



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:45 pm BST

PDB ID : 6PW3  
Title : LARP1 DM15 FYRE (F844Y, R847E) mutant bound to m7GpppG dinucleotide (capG)  
Authors : Lahr, R.M.; Berman, A.J.  
Deposited on : 2019-07-22  
Resolution : 2.34 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

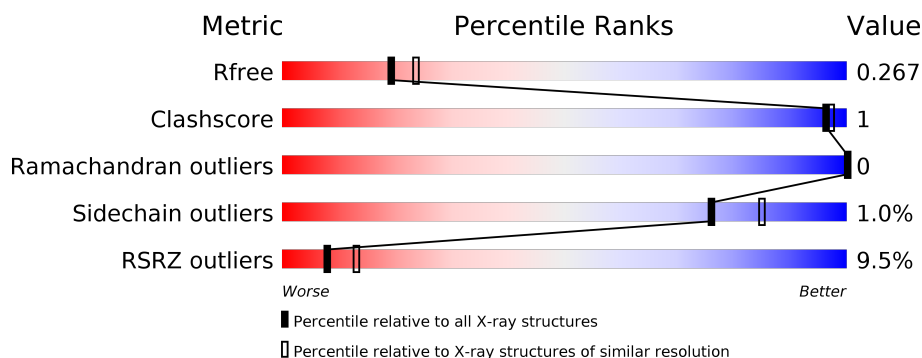
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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	162	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	162	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	162	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	162	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>12%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GTG	C	1001[A]	-	-	-	X
2	GTG	C	1001[B]	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9780 atoms, of which 4593 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 La-related protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	149	Total	C	H	N	O	S	0	1	0
			2482	843	1186	222	227	4			
1	A	144	Total	C	H	N	O	S	0	2	0
			2408	817	1151	213	223	4			
1	B	140	Total	C	H	N	O	S	0	0	0
			2362	798	1141	203	216	4			
1	D	143	Total	C	H	N	O	S	0	0	0
			2245	785	1034	205	217	4			

There are 52 discrepancies between the modelled and reference sequences:

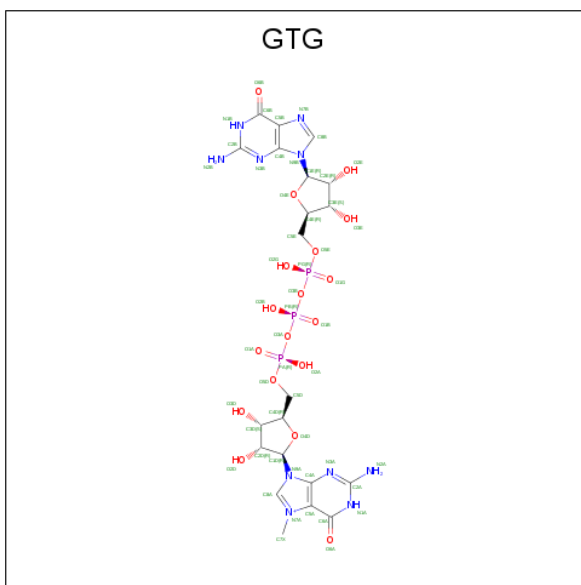
Chain	Residue	Modelled	Actual	Comment	Reference
C	785	GLY	-	expression tag	UNP Q6PKG0
C	786	HIS	-	expression tag	UNP Q6PKG0
C	787	SER	-	expression tag	UNP Q6PKG0
C	788	GLY	-	expression tag	UNP Q6PKG0
C	789	GLY	-	expression tag	UNP Q6PKG0
C	790	GLY	-	expression tag	UNP Q6PKG0
C	791	GLY	-	expression tag	UNP Q6PKG0
C	792	GLY	-	expression tag	UNP Q6PKG0
C	793	GLY	-	expression tag	UNP Q6PKG0
C	794	HIS	-	expression tag	UNP Q6PKG0
C	795	MET	-	expression tag	UNP Q6PKG0
C	844	TYR	PHE	engineered mutation	UNP Q6PKG0
C	847	GLU	ARG	engineered mutation	UNP Q6PKG0
A	785	GLY	-	expression tag	UNP Q6PKG0
A	786	HIS	-	expression tag	UNP Q6PKG0
A	787	SER	-	expression tag	UNP Q6PKG0
A	788	GLY	-	expression tag	UNP Q6PKG0
A	789	GLY	-	expression tag	UNP Q6PKG0
A	790	GLY	-	expression tag	UNP Q6PKG0
A	791	GLY	-	expression tag	UNP Q6PKG0
A	792	GLY	-	expression tag	UNP Q6PKG0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	793	GLY	-	expression tag	UNP Q6PKG0
A	794	HIS	-	expression tag	UNP Q6PKG0
A	795	MET	-	expression tag	UNP Q6PKG0
A	844	TYR	PHE	engineered mutation	UNP Q6PKG0
A	847	GLU	ARG	engineered mutation	UNP Q6PKG0
B	785	GLY	-	expression tag	UNP Q6PKG0
B	786	HIS	-	expression tag	UNP Q6PKG0
B	787	SER	-	expression tag	UNP Q6PKG0
B	788	GLY	-	expression tag	UNP Q6PKG0
B	789	GLY	-	expression tag	UNP Q6PKG0
B	790	GLY	-	expression tag	UNP Q6PKG0
B	791	GLY	-	expression tag	UNP Q6PKG0
B	792	GLY	-	expression tag	UNP Q6PKG0
B	793	GLY	-	expression tag	UNP Q6PKG0
B	794	HIS	-	expression tag	UNP Q6PKG0
B	795	MET	-	expression tag	UNP Q6PKG0
B	844	TYR	PHE	engineered mutation	UNP Q6PKG0
B	847	GLU	ARG	engineered mutation	UNP Q6PKG0
D	785	GLY	-	expression tag	UNP Q6PKG0
D	786	HIS	-	expression tag	UNP Q6PKG0
D	787	SER	-	expression tag	UNP Q6PKG0
D	788	GLY	-	expression tag	UNP Q6PKG0
D	789	GLY	-	expression tag	UNP Q6PKG0
D	790	GLY	-	expression tag	UNP Q6PKG0
D	791	GLY	-	expression tag	UNP Q6PKG0
D	792	GLY	-	expression tag	UNP Q6PKG0
D	793	GLY	-	expression tag	UNP Q6PKG0
D	794	HIS	-	expression tag	UNP Q6PKG0
D	795	MET	-	expression tag	UNP Q6PKG0
D	844	TYR	PHE	engineered mutation	UNP Q6PKG0
D	847	GLU	ARG	engineered mutation	UNP Q6PKG0

- Molecule 2 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (three-letter code: GTG) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>10</sub>O<sub>18</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total 158	C 42	H 54	N 20	O 36	P 6	0	1
2	B	1	Total 79	C 21	H 27	N 10	O 18	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

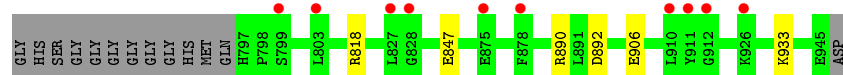
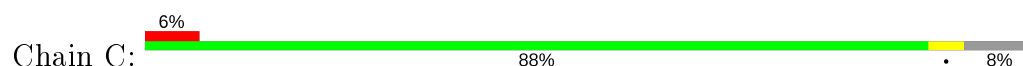
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	12	Total	O	0	0
			12	12		
4	A	15	Total	O	0	0
			15	15		
4	B	11	Total	O	0	0
			11	11		
4	D	7	Total	O	0	0
			7	7		

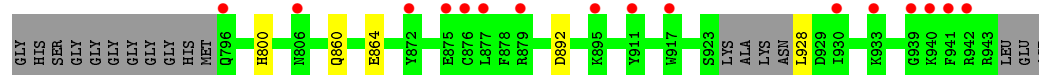
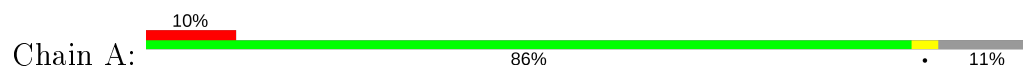
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

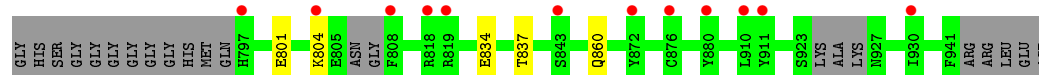
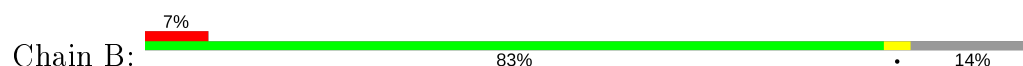
- Molecule 1: La-related protein 1



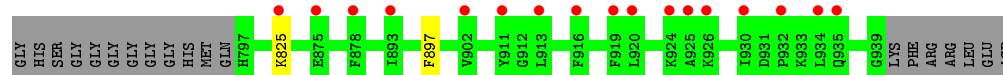
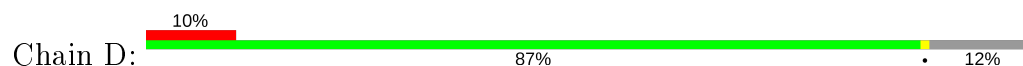
- Molecule 1: La-related protein 1



- Molecule 1: La-related protein 1



- Molecule 1: La-related protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.58Å 87.36Å 72.89Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	29.24 – 2.34 29.24 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.24-2.34) 94.3 (29.24-2.34)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.221 , 0.267 0.221 , 0.267	Depositor DCC
$R_{free}$ test set	1905 reflections (6.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: MG, GTG

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	0.25	0/1295	0.36	0/1733
1	B	0.24	0/1255	0.35	0/1678
1	C	0.24	0/1335	0.37	0/1786
1	D	0.24	0/1246	0.35	0/1673
All	All	0.24	0/5131	0.36	0/6870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	1257	1151	1182	3	0
1	B	1221	1141	1157	2	0
1	C	1296	1186	1240	3	0
1	D	1211	1034	1112	0	0
2	B	52	27	25	0	0
2	C	104	54	52	3	0
3	A	1	0	0	0	0
4	A	15	0	0	0	0
4	B	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	12	0	0	0	0
4	D	7	0	0	0	0
All	All	5187	4593	4768	10	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 1.

All (10) 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:847:GLU:OE2	2:C:1001[A]:GTG:N1B	2.35	0.58
1:A:860:GLN:NE2	1:A:864:GLU:OE2	2.38	0.53
2:C:1001[B]:GTG:H2B	2:C:1001[B]:GTG:N3B	2.29	0.48
1:B:801:GLU:OE1	1:B:804:LYS:HE3	2.14	0.47
1:A:928:LEU:N	1:A:928:LEU:HD12	2.30	0.47
2:C:1001[B]:GTG:N3B	2:C:1001[B]:GTG:C2E	2.78	0.46
1:C:890[B]:ARG:NH1	1:C:892:ASP:OD1	2.50	0.45
1:A:892:ASP:N	1:A:892:ASP:OD1	2.50	0.44
1:B:834:GLU:O	1:B:837:THR:OG1	2.32	0.43
1:C:906:GLU:OE2	1:C:933:LYS:NZ	2.38	0.42

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	142/162 (88%)	138 (97%)	4 (3%)	0	100	100
1	B	134/162 (83%)	133 (99%)	1 (1%)	0	100	100
1	C	148/162 (91%)	146 (99%)	2 (1%)	0	100	100
1	D	141/162 (87%)	137 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	565/648 (87%)	554 (98%)	11 (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	127/141 (90%)	126 (99%)	1 (1%)	81	89
1	B	125/141 (89%)	124 (99%)	1 (1%)	81	89
1	C	131/141 (93%)	130 (99%)	1 (1%)	81	89
1	D	118/141 (84%)	116 (98%)	2 (2%)	60	72
All	All	501/564 (89%)	496 (99%)	5 (1%)	76	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	818	ARG
1	A	800	HIS
1	B	860	GLN
1	D	825	LYS
1	D	897	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	811	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	GTG	B	1001	-	46,57,57	4.64	27 (58%)	51,90,90	2.73	14 (27%)
2	GTG	C	1001[A]	-	46,57,57	4.64	27 (58%)	51,90,90	2.72	14 (27%)
2	GTG	C	1001[B]	-	46,57,57	4.63	27 (58%)	51,90,90	2.53	15 (29%)

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	GTG	B	1001	-	-	9/24/64/64	0/6/6/6
2	GTG	C	1001[A]	-	-	13/24/64/64	0/6/6/6
2	GTG	C	1001[B]	-	-	10/24/64/64	0/6/6/6

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001[A]	GTG	C2D-C3D	-10.72	1.24	1.53
2	B	1001	GTG	C2D-C3D	-10.65	1.24	1.53
2	C	1001[B]	GTG	C2D-C3D	-10.64	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001[B]	GTG	C4B-N3B	9.25	1.50	1.35
2	C	1001[A]	GTG	C4B-N3B	9.19	1.50	1.35
2	B	1001	GTG	C4B-N3B	9.12	1.50	1.35
2	C	1001[B]	GTG	C4A-N3A	9.03	1.49	1.35
2	B	1001	GTG	C4A-N3A	9.02	1.49	1.35
2	C	1001[A]	GTG	C4A-N3A	9.02	1.49	1.35
2	B	1001	GTG	C2D-C1D	8.88	1.67	1.53
2	C	1001[A]	GTG	C2D-C1D	8.80	1.67	1.53
2	C	1001[B]	GTG	C2D-C1D	8.73	1.67	1.53
2	B	1001	GTG	C3E-C4E	-8.45	1.31	1.53
2	C	1001[A]	GTG	C3E-C4E	-8.43	1.31	1.53
2	C	1001[B]	GTG	C3E-C4E	-8.24	1.31	1.53
2	B	1001	GTG	O4E-C4E	7.68	1.62	1.45
2	C	1001[A]	GTG	O4E-C4E	7.61	1.62	1.45
2	C	1001[B]	GTG	O4E-C4E	7.57	1.61	1.45
2	C	1001[A]	GTG	O4E-C1E	-7.51	1.30	1.41
2	B	1001	GTG	C6B-C5B	7.30	1.53	1.41
2	C	1001[B]	GTG	C6B-C5B	7.30	1.53	1.41
2	C	1001[A]	GTG	C6B-C5B	7.25	1.53	1.41
2	C	1001[B]	GTG	C6A-C5A	7.25	1.53	1.41
2	B	1001	GTG	C6A-C5A	7.24	1.53	1.41
2	C	1001[B]	GTG	O4D-C1D	-7.20	1.31	1.41
2	C	1001[A]	GTG	C6A-C5A	7.20	1.53	1.41
2	B	1001	GTG	O4D-C1D	-7.20	1.31	1.41
2	B	1001	GTG	O4E-C1E	-7.10	1.31	1.41
2	C	1001[B]	GTG	O4E-C1E	-7.10	1.31	1.41
2	C	1001[A]	GTG	O4D-C1D	-6.98	1.31	1.41
2	B	1001	GTG	C6A-N1A	6.01	1.43	1.33
2	C	1001[B]	GTG	C6A-N1A	5.99	1.43	1.33
2	C	1001[A]	GTG	C6A-N1A	5.98	1.43	1.33
2	B	1001	GTG	C6B-N1B	5.95	1.43	1.33
2	C	1001[A]	GTG	C6B-N1B	5.95	1.43	1.33
2	C	1001[B]	GTG	C2B-N2B	5.87	1.45	1.33
2	C	1001[A]	GTG	C2B-N2B	5.87	1.45	1.33
2	C	1001[B]	GTG	C6B-N1B	5.86	1.43	1.33
2	B	1001	GTG	C2B-N2B	5.86	1.45	1.33
2	C	1001[B]	GTG	C2A-N2A	5.81	1.45	1.33
2	C	1001[A]	GTG	C2A-N2A	5.78	1.45	1.33
2	B	1001	GTG	C2A-N2A	5.78	1.45	1.33
2	C	1001[B]	GTG	C2A-N1A	5.13	1.44	1.35
2	B	1001	GTG	C2A-N1A	5.11	1.44	1.35
2	C	1001[A]	GTG	C2A-N1A	5.11	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	GTG	C2B-N1B	5.05	1.44	1.35
2	C	1001[A]	GTG	C2B-N1B	5.03	1.44	1.35
2	C	1001[B]	GTG	C2B-N1B	4.88	1.44	1.35
2	B	1001	GTG	C5D-C4D	-3.95	1.39	1.51
2	C	1001[B]	GTG	C5D-C4D	-3.88	1.39	1.51
2	C	1001[A]	GTG	C5D-C4D	-3.81	1.39	1.51
2	C	1001[B]	GTG	O3D-C3D	3.35	1.50	1.43
2	B	1001	GTG	O3D-C3D	3.32	1.50	1.43
2	C	1001[A]	GTG	O3D-C3D	3.31	1.50	1.43
2	C	1001[B]	GTG	C3D-C4D	3.18	1.61	1.53
2	B	1001	GTG	C3D-C4D	3.12	1.61	1.53
2	C	1001[A]	GTG	C3D-C4D	3.11	1.60	1.53
2	C	1001[B]	GTG	O3E-C3E	2.96	1.49	1.43
2	B	1001	GTG	O3E-C3E	2.95	1.49	1.43
2	C	1001[A]	GTG	O3E-C3E	2.94	1.49	1.43
2	C	1001[B]	GTG	O2E-C2E	-2.92	1.36	1.43
2	B	1001	GTG	O2E-C2E	-2.86	1.36	1.43
2	C	1001[A]	GTG	O2E-C2E	-2.85	1.36	1.43
2	C	1001[A]	GTG	O4D-C4D	2.68	1.51	1.45
2	C	1001[B]	GTG	O4D-C4D	2.67	1.51	1.45
2	C	1001[B]	GTG	C2A-N3A	2.55	1.46	1.34
2	C	1001[A]	GTG	C2A-N3A	2.55	1.46	1.34
2	B	1001	GTG	C2A-N3A	2.55	1.46	1.34
2	C	1001[A]	GTG	C2B-N3B	2.53	1.46	1.34
2	C	1001[B]	GTG	C2B-N3B	2.53	1.46	1.34
2	B	1001	GTG	C2B-N3B	2.53	1.46	1.34
2	B	1001	GTG	O4D-C4D	2.51	1.50	1.45
2	B	1001	GTG	O2D-C2D	2.32	1.48	1.43
2	C	1001[B]	GTG	O2D-C2D	2.30	1.48	1.43
2	B	1001	GTG	O6A-C6A	-2.29	1.18	1.24
2	C	1001[A]	GTG	O6A-C6A	-2.29	1.18	1.24
2	C	1001[A]	GTG	O2D-C2D	2.28	1.48	1.43
2	C	1001[B]	GTG	O6A-C6A	-2.28	1.18	1.24
2	C	1001[B]	GTG	O6B-C6B	-2.26	1.18	1.24
2	B	1001	GTG	O6B-C6B	-2.25	1.18	1.24
2	C	1001[A]	GTG	O6B-C6B	-2.25	1.18	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001[A]	GTG	C1E-N9B-C4B	-11.57	106.31	126.64
2	B	1001	GTG	C1E-N9B-C4B	-11.48	106.47	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	GTG	C1D-N9A-C4A	-8.15	112.33	126.64
2	C	1001[A]	GTG	C1D-N9A-C4A	-8.01	112.56	126.64
2	C	1001[B]	GTG	C1D-N9A-C4A	-7.92	112.72	126.64
2	C	1001[B]	GTG	C1E-N9B-C4B	-7.43	113.59	126.64
2	C	1001[B]	GTG	C2B-N3B-C4B	6.06	122.28	115.36
2	C	1001[B]	GTG	N3B-C2B-N1B	-5.61	119.74	127.22
2	C	1001[A]	GTG	N3B-C2B-N1B	-5.46	119.93	127.22
2	B	1001	GTG	N3B-C2B-N1B	-5.36	120.07	127.22
2	C	1001[B]	GTG	N3A-C2A-N1A	-5.35	120.08	127.22
2	C	1001[A]	GTG	N3A-C2A-N1A	-5.30	120.15	127.22
2	B	1001	GTG	N3A-C2A-N1A	-5.30	120.16	127.22
2	B	1001	GTG	C2B-N3B-C4B	4.72	120.75	115.36
2	C	1001[A]	GTG	C2B-N3B-C4B	4.68	120.70	115.36
2	C	1001[B]	GTG	C2A-N3A-C4A	4.21	120.16	115.36
2	C	1001[A]	GTG	C2A-N3A-C4A	4.19	120.15	115.36
2	B	1001	GTG	C2A-N3A-C4A	4.17	120.12	115.36
2	B	1001	GTG	C3D-C2D-C1D	4.16	107.24	100.98
2	C	1001[B]	GTG	C3D-C2D-C1D	3.89	106.84	100.98
2	C	1001[B]	GTG	C3E-C2E-C1E	3.30	105.94	100.98
2	B	1001	GTG	PB-O3A-PA	-3.18	121.92	132.83
2	C	1001[A]	GTG	C3D-C2D-C1D	3.08	105.62	100.98
2	C	1001[A]	GTG	C3E-C2E-C1E	3.01	105.51	100.98
2	B	1001	GTG	PG-O3B-PB	-2.84	123.08	132.83
2	C	1001[A]	GTG	PG-O3B-PB	-2.71	123.54	132.83
2	B	1001	GTG	C3E-C2E-C1E	2.67	105.00	100.98
2	C	1001[B]	GTG	PG-O3B-PB	-2.64	123.75	132.83
2	C	1001[A]	GTG	PB-O3A-PA	-2.56	124.06	132.83
2	C	1001[B]	GTG	PB-O3A-PA	-2.55	124.08	132.83
2	C	1001[A]	GTG	C5A-C6A-N1A	-2.50	120.01	123.43
2	C	1001[A]	GTG	C5B-C6B-N1B	-2.50	120.01	123.43
2	C	1001[B]	GTG	C5A-C6A-N1A	-2.47	120.06	123.43
2	B	1001	GTG	C5A-C6A-N1A	-2.46	120.06	123.43
2	B	1001	GTG	C5B-C6B-N1B	-2.45	120.08	123.43
2	C	1001[A]	GTG	C6B-N1B-C2B	2.36	119.69	115.93
2	C	1001[B]	GTG	C6A-N1A-C2A	2.35	119.66	115.93
2	C	1001[A]	GTG	C6A-N1A-C2A	2.33	119.63	115.93
2	B	1001	GTG	C6A-N1A-C2A	2.32	119.61	115.93
2	C	1001[B]	GTG	O4E-C1E-C2E	-2.26	103.62	106.93
2	B	1001	GTG	C6B-N1B-C2B	2.23	119.48	115.93
2	C	1001[B]	GTG	C5B-C6B-N1B	-2.20	120.43	123.43
2	C	1001[B]	GTG	C2E-C3E-C4E	2.18	106.88	102.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	GTG	C5D-O5D-PA-O3A
2	B	1001	GTG	C3D-C4D-C5D-O5D
2	C	1001[A]	GTG	C5D-O5D-PA-O1A
2	C	1001[A]	GTG	C5E-O5E-PG-O1G
2	C	1001[A]	GTG	C5E-O5E-PG-O2G
2	C	1001[B]	GTG	C5D-O5D-PA-O2A
2	C	1001[B]	GTG	C5D-O5D-PA-O3A
2	C	1001[B]	GTG	C5E-O5E-PG-O3B
2	C	1001[B]	GTG	C5E-O5E-PG-O2G
2	C	1001[B]	GTG	O4E-C4E-C5E-O5E
2	C	1001[B]	GTG	C3E-C4E-C5E-O5E
2	B	1001	GTG	O4D-C4D-C5D-O5D
2	B	1001	GTG	C4D-C5D-O5D-PA
2	C	1001[A]	GTG	C5D-O5D-PA-O3A
2	C	1001[A]	GTG	O4D-C4D-C5D-O5D
2	C	1001[B]	GTG	PB-O3A-PA-O2A
2	B	1001	GTG	C5D-O5D-PA-O1A
2	C	1001[A]	GTG	C5D-O5D-PA-O2A
2	C	1001[B]	GTG	C5D-O5D-PA-O1A
2	C	1001[B]	GTG	C5E-O5E-PG-O1G
2	C	1001[B]	GTG	C4E-C5E-O5E-PG
2	B	1001	GTG	PB-O3B-PG-O2G
2	C	1001[A]	GTG	PB-O3A-PA-O2A
2	C	1001[A]	GTG	C4D-C5D-O5D-PA
2	B	1001	GTG	C4E-C5E-O5E-PG
2	C	1001[A]	GTG	PG-O3B-PB-O3A
2	B	1001	GTG	O4E-C4E-C5E-O5E
2	B	1001	GTG	C3E-C4E-C5E-O5E
2	C	1001[A]	GTG	C5E-O5E-PG-O3B
2	C	1001[A]	GTG	PB-O3A-PA-O1A
2	C	1001[A]	GTG	PG-O3B-PB-O2B
2	C	1001[A]	GTG	O4E-C4E-C5E-O5E

There are no ring outliers.

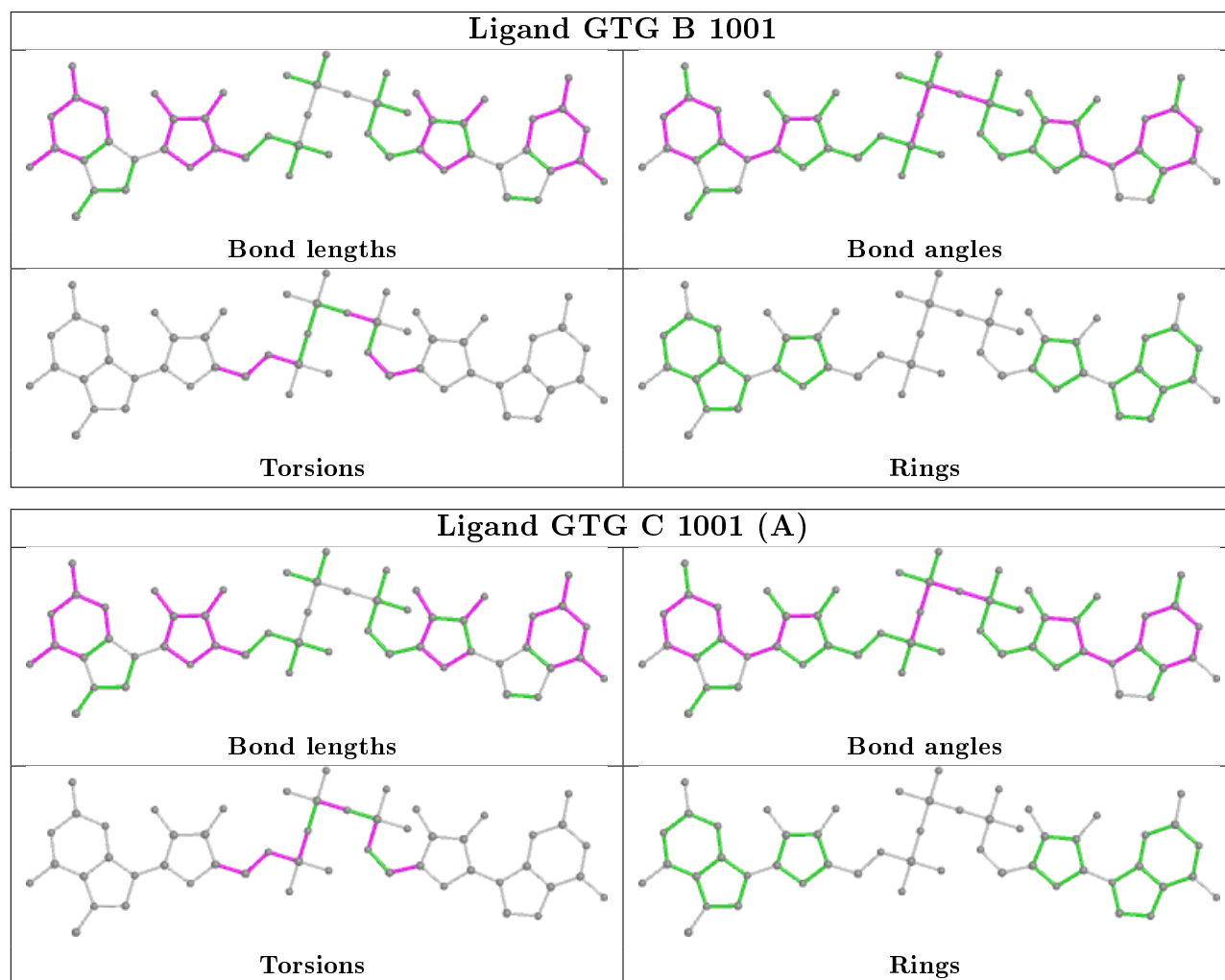
2 monomers are involved in 3 short contacts:

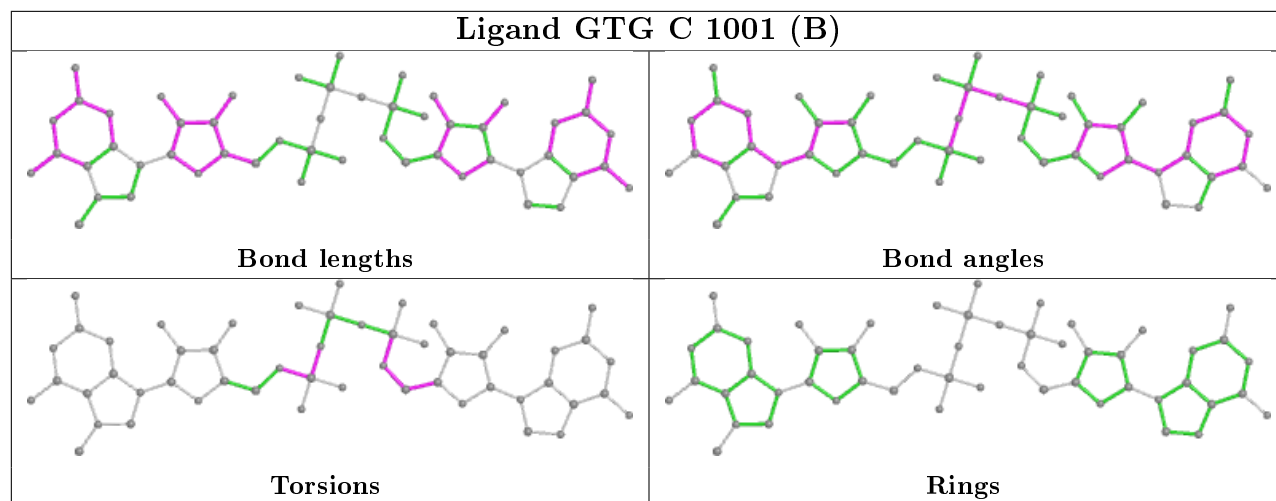
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001[A]	GTG	1	0
2	C	1001[B]	GTG	2	0

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, 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	144/162 (88%)	0.57	16 (11%) 5 9	41, 62, 94, 126	0
1	B	140/162 (86%)	0.58	12 (8%) 10 16	43, 67, 104, 122	0
1	C	149/162 (91%)	0.44	10 (6%) 17 25	42, 58, 88, 103	0
1	D	143/162 (88%)	0.76	17 (11%) 4 7	48, 74, 115, 129	0
All	All	576/648 (88%)	0.59	55 (9%) 8 13	41, 66, 104, 129	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	925	ALA	5.0
1	D	934	LEU	4.5
1	D	932	PRO	4.4
1	A	941	PHE	4.3
1	A	939	GLY	4.1
1	A	911	TYR	4.0
1	C	803	LEU	3.7
1	D	825	LYS	3.6
1	A	942	ARG	3.6
1	C	911	TYR	3.4
1	B	911	TYR	3.4
1	D	911	TYR	3.3
1	C	926	LYS	3.1
1	D	926	LYS	3.1
1	D	916	PHE	3.1
1	C	910	LEU	3.0
1	A	796	GLN	3.0
1	B	804	LYS	3.0
1	D	919	PHE	2.9
1	C	828	GLY	2.7
1	C	878	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	806	ASN	2.7
1	B	930	ILE	2.6
1	A	917	TRP	2.6
1	A	895	LYS	2.6
1	B	876	CYS	2.5
1	C	827	LEU	2.5
1	D	920	LEU	2.5
1	B	910	LEU	2.4
1	D	875	GLU	2.4
1	A	933	LYS	2.4
1	B	797	HIS	2.4
1	D	893	ILE	2.4
1	D	935	GLN	2.4
1	A	876	CYS	2.3
1	D	924	LYS	2.3
1	C	912	GLY	2.3
1	A	879	ARG	2.3
1	A	875	GLU	2.3
1	D	913	LEU	2.2
1	C	799	SER	2.2
1	B	818	ARG	2.2
1	B	819	ARG	2.2
1	B	872	TYR	2.2
1	A	940	LYS	2.1
1	B	843	SER	2.1
1	C	875	GLU	2.1
1	A	877	LEU	2.1
1	A	872	TYR	2.1
1	D	902	VAL	2.0
1	B	808	PHE	2.0
1	A	930	ILE	2.0
1	D	878	PHE	2.0
1	B	880	TYR	2.0
1	D	930	ILE	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands

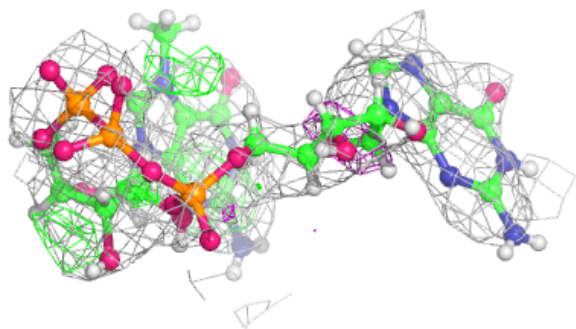
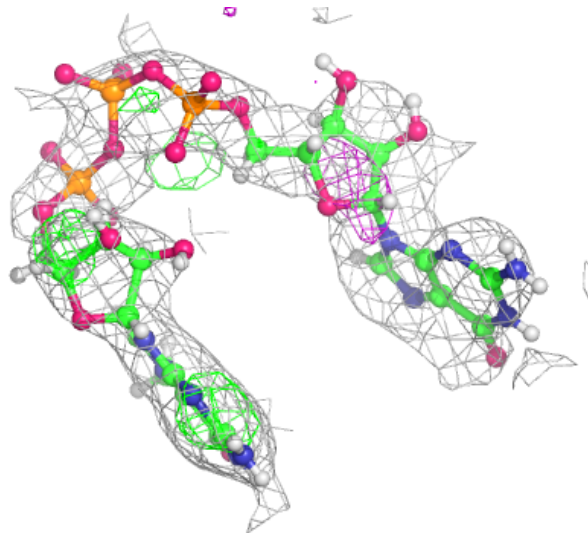
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GTG	C	1001[A]	52/52	0.65	0.41	58,77,97,98	79
2	GTG	C	1001[B]	52/52	0.65	0.41	64,81,97,100	79
2	GTG	B	1001	52/52	0.91	0.26	56,76,97,99	0
3	MG	A	1001	1/1	0.98	0.30	50,50,50,50	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.

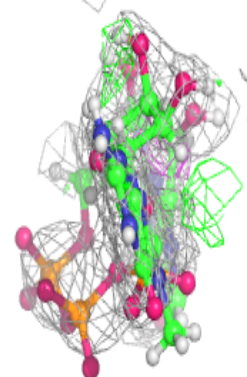
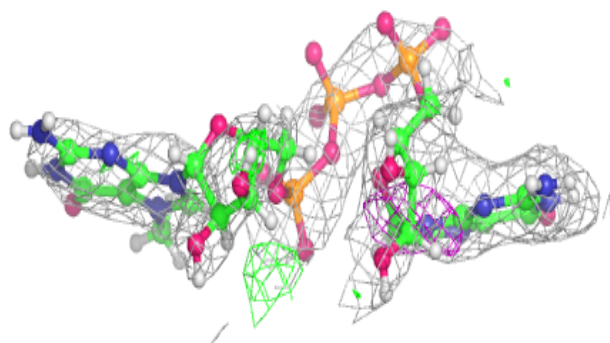
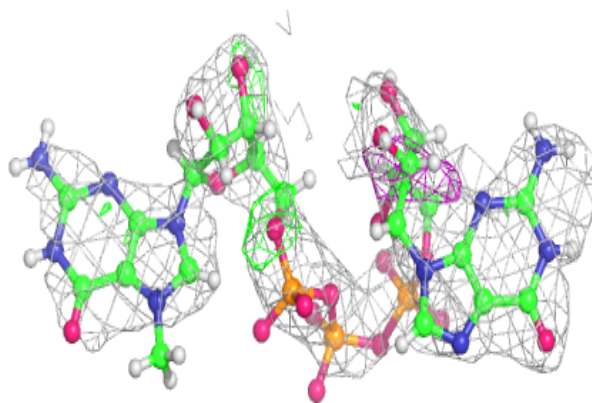
**Electron density around GTG C 1001 (A):**

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

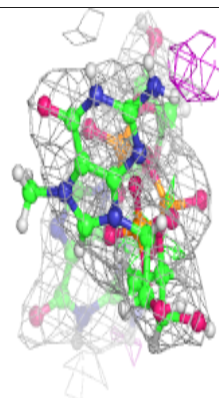
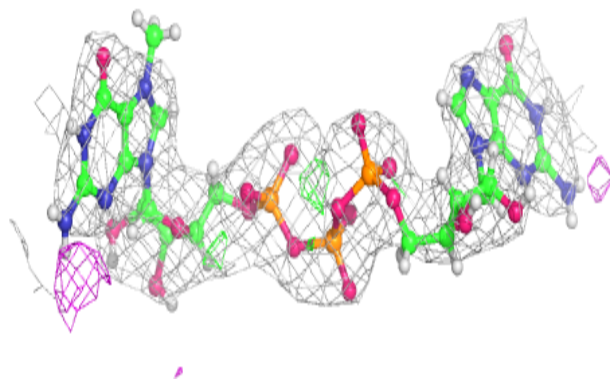
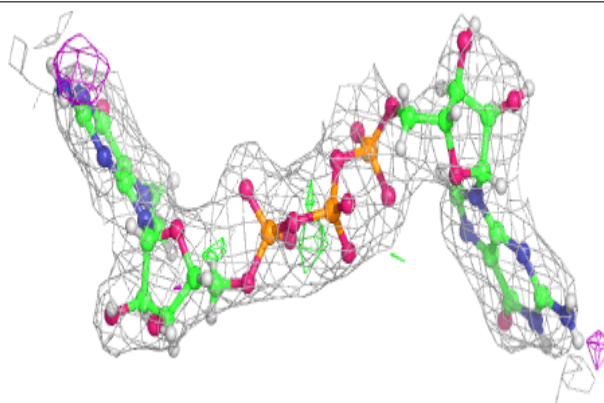


**Electron density around GTG C 1001 (B):**

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

**Electron density around GTG B 1001:**

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



## 6.5 Other polymers

There are no such residues in this entry.