



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

PDB ID : 3F2C  
Title : DNA Polymerase PolC from *Geobacillus kaustophilus* complex with DNA, dGTP and Mn  
Authors : Davies, D.R.; Evans, R.J.; Bullard, J.M.; Christensen, J.; Green, L.S.; Guiles, J.W.; Ribble, W.K.; Janjic, N.; Jarvis, T.C.  
Deposited on : 2008-10-29  
Resolution : 2.50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

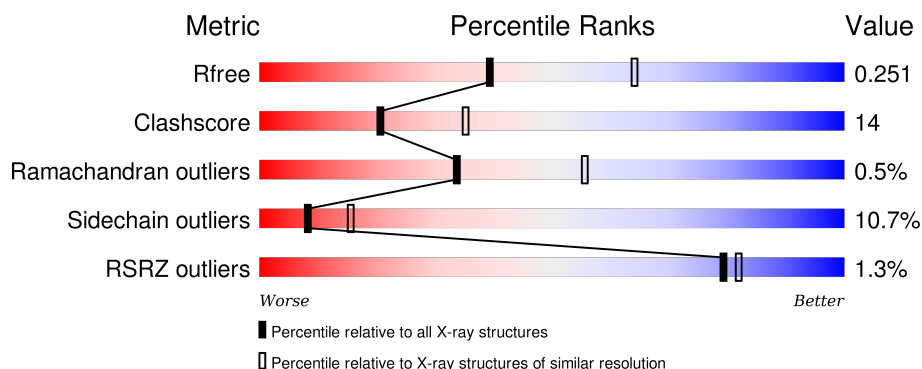
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	1041	<div> <div>68%</div> <div>23%</div> <div>5%</div> </div>
2	P	17	<div> <div>6%</div> <div>24%</div> <div>41%</div> <div>12%</div> <div>24%</div> </div>
3	T	22	<div> <div>45%</div> <div>14%</div> <div>23%</div> <div>18%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8622 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 GEOBACILLUS KAUSTOPHILUS DNA POLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	993	Total	C	N	O	S	0	0	0
			7796	4961	1318	1481	36			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	EXPRESSION TAG	UNP Q5L0J3
A	425	GLY	-	LINKER	UNP Q5L0J3
A	426	SER	-	LINKER	UNP Q5L0J3
A	427	GLY	-	LINKER	UNP Q5L0J3
A	428	SER	-	LINKER	UNP Q5L0J3
A	429	GLY	-	LINKER	UNP Q5L0J3
A	1445	SER	-	EXPRESSION TAG	UNP Q5L0J3
A	1446	GLY	-	EXPRESSION TAG	UNP Q5L0J3
A	1447	GLY	-	EXPRESSION TAG	UNP Q5L0J3
A	1448	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1449	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1450	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1451	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1452	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1453	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1454	HIS	-	EXPRESSION TAG	UNP Q5L0J3
A	1455	HIS	-	EXPRESSION TAG	UNP Q5L0J3

- Molecule 2 is a DNA chain called 5'-D(\*DCP\*DAP\*DGP\*DTP\*DGP\*DAP\*DGP\*DAP\*D CP\*DGP\*DGP\*DGP\*DCP\*DAP\*DAP\*DCP\*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			269	126	57	73	13			

- Molecule 3 is a DNA chain called 5'-D(\*DAP\*DTP\*DAP\*DAP\*DCP\*DGP\*DGP\*DTP\*D

TP\*DGP\*DCP\*DCP\*DCP\*DGP\*DTP\*DCP\*DTP\*DCP\*DAP\*DCP\*DTP\*DG)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	18	Total	C	N	O	P	0	0	0
			362	174	63	108	17			

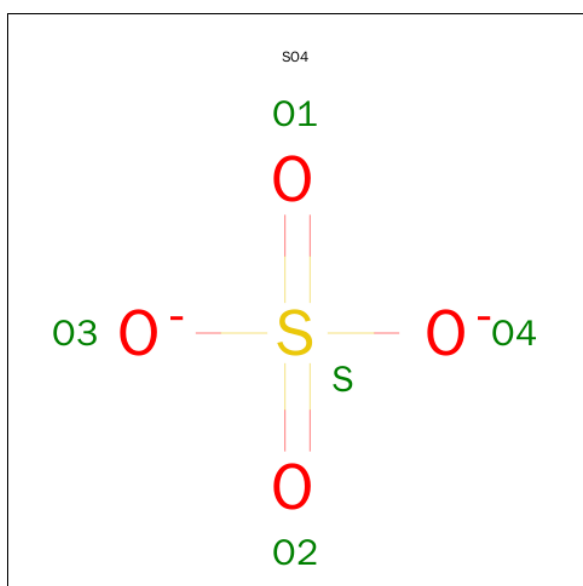
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mn	0	0
			3	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

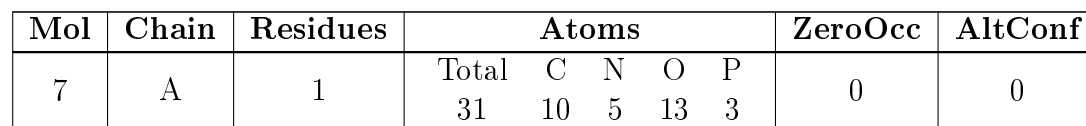
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

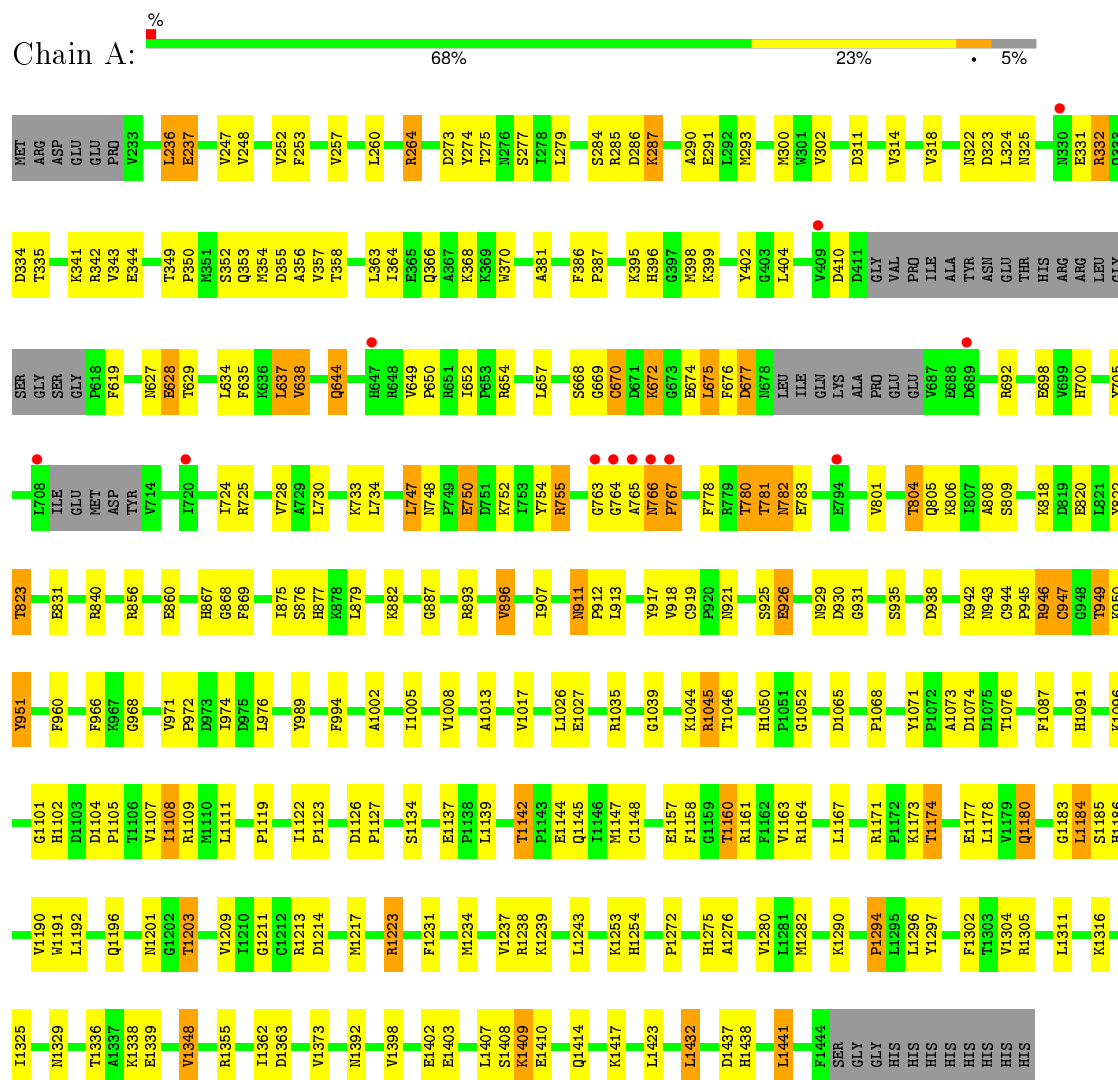


- | Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 8   | A     | 142      | Total O<br>142 142 | 0       | 0       |
| 8   | P     | 7        | Total O<br>7 7     | 0       | 0       |
| 8   | T     | 6        | Total O<br>6 6     | 0       | 0       |

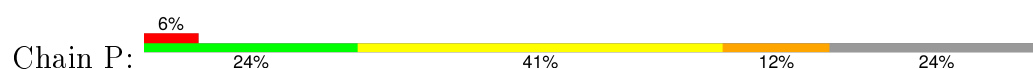
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: GEOBACILLUS KAUSTOPHILUS DNA POLC



#### • Molecule 2: 5'-D(\*DCP\*DAP\*DGP\*DTP\*DGP\*DAP\*DGP\*DAP\*DCP\*DGP\*DGP\*DGP\*D CP\*DAP\*DAP\*DCP\*DC)-3'





- Molecule 3: 5'-D(\*DAP\*DTP\*DAP\*DAP\*DCP\*DGP\*DGP\*DTP\*DTP\*DGP\*DCP\*DCP\*DCP\*DGP\*DTP\*DCP\*DTP\*DCP\*DAP\*DCP\*DTP\*DG)-3'

Chain T: 45% 14% 23% 18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.89Å 141.19Å 184.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.60 – 2.50 43.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.60-2.50) 98.9 (43.60-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.210 , 0.255 0.209 , 0.251	Depositor DCC
$R_{free}$ test set	2641 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51789 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MN, SO4, DGT

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	0.52	4/7960 (0.1%)	0.66	3/10776 (0.0%)
2	P	1.10	2/303 (0.7%)	1.84	7/465 (1.5%)
3	T	1.32	2/404 (0.5%)	2.25	20/621 (3.2%)
All	All	0.61	8/8667 (0.1%)	0.89	30/11862 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	8	DT	C4'-O4'	-17.10	1.27	1.45
1	A	725	ARG	CZ-NH1	9.41	1.45	1.33
1	A	725	ARG	CZ-NH2	9.02	1.44	1.33
1	A	725	ARG	CD-NE	8.91	1.61	1.46
1	A	725	ARG	NE-CZ	8.89	1.44	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	8	DT	O4'-C1'-N1	29.39	128.57	108.00
2	P	16	DC	O4'-C1'-N1	18.40	120.88	108.00
3	T	8	DT	N1-C1'-C2'	-12.45	88.94	112.60
3	T	8	DT	O4'-C4'-C3'	11.65	112.99	106.00
3	T	17	DT	O4'-C1'-N1	10.03	115.02	108.00

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	7796	0	7707	223	0
2	P	269	0	142	6	0
3	T	362	0	205	8	0
4	A	3	0	0	0	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	31	0	12	8	0
8	A	142	0	0	12	0
8	P	7	0	0	0	0
8	T	6	0	0	1	0
All	All	8622	0	8066	239	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 14.

The worst 5 of 239 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:A:947:CYS:SG	1:A:949:THR:OG1	2.05	1.15
1:A:877:HIS:CA	1:A:907:ILE:HD11	1.79	1.12
1:A:966:PHE:HE2	1:A:1217:MET:HE2	1.19	1.06
1:A:1217:MET:CE	1:A:1231:PHE:HB2	1.86	1.06
1:A:342:ARG:HB2	1:A:781:THR:HB	1.34	1.05

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	985/1041 (95%)	933 (95%)	47 (5%)	5 (0%)	34 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	PRO
1	A	670	CYS
1	A	1052	GLY
1	A	677	ASP
1	A	945	PRO

### 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	850/904 (94%)	759 (89%)	91 (11%)	8 15

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	823	THR
1	A	935	SER
1	A	1392	ASN
1	A	831	GLU
1	A	918	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	911	ASN
1	A	924	HIS
1	A	1254	HIS
1	A	805	GLN
1	A	1329	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
7	DGT	A	1456	4	25,33,33	1.15	2 (8%)	35,52,52	2.43	11 (31%)
6	SO4	A	5	-	4,4,4	0.19	0	6,6,6	0.12	0

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
7	DGT	A	1456	4	-	0/18/34/34	0/3/3/3
6	SO4	A	5	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1456	DGT	C5-C4	2.70	1.46	1.40
7	A	1456	DGT	C6-C5	3.55	1.48	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1456	DGT	C2'-C1'-N9	-6.23	99.02	114.16
7	A	1456	DGT	C5-C6-N1	-3.98	118.15	123.59
7	A	1456	DGT	N3-C2-N1	-3.92	121.47	127.44
7	A	1456	DGT	C6-C5-C4	-3.76	116.41	120.90
7	A	1456	DGT	C4-C5-N7	-3.62	106.14	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1456	DGT	8	0

## 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 [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<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	993/1041 (95%)	-0.08	12 (1%) 81 83	25, 38, 52, 73	0
2	P	13/17 (76%)	0.29	1 (7%) 16 18	25, 39, 73, 78	0
3	T	18/22 (81%)	-0.04	0 100 100	26, 41, 60, 60	0
All	All	1024/1080 (94%)	-0.08	13 (1%) 79 82	25, 38, 53, 78	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	PRO	5.7
1	A	765	ALA	3.7
1	A	708	LEU	3.5
1	A	647	HIS	3.4
1	A	330	ASN	3.4

### 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 carbohydrates 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. 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( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	5	5/5	0.88	0.17	-0.07	100,100,100,100	0
5	ZN	A	4	1/1	0.97	0.08	-1.72	67,67,67,67	0
7	DGT	A	1456	31/31	0.99	0.06	-4.20	20,23,25,26	0
4	MN	A	3	1/1	0.99	0.04	-6.37	61,61,61,61	0
4	MN	A	2	1/1	0.95	0.06	-	105,105,105,105	0
4	MN	A	1	1/1	0.99	0.02	-	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.