



# Full wwPDB X-ray Structure Validation Report

Jun 24, 2014 – 05:24 PM EDT

PDB ID : 4MFF  
Title : Structure of human DNA polymerase beta complexed with O6MG in the template base paired with incoming non-hydrolyzable TTP  
Authors : Koag, M.C.; Min, K.; Monzingo, A.F.; Lee, S.  
Deposited on : 2013-08-27  
Resolution : 2.55 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

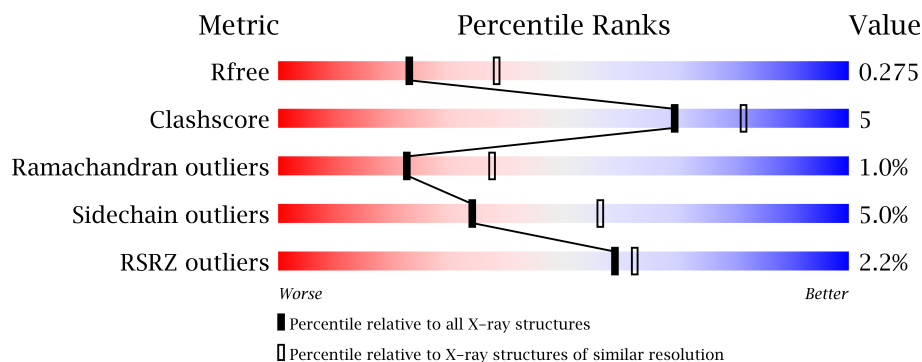
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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))
$R_{free}$	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	325	
2	T	16	
3	P	10	
4	D	5	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3276 atoms, of which 0 are hydrogen and 0 are deuterium.

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 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2559	1621	448	481	9			

- Molecule 2 is a DNA chain called template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	16	Total	C	N	O	P	0	0	0
			322	154	60	93	15			

- Molecule 3 is a DNA chain called up primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			205	98	40	58	9			

- Molecule 4 is a DNA chain called dn primer.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

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

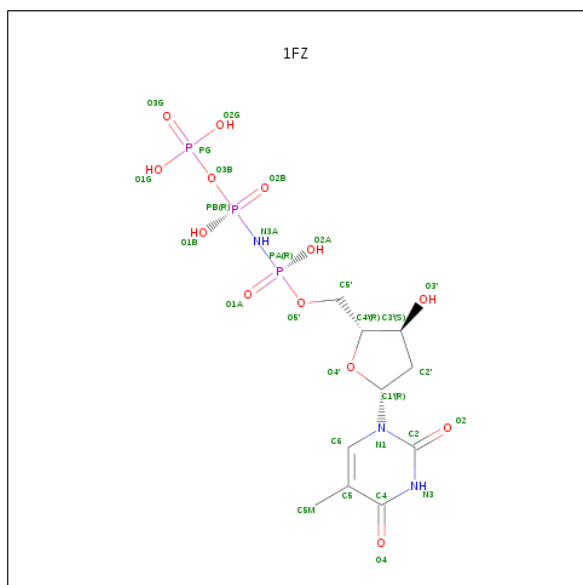
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

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

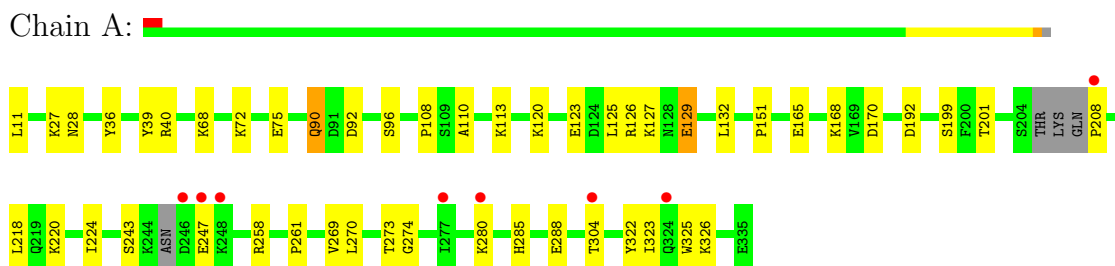
- Molecule 7 is 5'-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]AMINO}PHOSPHORYL]THYMIDINE (three-letter code: 1FZ) (formula:  $C_{10}H_{18}N_3O_{13}P_3$ ).



### 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: DNA polymerase beta



- Molecule 2: template



- Molecule 3: up primer



- Molecule 4: dn primer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.55Å 78.84Å 54.75Å 90.00° 105.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 19.09 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.55) 95.5 (19.09-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.222 , 0.294 0.210 , 0.275	Depositor DCC
$R_{free}$ test set	695 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 5.3	EDS
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 14368 reflections (0.014%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, 6OG, 1FZ

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	0.63	0/2606	0.77	1/3499 (0.0%)
2	T	0.48	0/333	1.11	2/508 (0.4%)
3	P	0.48	0/230	0.95	0/354
4	D	1.00	1/118 (0.8%)	0.86	0/179
All	All	0.62	1/3287 (0.0%)	0.83	3/4540 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	DG	OP3-P	-9.00	1.50	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	12	DT	O5'-P-OP1	-6.47	99.88	105.70
1	A	170	ASP	CB-CG-OD1	5.52	123.27	118.30
2	T	14	DA	P-O3'-C3'	5.42	126.20	119.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	0	2572	27	0
2	T	322	0	182	1	0
3	P	205	0	114	1	0
4	D	106	0	57	1	0
5	A	2	0	0	0	1
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	29	0	14	1	0
8	A	40	0	0	10	1
8	D	1	0	0	0	0
8	P	5	0	0	1	0
8	T	5	0	0	0	0
All	All	3276	0	2939	29	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (29) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:LYS:HD2	8:A:504:HOH:O	1.28	1.32
1:A:199:SER:HA	8:A:513:HOH:O	1.62	1.00
1:A:192:ASP:HB2	8:A:538:HOH:O	1.61	0.99
1:A:208:PRO:HA	8:A:506:HOH:O	1.72	0.89
2:T:15:DG:H2''	2:T:16:DC:OP2	1.82	0.79
1:A:110:ALA:HB2	8:P:105:HOH:O	1.85	0.75
1:A:165:GLU:HA	8:A:524:HOH:O	1.85	0.74
1:A:92:ASP:OD2	1:A:120:LYS:HE2	1.89	0.73
1:A:123:GLU:HG3	1:A:126:ARG:NH2	2.13	0.64
1:A:285:HIS:HD2	1:A:323:ILE:HD12	1.66	0.59
1:A:90:GLN:O	1:A:90:GLN:HG2	2.02	0.58
1:A:168:LYS:CB	8:A:524:HOH:O	2.52	0.57
1:A:168:LYS:HB3	8:A:524:HOH:O	2.04	0.57
1:A:36:TYR:CE1	1:A:40:ARG:HD2	2.43	0.53
1:A:168:LYS:CE	8:A:524:HOH:O	2.57	0.52
1:A:192:ASP:OD1	1:A:258:ARG:NH2	2.33	0.52
1:A:125:LEU:HD22	1:A:132:LEU:HD11	1.93	0.50
1:A:168:LYS:HE3	8:A:524:HOH:O	2.12	0.49
1:A:218:LEU:HB2	1:A:224:ILE:HD12	1.95	0.49
1:A:68:LYS:HB2	4:D:1:DG:H3'	1.96	0.48
1:A:274:GLY:HA3	7:A:404:1FZ:H8	1.96	0.46
3:P:9:DG:C6	3:P:10:DA:C6	3.04	0.45
1:A:75:GLU:HA	8:A:535:HOH:O	2.17	0.44
1:A:39:TYR:OH	1:A:72:LYS:HE3	2.16	0.43

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:GLN:HE21	1:A:90:GLN:C	2.21	0.43
1:A:285:HIS:O	1:A:288:GLU:HG2	2.19	0.43
1:A:28:ASN:HA	1:A:108:PRO:HB3	2.02	0.42
1:A:269:VAL:O	1:A:273:THR:OG1	2.27	0.42
1:A:201:THR:C	1:A:261:PRO:HB3	2.42	0.40

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-2	Distance(Å)	Clash(Å)
5:A:402:MG:MG	8:A:510:HOH:O[1.655]	1.68	0.52

## 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	315/325 (97%)	292 (93%)	20 (6%)	3 (1%)	22 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	TYR
1	A	247	GLU
1	A	129	GLU

### 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	278/286 (97%)	264 (95%)	14 (5%)	34 56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	90	GLN
1	A	96	SER
1	A	113	LYS
1	A	127	LYS
1	A	129	GLU
1	A	151	PRO
1	A	220	LYS
1	A	243	SER
1	A	270	LEU
1	A	280	LYS
1	A	304	THR
1	A	325	TRP
1	A	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
2	6OG	T	6	2	23,25,26	1.66	3 (13%)	33,36,39	2.72	10 (30%)

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	6OG	T	6	2	-	2/8/23/24	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	6	6OG	P-OP1	5.31	1.52	1.46
2	T	6	6OG	C5-C4	3.25	1.47	1.40
2	T	6	6OG	C4-N9	-2.85	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	6	6OG	C5-C4-N3	-6.31	118.80	126.07
2	T	6	6OG	C-O6-C6	6.19	123.84	117.27
2	T	6	6OG	C5-C6-N1	-5.70	116.40	123.82
2	T	6	6OG	N3-C4-N9	5.13	134.44	126.91
2	T	6	6OG	O6-C6-C5	4.95	123.82	116.14
2	T	6	6OG	C2-N1-C6	4.61	122.48	116.05
2	T	6	6OG	C2-N3-C4	4.18	120.31	115.30
2	T	6	6OG	C4-C5-N7	-3.33	106.19	109.41
2	T	6	6OG	N3-C2-N1	-2.57	123.78	127.55
2	T	6	6OG	C2'-C3'-C4'	2.42	108.10	102.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	6	6OG	C-O6-C6-C5
2	T	6	6OG	C-O6-C6-N1

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	1FZ	A	404	5	30,30,30	2.86	11 (36%)	39,47,47	2.64	6 (15%)

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	1FZ	A	404	5	-	0/16/34/34	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	404	1FZ	PA-N3A	9.74	1.72	1.64
7	A	404	1FZ	C6-N1	5.53	1.43	1.34
7	A	404	1FZ	C5M-C5	-5.41	1.40	1.51
7	A	404	1FZ	C4-N3	4.45	1.43	1.36
7	A	404	1FZ	PA-O1A	4.21	1.51	1.46
7	A	404	1FZ	O4'-C1'	3.03	1.49	1.42
7	A	404	1FZ	PA-O2A	2.78	1.64	1.56
7	A	404	1FZ	PB-N3A	2.27	1.66	1.64
7	A	404	1FZ	PB-O1B	2.25	1.63	1.56
7	A	404	1FZ	C2-N3	2.09	1.43	1.36
7	A	404	1FZ	PG-O2G	2.08	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	404	1FZ	PA-N3A-PB	-11.07	112.82	130.03
7	A	404	1FZ	C6-N1-C2	-8.96	119.86	122.41
7	A	404	1FZ	O1A-PA-N3A	3.96	117.81	111.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	404	1FZ	PG-O3B-PB	-3.81	118.96	132.05
7	A	404	1FZ	N3-C2-N1	3.14	118.59	115.97
7	A	404	1FZ	O4'-C1'-N1	2.30	111.79	107.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	321/325 (98%)	0.01	8 (2%) 54 58	7, 17, 46, 57	0
2	T	16/16 (100%)	-0.26	0 100 100	10, 20, 30, 32	0
3	P	10/10 (100%)	-0.31	0 100 100	12, 17, 26, 26	0
4	D	5/5 (100%)	-0.51	0 100 100	10, 11, 16, 20	0
All	All	352/356 (98%)	-0.02	8 (2%) 59 61	7, 17, 45, 57	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	3.5
1	A	304	THR	2.7
1	A	246	ASP	2.5
1	A	247	GLU	2.4
1	A	280	LYS	2.3
1	A	248	LYS	2.1
1	A	324	GLN	2.1
1	A	277	ILE	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	6OG	T	6	23/24	0.14	-0.13	22,30,33,33	0

### 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	1FZ	A	404	29/29	0.15	0.21	24,31,36,37	0
6	NA	D	101	1/1	0.14	-0.18	16,16,16,16	0
5	MG	A	402	1/1	0.09	-1.82	34,34,34,34	0
5	MG	A	401	1/1	0.05	-1.99	15,15,15,15	0
6	NA	A	403	1/1	0.07	-2.31	12,12,12,12	0

### 6.5 Other polymers

There are no such residues in this entry.