



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:10 AM UTC

PDB ID : 5A2Z / pdb_00005a2z
Title : Crystal structure of mtPAP in complex with GTP
Authors : Lapkouski, M.; Hallberg, B.M.
Deposited on : 2015-05-26
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

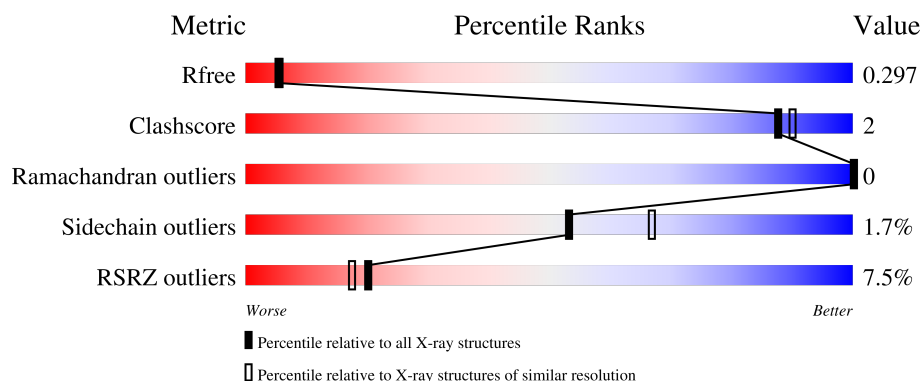
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	555	8% 78% 6% 16%
1	B	555	5% 77% 6% 17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7415 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 MITOCHONDRIAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3697	2375	620	681	21			
1	B	462	Total	C	N	O	S	0	0	0
			3651	2354	605	671	21			

There are 46 discrepancies between the modelled and reference sequences:

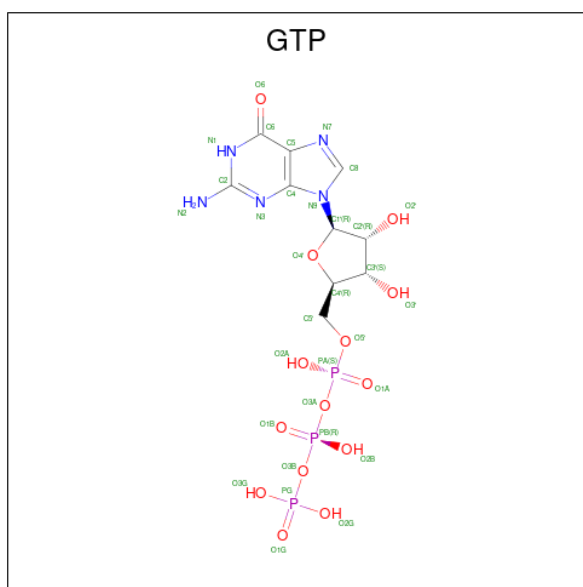
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	expression tag	UNP F1NBW0
A	15	HIS	-	expression tag	UNP F1NBW0
A	16	HIS	-	expression tag	UNP F1NBW0
A	17	HIS	-	expression tag	UNP F1NBW0
A	18	HIS	-	expression tag	UNP F1NBW0
A	19	HIS	-	expression tag	UNP F1NBW0
A	20	HIS	-	expression tag	UNP F1NBW0
A	21	SER	-	expression tag	UNP F1NBW0
A	22	SER	-	expression tag	UNP F1NBW0
A	23	GLY	-	expression tag	UNP F1NBW0
A	24	VAL	-	expression tag	UNP F1NBW0
A	25	ASP	-	expression tag	UNP F1NBW0
A	26	LEU	-	expression tag	UNP F1NBW0
A	27	GLY	-	expression tag	UNP F1NBW0
A	28	THR	-	expression tag	UNP F1NBW0
A	29	GLU	-	expression tag	UNP F1NBW0
A	30	ASN	-	expression tag	UNP F1NBW0
A	31	LEU	-	expression tag	UNP F1NBW0
A	32	TYR	-	expression tag	UNP F1NBW0
A	33	PHE	-	expression tag	UNP F1NBW0
A	34	GLN	-	expression tag	UNP F1NBW0
A	35	SER	-	expression tag	UNP F1NBW0
A	36	MET	-	expression tag	UNP F1NBW0
B	14	MET	-	expression tag	UNP F1NBW0
B	15	HIS	-	expression tag	UNP F1NBW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	HIS	-	expression tag	UNP F1NBW0
B	17	HIS	-	expression tag	UNP F1NBW0
B	18	HIS	-	expression tag	UNP F1NBW0
B	19	HIS	-	expression tag	UNP F1NBW0
B	20	HIS	-	expression tag	UNP F1NBW0
B	21	SER	-	expression tag	UNP F1NBW0
B	22	SER	-	expression tag	UNP F1NBW0
B	23	GLY	-	expression tag	UNP F1NBW0
B	24	VAL	-	expression tag	UNP F1NBW0
B	25	ASP	-	expression tag	UNP F1NBW0
B	26	LEU	-	expression tag	UNP F1NBW0
B	27	GLY	-	expression tag	UNP F1NBW0
B	28	THR	-	expression tag	UNP F1NBW0
B	29	GLU	-	expression tag	UNP F1NBW0
B	30	ASN	-	expression tag	UNP F1NBW0
B	31	LEU	-	expression tag	UNP F1NBW0
B	32	TYR	-	expression tag	UNP F1NBW0
B	33	PHE	-	expression tag	UNP F1NBW0
B	34	GLN	-	expression tag	UNP F1NBW0
B	35	SER	-	expression tag	UNP F1NBW0
B	36	MET	-	expression tag	UNP F1NBW0

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.75Å 94.36Å 192.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 2.45 39.67 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.67-2.45) 98.8 (39.67-2.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.260 , 0.295 0.260 , 0.297	Depositor DCC
R_{free} test set	2025 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7415	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/3785	0.74	4/5126 (0.1%)
1	B	0.45	2/3738 (0.1%)	0.75	6/5064 (0.1%)
All	All	0.44	2/7523 (0.0%)	0.75	10/10190 (0.1%)

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	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	HIS	CG-ND1	-5.47	1.32	1.38
1	B	104	HIS	CD2-NE2	-5.11	1.32	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLU	N-CA-C	13.20	133.02	111.37
1	B	408	ILE	CB-CA-C	10.96	121.82	111.30
1	B	476	GLN	CB-CA-C	-10.08	93.76	109.89
1	A	130	HIS	N-CA-CB	-9.72	96.31	110.80
1	B	99	GLU	N-CA-C	7.79	121.78	107.99
1	B	99	GLU	CB-CA-C	-7.22	99.02	110.79
1	A	130	HIS	N-CA-C	-6.38	104.04	113.61
1	B	476	GLN	N-CA-C	6.35	119.49	109.96
1	B	477	ASP	N-CA-C	6.16	119.67	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	GLN	N-CA-C	5.33	122.15	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	129	GLU	CA

There are no planarity outliers.

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	3697	0	3659	18	0
1	B	3651	0	3594	12	0
2	A	13	0	0	0	0
2	B	32	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	0	1	0
4	B	11	0	0	0	0
All	All	7415	0	7265	29	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 2.

All (29) 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:B:152:ALA:HB3	1:B:153:GLU:CB	2.12	0.78
1:B:231:PHE:O	1:B:352:ARG:NH2	2.30	0.65
1:A:85:TYR:OH	1:B:261:MET:SD	2.49	0.65
1:A:180:ILE:HG22	1:A:184:MET:CE	2.28	0.63
1:A:334:LEU:HD21	1:A:376:MET:CE	2.29	0.62
1:B:334:LEU:HD21	1:B:376:MET:CE	2.30	0.62
1:B:151:ALA:HB3	1:B:152:ALA:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HG22	1:A:184:MET:HE2	1.85	0.58
1:A:180:ILE:HG22	1:A:184:MET:HE3	1.95	0.48
1:A:399:LEU:HB2	1:A:416:VAL:CG2	2.45	0.47
1:A:275:THR:HG23	1:A:322:VAL:CG2	2.45	0.46
1:A:216:PHE:HB2	1:A:219:SER:OG	2.16	0.46
1:A:213:ARG:O	1:A:214:ALA:C	2.59	0.46
1:A:171:ILE:HB	1:A:172:PRO:HD3	1.98	0.45
1:B:171:ILE:HB	1:B:172:PRO:HD3	1.98	0.45
1:A:352:ARG:NH1	4:A:2007:HOH:O	2.49	0.45
1:B:275:THR:HG23	1:B:322:VAL:CG2	2.47	0.45
1:B:325:SER:O	1:B:329:ARG:HG2	2.17	0.45
1:B:152:ALA:CB	1:B:153:GLU:CB	2.93	0.43
1:A:399:LEU:HB2	1:A:416:VAL:HG21	2.01	0.43
1:B:216:PHE:HB2	1:B:219:SER:OG	2.19	0.43
1:B:312:GLN:N	1:B:313:PRO:CD	2.82	0.42
1:A:486:GLN:HB3	1:A:487:PRO:HD3	2.02	0.42
1:A:184:MET:HE2	1:A:435:LEU:HD22	2.02	0.41
1:A:325:SER:O	1:A:329:ARG:HG2	2.20	0.41
1:B:486:GLN:HB3	1:B:487:PRO:HD3	2.02	0.41
1:A:71:ILE:HD12	1:A:107:ILE:HG13	2.03	0.41
1:A:312:GLN:N	1:A:313:PRO:CD	2.84	0.40
1:A:124:ILE:O	1:A:125:PRO:C	2.64	0.40

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	462/555 (83%)	445 (96%)	17 (4%)	0	100	100
1	B	456/555 (82%)	443 (97%)	13 (3%)	0	100	100
All	All	918/1110 (83%)	888 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	411/497 (83%)	405 (98%)	6 (2%)	57	70
1	B	402/497 (81%)	394 (98%)	8 (2%)	48	63
All	All	813/994 (82%)	799 (98%)	14 (2%)	53	67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	SER
1	A	245	HIS
1	A	347	LEU
1	A	416	VAL
1	A	428	THR
1	A	513	ILE
1	B	150	GLN
1	B	181	SER
1	B	267	ARG
1	B	312	GLN
1	B	347	LEU
1	B	384	LYS
1	B	411	TYR
1	B	428	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	264	GLN
1	A	504	GLN
1	A	510	GLN
1	B	168	ASN

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Mol	Chain	Res	Type
1	B	264	GLN
1	B	312	GLN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	GTP	B	1528	3	33,34,34	1.29	5 (15%)	50,54,54	1.71	6 (12%)
2	GTP	A	1528	3	10,12,34	1.84	3 (30%)	17,20,54	1.22	1 (5%)

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	B	1528	3	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	A	1528	3	-	3/12/12/38	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1528	GTP	PG-O1G	3.62	1.61	1.50
2	B	1528	GTP	C5-C4	3.11	1.47	1.38
2	A	1528	GTP	PB-O3A	3.05	1.62	1.59
2	B	1528	GTP	PB-O3A	2.84	1.62	1.59
2	A	1528	GTP	PB-O3B	2.72	1.62	1.59
2	B	1528	GTP	PA-O3A	2.56	1.62	1.59
2	B	1528	GTP	PB-O3B	2.27	1.61	1.59
2	B	1528	GTP	C6-N1	-2.11	1.34	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1528	GTP	C5-C4-N3	-5.55	119.55	128.39
2	B	1528	GTP	C2-N3-C4	4.90	120.74	112.30
2	B	1528	GTP	C6-C5-N7	3.91	137.41	130.29
2	B	1528	GTP	N9-C4-N3	3.88	133.71	125.95
2	A	1528	GTP	O3G-PG-O2G	3.00	119.06	107.80
2	B	1528	GTP	C4-C5-N7	-2.88	106.10	110.67
2	B	1528	GTP	C8-N7-C5	2.07	107.95	104.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

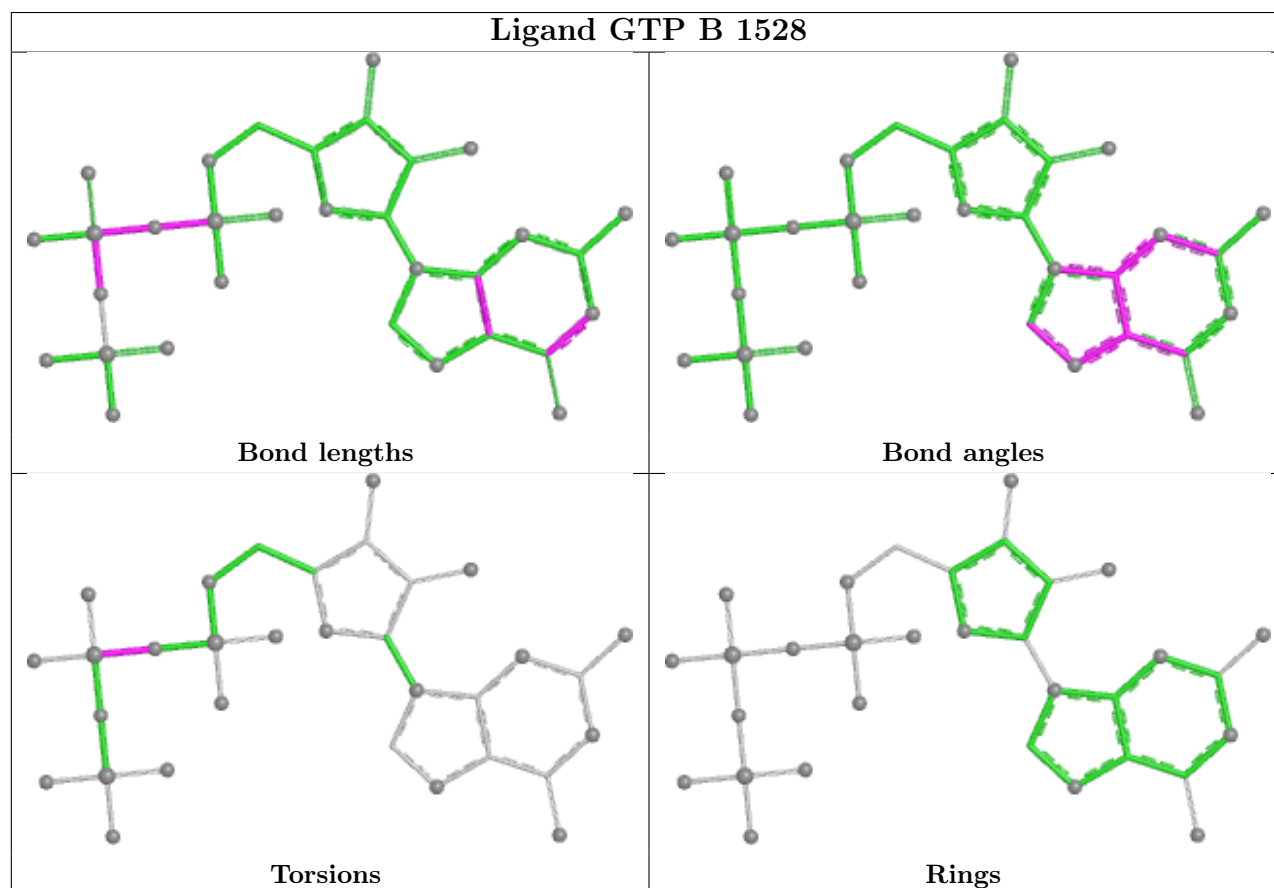
Mol	Chain	Res	Type	Atoms
2	A	1528	GTP	PB-O3A-PA-O2A
2	A	1528	GTP	PB-O3A-PA-O5'
2	B	1528	GTP	PA-O3A-PB-O2B
2	A	1528	GTP	PB-O3A-PA-O1A
2	B	1528	GTP	PA-O3A-PB-O1B

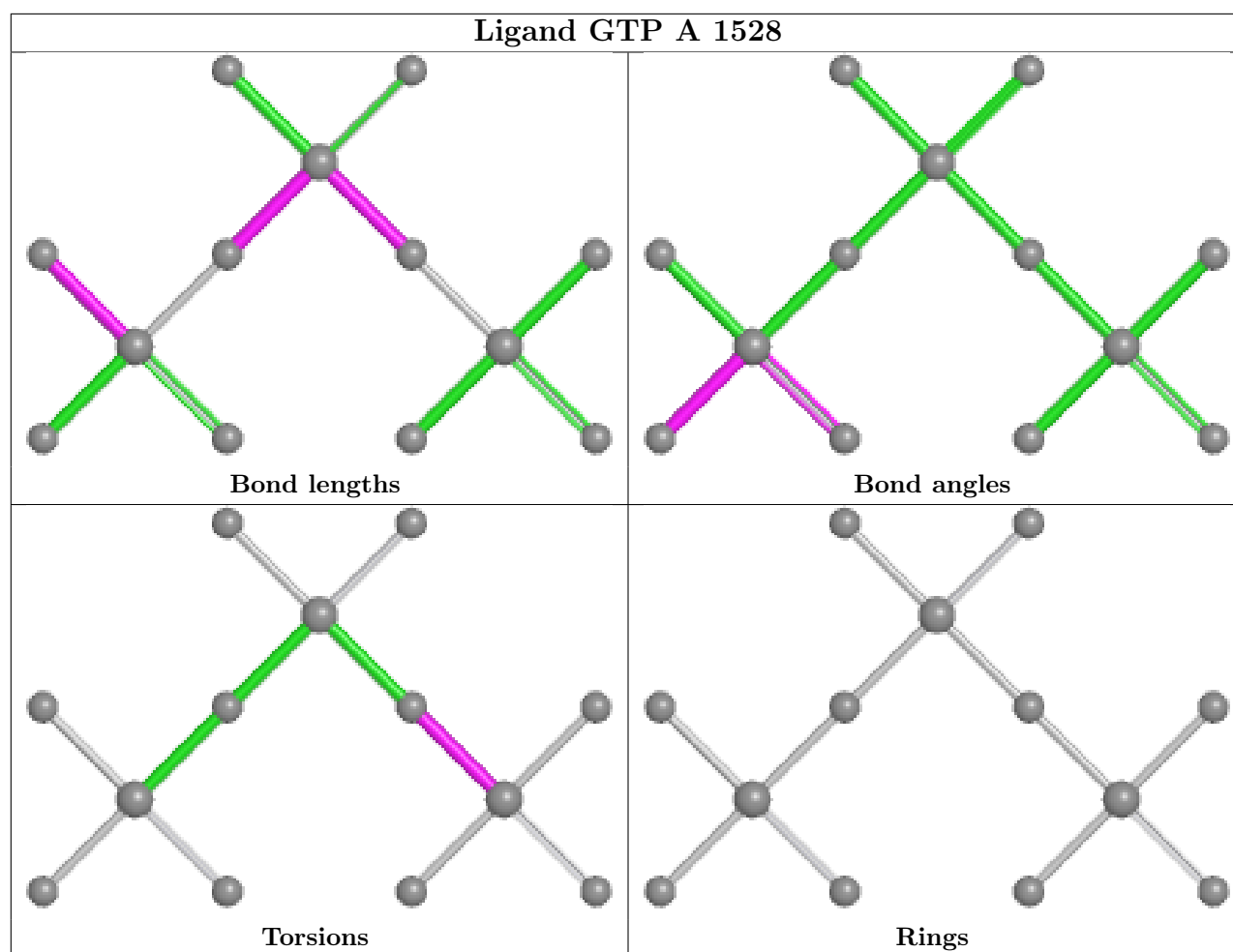
There are no ring outliers.

No monomer is involved in short contacts.

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	466/555 (83%)	0.77	44 (9%)	14 11	29, 51, 84, 98	0
1	B	462/555 (83%)	0.55	26 (5%)	30 27	26, 45, 72, 101	0
All	All	928/1110 (83%)	0.66	70 (7%)	20 17	26, 48, 80, 101	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	PHE	6.7
1	A	244	PHE	5.0
1	A	128	ALA	4.7
1	B	152	ALA	4.0
1	B	501	TRP	3.7
1	A	75	SER	3.6
1	B	241	PHE	3.6
1	B	411	TYR	3.4
1	A	508	LYS	3.3
1	A	408	ILE	3.1
1	B	268	LEU	3.0
1	A	290	GLY	3.0
1	A	245	HIS	2.9
1	A	74	PRO	2.9
1	B	514	ASN	2.9
1	A	411	TYR	2.9
1	A	402	GLU	2.8
1	A	410	GLY	2.8
1	A	178	ASP	2.8
1	B	323	SER	2.6
1	B	409	GLY	2.6
1	B	148	GLY	2.6
1	A	167	VAL	2.6
1	A	478	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	461	ASN	2.5
1	B	245	HIS	2.5
1	A	141	THR	2.5
1	A	465	SER	2.4
1	A	409	GLY	2.4
1	A	256	LYS	2.4
1	B	403	LYS	2.4
1	A	399	LEU	2.4
1	A	476	GLN	2.4
1	B	66	ASP	2.4
1	B	131	HIS	2.4
1	A	514	ASN	2.4
1	B	267	ARG	2.3
1	A	419	LEU	2.3
1	A	77	LEU	2.3
1	B	256	LYS	2.3
1	A	261	MET	2.3
1	A	407	VAL	2.3
1	B	509	THR	2.3
1	B	401	ASP	2.3
1	A	260	GLU	2.3
1	A	182	SER	2.2
1	B	408	ILE	2.2
1	A	127	ALA	2.2
1	A	395	GLN	2.2
1	A	512	MET	2.2
1	B	155	ARG	2.2
1	A	168	ASN	2.2
1	B	151	ALA	2.2
1	A	511	GLN	2.2
1	A	506	GLU	2.2
1	B	448	ARG	2.1
1	A	76	LYS	2.1
1	A	259	PHE	2.1
1	B	58	GLN	2.1
1	A	507	ASP	2.1
1	B	150	GLN	2.1
1	A	144	LEU	2.1
1	A	273	LEU	2.1
1	A	148	GLY	2.1
1	A	421	LYS	2.1
1	B	325	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	324	ASN	2.0
1	A	480	ILE	2.0
1	A	130	HIS	2.0
1	B	312	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

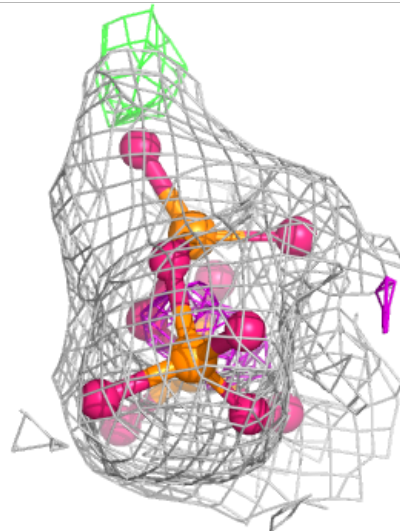
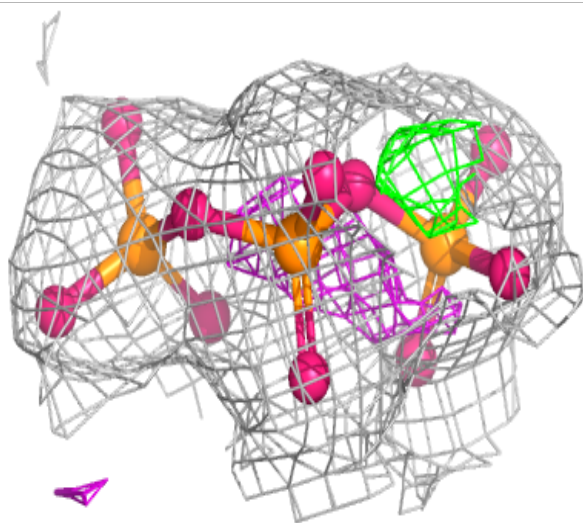
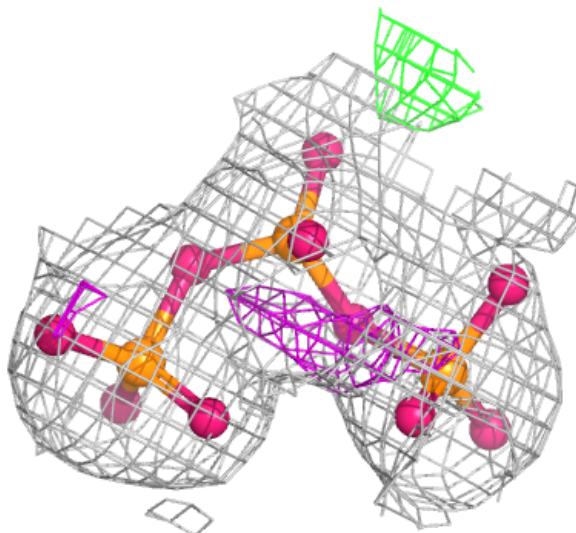
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTP	A	1528	13/32	0.78	0.12	75,78,82,83	0
2	GTP	B	1528	32/32	0.84	0.13	62,70,73,74	0
3	MG	A	1529	1/1	0.93	0.09	67,67,67,67	0
3	MG	B	1529	1/1	0.93	0.06	32,32,32,32	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.

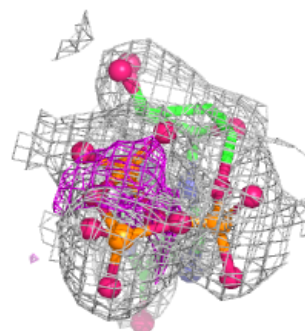
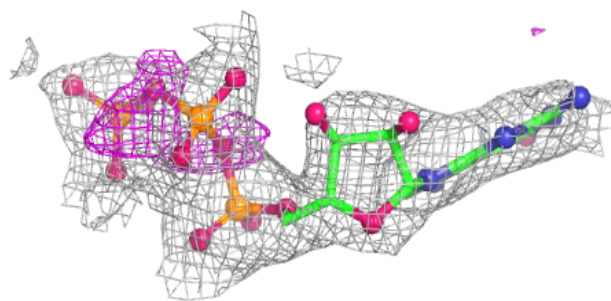
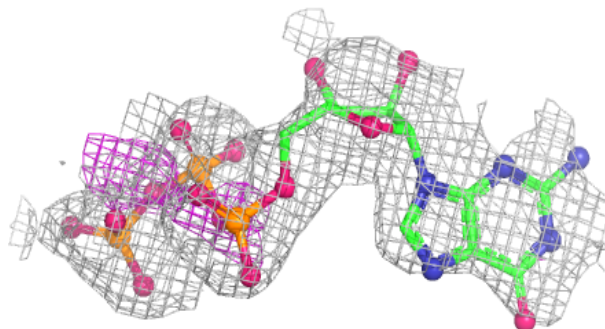
Electron density around GTP A 1528:

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



Electron density around GTP B 1528:

$2mF_o-DF_c$ (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.