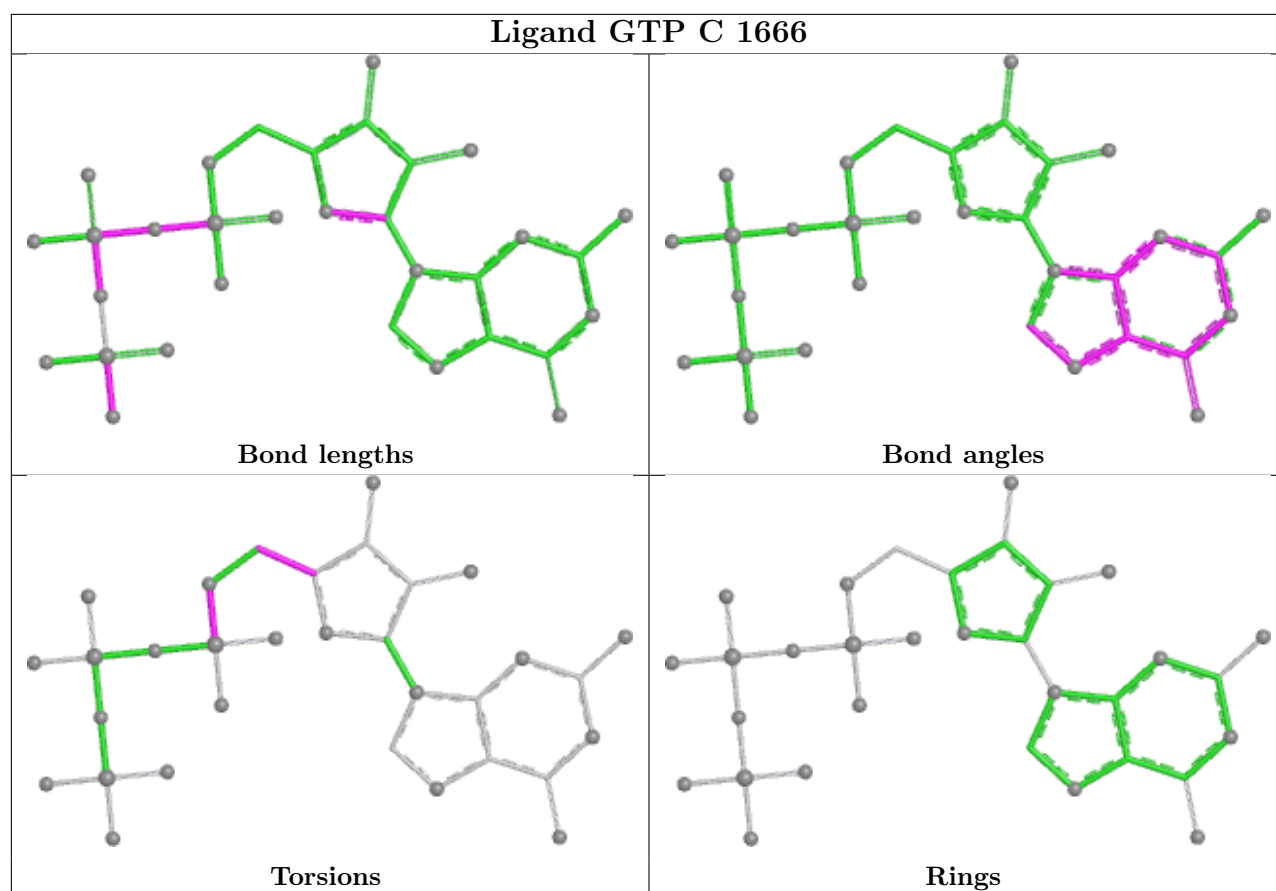
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1666



Ligand GTP B 1666





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	664/665 (99%)	-0.23	0 100 100	71, 94, 120, 146	0
1	B	664/665 (99%)	-0.21	1 (0%) 91 82	69, 92, 117, 174	0
1	C	664/665 (99%)	-0.21	1 (0%) 91 82	67, 97, 130, 201	0
2	E	4/4 (100%)	2.28	3 (75%) 0 0	225, 226, 228, 229	0
3	F	2/2 (100%)	1.39	0 100 100	181, 181, 181, 182	0
All	All	1998/2001 (99%)	-0.21	5 (0%) 90 76	67, 94, 124, 229	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	7	DC	2.9
1	B	453	ASP	2.4
2	E	4	DA	2.4
2	E	6	DT	2.3
1	C	609	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

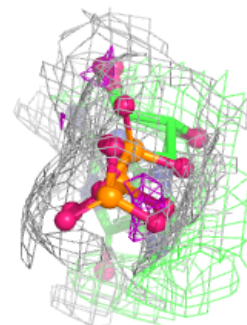
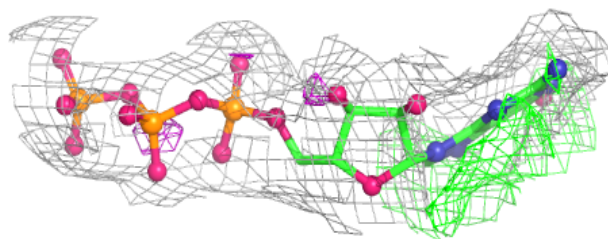
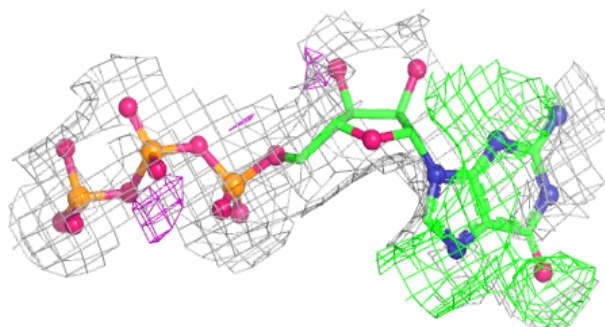
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	B	1666	32/32	0.31	0.16	170,174,176,178	0
5	GTP	C	1666	32/32	0.47	0.13	184,187,189,191	0
5	GTP	A	1666	32/32	0.62	0.13	183,186,189,191	0
4	MG	C	1665	1/1	0.86	0.11	68,68,68,68	0
4	MG	A	1665	1/1	0.94	0.12	63,63,63,63	0
4	MG	B	1665	1/1	0.98	0.06	63,63,63,63	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.

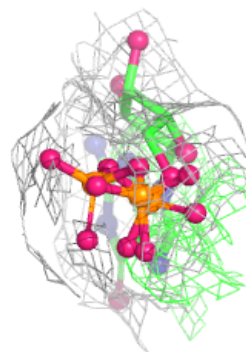
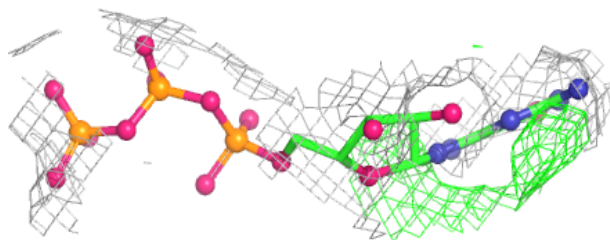
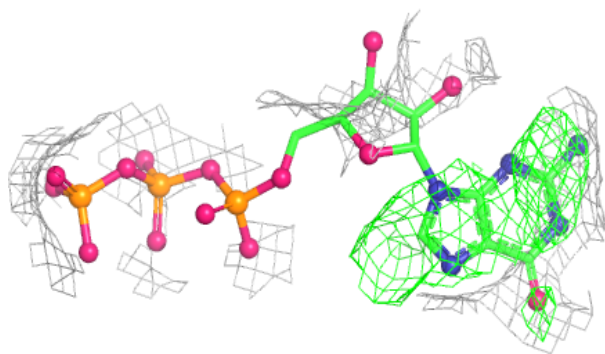
Electron density around GTP B 1666:

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

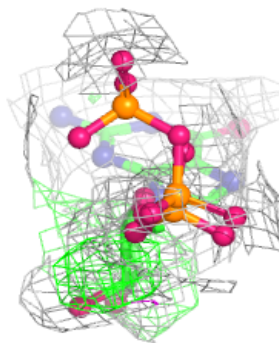
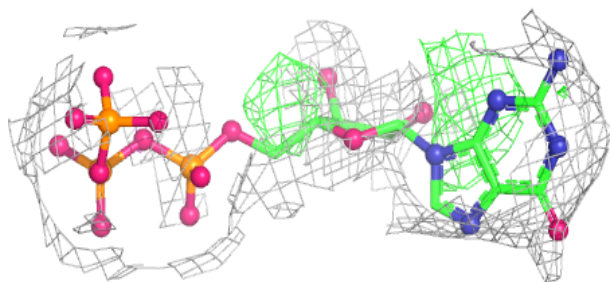
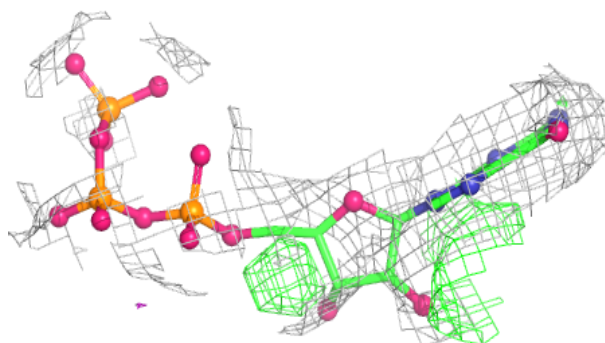


Electron density around GTP C 1666:

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

**Electron density around GTP A 1666:**

$2mF_o-DF_c$ (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.