



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 07:25 PM EDT

PDB ID : 8G2P
Title : Structure of Ternary Complex of cGAS with dsDNA and Bound ATP and GTP
Authors : Wu, S.; Sohn, J.
Deposited on : 2023-02-06
Resolution : 2.52 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

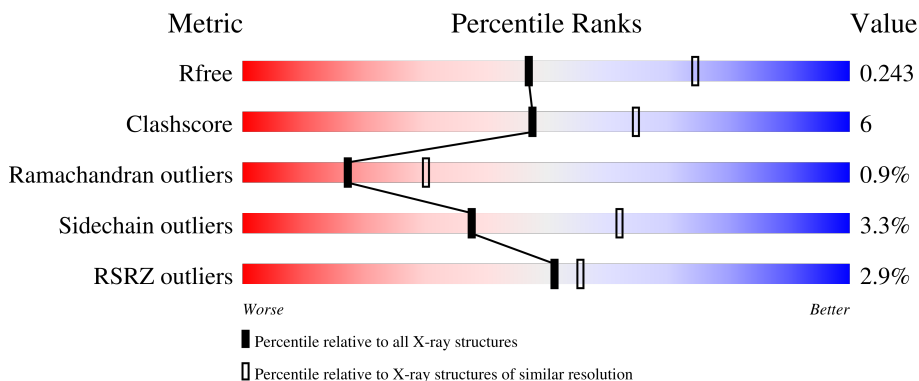
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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.



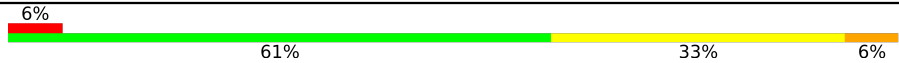
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	364	 3% 84% 10% • 5%
1	C	364	 2% 80% 12% • 5%
2	E	18	 67% 28% 6%
2	F	18	 72% 28%
2	I	18	 6% 72% 22% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	18	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment on the left labeled '6%', a large green segment labeled '61%', a yellow segment labeled '33%', and a small orange segment on the right labeled '6%'.</p>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14176 atoms, of which 6729 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
			Total	C	H	N	O	S			
1	A	347	5803	1850	2931	485	524	13	71	0	0
1	C	346	5796	1850	2930	485	518	13	69	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLY	-	expression tag	UNP Q8C6L5
A	145	THR	-	expression tag	UNP Q8C6L5
A	146	GLY	-	expression tag	UNP Q8C6L5
A	307	ASN	ASP	engineered mutation	UNP Q8C6L5
C	144	GLY	-	expression tag	UNP Q8C6L5
C	145	THR	-	expression tag	UNP Q8C6L5
C	146	GLY	-	expression tag	UNP Q8C6L5
C	307	ASN	ASP	engineered mutation	UNP Q8C6L5

- Molecule 2 is a DNA chain called Palindromic DNA18.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	E	18	571	177	205	66	106	17	1	0	0
2	F	18	571	177	205	66	106	17	1	0	0
2	I	18	571	177	205	66	106	17	1	0	0
2	J	18	571	177	205	66	106	17	1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	C	1	Total	C	H	N	O	P	2	0
			44	10	12	5	14	3		

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

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

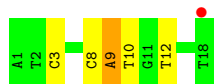
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	51	Total	O	0	0
			51	51		
7	C	46	Total	O	0	0
			46	46		
7	E	8	Total	O	0	0
			8	8		
7	F	5	Total	O	0	0
			5	5		
7	I	4	Total	O	0	0
			4	4		
7	J	1	Total	O	0	0
			1	1		

● Molecule 2: Palindromic DNA18



● Molecule 2: Palindromic DNA18



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.22Å 99.10Å 141.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.52 29.76 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.77-2.52) 99.5 (29.76-2.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.190 , 0.242 0.194 , 0.243	Depositor DCC
R_{free} test set	1895 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14176	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9067e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, MG, GTP

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	0.43	0/2932	0.77	2/3934 (0.1%)
1	C	0.42	0/2925	0.75	2/3922 (0.1%)
2	E	0.81	0/410	1.54	3/631 (0.5%)
2	F	0.78	0/410	1.36	3/631 (0.5%)
2	I	0.78	0/410	1.32	3/631 (0.5%)
2	J	0.78	0/410	1.46	3/631 (0.5%)
All	All	0.53	0/7497	0.96	16/10380 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	11	DG	OP1-P-OP2	6.78	129.77	119.60
2	J	1	DA	P-O3'-C3'	-6.75	111.60	119.70
2	E	1	DA	P-O3'-C3'	-6.44	111.97	119.70
2	I	8	DC	O4'-C1'-N1	5.99	112.19	108.00
1	C	410	LYS	CB-CA-C	-5.76	98.89	110.40
2	F	2	DT	O5'-P-OP2	-5.57	100.68	105.70
2	I	9	DA	C3'-C2'-C1'	5.56	109.17	102.50
2	F	1	DA	P-O3'-C3'	-5.32	113.32	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASP	CB-CA-C	-5.25	99.89	110.40
1	C	341	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	J	13	DA	P-O3'-C3'	-5.23	113.42	119.70
2	J	14	DC	C2'-C3'-O3'	-5.16	95.58	112.60
2	I	3	DC	O4'-C4'-C3'	5.08	109.05	106.00
2	F	4	DT	P-O3'-C3'	-5.08	113.61	119.70
2	E	16	DG	OP1-P-OP2	5.06	127.19	119.60
1	A	391	LYS	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Sidechain
1	C	267	ARG	Sidechain

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	2872	2931	2918	29	0
1	C	2866	2930	2918	44	0
2	E	366	205	206	3	0
2	F	366	205	206	2	0
2	I	366	205	206	4	0
2	J	366	205	206	4	0
3	A	31	12	12	0	0
3	C	31	12	12	0	0
4	A	32	12	12	1	0
4	C	32	12	12	3	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	1	0
7	A	51	0	0	3	0
7	C	46	0	0	13	0
7	E	8	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	5	0	0	0	0
7	I	4	0	0	0	0
7	J	1	0	0	0	0
All	All	7447	6729	6708	84	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 6.

All (84) 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:376:ASN:HB3	7:C:740:HOH:O	1.36	1.24
1:C:392:CYS:SG	6:C:604:ZN:ZN	1.27	1.22
1:A:301:PRO:HB2	1:A:302:GLU:OE2	1.47	1.12
1:C:391:LYS:O	7:C:701:HOH:O	1.70	1.08
1:C:391:LYS:C	7:C:701:HOH:O	1.91	1.08
1:A:301:PRO:CB	1:A:302:GLU:OE2	2.20	0.88
1:C:378:HIS:NE2	1:C:392:CYS:SG	2.54	0.80
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.52	0.74
1:C:372:LYS:NZ	2:J:12:DT:OP1	2.21	0.74
1:A:279:ASP:HB2	1:A:280:ILE:HG13	1.70	0.74
1:C:299:ARG:O	1:C:300:ASN:HB2	1.87	0.73
1:C:436:GLN:HG2	7:C:741:HOH:O	1.87	0.73
1:A:197:THR:HG21	1:A:215:MET:CE	2.19	0.73
1:C:350:LYS:O	1:C:351:ASN:HB2	1.89	0.72
1:C:290:GLY:O	1:C:350:LYS:O	2.09	0.70
1:A:249:SER:HA	1:A:252:LEU:HD12	1.73	0.69
2:F:14:DC:H2''	2:F:15:DA:N7	2.11	0.66
1:C:230:GLU:HG2	7:C:708:HOH:O	1.97	0.65
1:C:182:MET:CE	1:C:189:PHE:HB2	2.29	0.62
2:E:4:DT:H2''	2:E:5:DG:N7	2.15	0.61
1:C:300:ASN:HB2	1:C:301:PRO:HD2	1.83	0.60
4:C:602:GTP:O1G	7:C:702:HOH:O	2.17	0.60
1:A:246:ASN:OD1	1:A:248:LEU:N	2.34	0.58
1:A:185:ARG:O	1:A:186:GLU:C	2.42	0.57
1:A:343:GLU:HG3	7:A:751:HOH:O	2.05	0.57
1:C:182:MET:HE3	1:C:189:PHE:HB2	1.87	0.56
1:C:300:ASN:CB	1:C:301:PRO:CD	2.83	0.56
1:C:384:CYS:SG	1:C:392:CYS:SG	3.04	0.56
1:A:300:ASN:HB2	1:A:301:PRO:HD3	1.88	0.56
1:A:301:PRO:CG	1:A:302:GLU:OE2	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLN:NE2	1:C:192:VAL:O	2.41	0.53
2:I:9:DA:H2'	2:I:10:DT:C6	2.44	0.53
1:C:249:SER:O	1:C:252:LEU:HD12	2.09	0.52
1:C:299:ARG:O	1:C:300:ASN:CB	2.56	0.52
1:C:271:LYS:CE	7:C:745:HOH:O	2.59	0.51
2:F:14:DC:H2''	2:F:15:DA:C5	2.46	0.51
1:C:183:GLN:C	1:C:185:ARG:H	2.13	0.51
2:J:1:DA:H2'	2:J:2:DT:C6	2.46	0.51
1:C:364:ARG:NH2	4:C:602:GTP:N7	2.58	0.51
2:E:1:DA:H2'	2:E:2:DT:C6	2.46	0.50
1:C:254:GLY:O	1:C:256:VAL:N	2.45	0.50
1:A:183:GLN:NE2	1:A:192:VAL:O	2.45	0.50
1:A:246:ASN:OD1	1:A:246:ASN:C	2.51	0.49
1:C:202:GLU:OE1	7:C:703:HOH:O	2.18	0.49
1:C:292:PRO:HB2	1:C:348:VAL:HG13	1.94	0.49
1:C:223:ILE:HG22	1:C:225:LEU:HD13	1.95	0.49
1:C:165:SER:OG	2:J:10:DT:OP1	2.27	0.48
2:J:9:DA:H2'	2:J:10:DT:H71	1.95	0.48
1:A:197:THR:HG21	1:A:215:MET:HE1	1.95	0.48
1:A:300:ASN:CB	1:A:301:PRO:CD	2.92	0.48
1:A:161:ARG:HG3	1:A:161:ARG:NH1	2.25	0.47
1:A:170:THR:HG23	1:A:280:ILE:CD1	2.44	0.47
1:A:300:ASN:CB	1:A:301:PRO:HD3	2.45	0.47
1:C:219:GLU:OE2	1:C:315:LYS:HE2	2.14	0.47
1:C:414:GLU:OE1	1:C:488:PHE:CE2	2.68	0.47
2:E:2:DT:H3'	7:E:107:HOH:O	2.16	0.46
1:C:271:LYS:HE2	7:C:745:HOH:O	2.16	0.46
1:A:334:THR:HB	2:I:9:DA:OP1	2.16	0.46
1:A:350:LYS:HA	7:A:747:HOH:O	2.15	0.46
1:C:230:GLU:N	7:C:708:HOH:O	2.47	0.45
1:C:182:MET:CE	1:C:189:PHE:CB	2.94	0.45
1:A:170:THR:HG23	1:A:280:ILE:HD13	1.99	0.44
1:C:227:GLU:OE2	1:C:472:LYS:NZ	2.50	0.44
1:C:222:ARG:NH1	1:C:239:PHE:CZ	2.86	0.44
1:A:204:VAL:O	1:A:402:LYS:HE2	2.16	0.44
1:A:407:GLN:OE1	1:A:410:LYS:NZ	2.49	0.44
1:A:364:ARG:NH2	4:A:602:GTP:N7	2.65	0.44
1:A:148:ASP:N	7:A:702:HOH:O	2.49	0.44
1:C:301:PRO:HD2	7:C:737:HOH:O	2.18	0.44
1:C:178:LEU:O	1:C:182:MET:HG2	2.18	0.43
1:C:301:PRO:CD	7:C:737:HOH:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASN:HB3	1:C:201:TYR:CG	2.53	0.43
1:C:436:GLN:CG	7:C:741:HOH:O	2.58	0.43
1:C:195:LEU:HD22	1:C:197:THR:CG2	2.49	0.42
1:C:204:VAL:O	1:C:402:LYS:HE2	2.19	0.42
1:A:193:GLU:OE1	1:A:217:LYS:NZ	2.52	0.42
2:I:9:DA:H2'	2:I:10:DT:H71	2.01	0.42
4:C:602:GTP:O1G	4:C:602:GTP:O2A	2.38	0.42
1:C:351:ASN:HA	1:C:362:THR:HG22	2.00	0.42
1:A:290:GLY:O	1:A:350:LYS:C	2.59	0.41
1:C:350:LYS:O	1:C:351:ASN:CB	2.59	0.41
1:C:158:ARG:HG3	2:I:12:DT:OP1	2.21	0.41
1:A:153:VAL:O	1:A:157:LEU:HG	2.21	0.41
1:A:300:ASN:CG	1:A:301:PRO:CD	2.89	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	341/364 (94%)	328 (96%)	9 (3%)	4 (1%)	13	22
1	C	337/364 (93%)	322 (96%)	13 (4%)	2 (1%)	25	41
All	All	678/728 (93%)	650 (96%)	22 (3%)	6 (1%)	17	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	300	ASN
1	C	300	ASN
1	A	186	GLU
1	C	223	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	208	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	322/335 (96%)	315 (98%)	7 (2%)	52 75
1	C	321/335 (96%)	307 (96%)	14 (4%)	28 49
All	All	643/670 (96%)	622 (97%)	21 (3%)	38 62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	MET
1	A	207	SER
1	A	211	GLU
1	A	214	VAL
1	A	246	ASN
1	A	249	SER
1	A	362	THR
1	C	165	SER
1	C	183	GLN
1	C	186	GLU
1	C	195	LEU
1	C	211	GLU
1	C	215	MET
1	C	227	GLU
1	C	249	SER
1	C	252	LEU
1	C	320	ILE
1	C	348	VAL
1	C	350	LYS
1	C	391	LYS
1	C	392	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	C	246	ASN
1	C	307	ASN
1	C	498	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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$
4	GTP	A	602	-	26,34,34	1.13	3 (11%)	32,54,54	1.00	2 (6%)
3	ATP	A	601	5	26,33,33	0.61	0	31,52,52	0.87	1 (3%)
4	GTP	C	602	-	26,34,34	1.03	2 (7%)	32,54,54	1.13	2 (6%)
3	ATP	C	601	5	26,33,33	0.64	0	31,52,52	0.92	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	602	-	-	1/18/38/38	0/3/3/3
3	ATP	A	601	5	-	5/18/38/38	0/3/3/3
4	GTP	C	602	-	-	3/18/38/38	0/3/3/3
3	ATP	C	601	5	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	GTP	PG-O1G	3.30	1.61	1.50
4	C	602	GTP	C5-C6	-2.47	1.42	1.47
4	A	602	GTP	C6-N1	2.26	1.41	1.37
4	A	602	GTP	C5-C6	-2.12	1.43	1.47
4	C	602	GTP	PG-O1G	2.01	1.57	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	GTP	O2G-PG-O3B	-2.86	95.06	104.64
4	C	602	GTP	O2B-PB-O1B	2.13	122.79	112.24
3	A	601	ATP	O2A-PA-O1A	2.13	122.79	112.24
3	C	601	ATP	O2A-PA-O1A	2.05	122.39	112.24
4	A	602	GTP	O2A-PA-O1A	2.04	122.30	112.24
4	A	602	GTP	O3G-PG-O2G	2.03	115.39	107.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ATP	PB-O3B-PG-O3G
3	C	601	ATP	PB-O3B-PG-O2G
3	C	601	ATP	PB-O3B-PG-O3G
4	C	602	GTP	PB-O3A-PA-O2A
4	C	602	GTP	PB-O3A-PA-O1A
3	A	601	ATP	PB-O3B-PG-O2G
4	C	602	GTP	PB-O3B-PG-O2G
3	A	601	ATP	PA-O3A-PB-O1B
3	A	601	ATP	PA-O3A-PB-O2B
3	C	601	ATP	PA-O3A-PB-O1B
3	C	601	ATP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

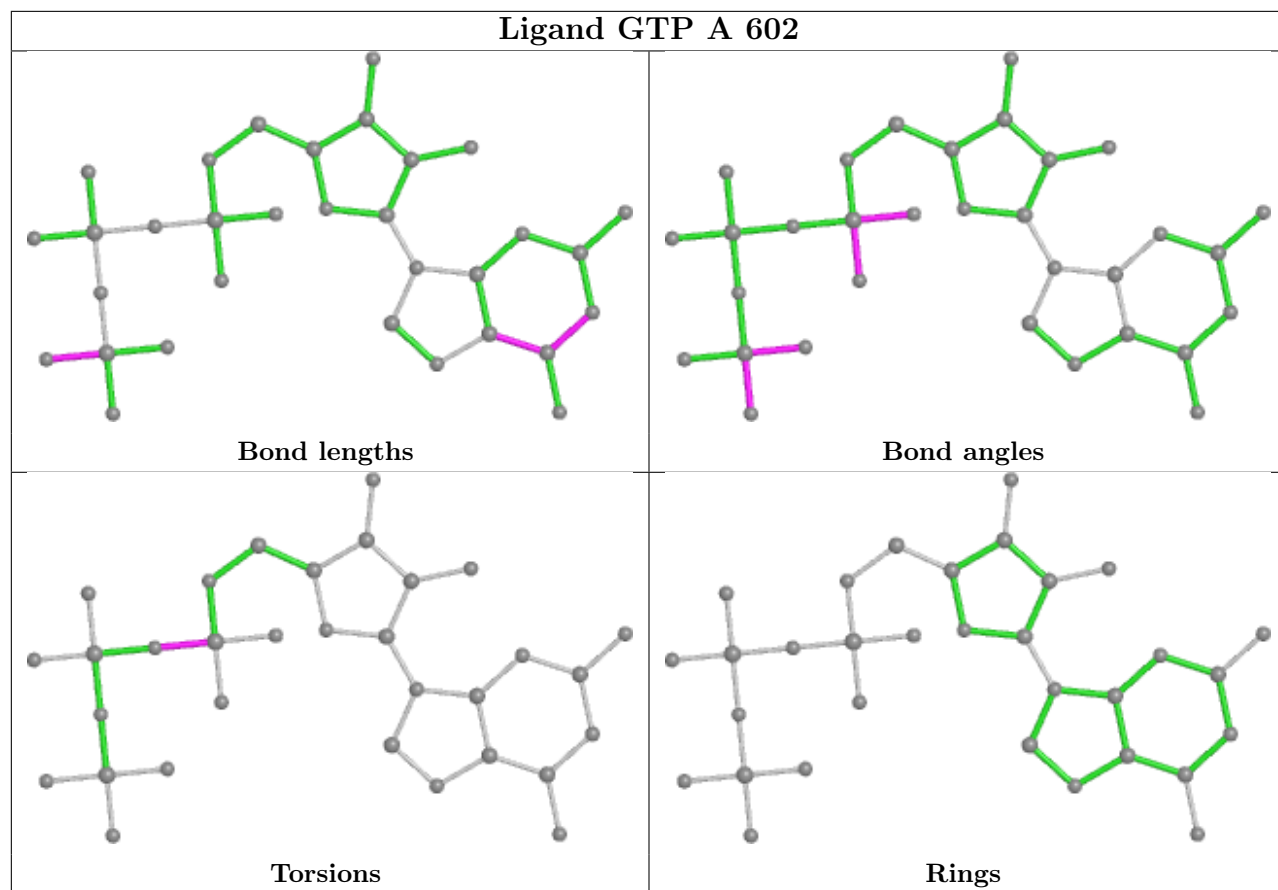
Mol	Chain	Res	Type	Atoms
4	A	602	GTP	PB-O3A-PA-O2A
3	A	601	ATP	PB-O3B-PG-O1G

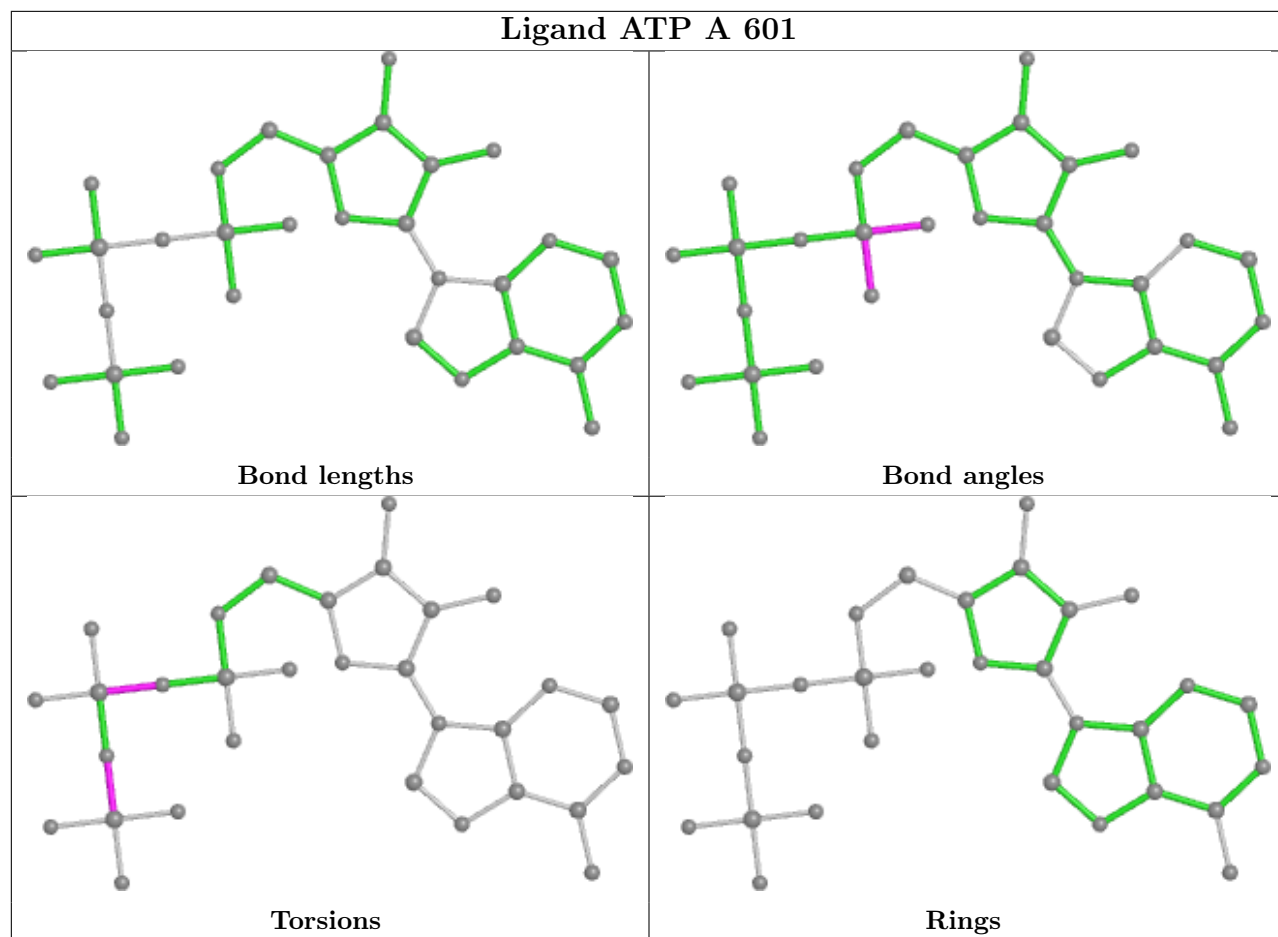
There are no ring outliers.

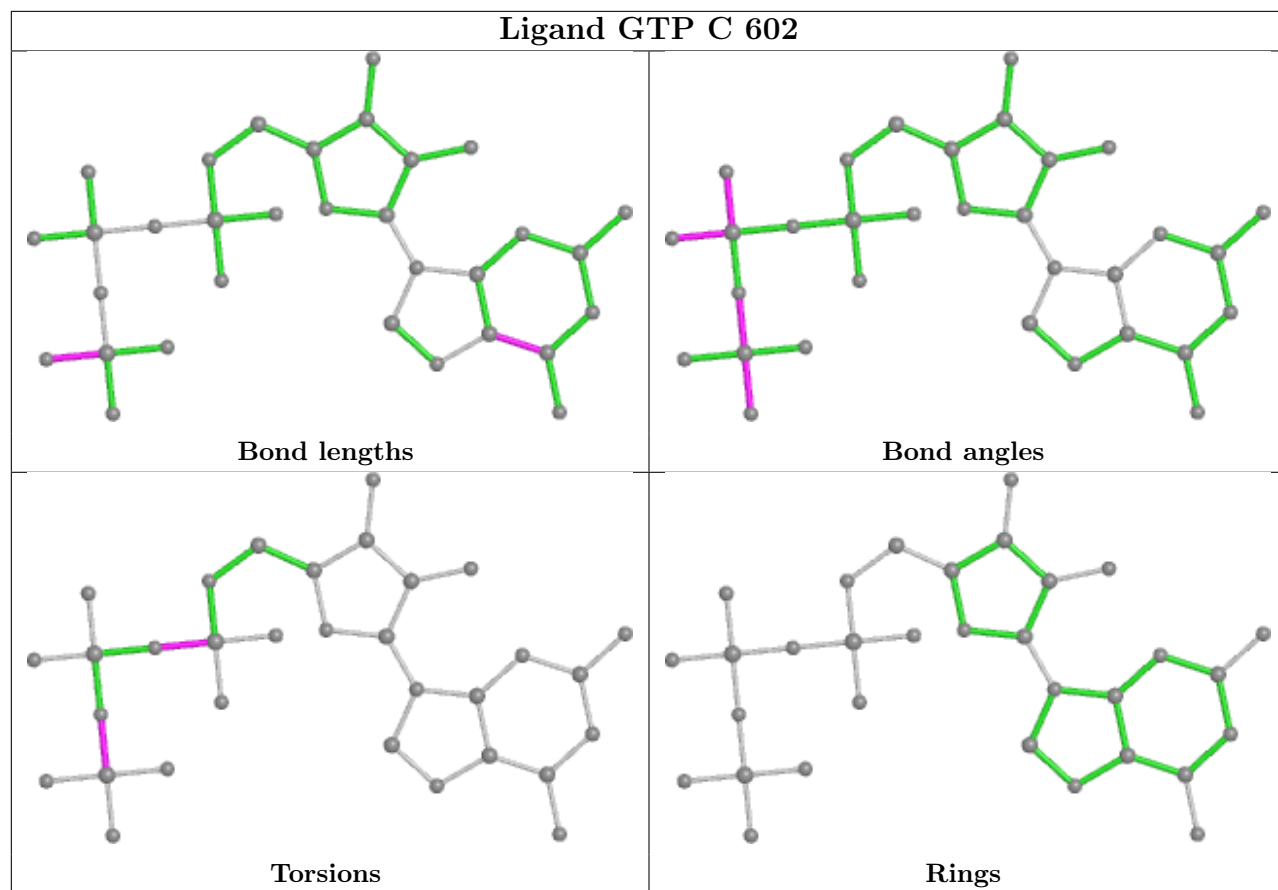
2 monomers are involved in 4 short contacts:

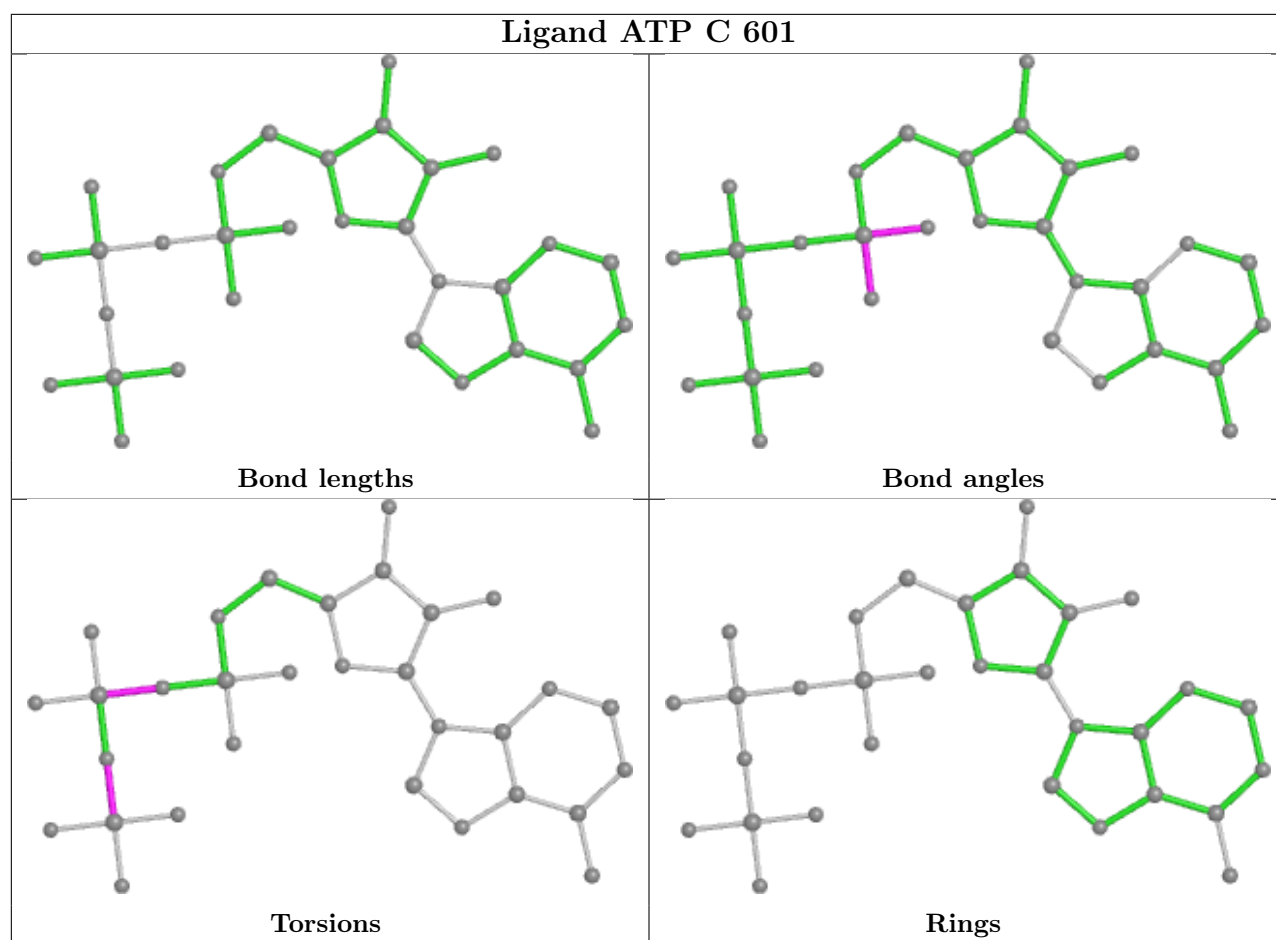
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	GTP	1	0
4	C	602	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	347/364 (95%)	0.03	11 (3%) 47 52	28, 55, 101, 146	0
1	C	346/364 (95%)	0.05	9 (2%) 56 59	33, 61, 110, 144	0
2	E	18/18 (100%)	0.05	0 100 100	41, 78, 191, 204	0
2	F	18/18 (100%)	0.10	0 100 100	40, 69, 153, 168	0
2	I	18/18 (100%)	0.15	1 (5%) 24 26	45, 70, 176, 190	0
2	J	18/18 (100%)	0.18	1 (5%) 24 26	48, 81, 174, 185	0
All	All	765/800 (95%)	0.05	22 (2%) 51 55	28, 59, 118, 204	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	358	PHE	4.7
1	A	245	GLY	3.3
1	A	507	LEU	3.2
1	C	507	LEU	3.2
1	A	286	LYS	3.1
1	A	301	PRO	3.0
1	A	222	ARG	2.9
1	A	254	GLY	2.9
1	A	186	GLU	2.8
1	C	301	PRO	2.6
1	C	428	PHE	2.5
1	A	413	GLN	2.5
1	A	246	ASN	2.5
1	C	495	TYR	2.4
1	A	185	ARG	2.4
1	C	250	HIS	2.3
1	A	398	LEU	2.2
2	J	18	DT	2.2
1	C	230	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	480	LEU	2.1
2	I	18	DT	2.1
1	C	229	TYR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

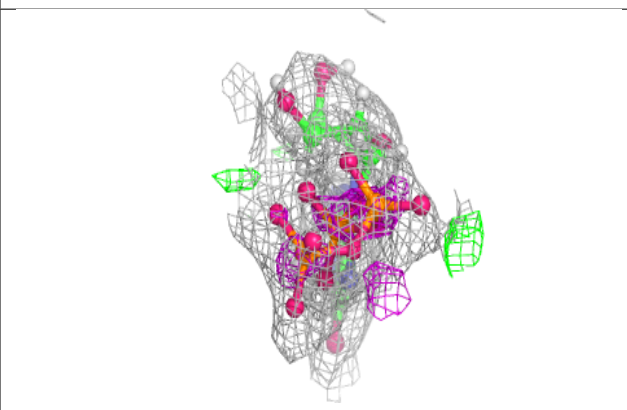
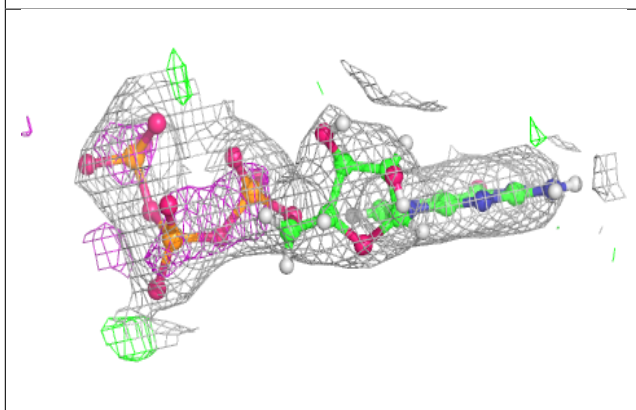
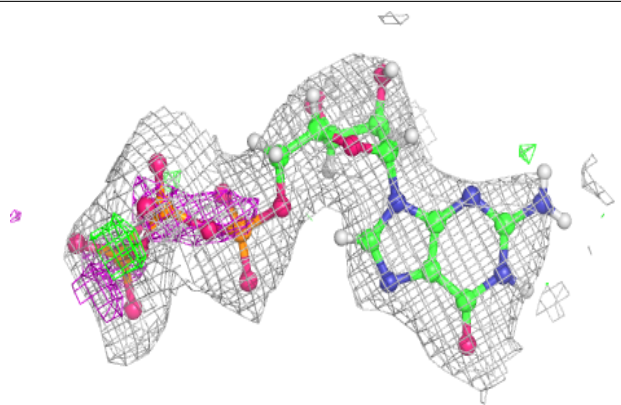
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	603	1/1	0.73	0.14	47,47,47,47	0
4	GTP	A	602	32/32	0.92	0.12	30,54,69,79	2
5	MG	C	603	1/1	0.93	0.10	45,45,45,45	0
4	GTP	C	602	32/32	0.94	0.12	30,49,63,73	2
3	ATP	A	601	31/31	0.98	0.14	30,47,53,55	2
3	ATP	C	601	31/31	0.98	0.14	30,44,48,51	2
6	ZN	C	604	1/1	0.99	0.07	45,45,45,45	0
6	ZN	A	604	1/1	1.00	0.14	38,38,38,38	0

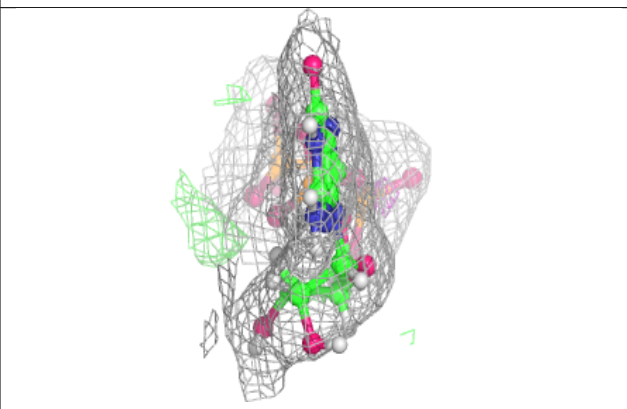
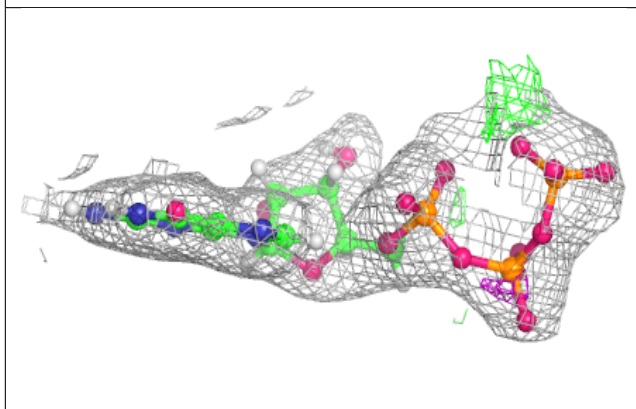
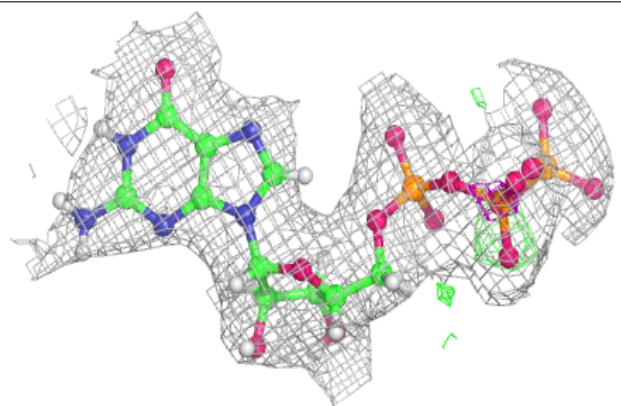
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

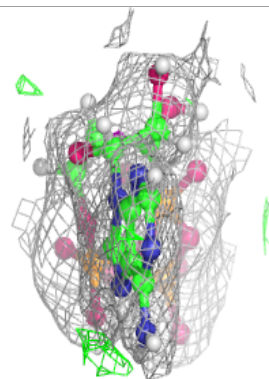
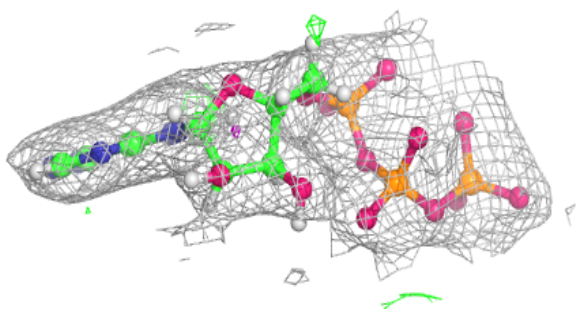
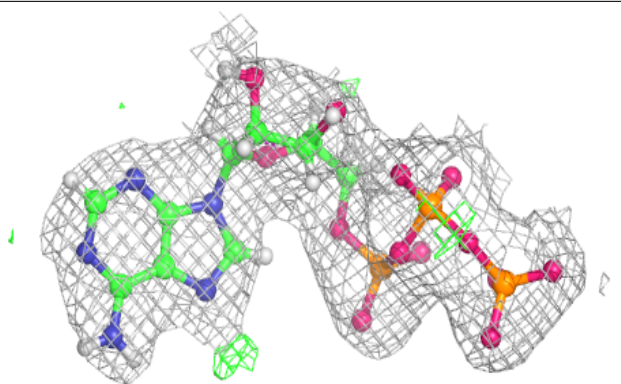
**Electron density around GTP C 602:**

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

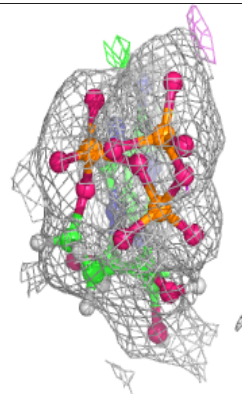
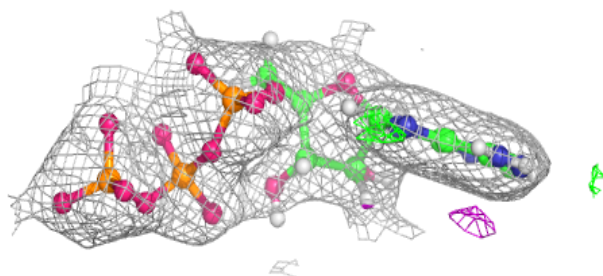
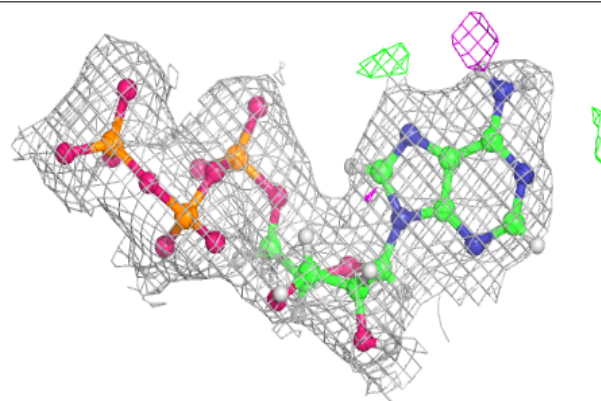


Electron density around ATP A 601:

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

**Electron density around ATP C 601:**

$2mF_o-DF_c$ (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.