



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2026 – 08:44 am BST

PDB ID : 8C63 / pdb_00008c63
Title : Crystal structure of arsenoplatin-1/B-DNA adduct obtained upon 4 h of soaking
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Deposited on : 2023-01-11
Resolution : 1.52 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	NOT EXECUTED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

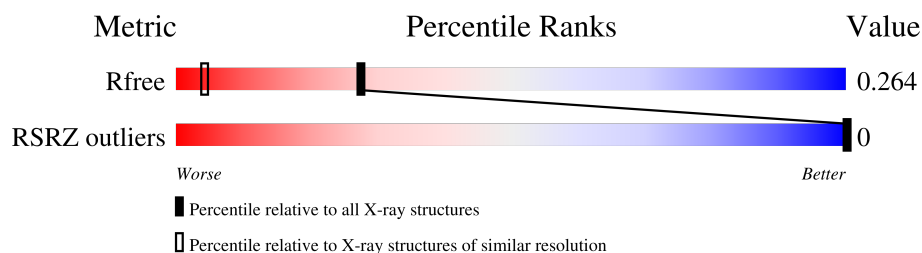
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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}	180053	5890 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A6R	B	101	-	-	-	X

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Xtriage (Phenix) was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	25.51Å 40.73Å 65.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.64 – 1.52 34.64 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.64-1.52) 99.7 (34.64-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.238 , 0.261 0.241 , 0.264	Depositor DCC
R_{free} test set	544 reflections (4.90%)	wwPDB-VP
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	569	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

3 Model quality [i](#)

3.1 Standard geometry [i](#)

MolProbity was not executed - this section is therefore empty.

3.2 Too-close contacts [i](#)

MolProbity was not executed - this section is therefore empty.

3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

MolProbity was not executed - this section is therefore empty.

3.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section is therefore empty.

3.3.3 RNA [i](#)

MolProbity was not executed - this section is therefore empty.

3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

validation-pack was not executed - this section is therefore empty.

3.5 Carbohydrates [i](#)

validation-pack was not executed - this section is therefore empty.

3.6 Ligand geometry [i](#)

validation-pack was not executed - this section is therefore empty.

3.7 Other polymers [i](#)

validation-pack was not executed - this section is therefore empty.

3.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 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	A	12/12 (100%)	0.45	0 100 100	28, 34, 36, 36	0
1	B	12/12 (100%)	0.71	0 100 100	27, 31, 37, 42	0
All	All	24/24 (100%)	0.58	0 100 100	27, 34, 36, 42	0

There are no RSRZ outliers to report.

4.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.4 Other polymers [i](#)

There are no such residues in this entry.