



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:23 PM UTC

PDB ID : 5T7E / pdb_00005t7e
Title : Crystal structure of Streptomyces hygroscopicus Bialaphos Resistance (BAR) protein in complex with Coenzyme A and L-phosphinothricin
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Deposited on : 2016-09-04
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	FAILED
Mogul	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

PERCENTILES INFOmissingINFO

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

1 Model quality [i](#)

1.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

1.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

1.3 Torsion angles [i](#)

1.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

1.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

1.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

Mogul failed to run properly - this section is therefore empty.

1.5 Carbohydrates [i](#)

Mogul failed to run properly - this section is therefore empty.

1.6 Ligand geometry [i](#)

Mogul failed to run properly - this section is therefore empty.

1.7 Other polymers [i](#)

Mogul failed to run properly - this section is therefore empty.

1.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

2 Fit of model and data

2.1 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, 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	1-A	174/189 (92%)	0.82	18 (10%) 12 10	12, 22, 33, 53	35 (20%)
1	1-B	42/189 (22%)	0.84	4 (9%) 14 12	15, 25, 32, 48	9 (21%)
All	All	216/378 (57%)	0.82	22 (10%) 12 10	12, 22, 33, 53	44 (20%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	101	GLY	8.1
1	1-A	10	ILE	5.2
1	1-A	100	THR	4.5
1	1-B	8	ALA	4.4
1	1-A	99	ARG	4.0
1	1-A	65	ASP	3.8
1	1-A	9	ASP	3.6
1	1-A	64	VAL	3.4
1	1-A	8	ALA	3.2
1	1-B	48	ASP	3.2
1	1-A	97	HIS	3.2
1	1-A	102	LEU	3.0
1	1-B	44	GLN	3.0
1	1-A	135	ARG	2.9
1	1-A	104	SER	2.9
1	1-A	180	VAL	2.8
1	1-A	66	GLY	2.6
1	1-A	40	PRO	2.6
1	1-A	98	GLN	2.6
1	1-A	181	THR	2.5
1	1-A	39	GLU	2.5
1	1-B	42	GLU	2.4

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

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

2.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

2.4 Other polymers [i](#)

There are no such residues in this entry.