



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 07:10 PM JST

PDB ID : 7BUJ / pdb_00007buj
Title : mcGAS bound with pppGpG
Authors : Wang, B.; Su, X.D.
Deposited on : 2020-04-07
Resolution : 2.13 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 : 1.8.5 (274361), CSD as541be (2020)
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

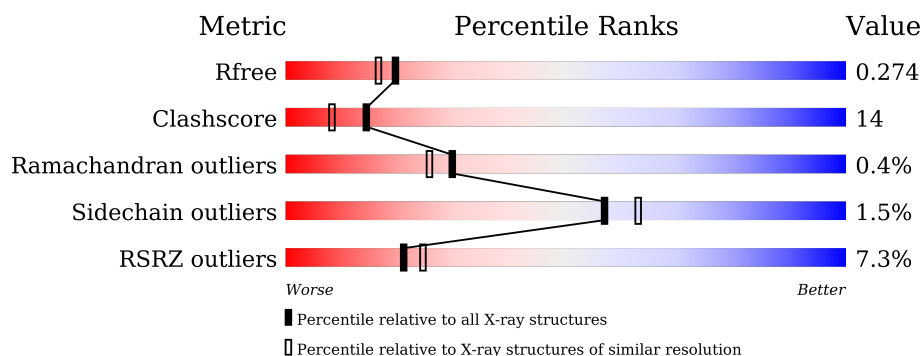
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	447	7% 58% 21% .. 19%
1	B	447	5% 61% 19% 19%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6269 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.

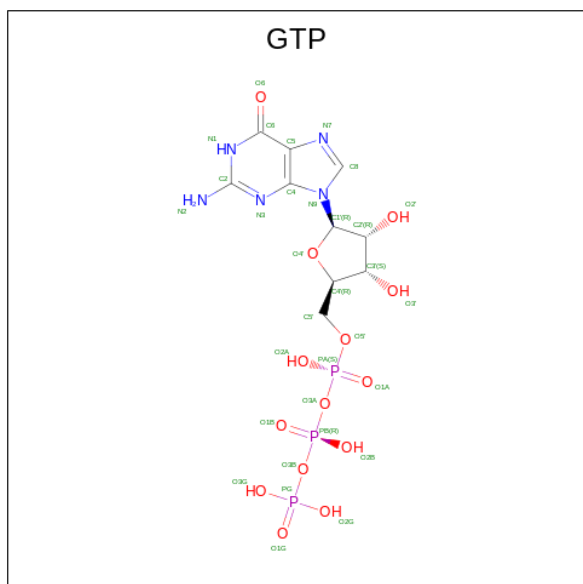
- Molecule 1 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2984	1919	508	544	13			
1	B	362	Total	C	N	O	S	0	0	0
			2993	1924	509	547	13			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

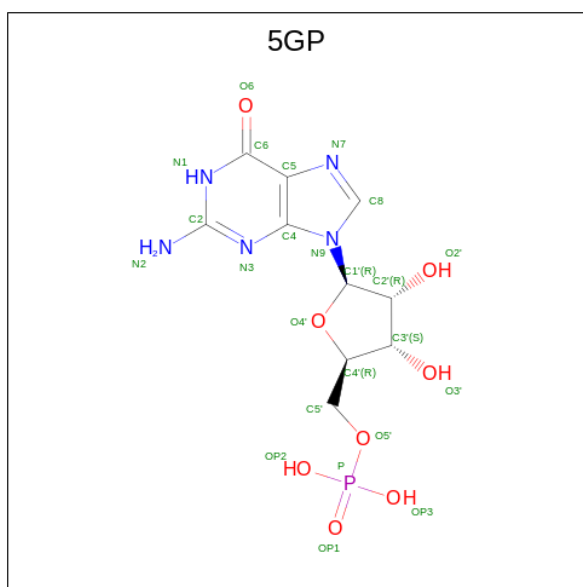


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is water.

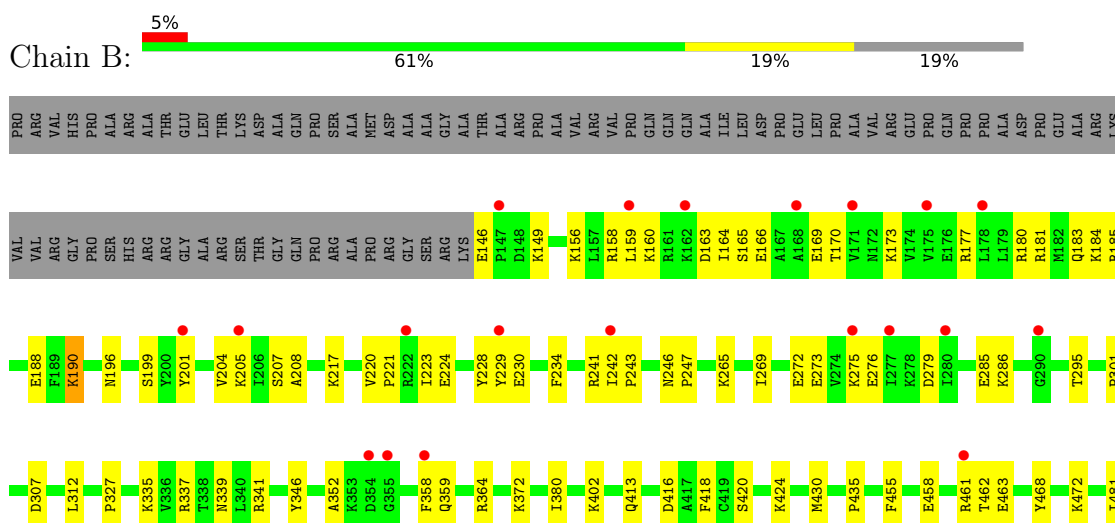
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		

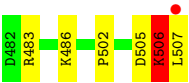
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	85	Total	O	0	0
			85	85		

- Molecule 1: Cyclic GMP-AMP synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.80Å 109.63Å 75.50Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	47.71 – 2.13 47.71 – 2.13	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.71-2.13) 96.8 (47.71-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.216 , 0.278 0.219 , 0.274	Depositor DCC
R_{free} test set	1984 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6269	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: 5GP, GTP, ZN, MN

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	0.65	3/3049 (0.1%)	0.77	6/4093 (0.1%)
1	B	0.47	1/3058 (0.0%)	0.60	1/4106 (0.0%)
All	All	0.57	4/6107 (0.1%)	0.69	7/8199 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	GLU	N-CA	-7.73	1.37	1.46
1	A	203	HIS	CA-C	-6.37	1.43	1.52
1	B	418	PHE	C-O	-5.70	1.16	1.23
1	A	406	GLU	C-O	-5.27	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLU	N-CA-C	-11.43	98.84	111.07
1	A	178	LEU	N-CA-C	-8.85	101.56	111.82
1	A	200	TYR	N-CA-C	5.92	120.04	112.34
1	B	506	LYS	N-CA-C	-5.71	99.04	109.56
1	A	300	ASN	N-CA-C	-5.15	98.43	109.81
1	A	203	HIS	N-CA-C	-5.12	105.19	111.75
1	A	170	THR	CB-CA-C	-5.12	103.08	110.96

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	2984	0	3034	100	0
1	B	2993	0	3039	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	11	2	0
3	B	32	0	11	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	12	1	0
5	B	23	0	11	0	0
6	A	91	0	0	10	0
6	B	85	0	0	8	0
All	All	6269	0	6118	172	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 14.

All (172) 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:300:ASN:CB	1:A:301:PRO:HD3	1.54	1.27
1:B:229:TYR:HB3	1:B:230:GLU:OE1	1.35	1.26
1:A:300:ASN:HB3	1:A:301:PRO:CD	1.66	1.21
1:A:159:LEU:HB2	1:A:203:HIS:CE1	1.93	1.02
1:B:352:ALA:O	1:B:359:GLN:HG3	1.68	0.93
1:A:177:ARG:HH12	1:B:180:ARG:CD	1.83	0.92
1:A:300:ASN:CB	1:A:301:PRO:CD	2.33	0.90
1:A:222:ARG:HD2	1:A:240:LYS:HD2	1.53	0.87
1:A:177:ARG:NE	1:A:180:ARG:HD2	1.93	0.83
1:A:161:ARG:HH11	1:A:164:ILE:HG21	1.45	0.81
1:B:158:ARG:HH22	1:B:205:LYS:HZ1	1.25	0.81
1:A:181:ARG:HH21	1:A:273:GLU:HB2	1.53	0.74
1:A:300:ASN:HB3	1:A:301:PRO:HD3	0.77	0.74
1:A:177:ARG:HH12	1:B:180:ARG:HD2	1.54	0.72
1:B:180:ARG:HE	1:B:184:LYS:HE3	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:TYR:CB	1:B:230:GLU:OE1	2.29	0.70
1:B:241:ARG:NH1	6:B:701:HOH:O	2.22	0.70
1:B:335:LYS:O	1:B:339:ASN:ND2	2.24	0.70
1:B:181:ARG:HH12	1:B:276:GLU:HB2	1.57	0.69
1:A:201:TYR:HA	1:A:204:VAL:HG23	1.75	0.69
1:A:397:CYS:SG	6:A:778:HOH:O	2.49	0.69
1:A:353:LYS:N	1:A:353:LYS:HD3	2.07	0.69
1:B:146:GLU:HB2	1:B:149:LYS:HB3	1.76	0.68
1:B:458:GLU:CD	1:B:461:ARG:HH21	2.02	0.67
1:A:177:ARG:HH12	1:B:180:ARG:HD3	1.58	0.67
1:A:186:GLU:O	1:A:186:GLU:HG2	1.95	0.67
1:A:161:ARG:HA	1:A:164:ILE:HD12	1.75	0.67
1:B:461:ARG:NH2	1:B:462:THR:HG23	2.09	0.67
1:B:164:ILE:HD12	1:B:204:VAL:HG21	1.78	0.65
1:B:177:ARG:HH22	1:B:279:ASP:HB2	1.62	0.65
1:B:463:GLU:HG2	1:B:486:LYS:HD3	1.79	0.65
1:B:430:MET:HE3	1:B:455:PHE:CD1	2.31	0.64
1:A:177:ARG:NH2	6:A:704:HOH:O	2.24	0.64
1:B:228:TYR:HE1	1:B:358:PHE:CD1	2.15	0.63
1:A:201:TYR:HA	1:A:204:VAL:CG2	2.29	0.62
1:B:160:LYS:HB2	1:B:163:ASP:HB2	1.82	0.62
1:A:200:TYR:C	1:A:202:GLU:H	2.06	0.62
1:A:169:GLU:O	1:A:173:LYS:HG2	2.00	0.61
1:B:185:ARG:NH2	1:B:272:GLU:OE1	2.33	0.61
1:A:159:LEU:HA	6:A:702:HOH:O	1.99	0.61
1:B:173:LYS:O	1:B:177:ARG:HG3	2.00	0.61
1:A:267:ARG:CZ	1:A:287:GLU:HB3	2.31	0.60
1:A:188:GLU:OE1	1:A:188:GLU:N	2.27	0.60
1:A:201:TYR:HD1	1:A:201:TYR:C	2.09	0.60
1:B:181:ARG:NH2	1:B:273:GLU:HB3	2.17	0.60
1:B:461:ARG:HH22	1:B:462:THR:HG23	1.65	0.60
1:A:265:LYS:N	1:A:265:LYS:HD2	2.17	0.60
1:B:502:PRO:O	1:B:505:ASP:HB2	2.02	0.59
1:B:159:LEU:HB3	1:B:164:ILE:HD11	1.84	0.59
1:A:402:LYS:NZ	1:A:420:SER:O	2.26	0.59
1:B:435:PRO:HB2	6:B:726:HOH:O	2.02	0.58
1:B:156:LYS:NZ	6:B:704:HOH:O	2.35	0.58
1:B:507:LEU:N	1:B:507:LEU:HD22	2.18	0.58
1:A:180:ARG:NH1	6:A:707:HOH:O	2.30	0.58
1:A:201:TYR:C	1:A:201:TYR:CD1	2.82	0.58
1:A:410:LYS:NZ	6:A:709:HOH:O	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LYS:NZ	6:B:705:HOH:O	2.37	0.58
1:A:204:VAL:O	1:A:204:VAL:HG12	2.04	0.57
1:B:243:PRO:HG2	1:B:246:ASN:HB2	1.86	0.57
1:B:341:ARG:HH11	1:B:341:ARG:HB3	1.68	0.57
1:B:265:LYS:O	1:B:269:ILE:HD12	2.04	0.57
1:A:376:ASN:ND2	6:A:710:HOH:O	2.38	0.57
1:A:174:VAL:O	1:A:178:LEU:HB2	2.05	0.55
1:A:178:LEU:O	1:A:182:MET:HG3	2.07	0.55
1:A:181:ARG:NH2	1:A:273:GLU:HB2	2.21	0.54
1:A:177:ARG:NH1	1:B:180:ARG:CD	2.64	0.54
1:B:430:MET:HA	1:B:430:MET:HE2	1.89	0.54
1:A:167:ALA:HB3	1:A:200:TYR:CE2	2.43	0.53
1:B:472:LYS:HB2	6:B:722:HOH:O	2.08	0.53
1:B:285:GLU:HB3	1:B:295:THR:OG1	2.09	0.53
1:A:177:ARG:NH1	1:B:180:ARG:HD3	2.22	0.53
1:A:322:THR:OG1	1:A:341:ARG:NH2	2.42	0.53
1:A:159:LEU:HD22	6:A:702:HOH:O	2.07	0.53
1:A:201:TYR:HD1	1:A:201:TYR:O	1.90	0.53
1:B:196:ASN:OD1	1:B:372:LYS:NZ	2.40	0.52
1:B:341:ARG:HB3	1:B:341:ARG:NH1	2.25	0.51
3:A:602:GTP:O1A	5:A:605:5GP:H3'	2.10	0.51
1:A:147:PRO:N	1:A:446:SER:HG	2.09	0.51
1:A:265:LYS:HA	1:A:268:LYS:HB3	1.93	0.51
1:A:353:LYS:N	1:A:353:LYS:CD	2.72	0.51
1:B:188:GLU:HG3	1:B:247:PRO:HB2	1.93	0.51
1:A:161:ARG:NH1	1:A:164:ILE:HG21	2.23	0.50
1:A:177:ARG:CZ	1:A:180:ARG:HD2	2.40	0.50
1:A:222:ARG:HG3	1:A:240:LYS:HG3	1.91	0.50
1:A:205:LYS:O	1:A:399:LYS:HB2	2.12	0.50
1:B:242:ILE:H	1:B:242:ILE:HD12	1.76	0.50
1:B:158:ARG:NH2	1:B:205:LYS:HZ1	2.02	0.50
1:B:402:LYS:HD3	1:B:420:SER:HA	1.94	0.49
1:A:200:TYR:C	1:A:202:GLU:N	2.69	0.49
1:B:169:GLU:O	1:B:173:LYS:HG2	2.12	0.49
1:B:220:VAL:HG11	1:B:312:LEU:HD22	1.95	0.49
1:A:217:LYS:HA	1:A:311:ALA:O	2.13	0.49
1:A:201:TYR:HB2	1:A:204:VAL:HB	1.95	0.48
1:A:265:LYS:HG3	1:A:268:LYS:HD3	1.94	0.48
1:A:276:GLU:O	1:A:277:ILE:HD12	2.13	0.48
1:A:394:ARG:HB3	1:A:431:TRP:CZ2	2.49	0.48
1:A:201:TYR:C	1:A:204:VAL:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:O	1:A:341:ARG:HG3	2.13	0.48
1:A:274:VAL:HG21	1:A:284:VAL:HG23	1.94	0.47
1:A:457:LEU:O	1:A:461:ARG:HG3	2.14	0.47
1:A:479:GLU:H	1:A:479:GLU:CD	2.22	0.47
1:B:413:GLN:HG2	1:B:416:ASP:OD2	2.14	0.47
1:B:160:LYS:O	1:B:164:ILE:HG12	2.14	0.47
1:B:228:TYR:HE1	1:B:358:PHE:CE1	2.33	0.47
1:B:234:PHE:CD1	1:B:352:ALA:HB2	2.50	0.47
1:A:292:PRO:HD3	1:A:350:LYS:HD3	1.96	0.47
1:B:380:ILE:HB	6:B:726:HOH:O	2.13	0.47
1:A:402:LYS:HE3	1:A:420:SER:OG	2.15	0.47
1:A:380:ILE:HG21	1:A:436:GLN:HE21	1.80	0.47
1:B:181:ARG:HH12	1:B:276:GLU:CB	2.26	0.47
1:A:202:GLU:C	1:A:204:VAL:N	2.73	0.46
1:B:430:MET:HE3	1:B:455:PHE:CG	2.50	0.46
1:A:162:LYS:HE3	1:A:166:GLU:HG3	1.96	0.46
1:A:181:ARG:HD2	1:A:184:LYS:CD	2.46	0.46
1:B:286:LYS:HA	1:B:286:LYS:HD2	1.72	0.46
1:A:285:GLU:HG2	1:A:295:THR:HB	1.97	0.46
1:A:201:TYR:CA	1:A:204:VAL:HB	2.46	0.46
1:A:181:ARG:HD2	1:A:184:LYS:HD3	1.97	0.45
1:A:218:LEU:HD21	1:A:248:LEU:HD21	1.98	0.45
1:B:221:PRO:O	1:B:223:ILE:HG23	2.15	0.45
1:A:162:LYS:HA	1:A:165:SER:HB2	1.98	0.45
1:B:188:GLU:OE2	1:B:265:LYS:HD3	2.17	0.45
1:B:483:ARG:HA	1:B:486:LYS:HD2	1.98	0.45
1:A:188:GLU:HA	1:A:247:PRO:HB2	1.98	0.45
1:A:201:TYR:CD1	1:A:201:TYR:O	2.69	0.45
1:B:228:TYR:CE1	1:B:358:PHE:CD1	3.02	0.45
1:A:300:ASN:HB2	1:A:301:PRO:HD3	1.78	0.45
1:A:258:SER:OG	1:A:261:LYS:HG3	2.17	0.44
1:A:271:LYS:NZ	6:A:716:HOH:O	2.50	0.44
1:A:364:ARG:NH2	3:A:602:GTP:O6	2.46	0.44
1:A:222:ARG:HD2	1:A:240:LYS:CD	2.37	0.44
1:A:238:LYS:HA	1:A:255:GLU:O	2.18	0.44
1:B:160:LYS:HB2	1:B:163:ASP:CB	2.47	0.44
1:B:234:PHE:CZ	1:B:364:ARG:HG3	2.52	0.44
1:B:337:ARG:O	1:B:341:ARG:HG3	2.17	0.44
1:A:185:ARG:HD2	1:A:190:LYS:NZ	2.32	0.44
1:A:159:LEU:HB2	1:A:203:HIS:HE1	1.67	0.44
1:A:211:GLU:HG2	1:A:305:SER:OG	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:CYS:HA	1:A:396:GLU:OE2	2.17	0.43
1:B:199:SER:OG	1:B:201:TYR:HB2	2.19	0.43
1:B:234:PHE:CE1	1:B:364:ARG:HG3	2.54	0.43
1:A:149:LYS:HA	1:A:152:LYS:HD3	2.01	0.43
1:B:402:LYS:HB3	1:B:402:LYS:HE3	1.79	0.43
1:A:492:LYS:HA	1:A:492:LYS:HD3	1.93	0.42
1:B:295:THR:HG22	1:B:307:ASP:OD1	2.19	0.42
1:A:394:ARG:HD3	1:A:431:TRP:CD1	2.54	0.42
1:A:151:LYS:HB2	1:A:151:LYS:HE2	1.76	0.42
1:A:417:ALA:HB1	1:A:481:ILE:HG12	2.01	0.42
1:B:165:SER:O	1:B:169:GLU:HG3	2.19	0.42
1:A:179:LEU:O	1:A:183:GLN:HG3	2.20	0.42
1:A:466:ASP:OD1	6:A:701:HOH:O	2.21	0.42
1:B:312:LEU:O	1:B:346:TYR:HA	2.20	0.42
1:A:402:LYS:NZ	1:A:423:VAL:HB	2.35	0.42
1:B:506:LYS:O	1:B:506:LYS:CG	2.67	0.42
1:A:179:LEU:HD13	1:A:216:PHE:CZ	2.54	0.42
1:B:183:GLN:O	1:B:190:LYS:HE3	2.21	0.41
1:A:447:SER:O	1:A:451:LYS:HG3	2.20	0.41
1:B:481:ILE:HB	1:B:486:LYS:HE3	2.02	0.41
1:A:200:TYR:O	1:A:202:GLU:N	2.54	0.41
1:A:234:PHE:CG	1:A:352:ALA:HB2	2.55	0.41
1:B:166:GLU:O	1:B:170:THR:HG22	2.20	0.41
1:B:424:LYS:NZ	6:B:714:HOH:O	2.53	0.41
1:A:436:GLN:NE2	1:A:437:ASP:H	2.19	0.41
1:B:230:GLU:OE1	1:B:230:GLU:N	2.49	0.41
1:B:380:ILE:HD12	6:B:726:HOH:O	2.20	0.41
1:A:244:ARG:H	1:A:244:ARG:HG3	1.72	0.41
1:A:413:GLN:HE21	1:A:413:GLN:HB2	1.59	0.40
1:A:383:THR:HB	1:A:389:GLY:HA3	2.03	0.40
1:B:207:SER:OG	1:B:208:ALA:N	2.55	0.40
1:A:335:LYS:HB2	1:A:335:LYS:HE2	1.92	0.40
1:B:327:PRO:HD2	1:B:468:TYR:CZ	2.57	0.40
1:A:158:ARG:O	6:A:702:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	359/447 (80%)	341 (95%)	16 (4%)	2 (1%)	21	15
1	B	360/447 (80%)	338 (94%)	21 (6%)	1 (0%)	36	33
All	All	719/894 (80%)	679 (94%)	37 (5%)	3 (0%)	30	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	PRO
1	B	301	PRO
1	A	201	TYR

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	334/400 (84%)	328 (98%)	6 (2%)	51	57
1	B	335/400 (84%)	331 (99%)	4 (1%)	63	69
All	All	669/800 (84%)	659 (98%)	10 (2%)	57	63

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

Mol	Chain	Res	Type
1	A	178	LEU
1	A	201	TYR
1	A	203	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	244	ARG
1	A	342	ARG
1	A	353	LYS
1	B	190	LYS
1	B	224	GLU
1	B	275	LYS
1	B	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	413	GLN
1	A	436	GLN
1	A	499	ASN
1	B	413	GLN
1	B	439	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	B	602	5,4	30,34,34	3.68	19 (63%)	46,54,54	1.87	10 (21%)
5	5GP	A	605	3	22,25,26	3.76	13 (59%)	33,37,40	1.84	10 (30%)
5	5GP	B	605	3	22,25,26	3.80	14 (63%)	33,37,40	1.96	8 (24%)
3	GTP	A	602	5,4	30,34,34	3.40	11 (36%)	46,54,54	1.70	10 (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
3	GTP	B	602	5,4	-	0/22/38/38	0/3/3/3
5	5GP	A	605	3	-	2/7/25/26	0/3/3/3
5	5GP	B	605	3	-	1/7/25/26	0/3/3/3
3	GTP	A	602	5,4	-	1/22/38/38	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	GTP	O4'-C4'	-9.04	1.24	1.45
5	A	605	5GP	C3'-C4'	-8.81	1.30	1.53
5	B	605	5GP	C3'-C4'	-8.42	1.31	1.53
3	A	602	GTP	O4'-C1'	8.39	1.61	1.42
5	B	605	5GP	O4'-C4'	7.63	1.62	1.45
5	A	605	5GP	O4'-C4'	7.32	1.61	1.45
3	B	602	GTP	C1'-N9	-7.03	1.27	1.47
3	A	602	GTP	O4'-C4'	-6.99	1.29	1.45
3	B	602	GTP	O4'-C1'	6.62	1.57	1.42
3	A	602	GTP	C4-N3	6.36	1.49	1.34
3	B	602	GTP	C2'-C3'	-6.35	1.36	1.53
5	B	605	5GP	C4-N3	6.15	1.48	1.34
5	A	605	5GP	C4-N3	5.98	1.48	1.34
3	A	602	GTP	C2'-C3'	-5.89	1.37	1.53
5	A	605	5GP	O4'-C1'	-5.64	1.28	1.42
5	B	605	5GP	C2-N3	5.57	1.46	1.33
5	B	605	5GP	O4'-C1'	-5.56	1.28	1.42
5	A	605	5GP	C2-N3	5.54	1.46	1.33
3	A	602	GTP	C2-N2	5.53	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GTP	C3'-C4'	5.44	1.66	1.53
3	A	602	GTP	C2-N3	5.32	1.46	1.33
3	B	602	GTP	C4-N3	5.05	1.46	1.34
3	B	602	GTP	C2-N3	4.87	1.44	1.33
3	A	602	GTP	C1'-N9	-4.77	1.33	1.47
3	B	602	GTP	C5-N7	-4.73	1.29	1.39
5	B	605	5GP	C2-N2	4.58	1.45	1.34
3	B	602	GTP	C3'-C4'	4.48	1.64	1.53
5	A	605	5GP	C2-N2	4.23	1.44	1.34
3	B	602	GTP	O6-C6	-4.22	1.15	1.23
3	B	602	GTP	C2-N2	3.98	1.43	1.34
5	A	605	5GP	O3'-C3'	3.80	1.51	1.43
5	B	605	5GP	C6-N1	3.19	1.44	1.38
5	B	605	5GP	C2-N1	3.17	1.45	1.37
5	A	605	5GP	C5-N7	-3.12	1.33	1.39
5	B	605	5GP	O3'-C3'	3.12	1.50	1.43
3	A	602	GTP	C5-C6	3.00	1.55	1.44
5	A	605	5GP	C2-N1	2.99	1.45	1.37
5	B	605	5GP	C5-N7	-2.85	1.33	1.39
3	B	602	GTP	C8-N9	-2.74	1.31	1.37
3	B	602	GTP	C4-N9	-2.74	1.30	1.38
3	A	602	GTP	C6-N1	2.68	1.43	1.38
5	B	605	5GP	O2'-C2'	-2.67	1.36	1.43
5	A	605	5GP	C5-C6	2.59	1.54	1.44
3	A	602	GTP	C2-N1	2.58	1.44	1.37
3	B	602	GTP	C5-C4	-2.58	1.31	1.38
3	B	602	GTP	PG-O3G	-2.54	1.45	1.54
3	B	602	GTP	PB-O2B	-2.52	1.43	1.55
5	B	605	5GP	O6-C6	-2.47	1.18	1.23
3	B	602	GTP	PG-O2G	-2.45	1.45	1.54
5	B	605	5GP	C5-C6	2.42	1.53	1.44
5	A	605	5GP	O5'-C5'	-2.36	1.39	1.44
3	B	602	GTP	PA-O1A	-2.27	1.42	1.50
3	B	602	GTP	O2'-C2'	2.20	1.48	1.43
5	B	605	5GP	O5'-C5'	-2.20	1.39	1.44
5	A	605	5GP	O2'-C2'	-2.13	1.38	1.43
3	B	602	GTP	PA-O2A	-2.09	1.45	1.55
5	A	605	5GP	C4-N9	-2.05	1.32	1.38

All (38) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GTP	C5-C4-N3	-5.50	119.54	128.46
5	B	605	5GP	C5-C4-N3	-4.98	120.37	128.46
3	A	602	GTP	C5-C4-N3	-4.77	120.72	128.46
5	A	605	5GP	C5-C4-N3	-4.72	120.81	128.46
5	B	605	5GP	C2-N3-C4	4.67	120.62	112.30
3	A	602	GTP	C2-N3-C4	4.43	120.19	112.30
3	B	602	GTP	C2-N1-C6	-4.43	117.02	125.10
3	B	602	GTP	C2-N3-C4	4.25	119.86	112.30
3	B	602	GTP	C5-C6-N1	3.72	122.63	113.19
5	A	605	5GP	C2-N3-C4	3.54	118.61	112.30
3	B	602	GTP	O6-C6-C5	-3.32	117.79	126.60
5	B	605	5GP	C2-N1-C6	-3.15	119.36	125.10
5	B	605	5GP	N9-C4-N3	3.06	132.09	125.94
3	B	602	GTP	N9-C4-N3	2.98	131.93	125.94
5	A	605	5GP	N9-C8-N7	-2.97	107.80	113.39
3	B	602	GTP	O2G-PG-O3B	2.96	114.55	104.64
5	A	605	5GP	N9-C4-N3	2.94	131.84	125.94
5	B	605	5GP	N9-C8-N7	-2.92	107.89	113.39
5	A	605	5GP	C2'-C1'-N9	-2.91	104.96	113.22
5	B	605	5GP	O6-C6-C5	-2.91	118.89	126.60
3	B	602	GTP	PB-O3B-PG	-2.77	123.31	132.83
5	B	605	5GP	C5-C6-N1	2.69	120.02	113.19
5	A	605	5GP	C2-N1-C6	-2.68	120.21	125.10
3	A	602	GTP	N9-C8-N7	-2.67	108.36	113.39
3	A	602	GTP	C2-N1-C6	-2.64	120.29	125.10
3	A	602	GTP	C3'-C2'-C1'	2.50	106.18	101.43
3	B	602	GTP	N9-C8-N7	-2.44	108.80	113.39
3	A	602	GTP	C5-C6-N1	2.33	119.11	113.19
3	B	602	GTP	O4'-C1'-N9	-2.25	103.21	108.36
5	A	605	5GP	C8-N7-C5	2.24	108.30	104.24
3	A	602	GTP	O2G-PG-O3B	2.23	112.10	104.64
5	A	605	5GP	C5-C6-N1	2.18	118.72	113.19
3	A	602	GTP	C5-C4-N9	2.17	109.57	105.63
3	A	602	GTP	C4-C5-N7	-2.16	107.30	110.72
5	A	605	5GP	O6-C6-C5	-2.16	120.88	126.60
5	B	605	5GP	C8-N7-C5	2.12	108.08	104.24
3	A	602	GTP	C8-N7-C5	2.06	107.97	104.24
5	A	605	5GP	O4'-C1'-N9	2.04	113.04	108.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

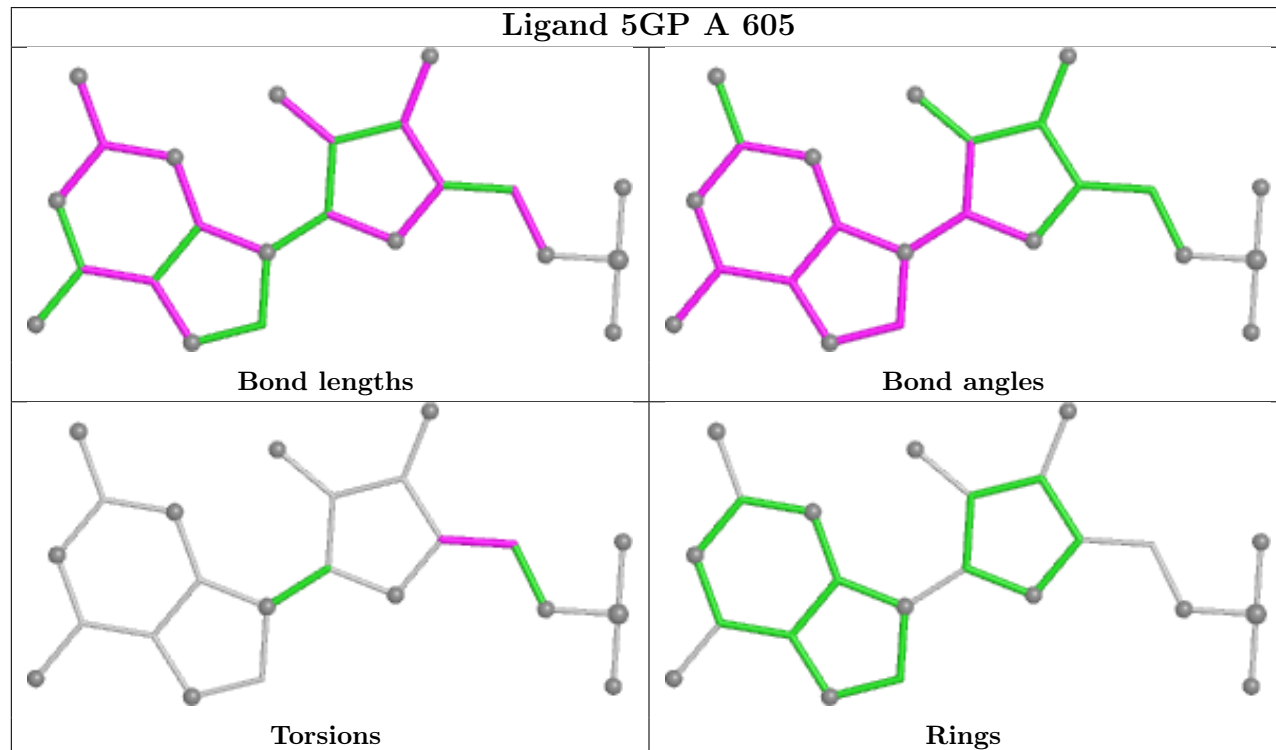
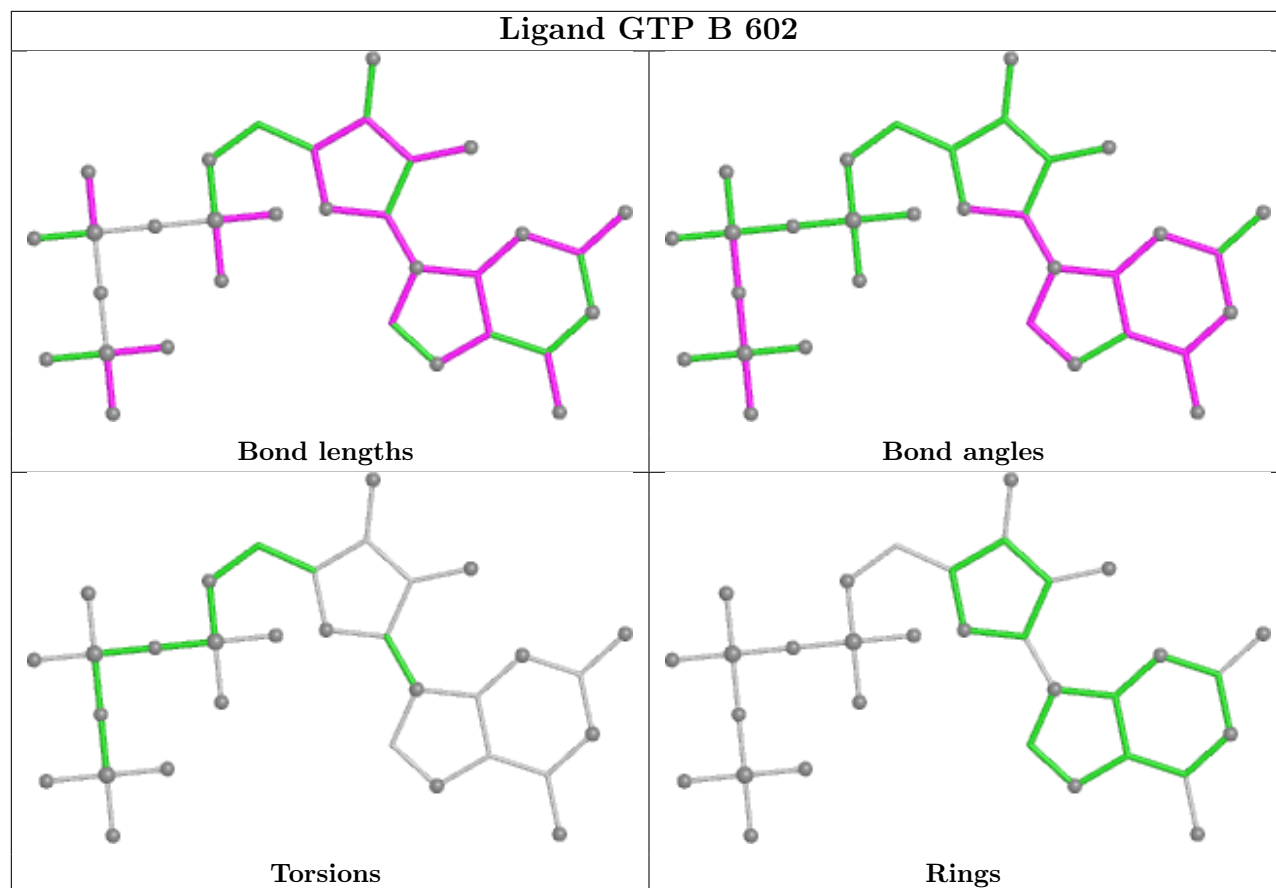
Mol	Chain	Res	Type	Atoms
5	A	605	5GP	O4'-C4'-C5'-O5'
5	A	605	5GP	C3'-C4'-C5'-O5'
3	A	602	GTP	PA-O3A-PB-O1B
5	B	605	5GP	O4'-C4'-C5'-O5'

There are no ring outliers.

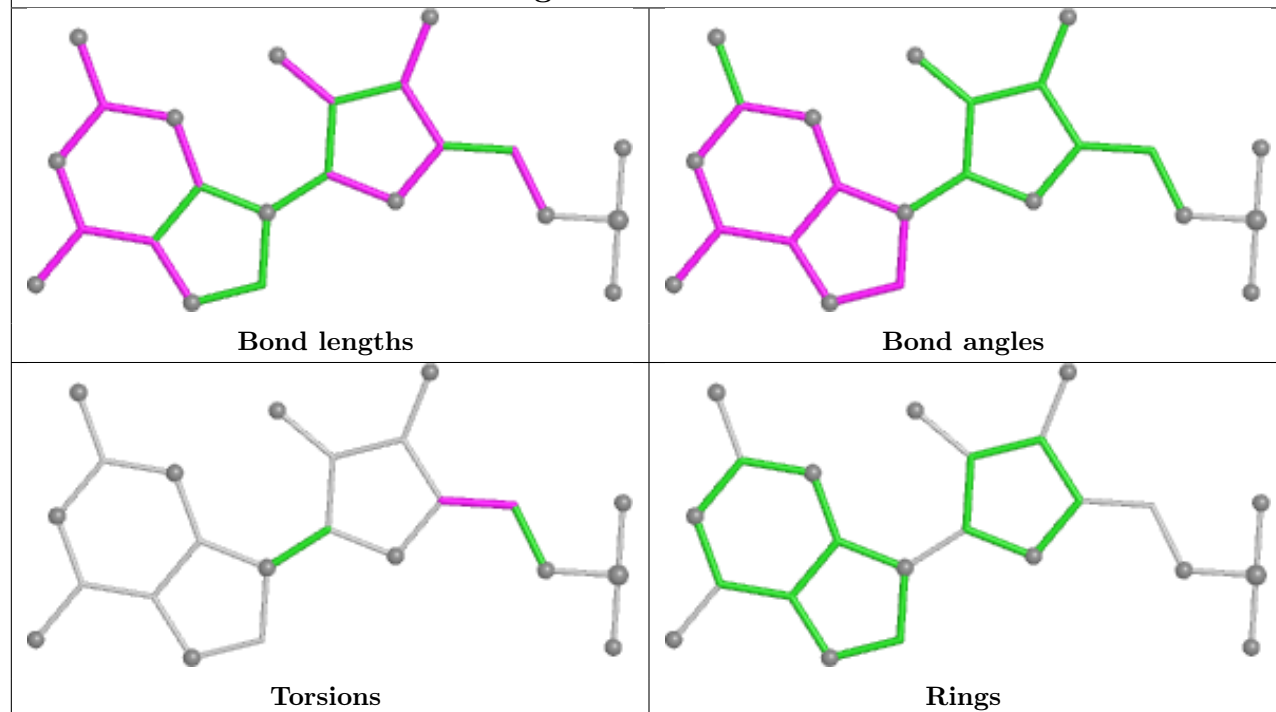
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	5GP	1	0
3	A	602	GTP	2	0

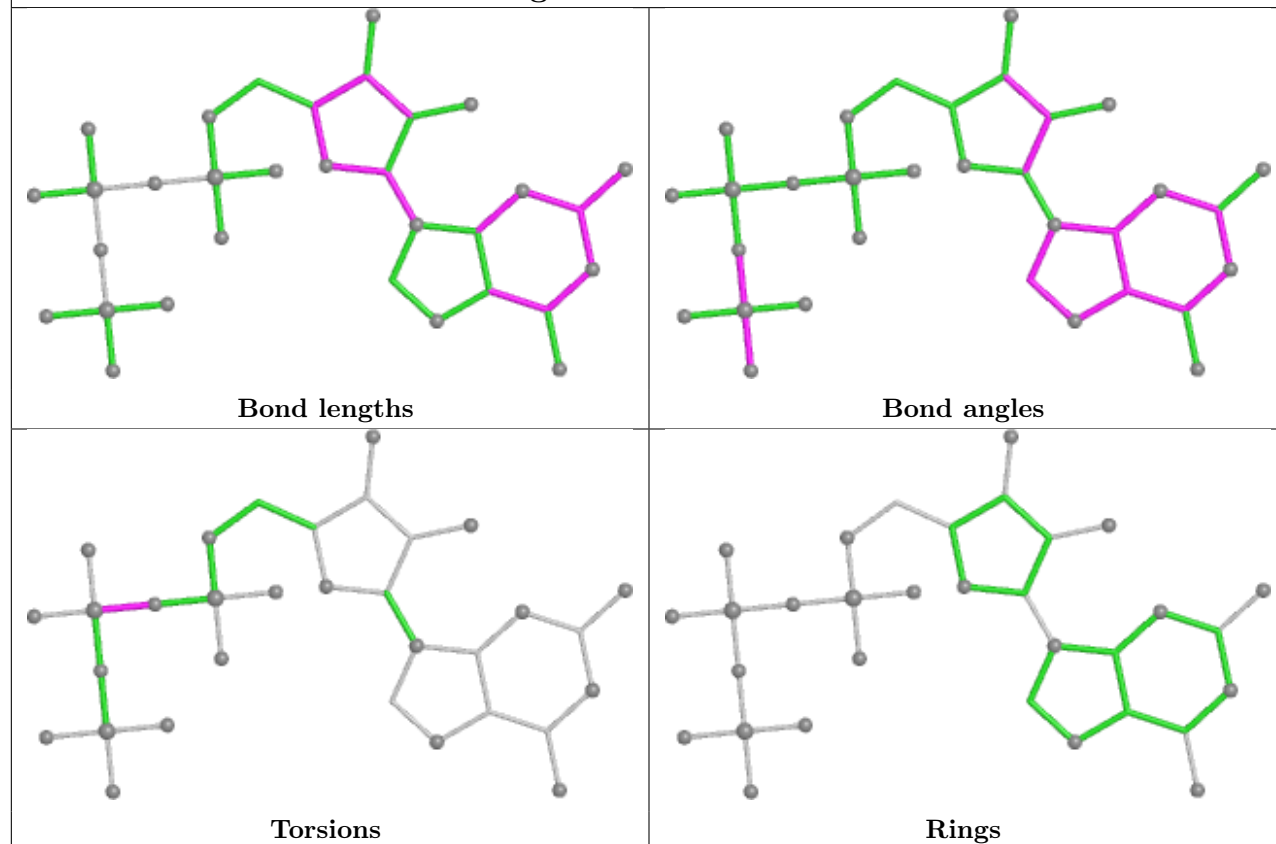
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 5GP B 605



Ligand GTP A 602



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, 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	361/447 (80%)	0.70	32 (8%) 15 17	35, 61, 105, 147	0
1	B	362/447 (80%)	0.58	21 (5%) 29 33	38, 59, 105, 145	0
All	All	723/894 (80%)	0.64	53 (7%) 21 24	35, 59, 105, 147	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	LEU	5.7
1	A	200	TYR	5.6
1	A	203	HIS	5.1
1	A	204	VAL	4.5
1	B	358	PHE	4.4
1	A	205	LYS	4.3
1	B	242	ILE	4.2
1	A	201	TYR	4.0
1	B	507	LEU	3.7
1	A	164	ILE	3.7
1	A	290	GLY	3.5
1	B	159	LEU	3.5
1	A	301	PRO	3.4
1	B	290	GLY	3.3
1	B	147	PRO	2.9
1	A	229	TYR	2.9
1	A	245	GLY	2.8
1	A	182	MET	2.8
1	A	355	GLY	2.8
1	A	277	ILE	2.8
1	A	161	ARG	2.7
1	A	198	GLY	2.7
1	B	280	ILE	2.7
1	A	356	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	275	LYS	2.7
1	A	358	PHE	2.6
1	A	147	PRO	2.6
1	A	274	VAL	2.6
1	A	160	LYS	2.6
1	A	242	ILE	2.5
1	A	252	LEU	2.4
1	B	277	ILE	2.4
1	A	357	SER	2.4
1	A	159	LEU	2.3
1	B	201	TYR	2.3
1	B	222	ARG	2.3
1	A	239	PHE	2.3
1	B	171	VAL	2.3
1	B	162	LYS	2.3
1	A	162	LYS	2.3
1	B	355	GLY	2.2
1	B	461	ARG	2.2
1	A	353	LYS	2.2
1	A	181	ARG	2.1
1	A	354	ASP	2.1
1	A	171	VAL	2.1
1	B	175	VAL	2.1
1	A	209	PRO	2.1
1	B	168	ALA	2.1
1	B	354	ASP	2.1
1	B	205	LYS	2.1
1	B	178	LEU	2.0
1	B	229	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

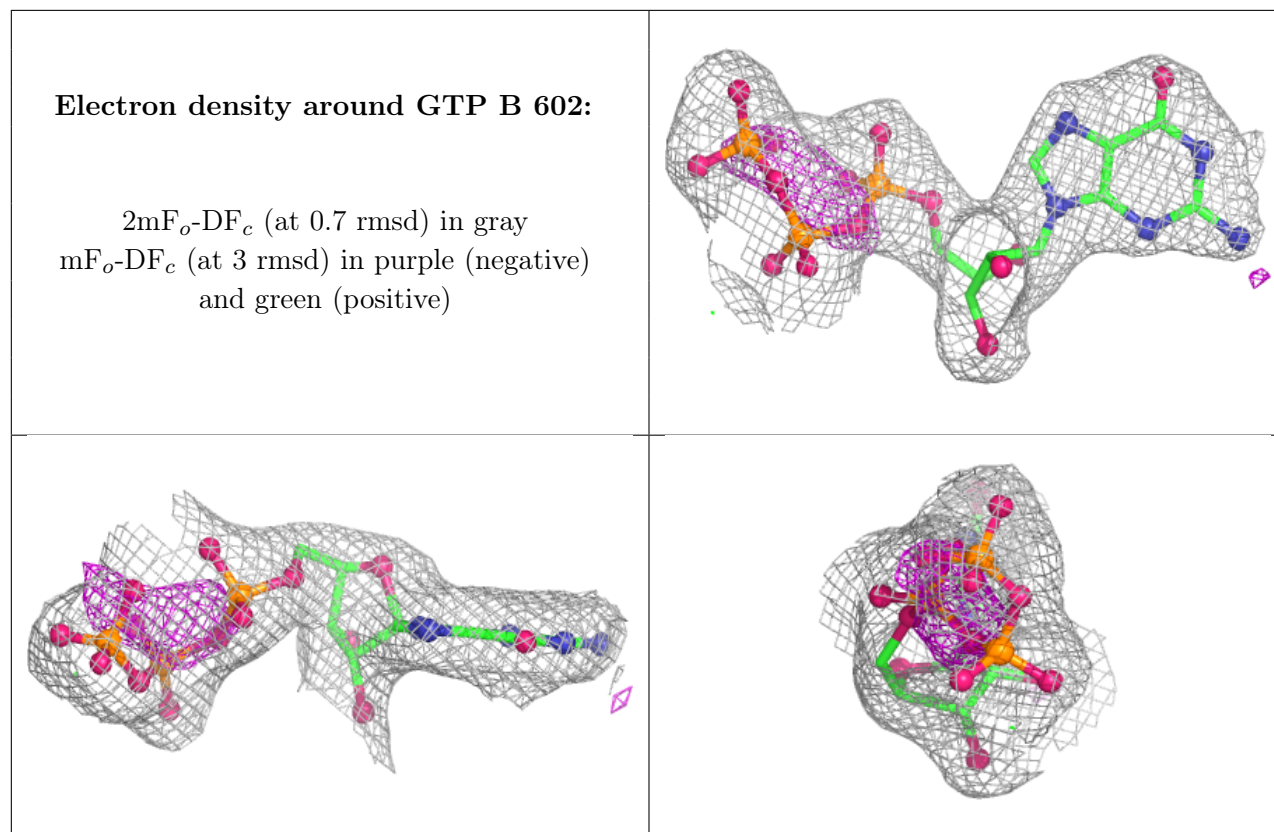
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

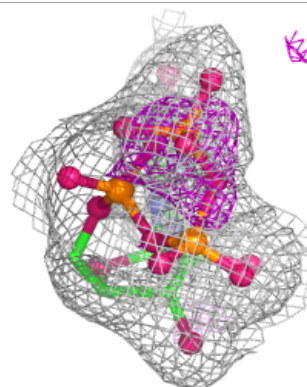
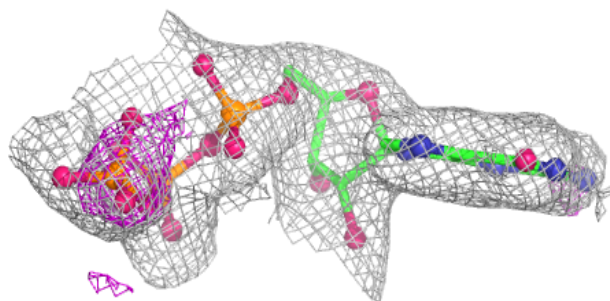
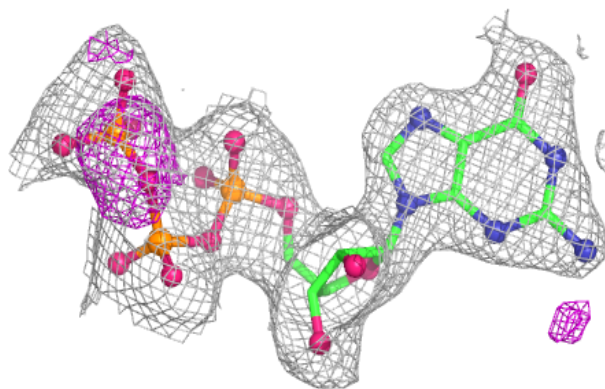
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MN	B	603	1/1	0.78	0.10	122,122,122,122	0
4	MN	A	604	1/1	0.87	0.09	105,105,105,105	0
3	GTP	B	602	32/32	0.89	0.09	61,68,80,81	0
4	MN	B	604	1/1	0.90	0.09	106,106,106,106	0
3	GTP	A	602	32/32	0.92	0.09	49,58,69,71	0
5	5GP	A	605	23/24	0.93	0.08	48,52,55,57	0
5	5GP	B	605	23/24	0.93	0.08	55,58,62,63	0
4	MN	A	603	1/1	0.96	0.06	94,94,94,94	0
2	ZN	B	601	1/1	0.99	0.03	45,45,45,45	0
2	ZN	A	601	1/1	1.00	0.02	46,46,46,46	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.

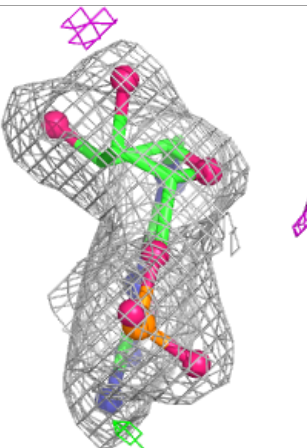
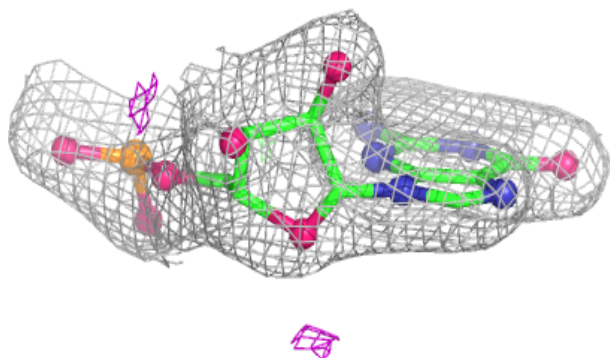
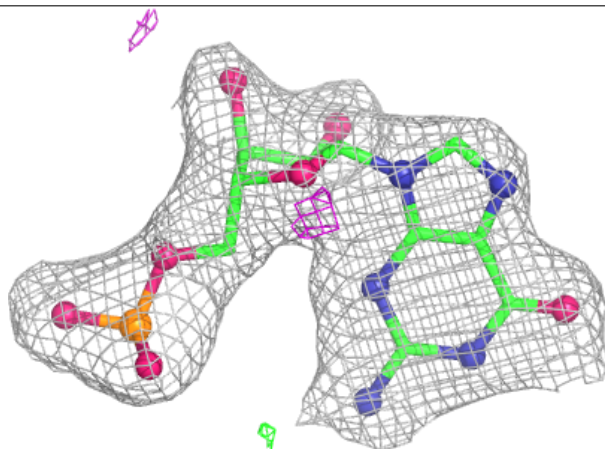


Electron density around GTP A 602:

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

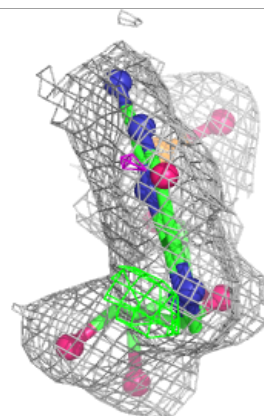
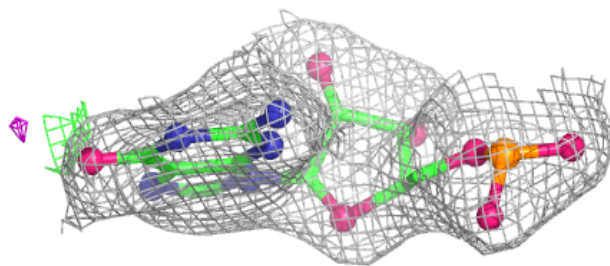
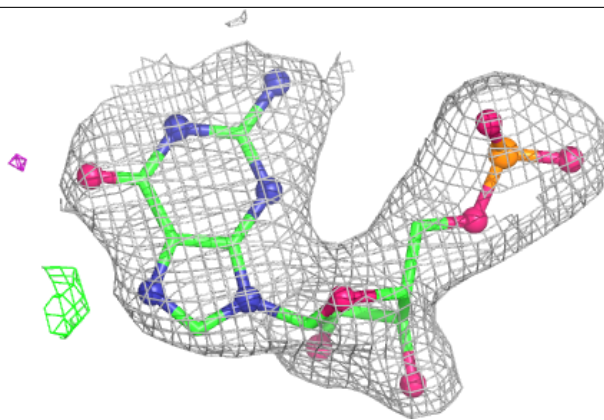
**Electron density around 5GP A 605:**

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



Electron density around 5GP B 605:

$2mF_o-DF_c$ (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.