

# wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2021 – 09:52 PM EDT

PDB ID : 1ST0

Title: Structure of DcpS bound to m7GpppG

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Deposited on : 2004-03-24

Resolution : 1.90 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.23.2buster-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)

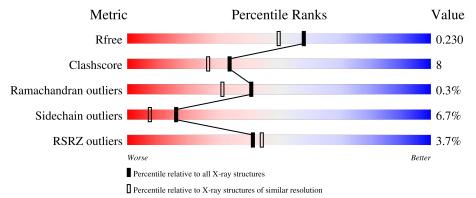
Validation Pipeline (wwPDB-VP) : 2.23.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.90 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\#\text{Entries, resolution range}(\text{\r{A}}))$		
$R_{free}$	130704	6207 (1.90-1.90)		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		
RSRZ outliers	127900	6082 (1.90-1.90)		

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 <=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	337	70%	15%	•	11%			
1	В	337	67%	18%		12%			



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5647 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.

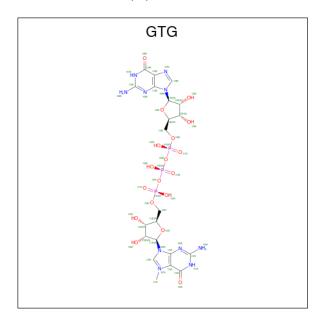
• Molecule 1 is a protein called mRNA decapping enzyme.

$\mathbf{Mol}$	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	R	297	Total C N O S		0	0	0			
1	Б	231	2439	1554	435	447	3		U	
1	Λ	300	Total	С	N	Ο	S	0	0	0
1	A	300	2458	1565	438	452	3	0	0	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ASN	HIS	engineered mutation	UNP Q96C86
В	277	ASN	HIS	engineered mutation	UNP Q96C86

• 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>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	В	1	Total	С	N	О	Р	0	0
		_	52	21	10	18	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	٨	1	Total	С	N	О	Р	0	0
2	2 A	1	52	21	10	18	3	U	0

• Molecule 3 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Y 3 3	0	0

• Molecule 4 is water.

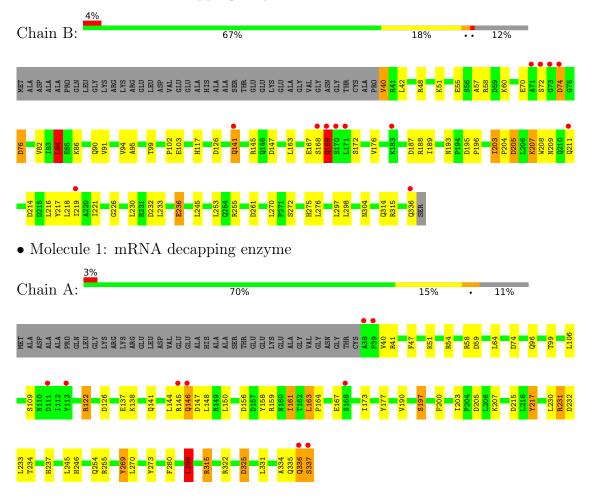
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	294	Total O 294 294	0	0
4	A	349	Total O 349 349	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: mRNA decapping enzyme





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	59.45Å 94.78Å 178.33Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 1.90	Depositor
rtesolution (A)	19.83 - 1.90	EDS
% Data completeness	99.1 (20.00-1.90)	Depositor
(in resolution range)	99.2 (19.83-1.90)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
P. P.	0.187 , 0.231	Depositor
$R, R_{free}$	0.187 , 0.230	DCC
$R_{free}$ test set	3991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 49.5	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: YT3, 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		nd lengths	Bond angles		
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	1.13	6/2515~(0.2%)	1.13	$12/3413 \ (0.4\%)$	
1	В	1.05	$2/2495 \ (0.1\%)$	1.07	$12/3386 \ (0.4\%)$	
All	All	1.09	8/5010 (0.2%)	1.10	$24/6799 \ (0.4\%)$	

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\text{\AA})$
1	A	190	VAL	CB-CG2	5.90	1.65	1.52
1	A	177	TYR	CD1-CE1	5.48	1.47	1.39
1	A	200	PHE	CE2-CZ	5.39	1.47	1.37
1	A	269	TYR	CE1-CZ	5.26	1.45	1.38
1	В	86	LYS	CE-NZ	5.21	1.62	1.49

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	231	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	A	231	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	В	261	ASP	CB-CG-OD2	8.23	125.70	118.30
1	В	84	LEU	CA-CB-CG	7.88	133.43	115.30
1	В	232	ASP	CB-CG-OD2	7.48	125.03	118.30

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2458	0	2445	44	0
1	В	2439	0	2428	46	0
2	A	52	0	26	1	0
2	В	52	0	26	3	0
3	A	3	0	0	0	1
4	A	349	0	0	12	0
4	В	294	0	0	12	0
All	All	5647	0	4925	84	1

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 8.

The worst 5 of 84 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:B:102:PRO:HA	4:B:942:HOH:O	1.26	1.33	
1:A:254:GLN:HG3	4:A:962:HOH:O	1.48	1.11	
1:B:205:ASP:HB2	1:B:219:ILE:CD1	1.84	1.06	
1:B:205:ASP:HB2	1:B:219:ILE:HD12	1.11	1.05	
1:B:91:VAL:HG23	4:A:829:HOH:O	1.62	0.97	

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-1 Atom-2		$egin{array}{c} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{array}{c} \begin{array}{c} \begin{array}{c$	
3:A:701:YT3:Y	3:A:702:YT3:Y[3_655]	2.07	0.13	

### 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	Perce	entiles
1	A	298/337 (88%)	285 (96%)	12 (4%)	1 (0%)	41	31
1	В	295/337~(88%)	284 (96%)	10 (3%)	1 (0%)	41	31
All	All	593/674 (88%)	569 (96%)	22 (4%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	169	GLN
1	A	145	ARG

#### 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	$269/295 \ (91\%)$	253 (94%)	16 (6%)	19 10		
1	В	$267/295 \ (90\%)$	247 (92%)	20 (8%)	13 5		
All	All	536/590 (91%)	500 (93%)	36 (7%)	16 7		

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LEU
1	A	337	SER
1	A	197	SER
1	A	270	LEU
1	В	217	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	249	GLN
1	A	336	GLN
1	A	314	GLN

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Mol	Chain	Res	Type
1	A	237	HIS

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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).

Mal Type Chain		Clasia.	Dec I	Res	Dag	Link	Во	ond leng	$\operatorname{ths}$	В	ond ang	gles
MIOI	$oxed{f Mol\ Type\ Ch}$	Chain	Lilik		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
2	GTG	A	651	-	46,57,57	1.89	9 (19%)	51,90,90	2.12	18 (35%)		
2	GTG	В	652	-	46,57,57	1.99	7 (15%)	51,90,90	2.07	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	A	651	-	-	9/24/64/64	0/6/6/6
2	GTG	В	652	-	-	9/24/64/64	0/6/6/6



The worst	5	of $1$	6	bond	length	outliers	are	listed	below.
THE WOLDS	$\cdot$	OII	v	DOM	10112011	Outilities	$\alpha r$	HOUCU	DOIOW.

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	В	652	GTG	C4A-N3A	7.13	1.46	1.35
2	В	652	GTG	C8B-N7B	6.93	1.47	1.34
2	В	652	GTG	C5E-C4E	-5.28	1.35	1.51
2	A	651	GTG	C4A-N3A	5.20	1.43	1.35
2	A	651	GTG	C5E-C4E	-4.88	1.36	1.51

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	651	GTG	N3B-C2B-N1B	-6.00	119.22	127.22
2	В	652	GTG	C6A-C5A-C4A	-5.98	115.09	120.80
2	В	652	GTG	N3A-C2A-N1A	-5.66	119.67	127.22
2	В	652	GTG	N3B-C2B-N1B	-4.51	121.20	127.22
2	A	651	GTG	C6A-N1A-C2A	4.41	122.94	115.93

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	652	GTG	C5E-O5E-PG-O3B
2	В	652	GTG	C5E-O5E-PG-O1G
2	В	652	GTG	C5E-O5E-PG-O2G
2	A	651	GTG	C5D-O5D-PA-O2A
2	A	651	GTG	C5E-O5E-PG-O1G

There are no ring outliers.

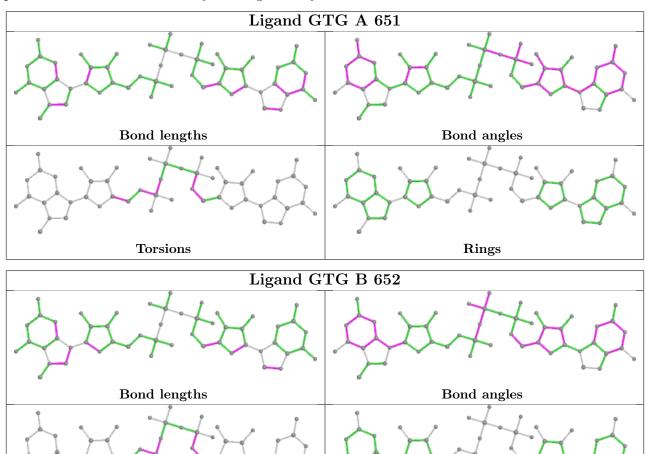
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	651	GTG	1	0
2	В	652	GTG	3	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 then 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.



Rings

### 5.7 Other polymers (i)

There are no such residues in this entry.

**Torsions** 

### 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	300/337 (89%)	-0.11	9 (3%) 50 53	17, 30, 55, 79	0
1	В	297/337 (88%)	0.11	13 (4%) 34 37	21, 37, 60, 76	0
All	All	597/674 (88%)	0.00	22 (3%) 41 44	17, 34, 57, 79	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	337	SER	7.8
1	A	38	ALA	6.5
1	A	336	GLN	4.7
1	В	71	ALA	4.4
1	В	73	GLY	4.4

### 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.

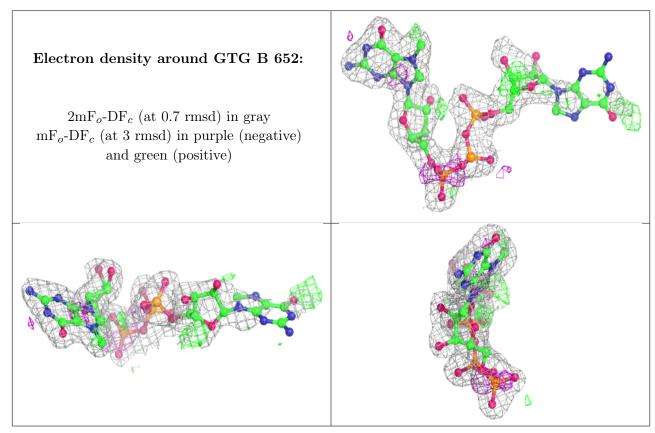
#### 6.4 Ligands (i)

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,  $95^{th}$  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.

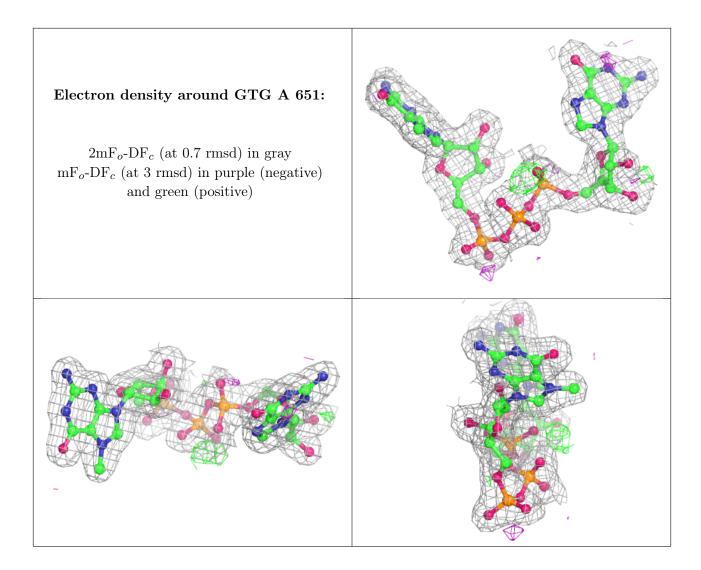


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GTG	В	652	52/52	0.93	0.17	35,52,89,90	11
2	GTG	A	651	52/52	0.98	0.07	17,25,39,41	0
3	YT3	A	701	1/1	0.98	0.09	55,55,55,55	0
3	YT3	A	702	1/1	0.98	0.13	94,94,94,94	0
3	YT3	A	703	1/1	0.98	0.20	66,66,66,66	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.

