



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:54 pm BST

PDB ID : 3UOB
Title : Crystal structure of Human Thymine DNA Glycosylase Bound to Substrate Analog 2'-deoxy-2'-beta-fluoro-cytidine
Authors : Zhang, L.; He, C.
Deposited on : 2011-11-16
Resolution : 3.01 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

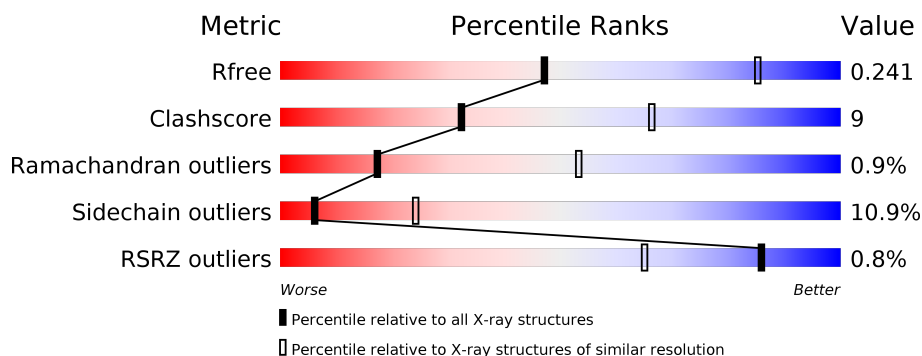
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 ≥ 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	
2	D	23	
3	A	201	
3	B	201	

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	1FC	D	11	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3764 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 5'-D(*CP*AP*GP*CP*TP*CP*TP*GP*TP*AP*CP*GP*TP*GP*AP*GP*CP*AP*GP*TP*GP*GP*A)-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 5'-D(*CP*CP*AP*CP*TP*GP*CP*TP*CP*AP*(1FC)P*GP*TP*AP*CP*AP*GP*AP*GP*CP*TP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	23	Total	C	F	N	O	P	0	0
			468	223	1	84	138	22		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	181	Total	C	N	O	S	0	0	0
			1447	933	248	257	9			
3	B	172	Total	C	N	O	S	0	0	0
			1376	890	234	244	8			

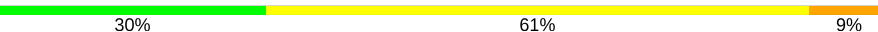
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	SER	-	EXPRESSION TAG	UNP Q13569
A	109	ASN	-	EXPRESSION TAG	UNP Q13569
A	110	ALA	-	EXPRESSION TAG	UNP Q13569
B	108	SER	-	EXPRESSION TAG	UNP Q13569
B	109	ASN	-	EXPRESSION TAG	UNP Q13569
B	110	ALA	-	EXPRESSION TAG	UNP Q13569

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 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.

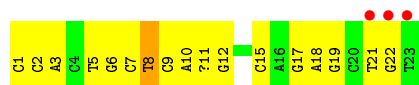
- Molecule 1: 5'-D(*CP*AP*GP*CP*TP*CP*TP*GP*TP*AP*CP*GP*TP*GP*AP*GP*CP*A P*GP*TP*GP*GP*A)-3'

Chain C: 



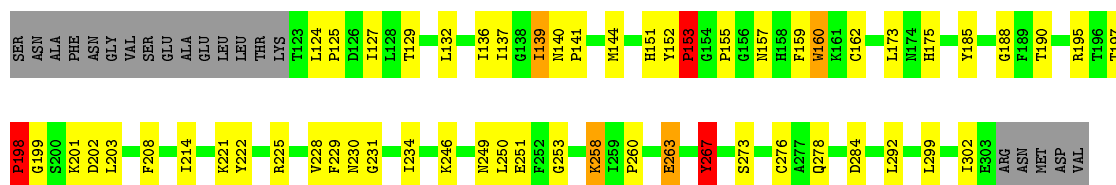
- Molecule 2: 5'-D(*CP*CP*AP*CP*TP*GP*CP*TP*CP*AP*(1FC)P*GP*TP*AP*CP*AP*G P*AP*GP*CP*TP*GP*T)-3'

Chain D: 



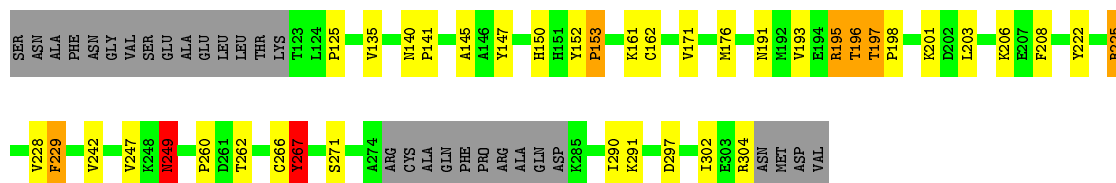
- Molecule 3: G/T mismatch-specific thymine DNA glycosylase

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	163.42Å 163.42Å 54.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.73 – 3.01 32.73 – 3.01	Depositor EDS
% Data completeness (in resolution range)	69.5 (32.73-3.01) 69.3 (32.73-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.219 , 0.276 0.236 , 0.241	Depositor DCC
R_{free} test set	598 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3764	wwPDB-VP
Average B, all atoms (Å ²)	103.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1FC

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	0.72	0/531	1.42	9/819 (1.1%)
2	D	0.72	0/497	1.35	5/762 (0.7%)
3	A	1.32	8/1484 (0.5%)	1.17	4/2001 (0.2%)
3	B	1.31	6/1410 (0.4%)	1.22	12/1899 (0.6%)
All	All	1.19	14/3922 (0.4%)	1.25	30/5481 (0.5%)

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	0	6
3	B	0	6
All	All	0	12

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	249	ASN	C-N	9.86	1.56	1.34
3	B	266	CYS	CB-SG	-8.36	1.68	1.82
3	B	247	VAL	C-N	8.13	1.52	1.34
3	A	162	CYS	CB-SG	-7.00	1.70	1.82
3	A	267	TYR	CB-CG	-6.50	1.41	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	267	TYR	CB-CG-CD2	11.11	127.67	121.00
3	B	267	TYR	CB-CG-CD1	-10.46	114.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	DG	O4'-C1'-N9	9.01	114.31	108.00
2	D	15	DC	O4'-C1'-N1	8.55	113.98	108.00
3	B	249	ASN	CA-C-N	-8.09	99.41	117.20

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	159	PHE	Sidechain
3	A	198	PRO	Mainchain,Peptide
3	A	208	PHE	Sidechain
3	A	225	ARG	Sidechain
3	A	267	TYR	Sidechain

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	18	0
2	D	468	0	259	21	0
3	A	1447	0	1456	32	0
3	B	1376	0	1391	6	0
All	All	3764	0	3366	61	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 9.

The worst 5 of 61 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)
2:D:11:1FC:H1	3:A:139:ILE:HD13	1.23	1.20
1:C:5:DT:OP1	3:A:246:LYS:NZ	2.02	0.93
2:D:11:1FC:C2'	3:A:139:ILE:HD13	2.08	0.82
3:A:197:THR:HB	3:A:198:PRO:HD2	1.61	0.82
2:D:11:1FC:O2	3:A:139:ILE:HD12	1.82	0.79

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	179/201 (89%)	167 (93%)	11 (6%)	1 (1%)	25	62
3	B	168/201 (84%)	158 (94%)	8 (5%)	2 (1%)	13	46
All	All	347/402 (86%)	325 (94%)	19 (6%)	3 (1%)	17	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	201	LYS
3	A	234	ILE
3	B	249	ASN

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	159/176 (90%)	143 (90%)	16 (10%)	7	27
3	B	152/176 (86%)	134 (88%)	18 (12%)	5	21
All	All	311/352 (88%)	277 (89%)	34 (11%)	6	24

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	284	ASP
3	B	191	ASN
3	B	297	ASP
3	B	161	LYS
3	A	201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	157	ASN
3	A	158	HIS
3	A	230	ASN
3	A	257	HIS
3	B	140	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	1FC	D	11	2	15,24,25	1.75	1 (6%)	15,35,38	2.29	5 (33%)

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	1FC	D	11	2	-	3/5/29/30	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	11	1FC	C5-C21	5.75	1.53	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	1FC	C2-N3-C4	4.36	121.28	116.02
2	D	11	1FC	F24-C2'-C3'	3.69	116.94	109.22
2	D	11	1FC	C2'-C3'-C4'	3.62	107.08	102.40
2	D	11	1FC	O4'-C1'-C2'	3.61	109.51	105.79
2	D	11	1FC	O3'-C3'-C4'	-3.11	102.05	111.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	11	1FC	C3'-C4'-C5'-O5'
2	D	11	1FC	C2'-C1'-N1-C6
2	D	11	1FC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	11	1FC	7	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, 95th 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 ²)	Q<0.9
1	C	23/23 (100%)	0.07	0 100 100	101, 141, 189, 196	0
2	D	22/23 (95%)	0.77	3 (13%) 3 1	87, 145, 193, 197	0
3	A	181/201 (90%)	-0.20	0 100 100	58, 85, 116, 131	0
3	B	172/201 (85%)	-0.31	0 100 100	61, 90, 122, 144	0
All	All	398/448 (88%)	-0.18	3 (0%) 86 65	58, 91, 160, 197	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	23	DT	4.2
2	D	22	DG	3.4
2	D	21	DT	2.3

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, 95th 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 ²)	Q<0.9
2	1FC	D	11	23/24	0.96	0.20	69,80,87,90	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.