



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 05:01 AM GMT

PDB ID : 1D67  
Title : THE MOLECULAR STRUCTURE OF AN IDARUBICIN-D(TGATCA)  
COMPLEX AT HIGH RESOLUTION  
Authors : Gallois, B.; Langlois D'Estaintot, B.; Brown, T.; Hunter, W.N.  
Deposited on : 1992-03-31  
Resolution : 1.60 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>

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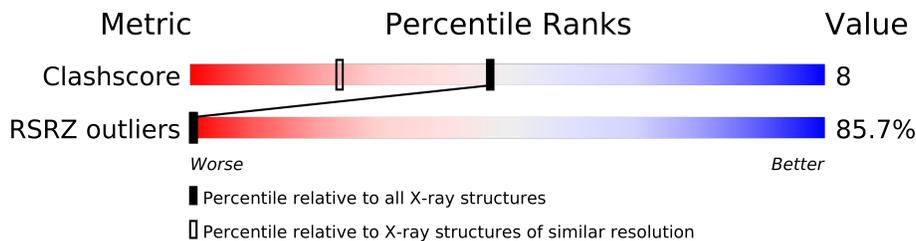
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
Clashscore	79885	2199 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	DM5	A	7	-	X

## 2 Entry composition i

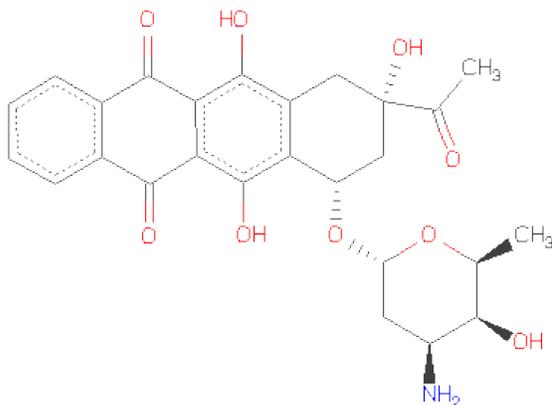
There are 3 unique types of molecules in this entry. The entry contains 191 atoms, of which 0 are hydrogen and 0 are deuterium.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	6	120	59	22	34	5	0	0	0

- Molecule 2 is IDARUBICIN (three-letter code: DM5) (formula: C<sub>26</sub>H<sub>27</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	36	26	1	9	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	35	Total 35 O 35	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	28.19Å 28.19Å 52.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.60 4.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.60) 67.8 (4.98-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.82 (at 1.60Å)	Xtrriage
Refinement program	NUCLSQ	Depositor
R, $R_{free}$	0.222 , (Not available) 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	7.6	Xtrriage
Anisotropy	0.527	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.55 , 82.2	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Outliers	8 of 2032 reflections (0.394%)	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows:

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

## 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: DM5

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	2.63	7/134 (5.2%)	3.24	14/205 (6.8%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	DA	C6-N1	11.39	1.43	1.35
1	A	2	DG	C6-N1	-8.05	1.33	1.39
1	A	4	DT	O4'-C1'	7.66	1.51	1.42
1	A	4	DT	C4'-O4'	-7.40	1.37	1.45
1	A	1	DT	C4'-O4'	-5.93	1.39	1.45
1	A	2	DG	N1-C2	-5.92	1.33	1.37
1	A	3	DA	C4'-O4'	-5.20	1.39	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	DC	O4'-C1'-N1	26.32	126.42	108.00
1	A	4	DT	O4'-C1'-N1	-8.70	101.91	108.00
1	A	2	DG	O4'-C1'-N9	8.42	113.89	108.00
1	A	1	DT	C2-N3-C4	-7.55	122.67	127.20
1	A	6	DA	C5-C6-N1	-6.75	114.33	117.70
1	A	4	DT	O4'-C1'-C2'	-6.63	100.59	105.90
1	A	1	DT	N3-C4-C5	6.27	118.96	115.20
1	A	2	DG	P-O5'-C5'	-5.82	111.59	120.90
1	A	1	DT	C5-C6-N1	-5.78	120.23	123.70
1	A	5	DC	O4'-C4'-C3'	5.72	109.43	106.00
1	A	5	DC	P-O5'-C5'	-5.29	112.43	120.90
1	A	2	DG	C6-N1-C2	5.21	128.23	125.10
1	A	3	DA	O5'-P-OP2	5.17	116.91	110.70
1	A	4	DT	C5-C4-O4	-5.04	121.37	124.90

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	120	0	69	2	0
2	A	36	0	26	0	0
3	A	35	0	0	2	0
All	All	191	0	95	2	0

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 8.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:DA:H1'	3:A:42:HOH:O	2.05	0.56
1:A:3:DA:N3	3:A:42:HOH:O	2.32	0.56

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

There are no protein chains in this entry.

### 5.3.2 Protein sidechains

There are no protein chains in this entry.

### 5.3.3 RNA

There are no RNA chains 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)

1 ligand 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	DM5	A	7	-	40,40,40	2.08	15 (37%)	63,63,63	2.46	19 (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	DM5	A	7	-	-	0/10/56/56	0/1/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	7	DM5	C2'-C3'	5.93	1.56	1.52
2	A	7	DM5	C4'-C5'	-3.85	1.44	1.52
2	A	7	DM5	O4'-C4'	3.83	1.52	1.43
2	A	7	DM5	C6'-C5'	-3.62	1.42	1.51
2	A	7	DM5	O13-C13	3.10	1.28	1.21
2	A	7	DM5	C17-C16	2.83	1.45	1.40
2	A	7	DM5	C18-C7	-2.72	1.35	1.41
2	A	7	DM5	C5-C6	2.58	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	7	DM5	O19-C19	2.49	1.27	1.22
2	A	7	DM5	O10-C1'	2.43	1.48	1.41
2	A	7	DM5	O10-C10	-2.41	1.40	1.44
2	A	7	DM5	C3-C2	-2.36	1.31	1.37
2	A	7	DM5	C20-C19	-2.35	1.43	1.48
2	A	7	DM5	C3-C4	-2.06	1.34	1.39
2	A	7	DM5	C2'-C1'	2.05	1.55	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	7	DM5	C4'-C3'-N3'	10.28	130.72	110.83
2	A	7	DM5	C1'-O10-C10	7.35	126.15	115.84
2	A	7	DM5	O4'-C4'-C3'	-5.16	97.56	109.66
2	A	7	DM5	C6'-C5'-C4'	-4.84	105.21	113.06
2	A	7	DM5	O13-C13-C14	-3.92	113.75	121.28
2	A	7	DM5	C2-C3-C4	3.48	125.96	120.17
2	A	7	DM5	O19-C19-C20	-3.45	115.53	120.82
2	A	7	DM5	O5'-C5'-C6'	3.25	113.88	106.70
2	A	7	DM5	O12-C12-C11	3.21	115.66	109.13
2	A	7	DM5	O10-C10-C11	3.18	117.70	110.17
2	A	7	DM5	O13-C13-C12	3.06	127.03	120.40
2	A	7	DM5	C11-C12-C15	-2.80	104.89	110.31
2	A	7	DM5	C15-C12-C13	-2.79	104.56	110.30
2	A	7	DM5	C8-C7-C6	-2.58	115.89	120.58
2	A	7	DM5	O10-C1'-C2'	2.58	113.11	108.44
2	A	7	DM5	O12-C12-C13	2.30	113.16	108.19
2	A	7	DM5	O5'-C1'-C2'	2.03	113.95	110.82
2	A	7	DM5	C3-C4-C5	-2.02	115.83	119.84
2	A	7	DM5	C2'-C3'-C4'	2.00	113.11	110.06

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	6/6 (100%)	8.05	6 (100%) <b>0</b> <b>0</b>	15, 18, 18, 19	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	DT	9.7
1	A	2	DG	8.6
1	A	4	DT	8.4
1	A	5	DC	8.1
1	A	6	DA	7.1
1	A	3	DA	6.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
2	DM5	A	7	36/36	0.67	0.45	8,15,23,26	0

## 6.5 Other polymers

There are no such residues in this entry.