



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2017 – 06:43 AM EDT

PDB ID : 3PML  
Title : crystal structure of a polymerase lambda variant with a dGTP analog opposite a templating T  
Authors : Bebenek, K.; Pedersen, L.C.; Kunkel, T.A.  
Deposited on : unknown  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

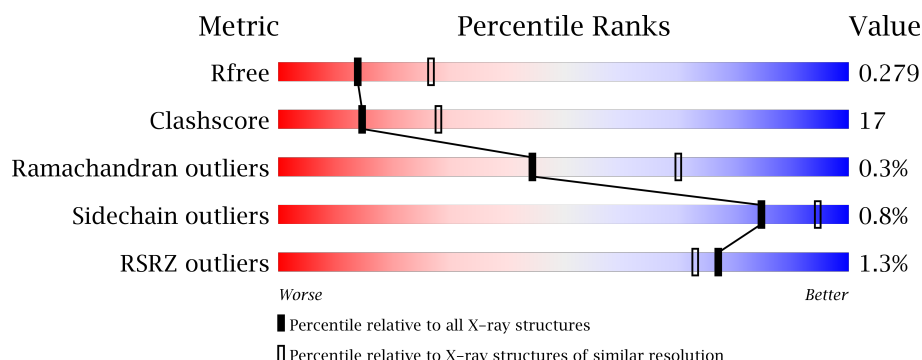
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	329	<div> <div>0.1%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>0.1%</div> </div> </div>
1	B	329	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div>1%</div> </div> </div>
2	C	11	<div> <div></div> <div> <div></div> <div>55%</div> <div>45%</div> </div> </div>
2	E	11	<div> <div></div> <div> <div></div> <div>27%</div> <div>73%</div> </div> </div>
3	D	4	<div> <div></div> <div> <div></div> <div>75%</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	4	 75%25%
4	F	6	 17%83%
4	H	6	 83%17%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6278 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 DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	2	0
			2528	1590	461	465	12			
1	B	324	Total	C	N	O	S	0	5	0
			2561	1611	467	471	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	LYS	SER	SEE REMARK 999	UNP Q9UGP5
A	464	GLY	GLN	SEE REMARK 999	UNP Q9UGP5
A	?	-	GLU	SEE REMARK 999	UNP Q9UGP5
A	?	-	GLU	SEE REMARK 999	UNP Q9UGP5
A	?	-	ASN	SEE REMARK 999	UNP Q9UGP5
A	?	-	GLY	SEE REMARK 999	UNP Q9UGP5
A	?	-	GLN	SEE REMARK 999	UNP Q9UGP5
A	470	GLU	GLN	SEE REMARK 999	UNP Q9UGP5
A	471	THR	GLN	SEE REMARK 999	UNP Q9UGP5
B	463	LYS	SER	SEE REMARK 999	UNP Q9UGP5
B	464	GLY	GLN	SEE REMARK 999	UNP Q9UGP5
B	?	-	GLU	SEE REMARK 999	UNP Q9UGP5
B	?	-	GLU	SEE REMARK 999	UNP Q9UGP5
B	?	-	ASN	SEE REMARK 999	UNP Q9UGP5
B	?	-	GLY	SEE REMARK 999	UNP Q9UGP5
B	?	-	GLN	SEE REMARK 999	UNP Q9UGP5
B	470	GLU	GLN	SEE REMARK 999	UNP Q9UGP5
B	471	THR	GLN	SEE REMARK 999	UNP Q9UGP5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			223	107	40	66	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	6	0
			325	156	57	97	15			

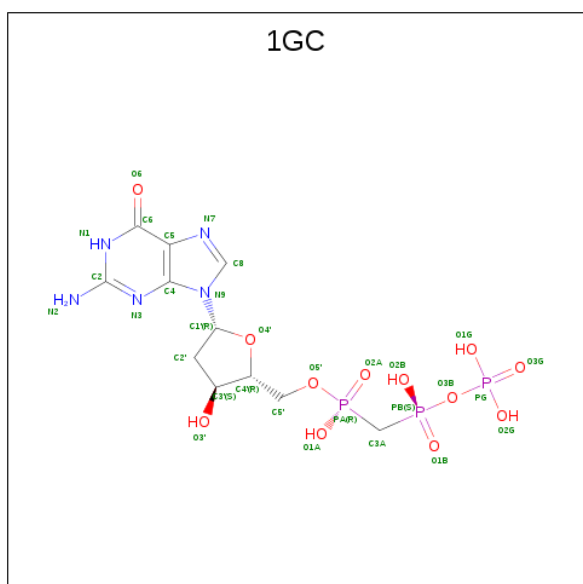
- Molecule 3 is a DNA chain called 5'-D(P\*GP\*CP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
3	G	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 4 is a DNA chain called 5'-D(\*CP\*AP\*GP\*TP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
4	H	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			

- Molecule 5 is 2'-deoxy-5'-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]guanosine (three-letter code: 1GC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Na	0	0
			2	2		
7	A	1	Total	Na	0	0
			1	1		

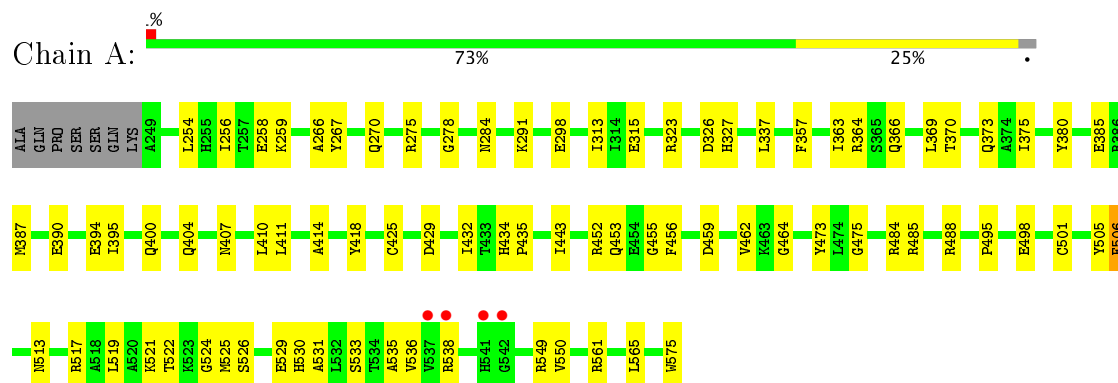
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	86	Total	O	0	0
			86	86		
8	B	57	Total	O	0	0
			57	57		
8	C	10	Total	O	0	0
			10	10		
8	E	2	Total	O	0	0
			2	2		
8	F	2	Total	O	0	0
			2	2		
8	H	11	Total	O	0	0
			11	11		

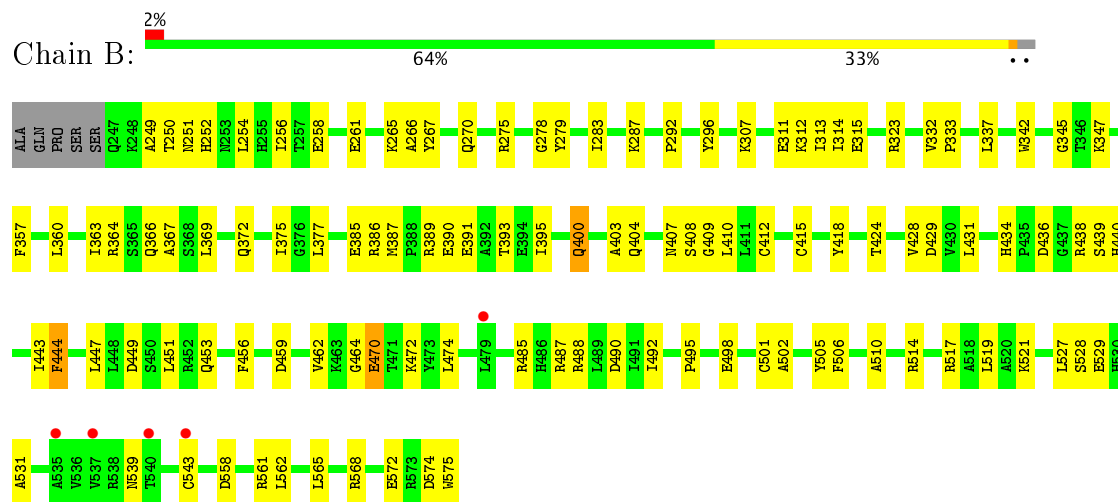
### 3 Residue-property plots

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: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda

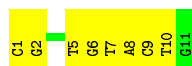


- Molecule 2: 5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*AP\*CP\*TP\*G)-3'

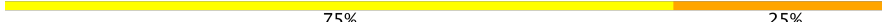


- Molecule 2: 5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*AP\*CP\*TP\*G)-3'

Chain E:  27% 73%



- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain D:  75% 25%



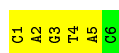
- Molecule 3: 5'-D(P\*GP\*CP\*CP\*G)-3'

Chain G:  75% 25%




- Molecule 4: 5'-D(\*CP\*AP\*GP\*TP\*AP\*C)-3'

Chain F:  17% 83%



- Molecule 4: 5'-D(\*CP\*AP\*GP\*TP\*AP\*C)-3'

Chain H:  83% 17%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.04Å 191.57Å 59.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.02 – 2.60 48.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (25.02-2.60) 95.6 (48.80-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.271 0.244 , 0.279	Depositor DCC
$R_{free}$ test set	1611 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 33.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.39% 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: NA, MG, 1GC

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	0.42	0/2580	0.61	0/3483
1	B	0.38	0/2614	0.59	0/3529
2	C	0.44	0/249	0.76	0/383
2	E	0.40	0/363	0.66	0/559
3	D	0.99	1/92 (1.1%)	0.89	0/138
3	G	1.03	1/92 (1.1%)	0.93	0/138
4	F	0.42	0/133	0.69	0/203
4	H	0.48	0/133	0.76	0/203
All	All	0.43	2/6256 (0.0%)	0.63	0/8636

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	DG	OP3-P	-7.30	1.52	1.61
3	D	1	DG	OP3-P	-7.11	1.52	1.61

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	2528	0	2512	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2561	0	2525	113	0
2	C	223	0	126	7	0
2	E	325	0	173	22	0
3	D	83	0	45	5	0
3	G	83	0	45	4	0
4	F	119	0	69	9	0
4	H	119	0	69	1	0
5	A	31	0	14	2	0
5	B	31	0	14	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	A	86	0	0	1	0
8	B	57	0	0	2	0
8	C	10	0	0	1	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
8	H	11	0	0	0	0
All	All	6278	0	5592	200	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 17.

The worst 5 of 200 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:519:LEU:CD2	1:B:565:LEU:HD11	1.54	1.37
1:B:519:LEU:HD23	1:B:565:LEU:HD11	1.21	1.09
1:B:519:LEU:CD2	1:B:565:LEU:CD1	2.42	0.97
5:B:702:1GC:HN1	2:E:5[B]:DT:H3	1.15	0.90
1:A:488:ARG:HH11	1:A:488:ARG:HG3	1.40	0.87

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	322/329 (98%)	301 (94%)	21 (6%)	0	100	100
1	B	327/329 (99%)	301 (92%)	24 (7%)	2 (1%)	28	53
All	All	649/658 (99%)	602 (93%)	45 (7%)	2 (0%)	44	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	249	ALA
1	B	408	SER

### 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	265/275 (96%)	264 (100%)	1 (0%)	93	98
1	B	266/275 (97%)	261 (98%)	5 (2%)	62	84
All	All	531/550 (96%)	525 (99%)	6 (1%)	85	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	400[B]	GLN
1	B	470[B]	GLU
1	B	444	PHE
1	B	400[A]	GLN

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Mol	Chain	Res	Type
1	B	470[A]	GLU

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

Mol	Chain	Res	Type
1	B	270	GLN
1	B	453	GLN
1	B	350	GLN
1	A	350	GLN
1	B	379	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 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	$\# Z  > 2$
5	1GC	A	701	6	27,33,33	2.07	7 (25%)	31,52,52	2.29	9 (29%)
5	1GC	B	702	6	27,33,33	2.30	6 (22%)	31,52,52	2.32	9 (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
5	1GC	A	701	6	-	0/15/34/34	0/3/3/3
5	1GC	B	702	6	-	0/15/34/34	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	1GC	PB-O3B	-7.48	1.49	1.58
5	A	701	1GC	PB-O3B	-6.60	1.50	1.58
5	B	702	1GC	PG-O3B	-6.05	1.50	1.60
5	A	701	1GC	PG-O3B	-4.94	1.52	1.60
5	B	702	1GC	PB-O2B	-3.00	1.49	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	1GC	C5-C6-N1	-8.39	111.54	123.48
5	A	701	1GC	C5-C6-N1	-8.28	111.69	123.48
5	B	702	1GC	PG-O3B-PB	-3.30	120.74	132.38
5	A	701	1GC	C2-N3-C4	-2.84	111.84	115.16
5	A	701	1GC	N3-C2-N1	-2.62	123.63	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	1GC	2	0
5	B	702	1GC	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	322/329 (97%)	-0.34	4 (1%) 79 75	28, 46, 75, 113	0
1	B	324/329 (98%)	-0.18	5 (1%) 74 69	29, 57, 85, 111	0
2	C	11/11 (100%)	-0.56	0 100 100	39, 52, 58, 59	0
2	E	11/11 (100%)	0.12	0 100 100	36, 54, 88, 90	0
3	D	4/4 (100%)	-0.74	0 100 100	35, 38, 47, 49	0
3	G	4/4 (100%)	-0.60	0 100 100	46, 52, 53, 53	0
4	F	6/6 (100%)	-0.51	0 100 100	47, 52, 77, 91	0
4	H	6/6 (100%)	-0.81	0 100 100	32, 38, 45, 57	0
All	All	688/700 (98%)	-0.27	9 (1%) 77 73	28, 50, 84, 113	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	ARG	3.9
1	B	540	THR	3.5
1	B	535	ALA	3.5
1	A	537	VAL	3.3
1	A	541	HIS	3.0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NA	A	5	1/1	0.89	0.15	1.20	35,35,35,35	0
5	1GC	A	701	31/31	0.98	0.13	-0.29	30,38,44,48	0
5	1GC	B	702	31/31	0.96	0.13	-0.47	55,59,64,65	0
7	NA	B	6	1/1	0.94	0.08	-1.65	73,73,73,73	0
7	NA	B	7	1/1	0.90	0.08	-2.84	48,48,48,48	0
6	MG	A	2	1/1	0.95	0.04	-	27,27,27,27	0
6	MG	B	3	1/1	0.97	0.06	-	52,52,52,52	0
6	MG	A	1	1/1	0.98	0.09	-	30,30,30,30	0
6	MG	B	4	1/1	0.94	0.10	-	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.