



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 10:02 AM EDT

PDB ID : 3RSB  
Title : Structure of the Archaeal GTP:AdoCbi-P Guanylyltransferase (CobY) from Methanocaldococcus jannaschii  
Authors : Newmister, S.A.; Otte, M.M.; Escalante-Semerena, J.C.; Rayment, I.  
Deposited on : 2011-05-02  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

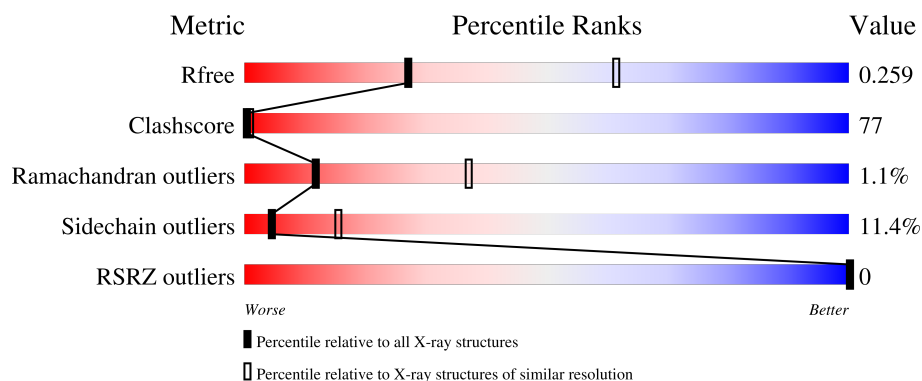
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	196	
1	B	196	
1	C	196	
1	D	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GTP	B	197	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5912 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 Adenosylcobinamide-phosphate guanylyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	Se	0	0	0
			1389	905	217	257	4	6			
1	B	185	Total	C	N	O	S	Se	0	0	0
			1440	934	226	270	4	6			
1	C	181	Total	C	N	O	S	Se	0	0	0
			1405	913	222	260	4	6			
1	D	180	Total	C	N	O	S	Se	0	0	0
			1400	910	221	259	4	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLY	engineered mutation	UNP Q58517
B	153	ASP	GLY	engineered mutation	UNP Q58517
C	153	ASP	GLY	engineered mutation	UNP Q58517
D	153	ASP	GLY	engineered mutation	UNP Q58517

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

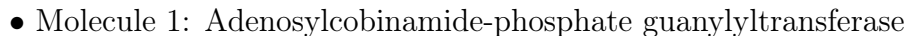
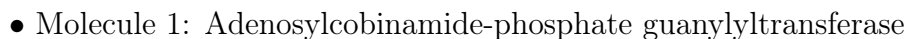


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	43	Total	O	0	0
			43	43		
3	C	29	Total	O	0	0
			29	29		
3	D	41	Total	O	0	0
			41	41		

- Molecule 1: Adenosylcobinamide-phosphate guanylyltransferase





● Molecule 1: Adenosylcobinamide-phosphate guanylyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.60Å 63.60Å 222.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.57 – 2.80 19.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.57-2.80) 92.7 (19.57-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.256 , 0.279 0.249 , 0.259	Depositor DCC
$R_{free}$ test set	1179 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.074 for h,-h-k,-l 0.051 for -k,-h,-l	Xtriage
Reported twinning fraction	0.838 for H, K, L 0.083 for -H, H+K, -L 0.079 for K, H, -L	Depositor
Outliers	0 of 22907 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.76	8/1407 (0.6%)	1.16	4/1894 (0.2%)
1	B	1.93	15/1460 (1.0%)	1.13	5/1968 (0.3%)
1	C	1.75	7/1425 (0.5%)	1.09	1/1919 (0.1%)
1	D	1.87	13/1419 (0.9%)	1.11	4/1910 (0.2%)
All	All	1.83	43/5711 (0.8%)	1.12	14/7691 (0.2%)

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	CYS	CB-SG	-9.17	1.66	1.82
1	B	87	CYS	CB-SG	-7.99	1.68	1.82
1	B	139	TYR	CD2-CE2	-7.72	1.27	1.39
1	D	1	MSE	CG-SE	-7.59	1.69	1.95
1	B	139	TYR	CD1-CE1	-7.41	1.28	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASN	N-CA-C	-8.80	87.24	111.00
1	B	139	TYR	C-N-CD	-7.42	104.27	120.60
1	D	155	ASN	N-CA-C	-6.56	93.28	111.00
1	D	158	SER	N-CA-C	-6.26	94.11	111.00
1	B	71	VAL	CB-CA-C	-5.87	100.24	111.40

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	1389	0	1440	292	1
1	B	1440	0	1488	191	1
1	C	1405	0	1448	285	1
1	D	1400	0	1453	148	5
2	A	32	0	12	7	0
2	B	32	0	12	10	0
2	C	32	0	12	6	0
2	D	32	0	12	6	0
3	A	37	0	0	14	5
3	B	43	0	0	8	0
3	C	29	0	0	4	1
3	D	41	0	0	4	0
All	All	5912	0	5877	901	7

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 77.

The worst 5 of 901 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:171:ILE:HG22	1:C:173:GLU:CG	1.27	1.64
1:C:171:ILE:CG2	1:C:173:GLU:HG3	1.26	1.63
1:C:133:MSE:HG3	1:C:168:ILE:CD1	1.19	1.60
1:A:116:TYR:CG	1:A:169:MSE:CE	1.91	1.50
1:C:18:GLU:C	1:C:20:PRO:CD	1.76	1.50

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:TYR:OH	3:A:211:HOH:O[2_545]	1.32	0.88
1:C:144:ILE:CD1	3:A:218:HOH:O[1_445]	1.76	0.44
1:D:90:TYR:CA	3:A:201:HOH:O[2_545]	2.06	0.14
1:D:90:TYR:CZ	3:A:211:HOH:O[2_545]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLY:O	3:A:201:HOH:O[2_545]	2.12	0.08

## 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	169/196 (86%)	159 (94%)	8 (5%)	2 (1%)	11	34
1	B	181/196 (92%)	171 (94%)	9 (5%)	1 (1%)	22	51
1	C	177/196 (90%)	167 (94%)	7 (4%)	3 (2%)	7	26
1	D	174/196 (89%)	165 (95%)	7 (4%)	2 (1%)	12	37
All	All	701/784 (89%)	662 (94%)	31 (4%)	8 (1%)	12	37

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	53	THR
1	D	53	THR
1	D	140	PRO
1	B	140	PRO
1	A	140	PRO

### 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	159/169 (94%)	137 (86%)	22 (14%)	3	10
1	B	164/169 (97%)	146 (89%)	18 (11%)	5	17
1	C	159/169 (94%)	137 (86%)	22 (14%)	3	10
1	D	159/169 (94%)	148 (93%)	11 (7%)	13	37
All	All	641/676 (95%)	568 (89%)	73 (11%)	4	15

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	173	GLU
1	D	171	ILE
1	C	178	ILE
1	D	52	ASN
1	B	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	ASN
1	C	104	ASN
1	B	104	ASN
1	B	69	ASN
1	C	43	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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
2	GTP	A	197	-	29,34,34	1.23	2 (6%)	35,54,54	1.36	5 (14%)
2	GTP	C	197	-	29,34,34	1.23	2 (6%)	35,54,54	1.37	5 (14%)
2	GTP	D	197	-	29,34,34	1.24	2 (6%)	35,54,54	1.36	5 (14%)
2	GTP	B	197	-	29,34,34	1.23	2 (6%)	35,54,54	1.36	5 (14%)

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
2	GTP	A	197	-	-	8/18/38/38	0/3/3/3
2	GTP	C	197	-	-	7/18/38/38	0/3/3/3
2	GTP	D	197	-	-	10/18/38/38	0/3/3/3
2	GTP	B	197	-	-	7/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	197	GTP	C5-C6	-4.11	1.39	1.47
2	D	197	GTP	C5-C6	-4.11	1.39	1.47
2	B	197	GTP	C5-C6	-4.08	1.39	1.47
2	A	197	GTP	C5-C6	-4.07	1.39	1.47
2	D	197	GTP	C2-N3	2.22	1.38	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	197	GTP	C8-N7-C5	3.66	108.78	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	197	GTP	C8-N7-C5	3.64	108.74	102.55
2	B	197	GTP	C8-N7-C5	3.63	108.74	102.55
2	D	197	GTP	C8-N7-C5	3.62	108.71	102.55
2	D	197	GTP	C5-C6-N1	2.93	119.66	114.07

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

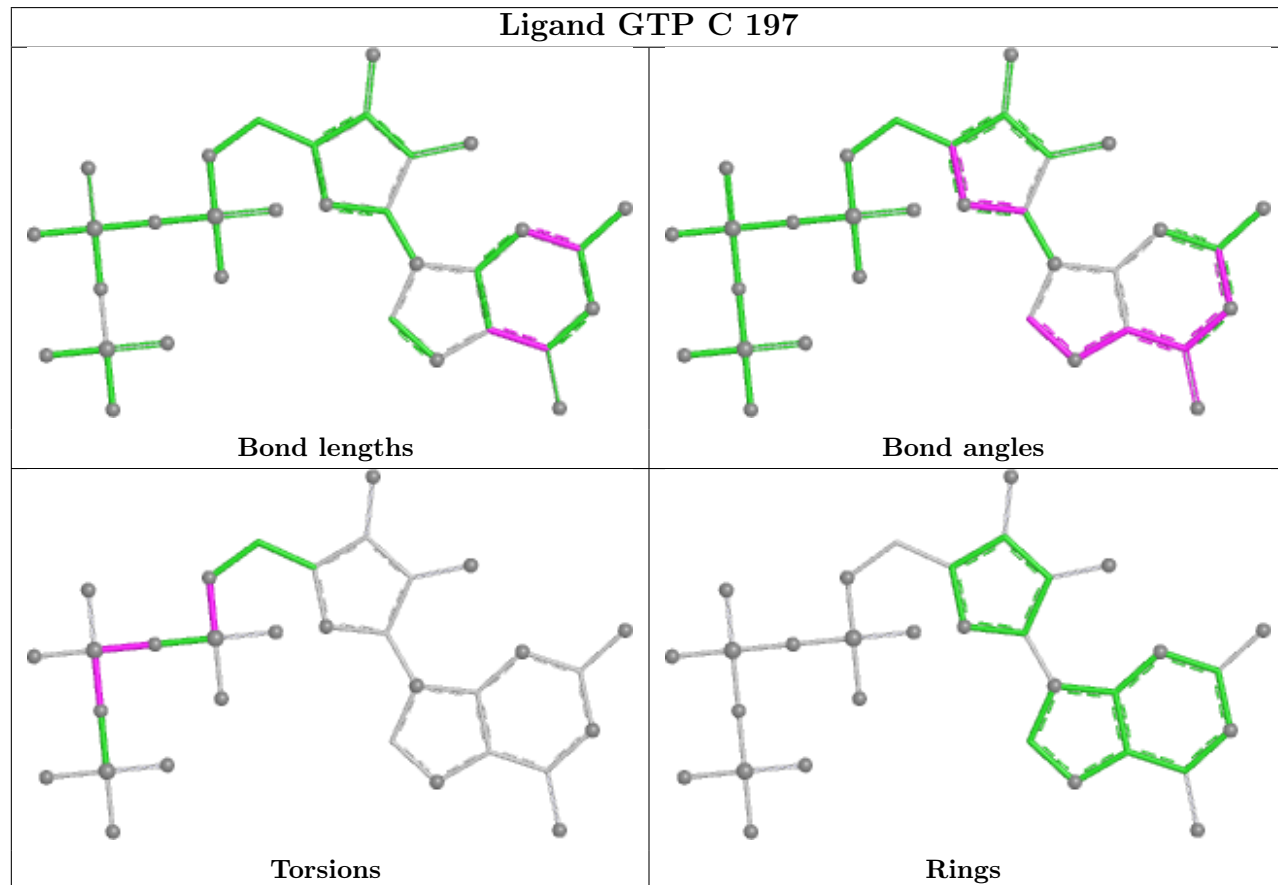
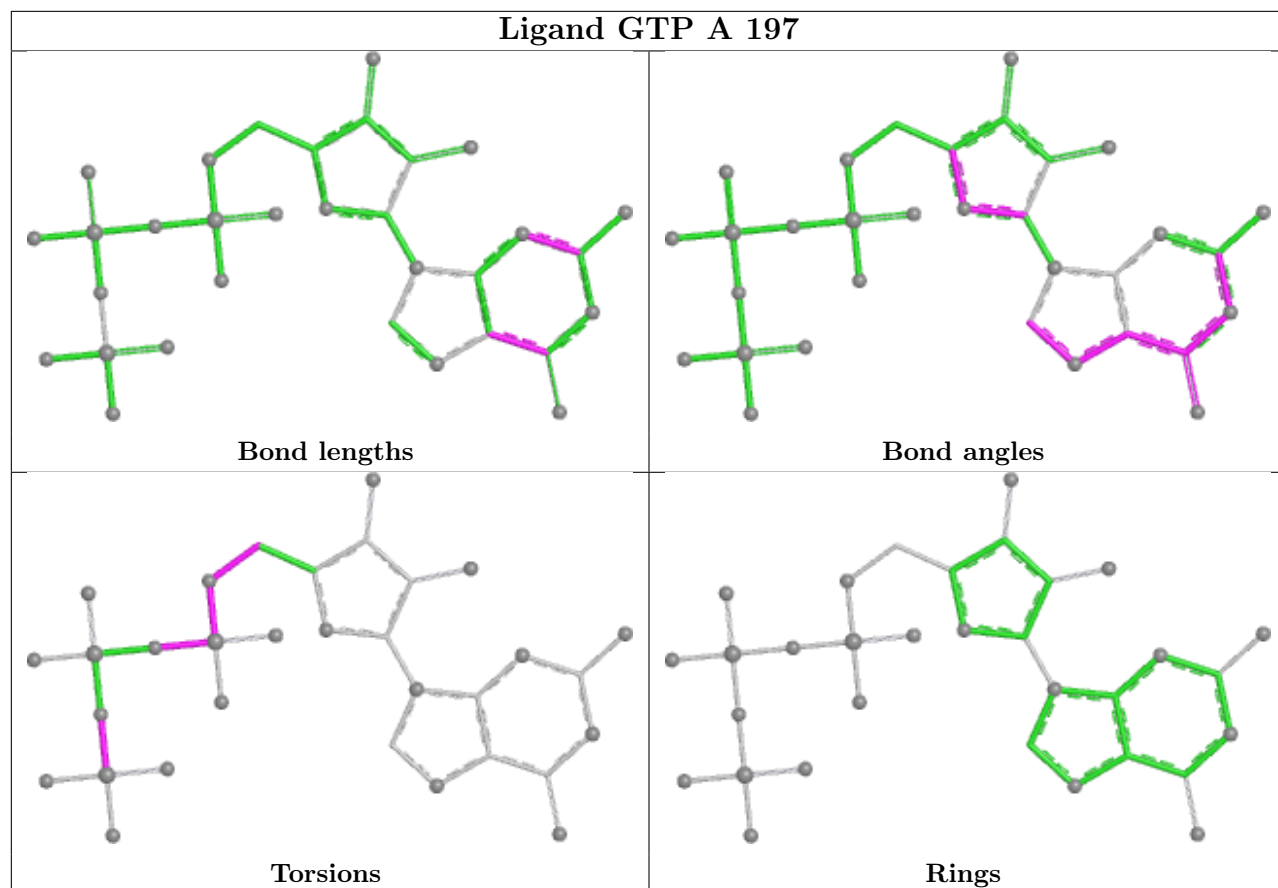
Mol	Chain	Res	Type	Atoms
2	A	197	GTP	PB-O3B-PG-O2G
2	A	197	GTP	C5'-O5'-PA-O3A
2	A	197	GTP	C5'-O5'-PA-O1A
2	A	197	GTP	C5'-O5'-PA-O2A
2	B	197	GTP	C5'-O5'-PA-O3A

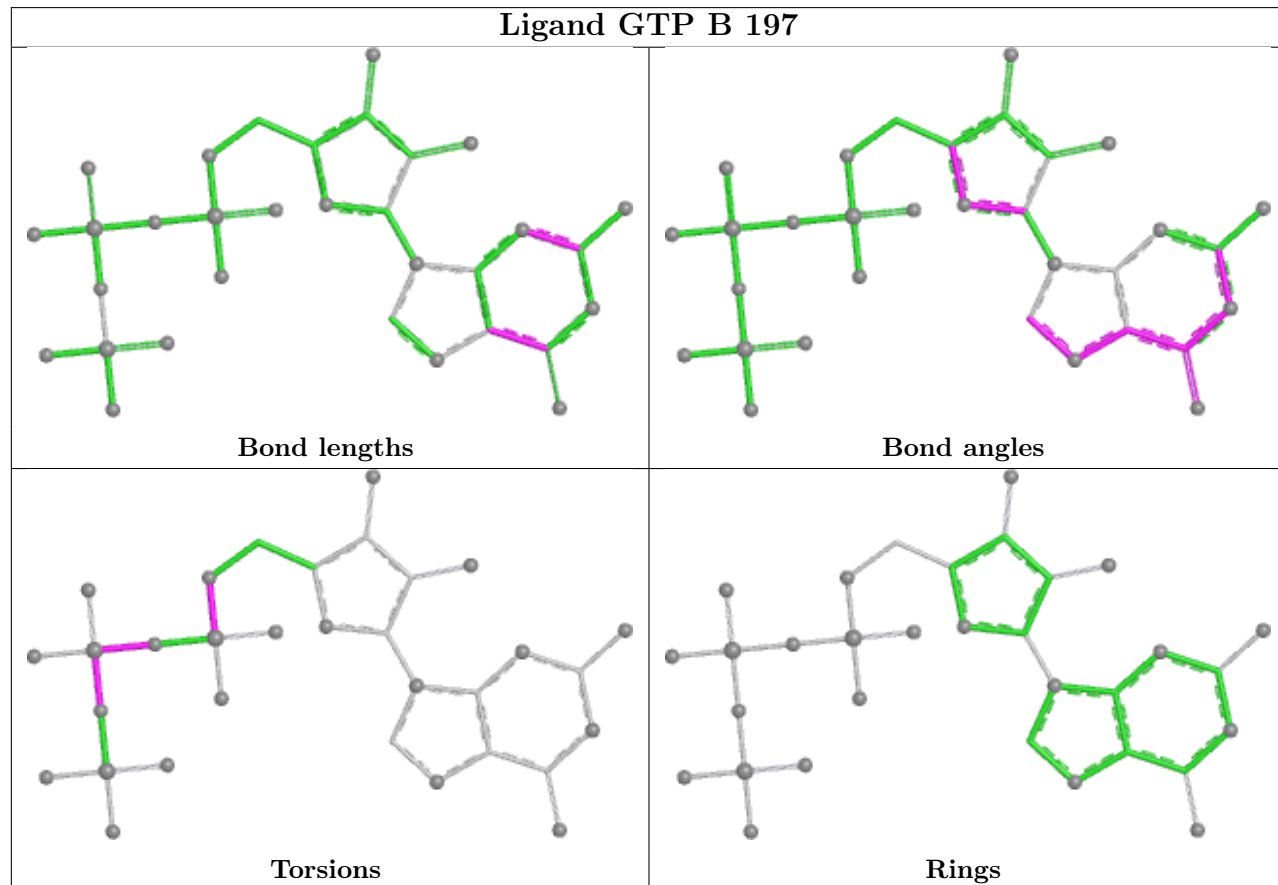
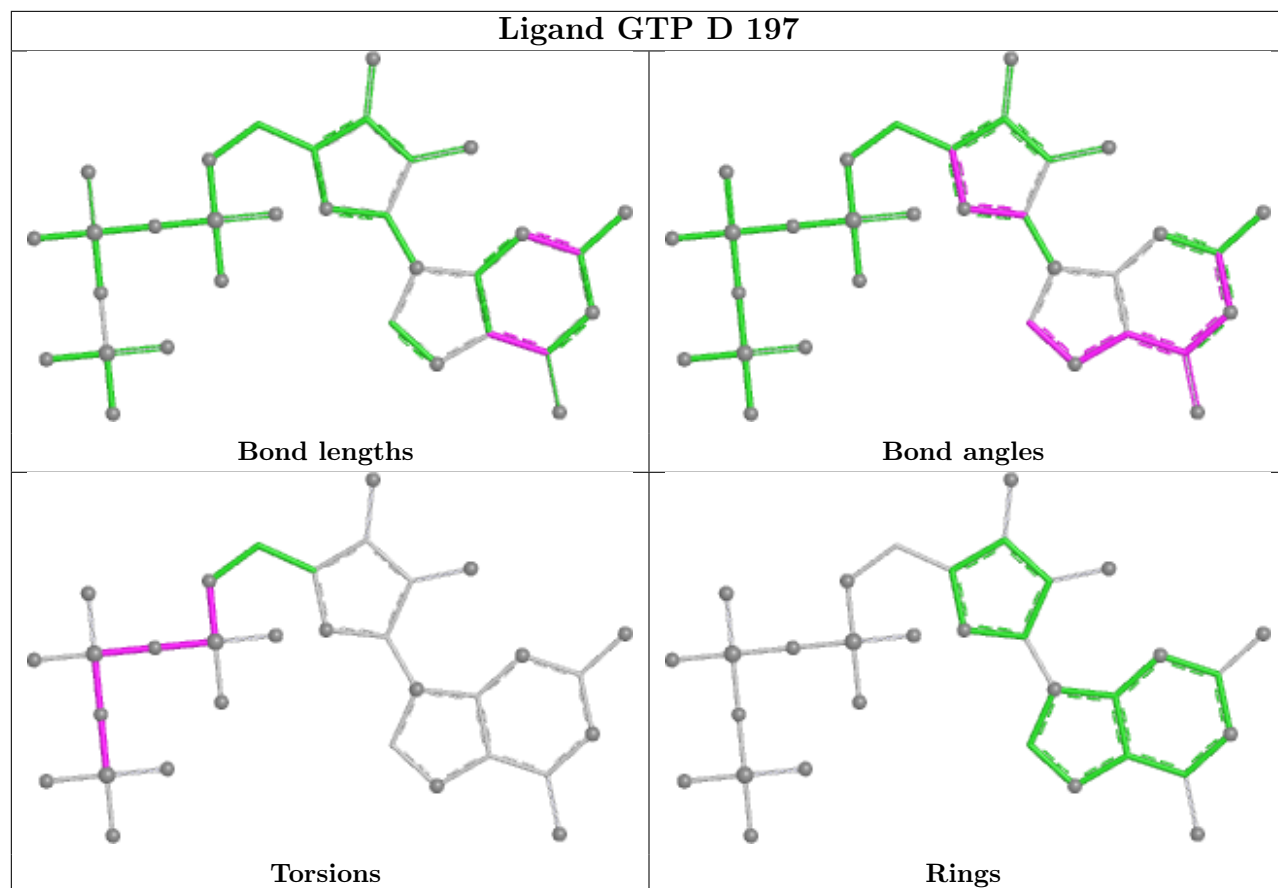
There are no ring outliers.

4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	197	GTP	7	0
2	C	197	GTP	6	0
2	D	197	GTP	6	0
2	B	197	GTP	10	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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	171/196 (87%)	-1.83	0 100 100	41, 51, 57, 58	0
1	B	179/196 (91%)	-1.85	0 100 100	37, 43, 49, 52	0
1	C	175/196 (89%)	-1.83	0 100 100	43, 52, 57, 61	0
1	D	174/196 (88%)	-1.87	0 100 100	39, 45, 54, 59	0
All	All	699/784 (89%)	-1.84	0 100 100	37, 47, 57, 61	0

There are no RSRZ outliers to report.

### 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](#)

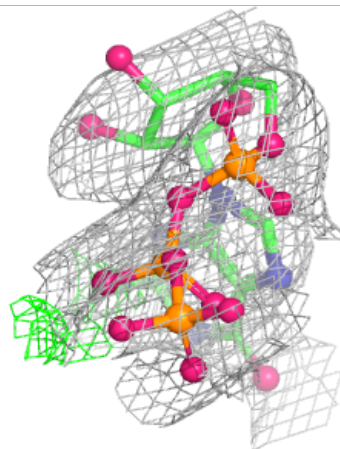
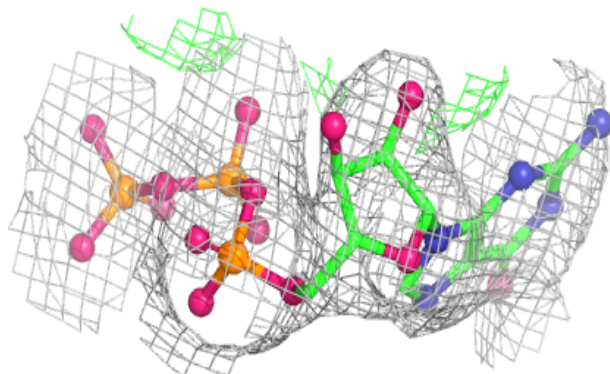
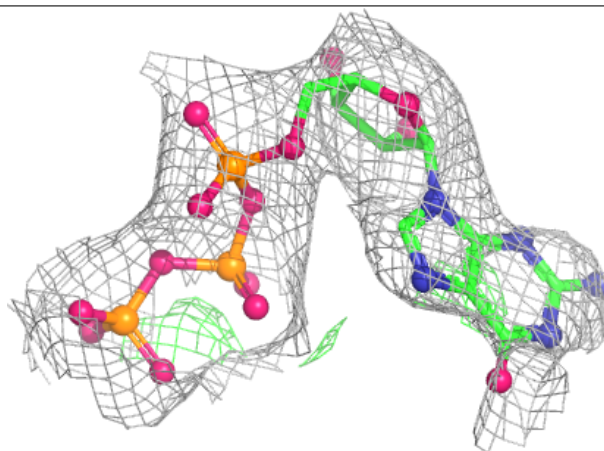
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GTP	A	197	32/32	0.99	0.03	63,63,64,64	0
2	GTP	D	197	32/32	0.99	0.03	40,40,40,40	0
2	GTP	C	197	32/32	1.00	0.02	43,44,45,45	0
2	GTP	B	197	32/32	1.00	0.02	42,43,44,44	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.

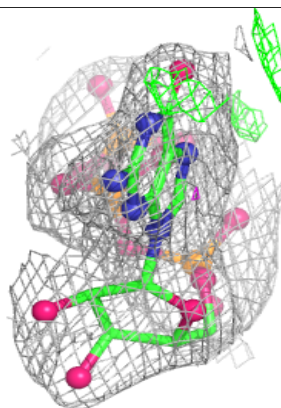
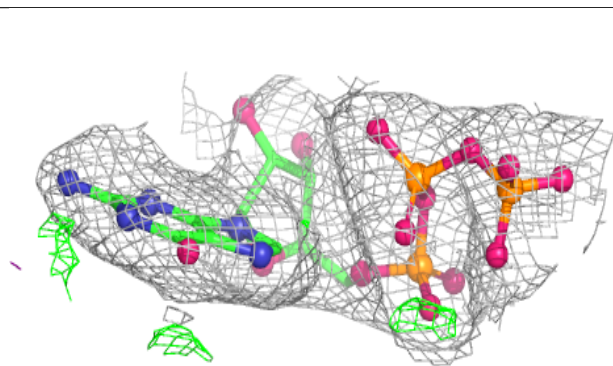
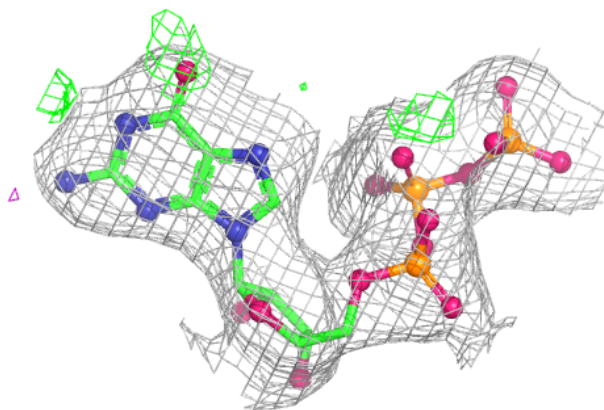
**Electron density around GTP A 197:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



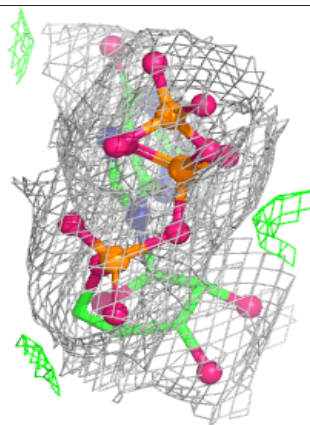
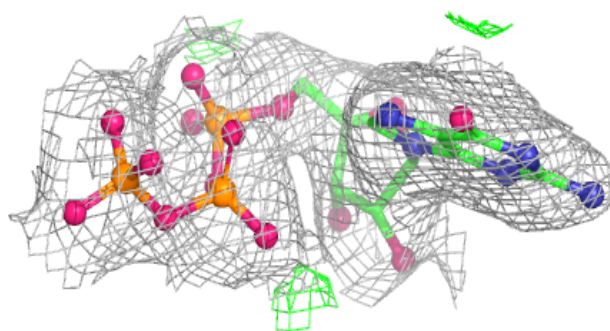
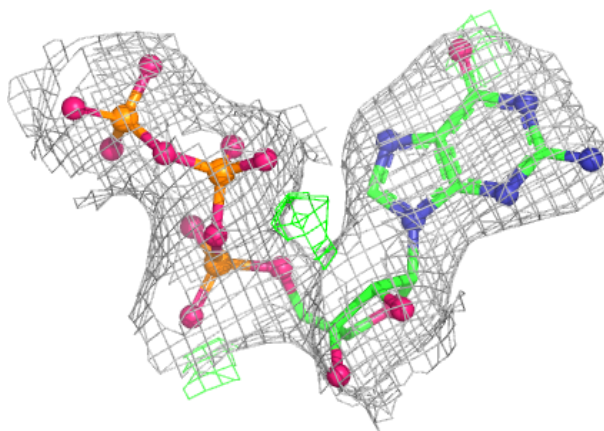
**Electron density around GTP D 197:**

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

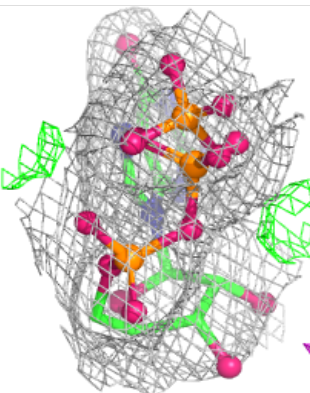
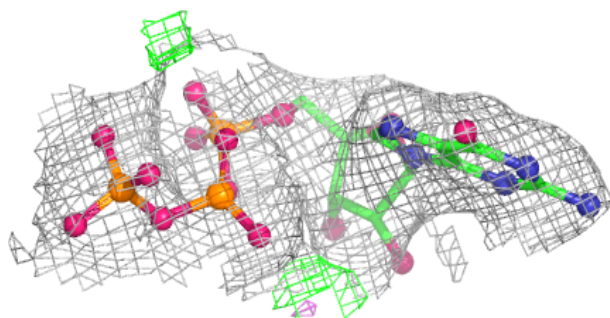
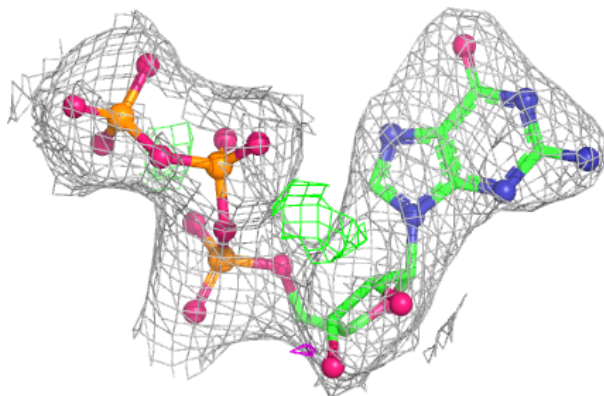


**Electron density around GTP C 197:**

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

**Electron density around GTP B 197:**

$2mF_o-DF_c$  (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.