



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 10:17 PM EDT

PDB ID : 6MHL
Title : Crystal structure of ketosynthase twelve from bacillaene polyketide synthase in *Bacillus amyloliquefaciens*
Authors : Meinke, J.L.; Keatinge-Clay, A.T.
Deposited on : 2018-09-18
Resolution : 1.82 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**
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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 9266 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 Hybrid NRPS/PKS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	561	Total	C	N	O	S	0	0	0
			4366	2755	750	848	13			
1	B	561	Total	C	N	O	S	0	0	0
			4365	2755	748	848	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q1RS70
A	-19	GLY	-	expression tag	UNP Q1RS70
A	-18	SER	-	expression tag	UNP Q1RS70
A	-17	SER	-	expression tag	UNP Q1RS70
A	-16	HIS	-	expression tag	UNP Q1RS70
A	-15	HIS	-	expression tag	UNP Q1RS70
A	-14	HIS	-	expression tag	UNP Q1RS70
A	-13	HIS	-	expression tag	UNP Q1RS70
A	-12	HIS	-	expression tag	UNP Q1RS70
A	-11	HIS	-	expression tag	UNP Q1RS70
A	-10	SER	-	expression tag	UNP Q1RS70
A	-9	SER	-	expression tag	UNP Q1RS70
A	-8	GLY	-	expression tag	UNP Q1RS70
A	-7	LEU	-	expression tag	UNP Q1RS70
A	-6	VAL	-	expression tag	UNP Q1RS70
A	-5	PRO	-	expression tag	UNP Q1RS70
A	-4	ARG	-	expression tag	UNP Q1RS70
A	-3	GLY	-	expression tag	UNP Q1RS70
A	-2	SER	-	expression tag	UNP Q1RS70
A	-1	HIS	-	expression tag	UNP Q1RS70
B	-20	MET	-	initiating methionine	UNP Q1RS70
B	-19	GLY	-	expression tag	UNP Q1RS70
B	-18	SER	-	expression tag	UNP Q1RS70
B	-17	SER	-	expression tag	UNP Q1RS70
B	-16	HIS	-	expression tag	UNP Q1RS70

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q1RS70
B	-14	HIS	-	expression tag	UNP Q1RS70
B	-13	HIS	-	expression tag	UNP Q1RS70
B	-12	HIS	-	expression tag	UNP Q1RS70
B	-11	HIS	-	expression tag	UNP Q1RS70
B	-10	SER	-	expression tag	UNP Q1RS70
B	-9	SER	-	expression tag	UNP Q1RS70
B	-8	GLY	-	expression tag	UNP Q1RS70
B	-7	LEU	-	expression tag	UNP Q1RS70
B	-6	VAL	-	expression tag	UNP Q1RS70
B	-5	PRO	-	expression tag	UNP Q1RS70
B	-4	ARG	-	expression tag	UNP Q1RS70
B	-3	GLY	-	expression tag	UNP Q1RS70
B	-2	SER	-	expression tag	UNP Q1RS70
B	-1	HIS	-	expression tag	UNP Q1RS70

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	247	Total O 247 247	0	0
2	B	288	Total O 288 288	0	0

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

3 Data and refinement statistics

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	132.22Å 85.13Å 134.30Å 90.00° 110.55° 90.00°	Depositor
Resolution (Å)	50.00 – 1.82	Depositor
% Data completeness (in resolution range)	99.9 (50.00-1.82)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.188 , 0.219	Depositor
Wilson B-factor (Å ²)	21.3	Xtrriage
Anisotropy	0.031	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9266	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

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

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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