



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 06:58 am BST

PDB ID : 2RBA  
Title : Structure of Human Thymine DNA Glycosylase Bound to Abasic and Undamaged DNA  
Authors : Maiti, A.; Pozharski, E.; Drohat, A.C.  
Deposited on : 2007-09-18  
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

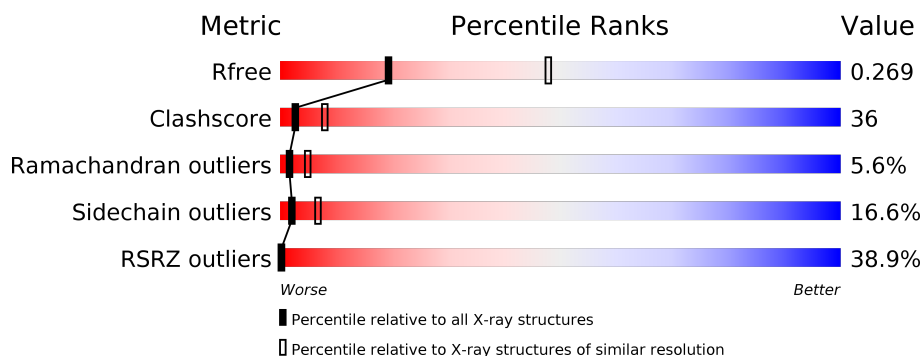
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. 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	C	23	<div> <div>39%</div> <div> <div>13%</div> <div>39%</div> <div>48%</div> </div> </div>
2	D	23	<div> <div>39%</div> <div> <div>17%</div> <div>78%</div> </div> </div>
3	A	204	<div> <div>32%</div> <div> <div>33%</div> <div>41%</div> <div>14%</div> <div>11%</div> </div> </div>
3	B	204	<div> <div>37%</div> <div> <div>43%</div> <div>38%</div> <div>7%</div> <div>11%</div> </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
2	3DR	D	11	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3845 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(\*DCP\*DAP\*DGP\*DCP\*DTP\*DCP\*DTP\*DCP\*DTP\*DAP\*DCP\*DGP\*DTP\*DGP\*DAP\*DGP\*DCP\*DAP\*DGP\*DTP\*DGP\*DGP\*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			473	225	90	136	22			

- Molecule 2 is a DNA chain called DNA (5'-D(\*DCP\*DCP\*DAP\*DCP\*DTP\*DGP\*DCP\*DTP\*DCP\*DAP\*(3DR)P\*DGP\*DTP\*DAP\*DCP\*DAP\*DGP\*DAP\*DGP\*DCP\*DTP\*DG P\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	23	Total	C	N	O	P	0	0	0
			456	218	81	135	22			

- Molecule 3 is a protein called G/T mismatch-specific thymine DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	182	Total	C	N	O	S	0	0	0
			1458	939	252	258	9			
3	B	182	Total	C	N	O	S	0	0	0
			1458	939	252	258	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	EXPRESSION TAG	UNP Q13569
A	106	SER	-	EXPRESSION TAG	UNP Q13569
A	107	HIS	-	EXPRESSION TAG	UNP Q13569
A	108	MET	-	EXPRESSION TAG	UNP Q13569
A	109	ALA	-	EXPRESSION TAG	UNP Q13569
A	110	SER	-	EXPRESSION TAG	UNP Q13569
B	105	GLY	-	EXPRESSION TAG	UNP Q13569
B	106	SER	-	EXPRESSION TAG	UNP Q13569

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Chain	Residue	Modelled	Actual	Comment	Reference
B	107	HIS	-	EXPRESSION TAG	UNP Q13569
B	108	MET	-	EXPRESSION TAG	UNP Q13569
B	109	ALA	-	EXPRESSION TAG	UNP Q13569
B	110	SER	-	EXPRESSION TAG	UNP Q13569

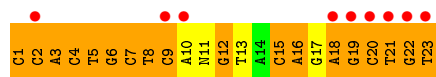
### 3 Residue-property plots

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.

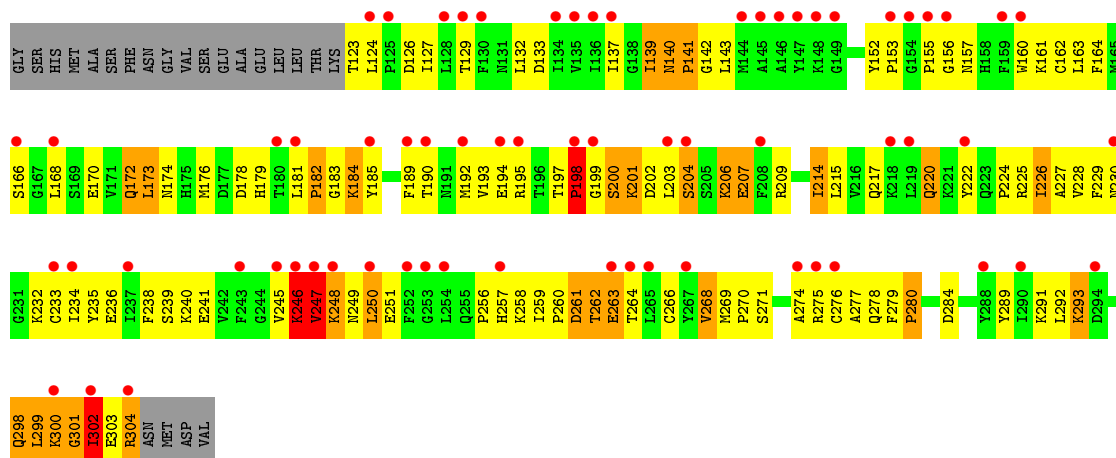
- Molecule 1: DNA (5'-D(\*DCP\*DAP\*DGP\*DCP\*DTP\*DCP\*DTP\*DGP\*DTP\*DAP\*DCP\*DCP\*DTP\*DGP\*DAP\*DGP\*DCP\*DAP\*DGP\*DTP\*DGP\*DGP\*DA)-3')



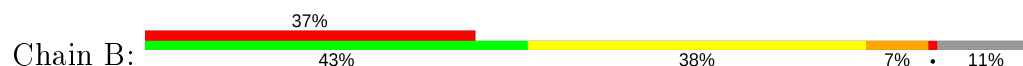
- Molecule 2: DNA (5'-D(\*DCP\*DCP\*DAP\*DCP\*DTP\*DGP\*DCP\*DTP\*DCP\*DAP\*(3DR)P\*DGP\*DTP\*DAP\*DCP\*DAP\*DGP\*DAP\*DGP\*DCP\*DTP\*DGP\*DT)-3')

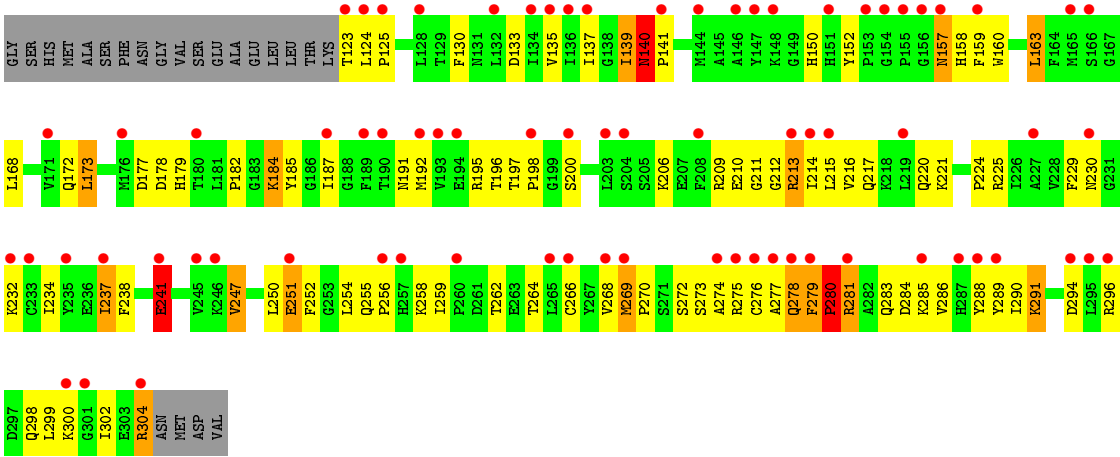


- Molecule 3: G/T mismatch-specific thymine DNA glycosylase



- Molecule 3: G/T mismatch-specific thymine DNA glycosylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.13 Å   162.13 Å   56.14 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.79 35.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.79) 97.6 (35.10-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, $R_{free}$	0.230 , 0.276 0.225 , 0.269	Depositor DCC
$R_{free}$ test set	1048 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 178.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	C	1.10	0/531	1.98	23/819 (2.8%)
2	D	1.15	0/497	2.29	42/762 (5.5%)
3	A	1.18	6/1495 (0.4%)	1.21	8/2015 (0.4%)
3	B	0.91	1/1495 (0.1%)	0.93	0/2015
All	All	1.07	7/4018 (0.2%)	1.46	73/5611 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	1	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	LYS	CD-CE	12.25	1.81	1.51
3	A	268	VAL	CA-CB	-7.35	1.39	1.54
3	B	266	CYS	CB-SG	-6.82	1.70	1.82
3	A	247	VAL	C-O	6.78	1.36	1.23
3	A	266	CYS	CB-SG	-6.59	1.71	1.82

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	DG	O4'-C4'-C3'	-12.97	98.22	106.00
1	C	17	DC	O4'-C1'-N1	12.81	116.97	108.00
2	D	7	DC	O4'-C1'-N1	10.12	115.08	108.00
1	C	15	DA	O4'-C1'-N9	-8.76	101.87	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	4	DC	O4'-C1'-N1	8.59	114.01	108.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	302	ILE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	156	GLY	Peptide
3	A	198	PRO	Peptide

## 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	C	473	0	260	27	0
2	D	456	0	257	28	0
3	A	1458	0	1469	114	0
3	B	1458	0	1469	110	0
All	All	3845	0	3455	263	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 36.

The worst 5 of 263 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:A:246:LYS:CE	3:A:246:LYS:CD	1.81	1.55
3:A:301:GLY:CA	3:A:303:GLU:HB2	1.68	1.22
3:A:301:GLY:HA2	3:A:303:GLU:CB	1.76	1.13
3:A:302:ILE:HG13	3:A:303:GLU:HG2	1.13	1.08
3:B:269:MET:HE1	3:B:288:TYR:HB3	1.36	1.06

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	
3	A	180/204 (88%)	128 (71%)	39 (22%)	13 (7%)	1	2
3	B	180/204 (88%)	147 (82%)	26 (14%)	7 (4%)	3	10
All	All	360/408 (88%)	275 (76%)	65 (18%)	20 (6%)	2	5

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	182	PRO
3	A	183	GLY
3	A	200	SER
3	A	206	LYS
3	A	207	GLU

### 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	
3	A	160/178 (90%)	133 (83%)	27 (17%)	2	6
3	B	160/178 (90%)	134 (84%)	26 (16%)	2	7
All	All	320/356 (90%)	267 (83%)	53 (17%)	2	7

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	298	GLN

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Mol	Chain	Res	Type
3	B	140	ASN
3	B	279	PHE
3	A	300	LYS
3	A	304	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	150	HIS
3	B	179	HIS
3	B	158	HIS
3	A	298	GLN
3	B	157	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	3DR	D	11	2	8,11,12	0.56	0	9,14,17	1.34	1 (11%)

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	3DR	D	11	2	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	11	3DR	O4'-C4'-C3'	2.97	108.09	103.73

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
2	D	11	3DR	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	C	23/23 (100%)	1.89	9 (39%) 0 0	77, 143, 198, 202	0
2	D	22/23 (95%)	1.73	9 (40%) 0 0	88, 151, 198, 203	0
3	A	182/204 (89%)	2.06	66 (36%) 0 0	72, 94, 108, 117	0
3	B	182/204 (89%)	2.16	75 (41%) 0 0	78, 99, 135, 154	0
All	All	409/454 (90%)	2.07	159 (38%) 0 0	72, 97, 162, 203	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	203	LEU	14.8
3	B	203	LEU	12.5
3	A	154	GLY	9.8
3	A	147	TYR	9.4
3	A	155	PRO	9.2

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	3DR	D	11	11/12	0.45	0.60	124,131,137,140	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.