



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2016 – 12:45 PM EDT

PDB ID : 4Z6C  
Title : Structure of human DNA polymerase beta 279NA mutant complexed with G in the template base paired with incoming non-hydrolyzable CTP  
Authors : Koag, M.-C.; Lee, S.  
Deposited on : 2015-04-04  
Resolution : 2.68 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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) : rb-20027107

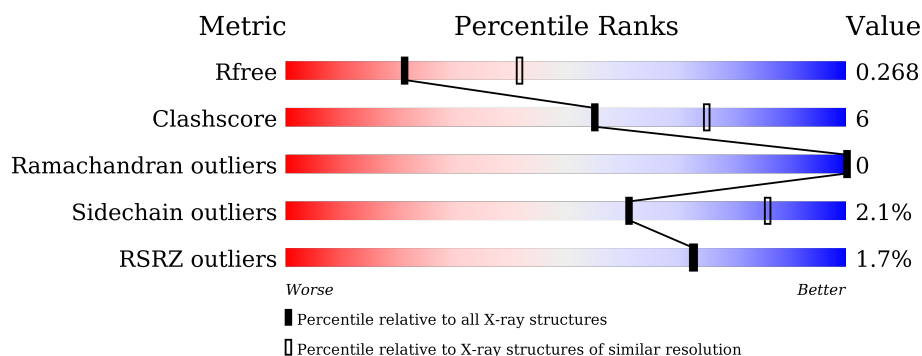
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	T	16	<div> <div></div> <div>69%31%</div> </div>
2	P	10	<div> <div></div> <div>70%30%</div> </div>
3	D	5	<div> <div>20%</div> <div>20%80%</div> </div>
4	A	335	<div> <div>%</div> <div>84%12%..</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
6	NA	P	102	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3305 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 DNA chain called DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*TP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	16	Total	C	N	O	P	0	0	0
			321	153	60	93	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	0	0
			204	97	40	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	P	0	0	0
			106	49	20	32	5			

- Molecule 4 is a protein called DNA polymerase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	325	Total	C	N	O	S	0	0	0
			2593	1639	453	492	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	ASN	engineered mutation	UNP P06746

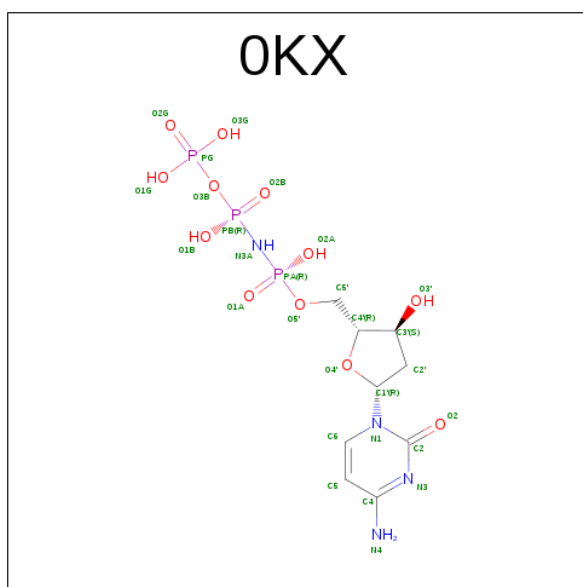
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	1	Total Na 1 1	0	0
6	D	1	Total Na 1 1	0	0

- Molecule 7 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]cytidine (three-letter code: 0KX) (formula: C<sub>9</sub>H<sub>17</sub>N<sub>4</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O P 28 9 4 12 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	T	7	Total O 7 7	0	0
8	P	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	O	0	0
			2	2		
8	A	37	Total	O	0	0
			37	37		



- Molecule 1: DNA (5'-D(\*CP\*CP\*GP\*AP\*CP\*GP\*TP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3')



- |    |    |    |    |    |    |     |
|----|----|----|----|----|----|-----|
| G1 | C2 | T3 | G4 | A5 | T6 | A10 |
|----|----|----|----|----|----|-----|

- |    |    |    |    |    |
|----|----|----|----|----|
| G1 | T2 | C3 | G4 | G5 |
|----|----|----|----|----|

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- Figure 1: Schematic representation of the 1200 amino acid residues of the protein. The protein is represented as a horizontal bar divided into segments. The segments are labeled with three-letter codes: MET, SER, LYS, ARG, LYS, ALA, PRO, GLU, GLU, T10, V45, Y49, H51, D91, S94, F99, R102, K120, T121, L122, D123, D124, L125, K126, K127, H135, E147, E153, E154, Q157, C178, F200, E203, S204, T205, K206, Q207, P208, L228, K244, N245, ASP. The segments are color-coded: MET (grey), SER (light blue), LYS (light blue), ARG (light blue), LYS (light blue), ALA (light blue), PRO (light blue), GLU (light blue), GLU (light blue), T10 (light blue), V45 (light blue), Y49 (light blue), H51 (light blue), D91 (light blue), S94 (light blue), F99 (light blue), R102 (light blue), K120 (light blue), T121 (light blue), L122 (light blue), D123 (light blue), D124 (light blue), L125 (light blue), K126 (light blue), K127 (light blue), H135 (light blue), E147 (light blue), E153 (light blue), E154 (light blue), Q157 (light blue), C178 (light blue), F200 (light blue), E203 (light blue), S204 (light blue), T205 (light blue), K206 (light blue), Q207 (light blue), P208 (light blue), L228 (light blue), K244 (light blue), N245 (light blue), ASP (light blue). The segments are connected by lines, and the entire bar is enclosed in a box.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.18 Å   79.27 Å   54.37 Å 90.00°   105.96°   90.00°	Depositor
Resolution (Å)	20.00 – 2.68 20.00 – 2.68	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-2.68) 96.5 (20.00-2.68)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.67 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.201 , 0.272 0.200 , 0.268	Depositor DCC
$R_{free}$ test set	517 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.7	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 11098 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% 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: NA, 0KX, MG

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	T	0.49	0/359	0.90	0/551
2	P	0.54	0/229	1.01	0/352
3	D	1.10	1/118 (0.8%)	1.09	0/179
4	A	0.27	0/2641	0.43	0/3549
All	All	0.38	1/3347 (0.0%)	0.60	0/4631

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	DG	OP3-P	-10.51	1.48	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	T	321	0	180	4	0
2	P	204	0	111	2	0
3	D	106	0	57	3	0
4	A	2593	0	2600	28	0
5	A	1	0	0	0	0
5	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
6	P	1	0	0	0	0
7	A	28	0	16	0	0
8	A	37	0	0	0	0
8	D	2	0	0	0	0
8	P	3	0	0	0	0
8	T	7	0	0	0	0
All	All	3305	0	2964	35	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 6.

All (35) 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)
4:A:277:ILE:HG13	4:A:335:GLU:OXT	1.78	0.83
4:A:330:PRO:HA	4:A:333:ARG:HD2	1.72	0.71
4:A:123:GLU:HG2	4:A:127:LYS:HE3	1.76	0.66
4:A:277:ILE:CG1	4:A:335:GLU:OXT	2.46	0.64
4:A:304:THR:HG23	4:A:304:THR:O	1.99	0.61
3:D:3:DC:H2''	3:D:4:DG:OP2	2.00	0.60
4:A:123:GLU:CG	4:A:127:LYS:HE3	2.37	0.54
4:A:178:CYS:HB2	4:A:272:PHE:CD2	2.43	0.54
4:A:328:ARG:NH2	4:A:332:ASP:O	2.40	0.53
4:A:304:THR:CG2	4:A:306:VAL:H	2.22	0.52
4:A:290:GLY:O	4:A:301:LEU:N	2.37	0.52
4:A:49:TYR:CE2	4:A:51:HIS:HB2	2.45	0.51
1:T:14:DA:H2''	1:T:15:DG:H5''	1.93	0.51
2:P:5:DA:H2''	2:P:6:DT:H5'	1.92	0.50
4:A:135:HIS:CD2	4:A:228:LEU:HD22	2.47	0.49
1:T:14:DA:N1	2:P:3:DT:C5	2.81	0.49
4:A:102:ARG:NH2	4:A:147:GLU:OE1	2.45	0.49
3:D:4:DG:H2''	3:D:5:DG:H2'	1.95	0.48
4:A:121:THR:OG1	4:A:124:ASP:N	2.37	0.48
4:A:304:THR:HG22	4:A:306:VAL:H	1.77	0.48
4:A:251:PRO:HG2	4:A:253:ARG:CZ	2.45	0.47
4:A:153:GLU:O	4:A:157:GLN:NE2	2.38	0.46
4:A:120:LYS:HE2	4:A:120:LYS:HB3	1.72	0.45
1:T:6:DG:OP2	4:A:280:LYS:NZ	2.36	0.44
4:A:200:PHE:CZ	4:A:261:PRO:HG3	2.52	0.44
4:A:203:GLU:O	4:A:204:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:DG:H2''	3:D:5:DG:C2'	2.49	0.43
4:A:91:ASP:HB3	4:A:94:SER:HB2	2.00	0.43
1:T:2:DC:H2''	1:T:3:DG:C8	2.53	0.43
4:A:122:LEU:O	4:A:126:ARG:HG3	2.18	0.42
4:A:289:LYS:HB2	4:A:291:PHE:HD2	1.86	0.41
4:A:99:PHE:HZ	4:A:122:LEU:HD13	1.85	0.41
4:A:122:LEU:HD12	4:A:122:LEU:HA	1.85	0.40
4:A:154:GLU:HA	4:A:157:GLN:NE2	2.37	0.40
4:A:277:ILE:H	4:A:277:ILE:HG12	1.63	0.40

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	
4	A	321/335 (96%)	309 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
4	A	282/294 (96%)	276 (98%)	6 (2%)	61	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	45	VAL
4	A	244	LYS
4	A	245	ASN
4	A	272	PHE
4	A	277	ILE
4	A	304	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 5 ligands modelled in this entry, 4 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	$\# Z  > 2$
7	0KX	A	402	5	25,29,29	2.00	7 (28%)	28,45,45	2.25	5 (17%)

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	0KX	A	402	5	-	0/14/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	402	0KX	PB-O3B	-3.90	1.54	1.59
7	A	402	0KX	PG-O3G	2.63	1.63	1.54
7	A	402	0KX	PB-O1B	2.71	1.64	1.56
7	A	402	0KX	PB-O2B	3.61	1.50	1.46
7	A	402	0KX	C4-N3	3.68	1.42	1.35
7	A	402	0KX	C6-N1	3.72	1.40	1.35
7	A	402	0KX	PA-O1A	3.82	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	0KX	C2'-C3'-C4'	-2.84	97.00	102.77
7	A	402	0KX	PG-O3B-PB	-2.72	122.83	132.71
7	A	402	0KX	O2A-PA-O5'	-2.44	99.42	106.72
7	A	402	0KX	O2A-PA-O1A	3.97	117.83	110.02
7	A	402	0KX	C6-C5-C4	9.28	121.07	117.44

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 [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	T	16/16 (100%)	-0.14	0 <span>100</span> <span>100</span>	25, 38, 60, 68	0
2	P	10/10 (100%)	-0.12	0 <span>100</span> <span>100</span>	27, 36, 40, 43	0
3	D	5/5 (100%)	1.01	1 (20%) <span>1</span> <span>1</span>	26, 31, 65, 85	0
4	A	325/335 (97%)	-0.14	5 (1%) <span>76</span> <span>75</span>	19, 31, 56, 83	2 (0%)
All	All	356/366 (97%)	-0.12	6 (1%) <span>73</span> <span>72</span>	19, 31, 58, 85	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	5	DG	5.3
4	A	245	ASN	3.2
4	A	244	LYS	3.1
4	A	10	THR	3.0
4	A	206	LYS	2.9
4	A	208	PRO	2.1

### 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(Å <sup>2</sup> )	Q<0.9
6	NA	P	102	1/1	0.82	0.19	2.13	25,25,25,25	0
7	0KX	A	402	28/28	0.97	0.10	-1.06	21,24,26,28	0
6	NA	D	101	1/1	0.83	0.09	-2.68	30,30,30,30	0
5	MG	P	101	1/1	0.82	0.10	-3.87	26,26,26,26	0
5	MG	A	401	1/1	0.98	0.12	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.