



Full wwPDB X-ray Structure Validation Report

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PDB ID : 4BPF
Title : High resolution crystal structure of Bacillus subtilis DltC S36A
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Deposited on : 2013-05-26
Resolution : 1.01 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

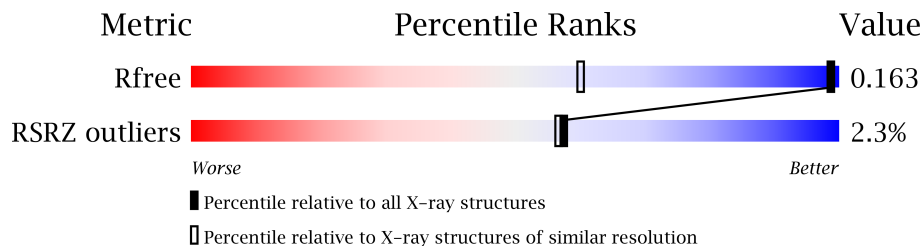
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
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) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 1.01 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}	66092	1167 (1.14-0.90)
RSRZ outliers	66119	1167 (1.14-0.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note MolProbity failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	86	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2027 atoms, of which 1062 are hydrogens 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 protein called D-ALANINE--POLY(PHOSPHORIBITOL)LIGASE SUB-UNIT 2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	86	Total	C	H	N	O	S	Se	0	18	0
			1654	535	826	137	153	1	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ARG	-	EXPRESSION TAG	UNP P39579
A	80	SER	-	EXPRESSION TAG	UNP P39579
A	81	HIS	-	EXPRESSION TAG	UNP P39579
A	82	HIS	-	EXPRESSION TAG	UNP P39579
A	83	HIS	-	EXPRESSION TAG	UNP P39579
A	84	HIS	-	EXPRESSION TAG	UNP P39579
A	85	HIS	-	EXPRESSION TAG	UNP P39579
A	86	HIS	-	EXPRESSION TAG	UNP P39579
A	36	ALA	SER	ENGINEERED MUTATION	UNP P39579

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	137	Total	H	O	0	0
			373	236	137		

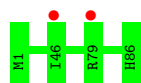
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note MolProbity failed to run properly.

- Molecule 1: D-ALANINE--POLY(PHOSPHORIBITOL)LIGASE SUBUNIT 2

Chain A:  



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	34.59Å 37.22Å 37.68Å 90.00° 114.79° 90.00°	Depositor
Resolution (Å)	17.28 – 1.01 17.28 – 1.01	Depositor EDS
% Data completeness (in resolution range)	96.3 (17.28-1.01) 96.3 (17.28-1.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.129 , 0.156 0.137 , 0.163	Depositor DCC
R_{free} test set	1381 reflections (3.14%)	DCC
Wilson B-factor (Å ²)	8.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 44007 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2027	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.2 Close contacts ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.3 RNA ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

MolProbity failed to run properly - this section will therefore be empty.

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, 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	86/86 (100%)	0.16	2 (2%) 57 57	6, 10, 17, 25	2 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79[A]	ARG	3.7
1	A	46[A]	ILE	2.8

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.