



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:37 AM UTC

PDB ID : 7Y7R / pdb_00007y7r
Title : QDE-1 in complex with DNA template, RNA primer and 3'-dGTP
Authors : Cui, R.X.; Gan, J.H.; Ma, J.B.
Deposited on : 2022-06-22
Resolution : 2.10 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

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:

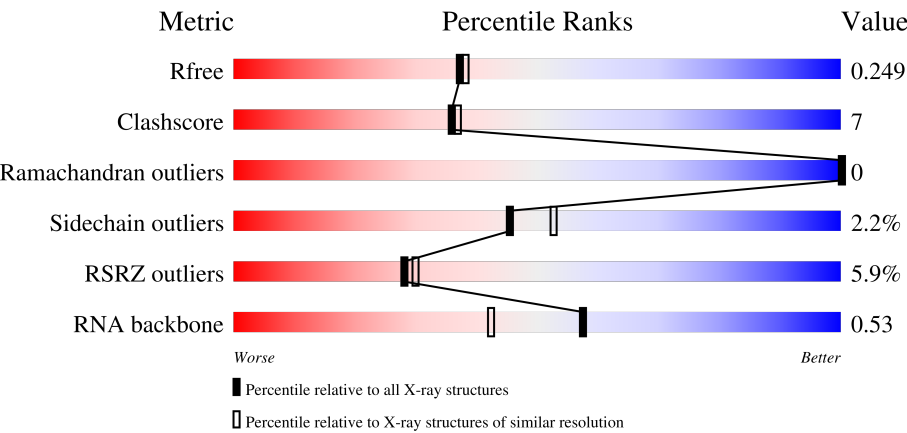
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



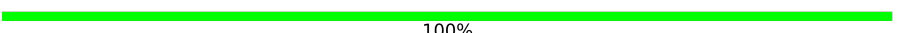
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

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	1026	2% 75% 16% 8%
1	B	1026	8% 71% 16% 13%
2	C	14	57% 14% 29%
2	E	14	14% 64% 21% 14%

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Mol	Chain	Length	Quality of chain
2	H	14	 50%50%
3	D	7	 71%29%
3	F	7	 43%29%29%
3	G	7	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16197 atoms, of which 26 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	941	Total	C	N	O	S	0	6	0
			7567	4838	1315	1377	37			
1	B	897	Total	C	N	O	S	0	5	0
			7024	4458	1239	1294	33			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*AP*CP*TP*AP*CP*CP*GP*TP*CP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			205	97	38	60	10			
2	E	12	Total	C	N	O	P	0	0	0
			245	116	46	71	12			
2	H	7	Total	C	N	O	P	0	0	0
			142	68	28	40	6			

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	P	0	0	0
			144	66	26	46	6			
3	F	5	Total	C	N	O	P	0	0	0
			107	48	21	33	5			
3	G	7	Total	C	N	O	P	0	0	0
			144	66	26	46	6			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

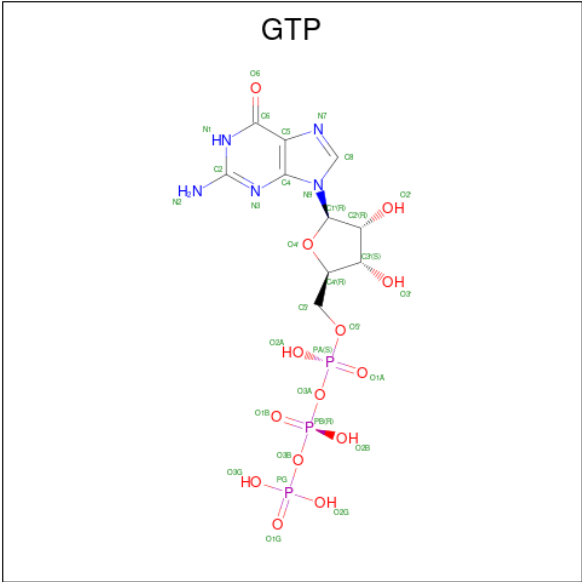
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

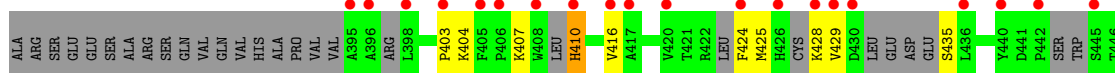
- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

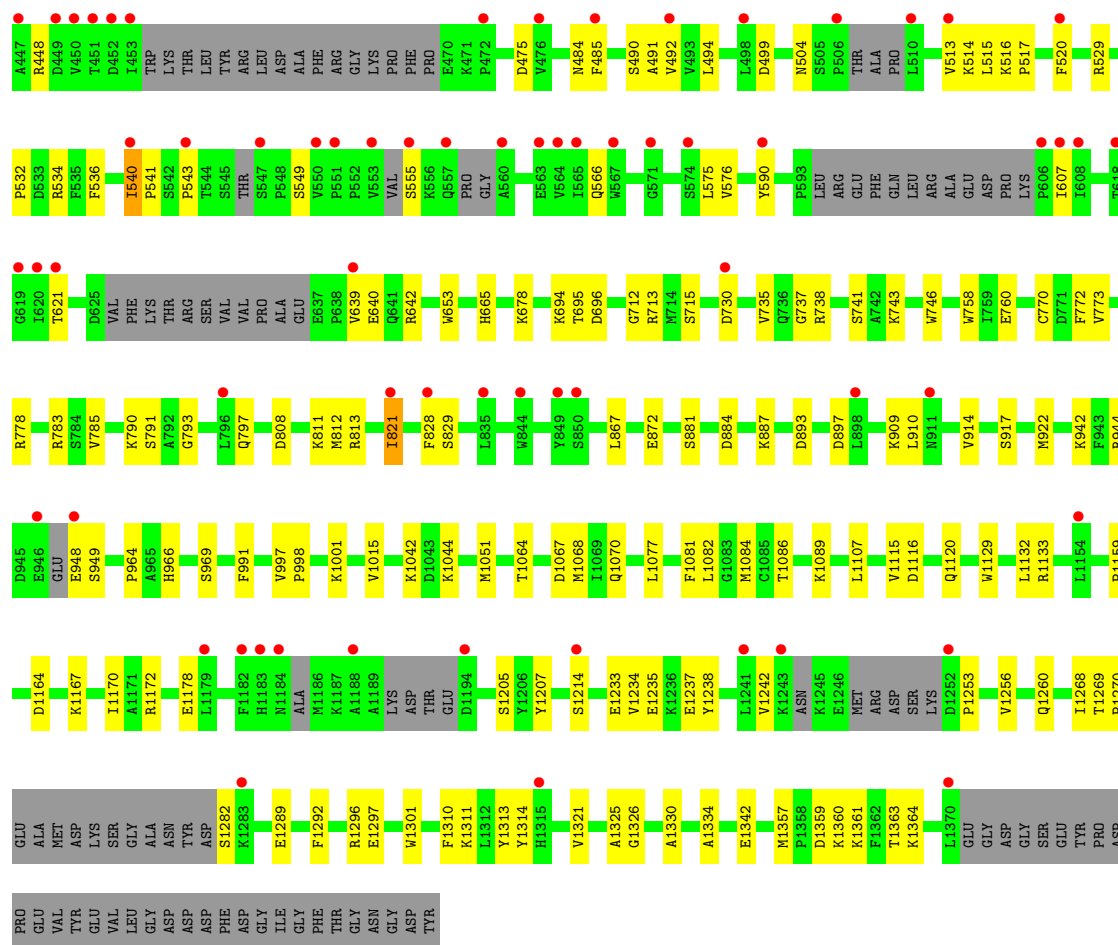


- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	266	Total 266	O 266	0	0
9	B	209	Total 209	O 209	0	0
9	C	11	Total 11	O 11	0	0
9	D	7	Total 7	O 7	0	0
9	E	6	Total 6	O 6	0	0
9	F	7	Total 7	O 7	0	0

- Molecule 1: RNA-dependent RNA polymerase





- Molecule 2: DNA (5'-D(*GP*AP*AP*CP*TP*AP*CP*CP*GP*TP*CP*GP*GP*A)-3')

Chain C: 57% 14% 29%



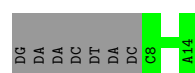
- Molecule 2: DNA (5'-D(*GP*AP*AP*CP*TP*AP*CP*CP*GP*TP*CP*GP*GP*A)-3')

Chain E: 14% 64% 21% 14%



- Molecule 2: DNA (5'-D(*GP*AP*AP*CP*TP*AP*CP*CP*GP*TP*CP*GP*GP*A)-3')

Chain H: 50% 50%



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain D:  71% 29%



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain F:  43% 29% 29%



- Molecule 3: RNA (5'-R(*UP*CP*CP*GP*AP*CP*G)-3')

Chain G:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.37Å 122.17Å 114.92Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	49.57 – 2.10 49.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.57-2.10) 93.4 (49.57-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.249	Depositor DCC
R_{free} test set	7165 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16197	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.26 % 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 2.2690e-03. 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

5.1 Standard geometry

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

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	0.35	0/7756	0.54	3/10495 (0.0%)
1	B	0.43	0/7174	0.63	1/9673 (0.0%)
2	C	0.31	0/229	0.43	0/351
2	E	0.26	0/274	0.36	0/420
2	H	0.26	0/159	0.39	0/244
3	D	0.22	0/160	0.34	0/247
3	F	0.19	0/119	0.37	0/183
3	G	0.13	0/160	0.23	0/247
All	All	0.38	0/16031	0.57	4/21860 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	PRO	CA-N-CD	-7.25	101.86	112.00
1	A	548	PRO	N-CD-CG	-5.87	94.39	103.20
1	A	548	PRO	CA-CB-CG	-5.56	93.93	104.50
1	B	1363	THR	CA-CB-OG1	-5.23	101.75	109.60

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	7567	0	7457	120	0
1	B	7024	0	6780	108	0
2	C	205	0	113	3	0
2	E	245	0	135	2	0
2	H	142	0	80	0	0
3	D	144	0	76	3	0
3	F	107	0	54	2	0
3	G	144	0	76	0	0
4	A	7	10	10	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	10	0	0
7	B	31	0	10	1	0
8	B	12	16	16	2	0
9	A	266	0	0	5	0
9	B	209	0	0	1	0
9	C	11	0	0	0	0
9	D	7	0	0	1	0
9	E	6	0	0	0	0
9	F	7	0	0	0	0
All	All	16171	26	14817	222	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 7.

The worst 5 of 222 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:485:PHE:CD1	1:B:492:VAL:HB	2.05	0.92
1:B:485:PHE:HD1	1:B:492:VAL:HB	1.37	0.89
1:A:847:GLU:OE2	1:A:1360:LYS:HE2	1.74	0.86
1:A:552:PRO:HD2	1:A:553:VAL:H	1.45	0.81
1:A:1269:THR:HG23	1:A:1270:PRO:HD2	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	933/1026 (91%)	914 (98%)	19 (2%)	0	100	100
1	B	862/1026 (84%)	841 (98%)	21 (2%)	0	100	100
All	All	1795/2052 (88%)	1755 (98%)	40 (2%)	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	814/894 (91%)	801 (98%)	13 (2%)	55	64
1	B	734/894 (82%)	712 (97%)	22 (3%)	36	41
All	All	1548/1788 (87%)	1513 (98%)	35 (2%)	45	51

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	743[A]	LYS
1	B	743[B]	LYS
1	B	1172	ARG
1	A	1370	LEU
1	A	1369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	876	ASN
1	B	1184	ASN
1	A	1063	GLN
1	A	1120	GLN
1	A	1183	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	5/7 (71%)	0	0
3	F	3/7 (42%)	0	0
3	G	5/7 (71%)	0	0
All	All	13/21 (61%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\# Z > 2$
8	GOL	B	1502	-	5,5,5	1.09	1 (20%)	5,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	B	1501	-	5,5,5	0.74	0	5,5,5	1.05	0
4	PEG	A	1501	-	6,6,6	0.51	0	5,5,5	0.32	0
7	GTP	B	1506	5,6	31,33,34	1.10	3 (9%)	44,52,54	1.70	10 (22%)
7	GTP	A	1505	5	31,33,34	1.02	2 (6%)	44,52,54	1.75	9 (20%)

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
8	GOL	B	1502	-	-	2/4/4/4	-
8	GOL	B	1501	-	-	0/4/4/4	-
4	PEG	A	1501	-	-	1/4/4/4	-
7	GTP	B	1506	5,6	-	1/22/34/38	0/3/3/3
7	GTP	A	1505	5	-	1/22/34/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1506	GTP	PB-O3B	3.34	1.63	1.59
7	A	1505	GTP	PB-O3B	3.00	1.62	1.59
7	B	1506	GTP	PB-O3A	2.16	1.61	1.59
7	A	1505	GTP	C2-N3	2.07	1.38	1.33
8	B	1502	GOL	O2-C2	-2.03	1.37	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1505	GTP	C5-C4-N3	-5.12	120.23	128.39
7	B	1506	GTP	C2-N3-C4	5.03	120.97	112.30
7	A	1505	GTP	C2-N3-C4	4.92	120.78	112.30
7	B	1506	GTP	C5-C4-N3	-4.88	120.62	128.39
7	A	1505	GTP	N9-C4-N3	3.32	132.60	125.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1505	GTP	C5'-O5'-PA-O1A
8	B	1502	GOL	C1-C2-C3-O3

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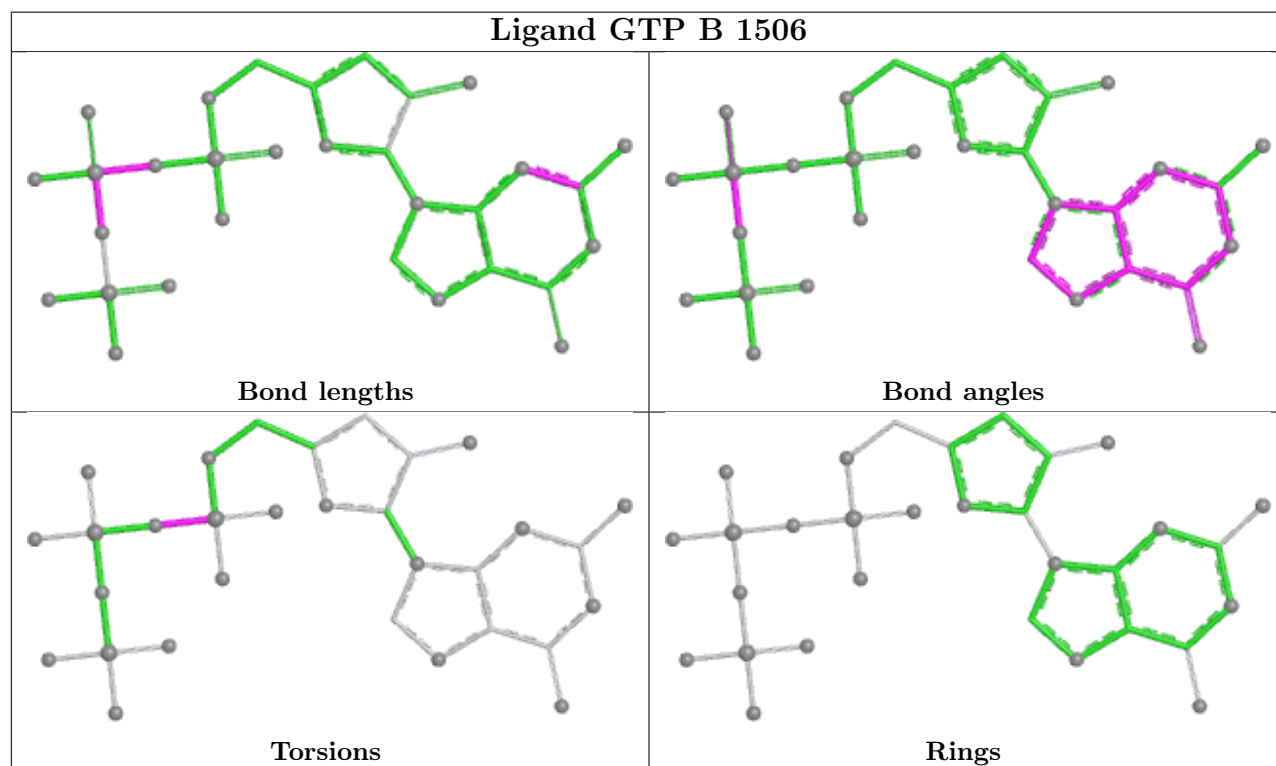
Mol	Chain	Res	Type	Atoms
7	B	1506	GTP	PB-O3A-PA-O5'
8	B	1502	GOL	O2-C2-C3-O3
4	A	1501	PEG	C1-C2-O2-C3

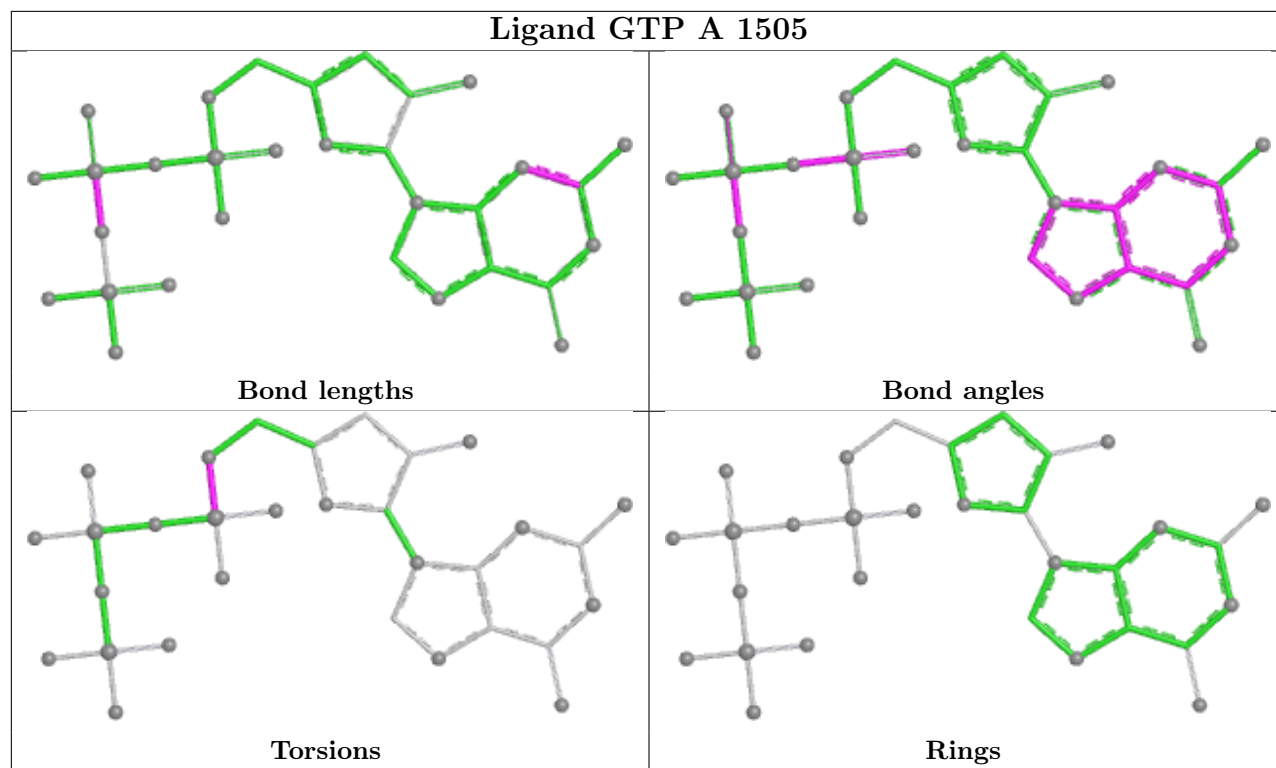
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1501	GOL	2	0
7	B	1506	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 ⓘ

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	941/1026 (91%)	0.15	24 (2%) 57 60	12, 47, 83, 114	6 (0%)
1	B	897/1026 (87%)	0.44	85 (9%) 14 14	17, 50, 96, 117	5 (0%)
2	C	10/14 (71%)	0.21	0 100 100	41, 60, 111, 136	0
2	E	12/14 (85%)	0.75	2 (16%) 4 4	52, 59, 121, 143	2 (16%)
2	H	7/14 (50%)	0.95	0 100 100	64, 88, 101, 117	6 (85%)
3	D	7/7 (100%)	-0.16	0 100 100	36, 64, 114, 125	0
3	F	5/7 (71%)	0.05	0 100 100	46, 61, 102, 129	0
3	G	7/7 (100%)	1.20	0 100 100	50, 63, 72, 75	7 (100%)
All	All	1886/2115 (89%)	0.30	111 (5%) 28 30	12, 49, 93, 143	26 (1%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	442	PRO	5.2
1	B	557	GLN	4.5
1	B	408	TRP	4.4
1	B	452	ASP	4.2
1	B	520	PHE	4.2

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

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

6.3 Carbohydrates ⓘ

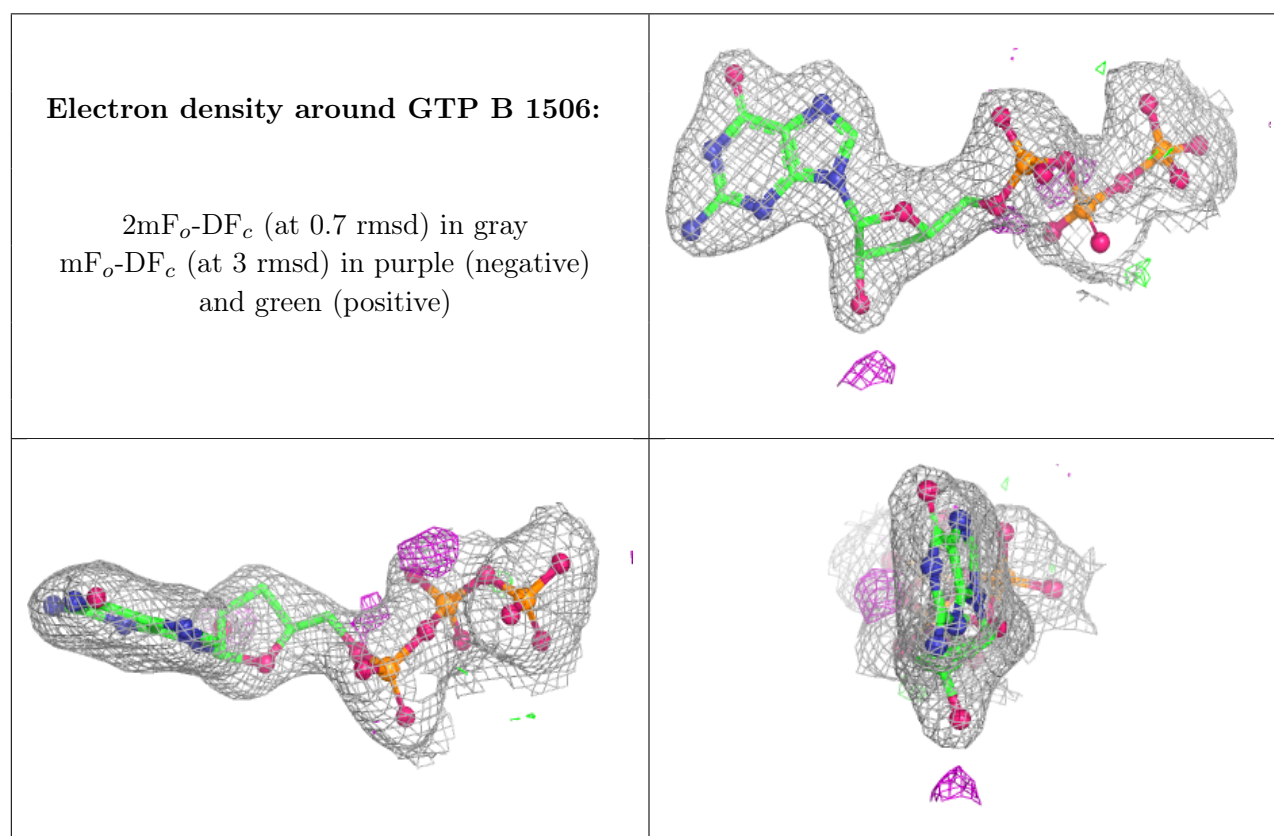
There are no oligosaccharides in this entry.

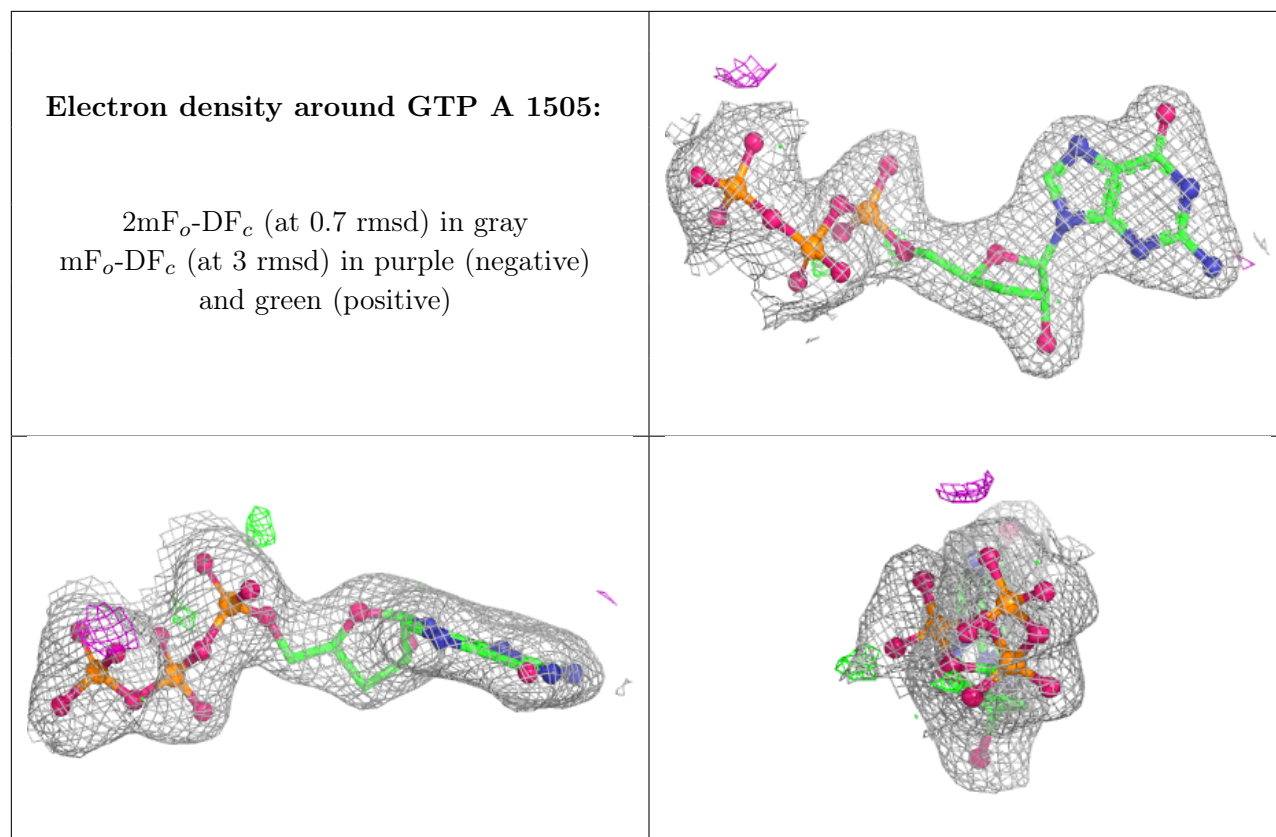
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	1502	6/6	0.87	0.14	54,78,93,101	0
8	GOL	B	1501	6/6	0.92	0.11	65,78,85,87	0
4	PEG	A	1501	7/7	0.93	0.09	53,64,74,74	0
7	GTP	B	1506	31/32	0.97	0.07	28,47,57,57	0
7	GTP	A	1505	31/32	0.98	0.05	25,37,49,54	0
6	MG	A	1504	1/1	0.98	0.06	33,33,33,33	0
6	MG	B	1505	1/1	0.99	0.02	25,25,25,25	0
5	CA	A	1503	1/1	0.99	0.03	35,35,35,35	0
5	CA	B	1503	1/1	0.99	0.02	31,31,31,31	0
5	CA	B	1504	1/1	0.99	0.03	33,33,33,33	0
5	CA	A	1502	1/1	0.99	0.02	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.