



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 07:20 AM EDT

PDB ID : 4PYG  
Title : Transglutaminase2 complexed with GTP  
Authors : Park, H.H.; Jang, T.H.  
Deposited on : 2014-03-27  
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

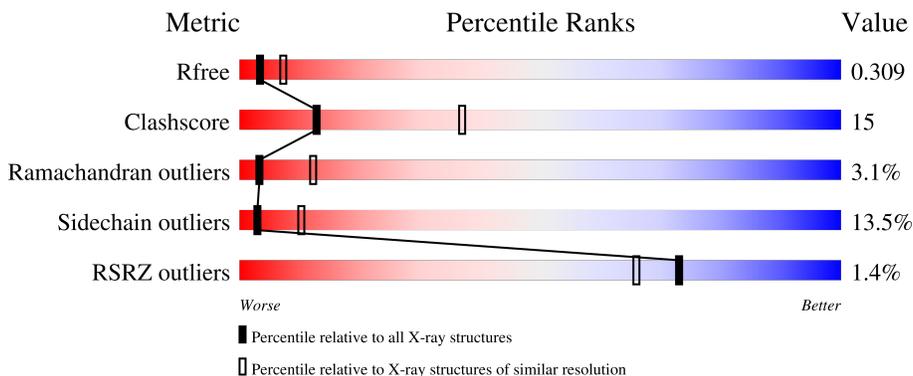
# 1 Overall quality at a glance

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	695	
1	B	695	
1	E	695	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 16462 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 Protein-glutamine gamma-glutamyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	685	5419	3424	933	1032	30	0	0	0
1	B	685	5419	3424	933	1032	30	0	0	0
1	E	685	5419	3424	933	1032	30	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

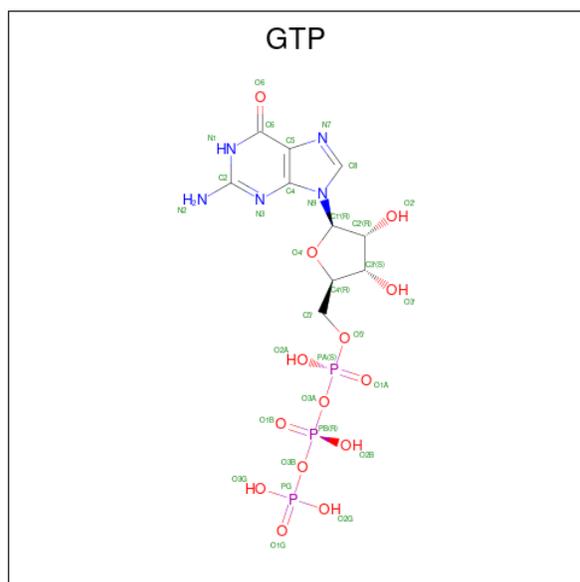
Chain	Residue	Modelled	Actual	Comment	Reference
A	688	LEU	-	expression tag	UNP P21980
A	689	GLU	-	expression tag	UNP P21980
A	690	HIS	-	expression tag	UNP P21980
A	691	HIS	-	expression tag	UNP P21980
A	692	HIS	-	expression tag	UNP P21980
A	693	HIS	-	expression tag	UNP P21980
A	694	HIS	-	expression tag	UNP P21980
A	695	HIS	-	expression tag	UNP P21980
B	688	LEU	-	expression tag	UNP P21980
B	689	GLU	-	expression tag	UNP P21980
B	690	HIS	-	expression tag	UNP P21980
B	691	HIS	-	expression tag	UNP P21980
B	692	HIS	-	expression tag	UNP P21980
B	693	HIS	-	expression tag	UNP P21980
B	694	HIS	-	expression tag	UNP P21980
B	695	HIS	-	expression tag	UNP P21980
E	688	LEU	-	expression tag	UNP P21980
E	689	GLU	-	expression tag	UNP P21980
E	690	HIS	-	expression tag	UNP P21980
E	691	HIS	-	expression tag	UNP P21980
E	692	HIS	-	expression tag	UNP P21980
E	693	HIS	-	expression tag	UNP P21980
E	694	HIS	-	expression tag	UNP P21980

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Chain	Residue	Modelled	Actual	Comment	Reference
E	695	HIS	-	expression tag	UNP P21980

- 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	
			Total	C	N	O			P
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	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	34	Total	O	0	0
			34	34		
3	B	42	Total	O	0	0
			42	42		
3	E	33	Total	O	0	0
			33	33		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.55Å 216.22Å 165.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.92 – 2.80 39.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.92-2.80) 99.4 (39.92-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.88 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.236 , 0.319 0.230 , 0.309	Depositor DCC
$R_{free}$ test set	2961 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.1	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	0.68	1/5537 (0.0%)	0.80	3/7515 (0.0%)
1	B	0.65	0/5537	0.77	1/7515 (0.0%)
1	E	0.66	0/5537	0.76	0/7515
All	All	0.66	1/16611 (0.0%)	0.78	4/22545 (0.0%)

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	2
1	B	0	1
1	E	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	CYS	CB-SG	-5.28	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	424	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	5	LEU	CA-CB-CG	5.66	128.33	115.30
1	A	230	CYS	CA-CB-SG	5.20	123.35	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	LYS	Peptide
1	A	645	GLY	Peptide
1	B	645	GLY	Peptide
1	E	13	GLU	Peptide
1	E	273	LYS	Peptide

## 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	5419	0	5312	146	0
1	B	5419	0	5312	187	0
1	E	5419	0	5312	165	0
2	A	32	0	12	1	0
2	B	32	0	12	1	0
2	E	32	0	12	0	0
3	A	34	0	0	1	0
3	B	42	0	0	5	0
3	E	33	0	0	0	0
All	All	16462	0	15972	483	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 15.

The worst 5 of 483 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:346:ASP:OD1	1:A:387:LYS:HE3	1.50	1.10
1:A:463:ASN:O	1:A:464:LYS:HG2	1.57	1.04
1:E:55:ASP:HA	1:E:123:THR:OG1	1.64	0.95
1:E:344:ARG:HH21	1:E:387:LYS:HZ3	1.13	0.93
1:E:225:SER:HB2	1:E:357:LEU:HD23	1.48	0.92

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	683/695 (98%)	605 (89%)	54 (8%)	24 (4%)	3	10
1	B	683/695 (98%)	582 (85%)	81 (12%)	20 (3%)	3	13
1	E	683/695 (98%)	595 (87%)	69 (10%)	19 (3%)	4	14
All	All	2049/2085 (98%)	1782 (87%)	204 (10%)	63 (3%)	3	12

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	82	ALA
1	A	122	SER
1	A	233	ASP
1	A	274	TYR

### 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	595/605 (98%)	515 (87%)	80 (13%)	3	10
1	B	595/605 (98%)	514 (86%)	81 (14%)	3	10
1	E	595/605 (98%)	515 (87%)	80 (13%)	3	10
All	All	1785/1815 (98%)	1544 (86%)	241 (14%)	3	10

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	257	SER
1	E	499	THR
1	B	564	ARG
1	E	470	GLU
1	E	630	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	234	GLN
1	E	481	GLN
1	E	413	HIS
1	B	461	HIS
1	E	231	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](#)

3 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	701	-	29,34,34	1.89	3 (10%)	35,54,54	1.77	8 (22%)
2	GTP	E	701	-	29,34,34	1.83	5 (17%)	35,54,54	1.80	8 (22%)
2	GTP	B	701	-	29,34,34	1.73	3 (10%)	35,54,54	1.93	14 (40%)

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	701	-	-	3/18/38/38	0/3/3/3
2	GTP	E	701	-	-	3/18/38/38	0/3/3/3
2	GTP	B	701	-	-	1/18/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GTP	C5-C6	-6.60	1.34	1.47
2	E	701	GTP	C5-C6	-6.54	1.34	1.47
2	A	701	GTP	C5-C6	-6.49	1.34	1.47
2	A	701	GTP	PB-O3A	-3.98	1.55	1.59
2	B	701	GTP	C5-C4	-3.70	1.33	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GTP	O4'-C1'-N9	-4.26	103.09	108.75
2	B	701	GTP	C8-N7-C5	3.81	109.04	102.55
2	E	701	GTP	O2A-PA-O3A	3.77	117.45	107.27
2	E	701	GTP	C2-N1-C6	-3.69	118.36	125.11
2	B	701	GTP	O3A-PB-O1B	-3.55	100.02	110.70

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GTP	C5'-O5'-PA-O1A
2	E	701	GTP	C5'-O5'-PA-O1A
2	A	701	GTP	C5'-O5'-PA-O3A
2	A	701	GTP	C5'-O5'-PA-O2A

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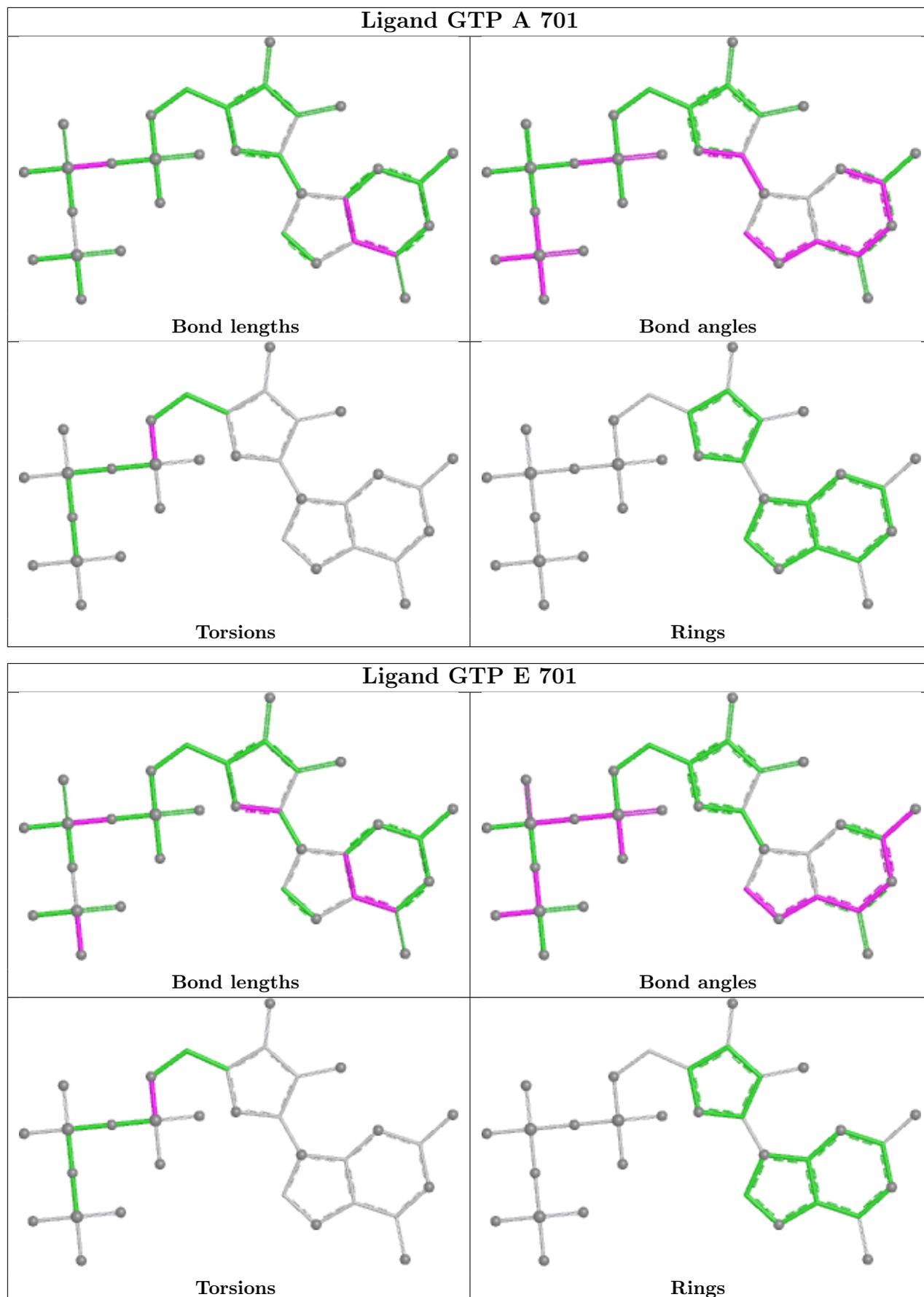
Mol	Chain	Res	Type	Atoms
2	E	701	GTP	C5'-O5'-PA-O3A

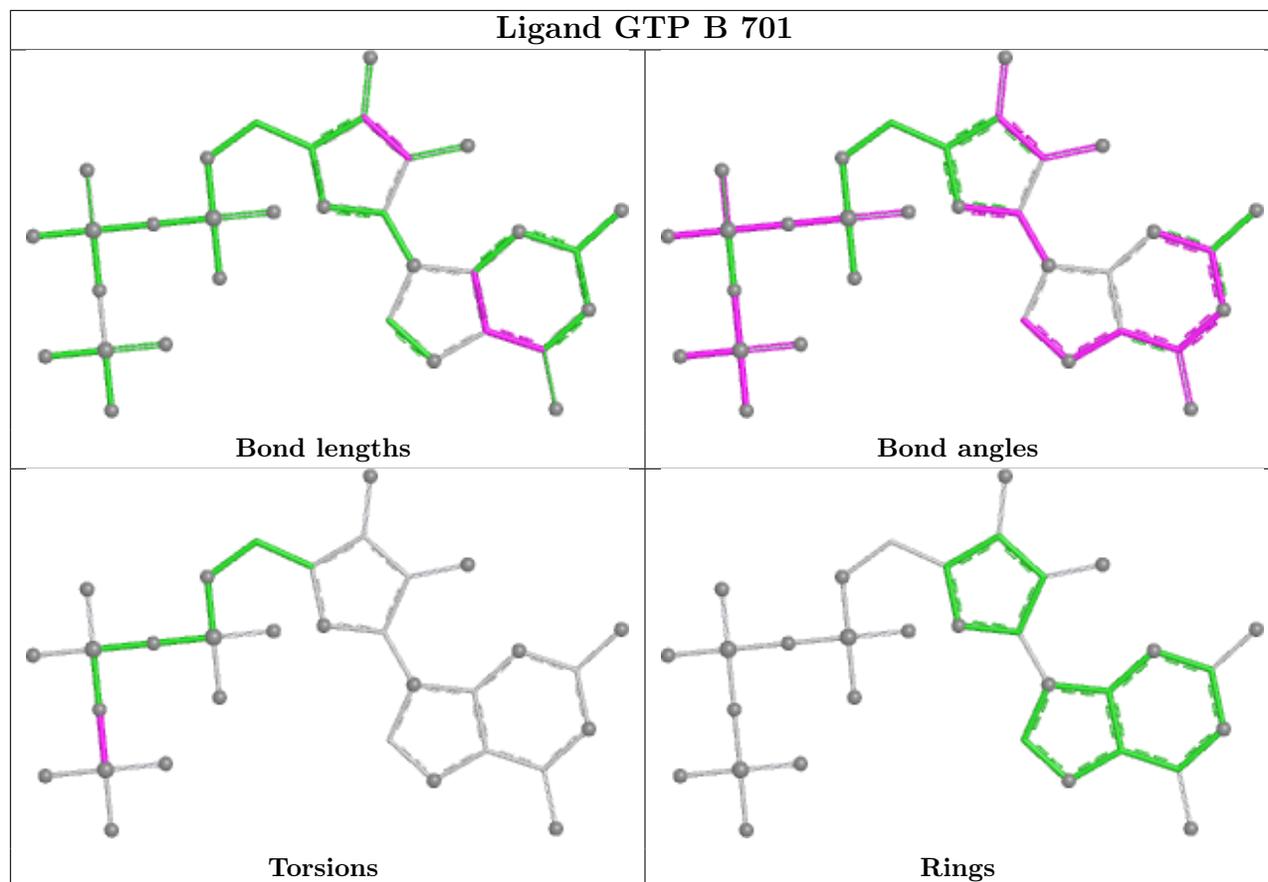
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GTP	1	0
2	B	701	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	685/695 (98%)	-0.23	9 (1%) 74 67	41, 66, 99, 121	0
1	B	685/695 (98%)	-0.02	11 (1%) 70 63	44, 78, 119, 135	0
1	E	685/695 (98%)	-0.03	9 (1%) 74 67	43, 77, 106, 126	0
All	All	2055/2085 (98%)	-0.10	29 (1%) 73 66	41, 73, 113, 135	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	TYR	4.4
1	E	688	LEU	4.2
1	A	465	LEU	3.5
1	A	121	ALA	3.5
1	E	121	ALA	3.3

### 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](#)

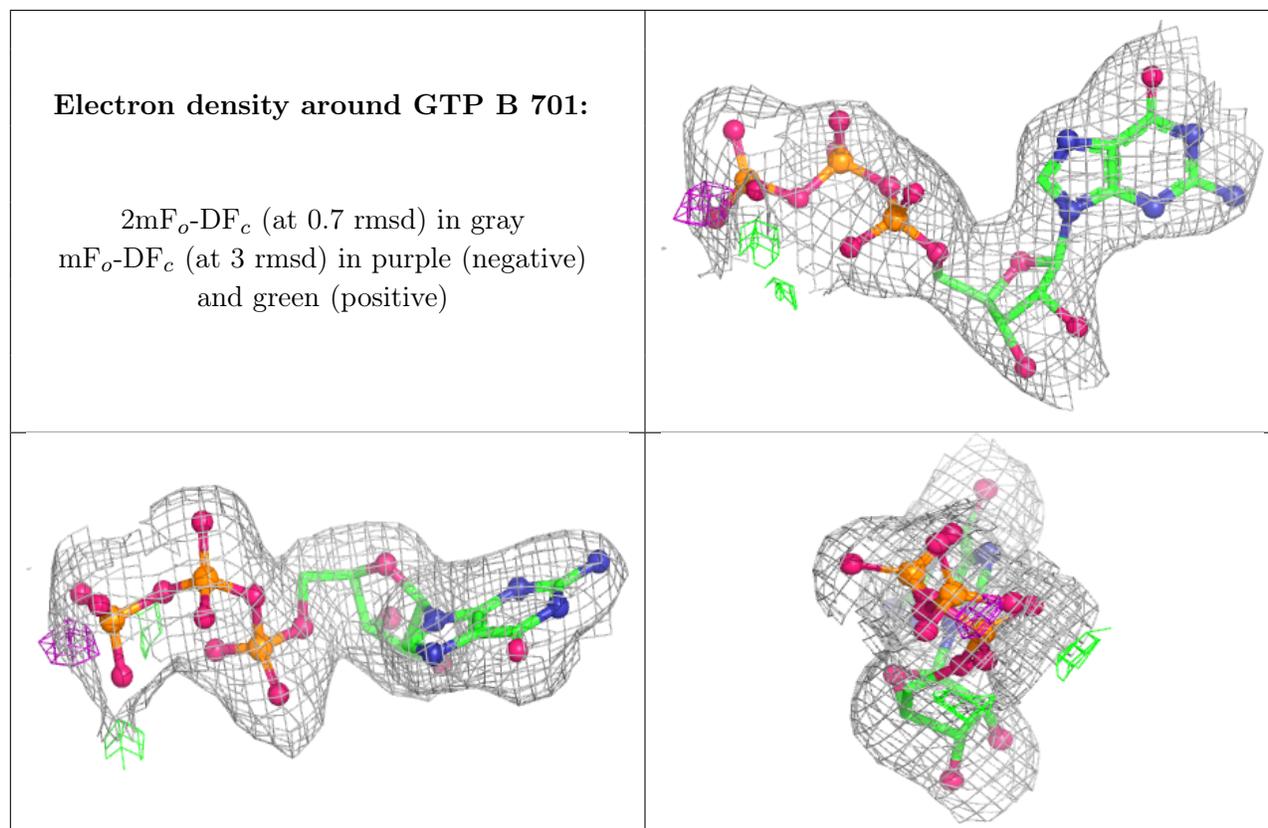
There are no monosaccharides in this entry.

### 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.

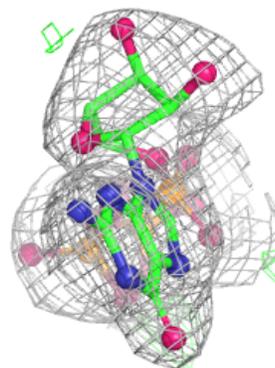
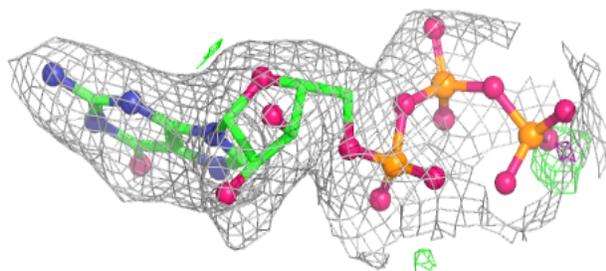
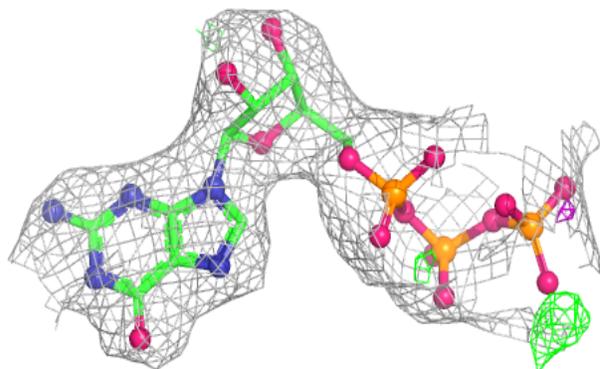
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GTP	B	701	32/32	0.92	0.07	63,67,79,80	0
2	GTP	A	701	32/32	0.93	0.06	45,53,80,81	0
2	GTP	E	701	32/32	0.94	0.06	45,63,75,75	0

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.

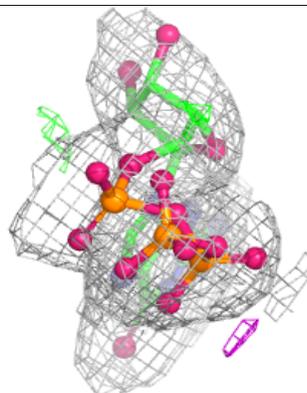
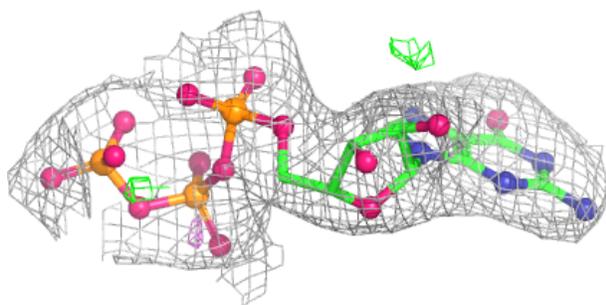
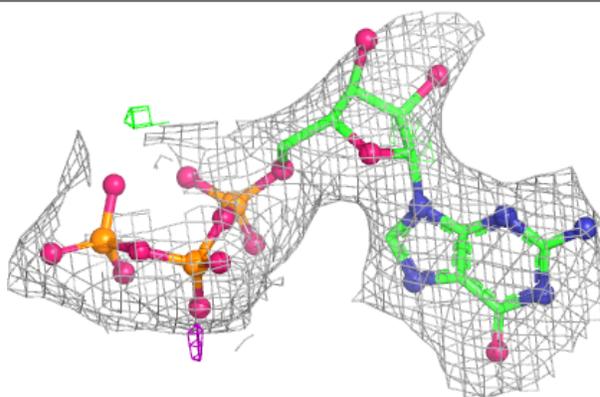


**Electron density around GTP A 701:**

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

**Electron density around GTP E 701:**

$2mF_o-DF_c$  (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.