



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:54 PM GMT

PDB ID : 4DU4  
Title : RB69 DNA Polymerase Ternary Complex with dATP Opposite dT with 3-Deaza-adenine at the N-3 Position of Primer Strand  
Authors : Xia, S.; Wang, J.; Konigsberg, W.H.  
Deposited on : 2012-02-21  
Resolution : 2.28 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

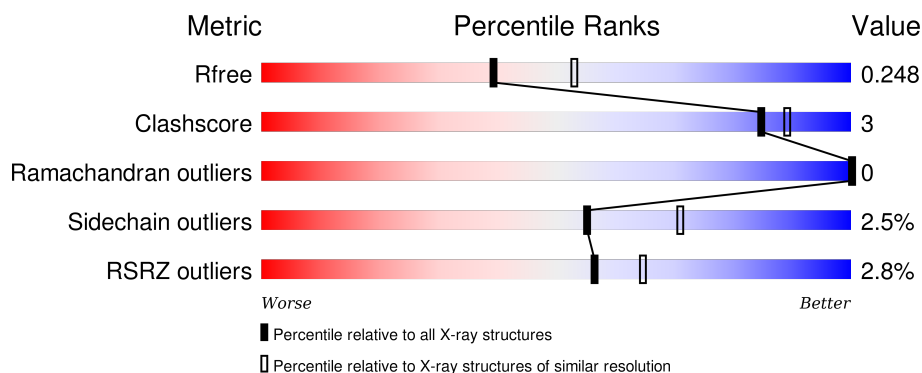
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	903	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>
2	T	17	<div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
3	P	13	<div> <div>8%</div> <div>69%</div> <div>23%</div> <div>8%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8212 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	1	0
			7371	4733	1228	1377	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087

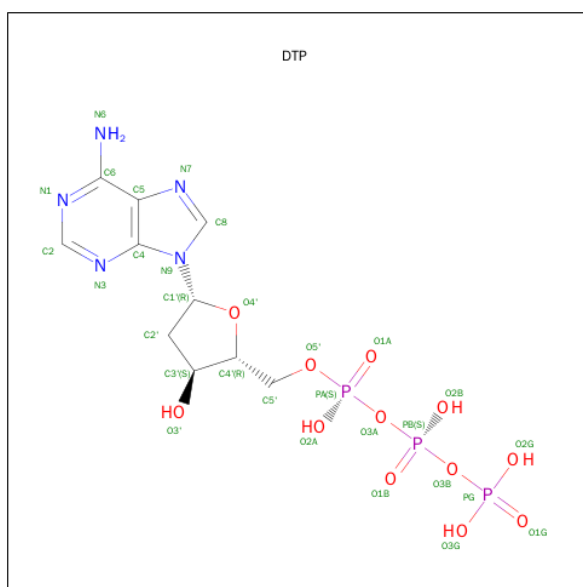
- Molecule 2 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	17	Total	C	N	O	P	0	0	0
			349	165	63	104	17			

- Molecule 3 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			263	127	50	74	12			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	Ca	0	0
			7	7		

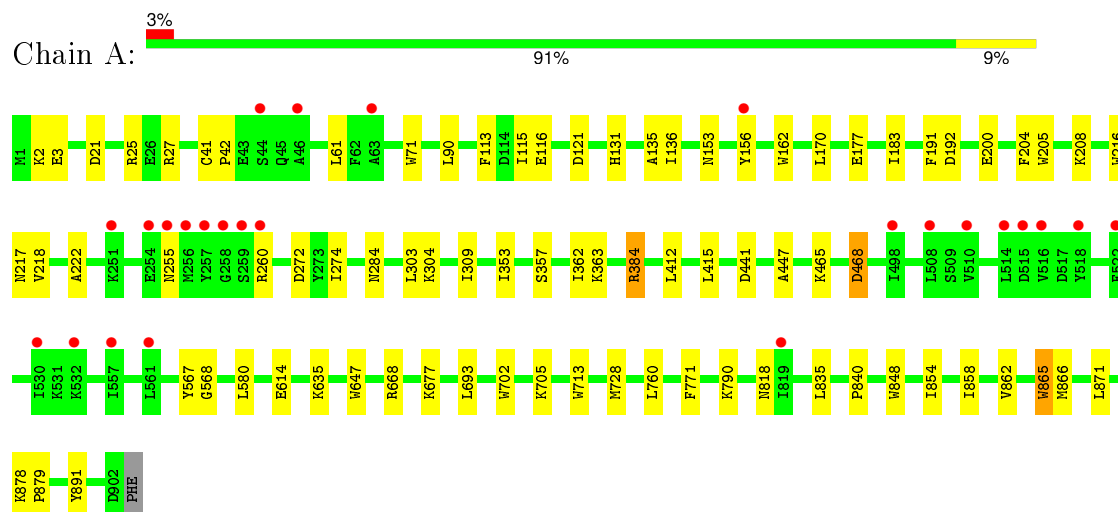
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	172	Total	O	0	5
			177	177		
6	T	10	Total	O	0	0
			10	10		
6	P	5	Total	O	0	0
			5	5		

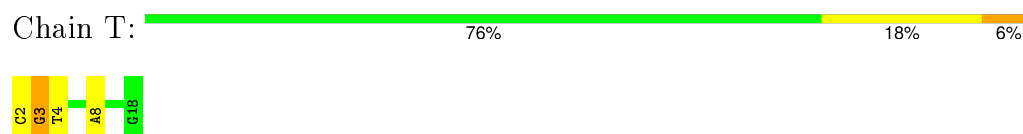
### 3 Residue-property plots [i](#)

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

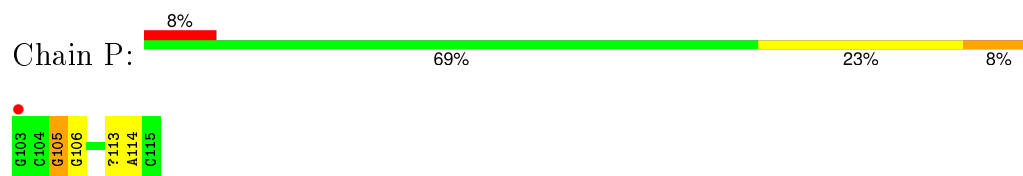
#### • Molecule 1: DNA polymerase



#### • Molecule 2: DNA template



#### • Molecule 3: DNA primer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.14Å 119.50Å 130.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.28 46.20 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.20-2.28) 98.2 (46.20-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.249 0.192 , 0.248	Depositor DCC
$R_{free}$ test set	2859 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 55288 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, CA, DTP, 4DU

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	0.46	7/7554 (0.1%)	0.55	0/10207
2	T	0.33	0/390	0.89	2/600 (0.3%)
3	P	0.31	0/250	0.81	1/382 (0.3%)
All	All	0.46	7/8194 (0.1%)	0.58	3/11189 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	TRP	CD2-CE2	5.44	1.47	1.41
1	A	205	TRP	CD2-CE2	5.20	1.47	1.41
1	A	713	TRP	CD2-CE2	5.18	1.47	1.41
1	A	162	TRP	CD2-CE2	5.13	1.47	1.41
1	A	702	TRP	CD2-CE2	5.07	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2	DC	P-O3'-C3'	6.49	127.48	119.70
2	T	3	DG	O3'-P-O5'	6.23	115.83	104.00
3	P	105	DG	P-O3'-C3'	5.30	126.06	119.70

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	7371	0	7271	42	0
2	T	349	0	192	5	0
3	P	263	0	148	6	0
4	A	30	0	12	0	0
5	A	7	0	0	0	0
6	A	177	0	0	3	0
6	P	5	0	0	0	0
6	T	10	0	0	0	0
All	All	8212	0	7623	46	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 3.

The worst 5 of 46 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)
3:P:105:DG:H2'	3:P:106:DG:C8	2.16	0.80
1:A:771:PHE:HZ	1:A:871:LEU:HD22	1.47	0.79
1:A:170:LEU:HA	1:A:177:GLU:HG3	1.75	0.68
1:A:362:ILE:HD12	2:T:4:DT:OP2	1.94	0.68
1:A:284:ASN:ND2	3:P:113:4DU:OP1	2.21	0.67

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	901/903 (100%)	874 (97%)	27 (3%)	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	800/800 (100%)	779 (97%)	21 (3%)	54 69

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	ARG
1	A	567	TYR
1	A	693	LEU
1	A	309	ILE
1	A	790	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	354	GLN
1	A	679	HIS
1	A	333	GLN
1	A	546	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
3	4DU	P	113	3	16,23,24	1.05	2 (12%)	20,33,36	2.84	4 (20%)
3	DOC	P	115	3,2	11,19,20	0.75	0	14,26,29	1.05	1 (7%)

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
3	4DU	P	113	3	-	0/3/21/22	0/3/3/3
3	DOC	P	115	3,2	-	0/3/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	113	4DU	C3-C4	-2.90	1.34	1.41
3	P	113	4DU	C3-C2	-2.25	1.33	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	113	4DU	C2-C3-C4	-9.52	110.74	119.64
3	P	113	4DU	C3-C4-N9	-4.13	127.36	131.94
3	P	115	DOC	C2-N3-C4	3.10	119.98	115.61
3	P	113	4DU	C3-C4-C5	3.24	126.78	121.39
3	P	113	4DU	C3-C2-N1	6.04	129.25	123.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	113	4DU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\# Z  > 2$
4	DTP	A	1001	5	24,32,32	1.01	1 (4%)	32,50,50	2.01	7 (21%)

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
4	DTP	A	1001	5	-	0/18/34/34	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	DTP	C5-C4	3.27	1.47	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	DTP	N3-C2-N1	-8.43	122.44	128.89
4	A	1001	DTP	C2'-C1'-N9	-3.77	104.98	114.16
4	A	1001	DTP	C4-C5-N7	-2.67	107.03	109.48
4	A	1001	DTP	C1'-N9-C4	-2.13	123.55	127.16
4	A	1001	DTP	O4'-C1'-N9	2.13	111.40	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	902/903 (99%)	0.08	25 (2%) 56 65	41, 58, 91, 190	1 (0%)
2	T	17/17 (100%)	-0.08	0 100 100	47, 60, 91, 103	0
3	P	11/13 (84%)	0.70	1 (9%) 11 16	51, 86, 112, 119	0
All	All	930/933 (99%)	0.09	26 (2%) 56 65	41, 58, 93, 190	1 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	MET	15.5
1	A	257	TYR	11.1
1	A	258	GLY	8.1
1	A	44	SER	6.4
1	A	255	ASN	4.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
3	DOC	P	115	18/19	0.98	0.19	-	46,49,54,57	0
3	4DU	P	113	21/22	0.98	0.20	-	47,53,62,64	0

### 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(Å <sup>2</sup> )	Q<0.9
4	DTP	A	1001	30/30	0.98	0.22	1.31	43,46,50,53	0
5	CA	A	1002	1/1	0.98	0.17	-0.20	47,47,47,47	0
5	CA	A	1004	1/1	0.86	0.05	-1.91	93,93,93,93	0
5	CA	A	1006	1/1	0.78	0.11	-	88,88,88,88	0
5	CA	A	1007	1/1	0.51	0.10	-	132,132,132,132	0
5	CA	A	1005	1/1	0.94	0.24	-	86,86,86,86	0
5	CA	A	1003	1/1	0.94	0.23	-	60,60,60,60	0
5	CA	A	1008	1/1	0.83	0.06	-	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.