Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 11:58 PM EDT

PDB ID	:	6OBT
Title	:	Structural insights into dehydratase substrate selection for the borrelidin and fluvirucin polyketide synthases
Authors	:	McAndrew, R.P.; Barajas, J.F.; Pereira, J.H.; Keasling, J.D.; Adams, P.D.
Deposited on	:	2019-03-21
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
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2080 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 protein called Borrelidin polyketide synthase, type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2032	1286	359	382	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q70I00
A	2	GLY	-	expression tag	UNP Q70I00
A	3	SER	-	expression tag	UNP Q70I00
A	4	SER	-	expression tag	UNP Q70I00
A	5	HIS	-	expression tag	UNP Q70I00
A	6	HIS	-	expression tag	UNP Q70I00
A	7	HIS	-	expression tag	UNP Q70I00
A	8	HIS	-	expression tag	UNP Q70I00
A	9	HIS	-	expression tag	UNP Q70I00
A	10	HIS	-	expression tag	UNP Q70I00
A	11	ASP	-	expression tag	UNP Q70I00
A	12	TYR	-	expression tag	UNP Q70I00
A	13	ASP	-	expression tag	UNP Q70I00
A	14	ILE	-	expression tag	UNP Q70I00
A	15	PRO	-	expression tag	UNP Q70I00
A	16	THR	-	expression tag	UNP Q70I00
A	17	THR	-	expression tag	UNP Q70I00
A	18	GLU	-	expression tag	UNP Q70I00
A	19	ASN	-	expression tag	UNP Q70I00
A	20	LEU	-	expression tag	UNP Q70I00
A	21	TYR	-	expression tag	UNP Q70I00
A	22	PHE	-	expression tag	UNP Q70I00
A	23	GLN	-	expression tag	UNP Q70I00
A	24	GLY	-	expression tag	UNP Q70I00
A	25	HIS	-	expression tag	UNP Q70I00
A	26	MET	-	expression tag	UNP Q70I00
A	349	VAL	-	expression tag	UNP Q70I00

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Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LEU	-	expression tag	UNP Q70I00
A	351	ARG	-	expression tag	UNP Q70I00
A	352	SER	-	expression tag	UNP Q70I00
A	353	ALA	-	expression tag	UNP Q70I00
A	353A	ALA	-	expression tag	UNP Q70I00
A	353B	ALA	-	expression tag	UNP Q70I00
A	353C	ARG	-	expression tag	UNP Q70I00
A	353D	ARG	-	expression tag	UNP Q70I00
A	354	THR	-	expression tag	UNP Q70I00
A	355	GLY	-	expression tag	UNP Q70I00
A	356	ALA	-	expression tag	UNP Q70I00
A	357	ARG	-	expression tag	UNP Q70I00
A	358	ARG	-	expression tag	UNP Q70I00
A	359	GLN	-	expression tag	UNP Q70I00
A	360	ALA	-	expression tag	UNP Q70I00

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		

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

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.21Å 63.35Å 40.67Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	30.89 – 1.80	Depositor
% Data completeness (in resolution range)	98.3 (30.89-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.15rc3_3435, PHENIX 1.15rc3_3435	Depositor
R, R_{free}	0.203 , 0.232	Depositor
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.661	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2080	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	239:ALA	C	301:CYS	N	2.94

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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