



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 12:53 pm BST

PDB ID : 6MHK  
Title : Crystal structure of ketosynthase nine from bacillaene polyketide synthase in *Bacillus amyloliquefaciens*  
Authors : Meinke, J.L.; Keatinge-Clay, A.T.  
Deposited on : 2018-09-18  
Resolution : 1.93 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

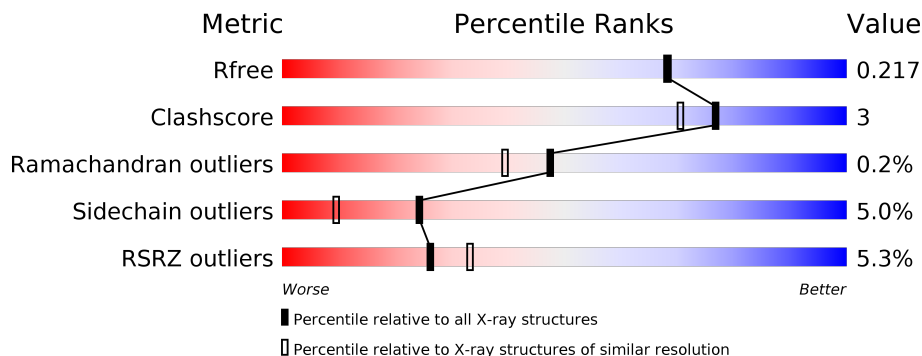
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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))
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	614	 6% 77% 9% • 13%
1	B	614	 4% 78% 8% • 13%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8679 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 Polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4144	2628	715	787	14	0	0	0
1	B	534	4134	2620	711	789	14	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q1RS71
A	-21	GLY	-	expression tag	UNP Q1RS71
A	-20	SER	-	expression tag	UNP Q1RS71
A	-19	SER	-	expression tag	UNP Q1RS71
A	-18	HIS	-	expression tag	UNP Q1RS71
A	-17	HIS	-	expression tag	UNP Q1RS71
A	-16	HIS	-	expression tag	UNP Q1RS71
A	-15	HIS	-	expression tag	UNP Q1RS71
A	-14	HIS	-	expression tag	UNP Q1RS71
A	-13	HIS	-	expression tag	UNP Q1RS71
A	-12	SER	-	expression tag	UNP Q1RS71
A	-11	SER	-	expression tag	UNP Q1RS71
A	-10	GLY	-	expression tag	UNP Q1RS71
A	-9	LEU	-	expression tag	UNP Q1RS71
A	-8	VAL	-	expression tag	UNP Q1RS71
A	-7	PRO	-	expression tag	UNP Q1RS71
A	-6	ARG	-	expression tag	UNP Q1RS71
A	-5	GLY	-	expression tag	UNP Q1RS71
A	-4	SER	-	expression tag	UNP Q1RS71
A	-3	SER	-	expression tag	UNP Q1RS71
B	-22	MET	-	initiating methionine	UNP Q1RS71
B	-21	GLY	-	expression tag	UNP Q1RS71
B	-20	SER	-	expression tag	UNP Q1RS71
B	-19	SER	-	expression tag	UNP Q1RS71
B	-18	HIS	-	expression tag	UNP Q1RS71

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	HIS	-	expression tag	UNP Q1RS71
B	-16	HIS	-	expression tag	UNP Q1RS71
B	-15	HIS	-	expression tag	UNP Q1RS71
B	-14	HIS	-	expression tag	UNP Q1RS71
B	-13	HIS	-	expression tag	UNP Q1RS71
B	-12	SER	-	expression tag	UNP Q1RS71
B	-11	SER	-	expression tag	UNP Q1RS71
B	-10	GLY	-	expression tag	UNP Q1RS71
B	-9	LEU	-	expression tag	UNP Q1RS71
B	-8	VAL	-	expression tag	UNP Q1RS71
B	-7	PRO	-	expression tag	UNP Q1RS71
B	-6	ARG	-	expression tag	UNP Q1RS71
B	-5	GLY	-	expression tag	UNP Q1RS71
B	-4	SER	-	expression tag	UNP Q1RS71
B	-3	SER	-	expression tag	UNP Q1RS71


- Molecule 2 is water.

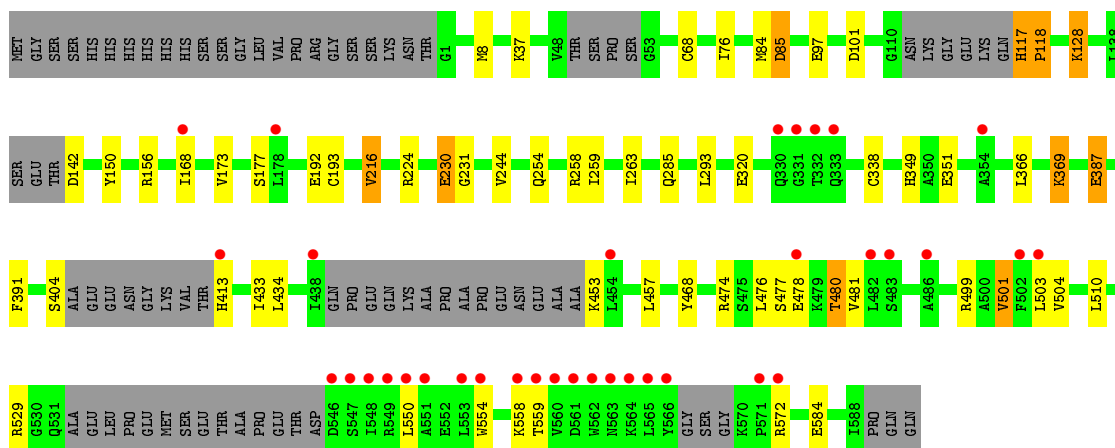
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	187	Total O 187 187	0	0
2	B	214	Total O 214 214	0	0

### 3 Residue-property plots [i](#)


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

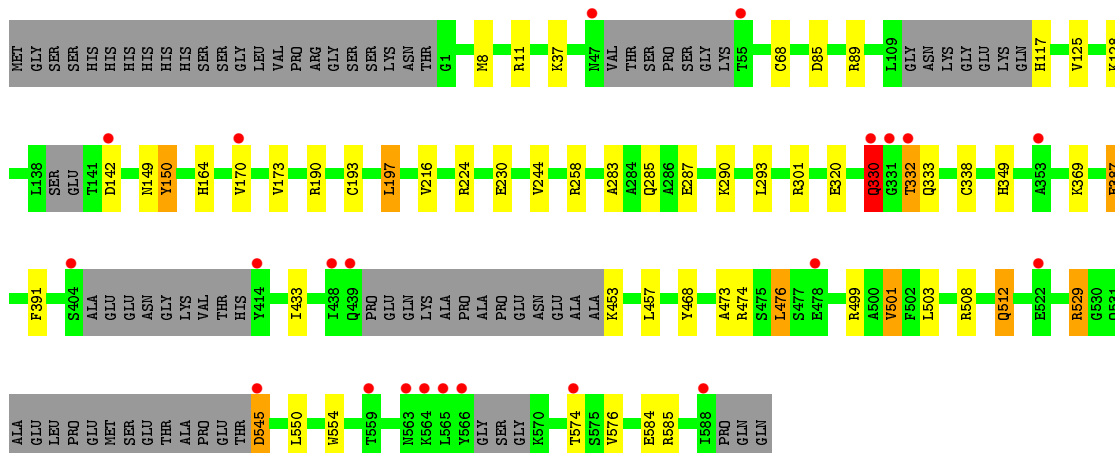
- Molecule 1: Polyketide synthase

Chain A: 



- Molecule 1: Polyketide synthase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.86Å 116.49Å 141.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93 47.93 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.93) 98.7 (47.93-1.88)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.88Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.182 , 0.210 0.191 , 0.217	Depositor DCC
$R_{free}$ test set	5231 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.05	5/4235 (0.1%)	0.97	14/5726 (0.2%)
1	B	1.05	1/4224 (0.0%)	1.00	16/5713 (0.3%)
All	All	1.05	6/8459 (0.1%)	0.98	30/11439 (0.3%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	CYS	CB-SG	-7.92	1.68	1.82
1	A	351	GLU	CD-OE1	-5.86	1.19	1.25
1	A	192	GLU	CD-OE2	-5.28	1.19	1.25
1	A	177	SER	CB-OG	-5.14	1.35	1.42
1	B	150	TYR	CE2-CZ	-5.12	1.31	1.38

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	A	529	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	529	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	B	529	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	B	197	LEU	CB-CG-CD1	7.16	123.17	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4144	0	4083	27	0
1	B	4134	0	4067	25	0
2	A	187	0	0	0	0
2	B	214	0	0	2	0
All	All	8679	0	8150	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HD3	1:B:332:THR:HG21	1.56	0.86
1:B:117:HIS:N	1:B:164:HIS:HD1	1.73	0.85
1:A:504:VAL:HG11	1:A:510:LEU:HB2	1.75	0.67
1:A:477:SER:H	1:A:480:THR:CG2	2.07	0.66
1:B:290:LYS:HE2	1:B:330:GLN:NE2	2.14	0.63

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	520/614 (85%)	512 (98%)	7 (1%)	1 (0%)	47 39
1	B	518/614 (84%)	511 (99%)	6 (1%)	1 (0%)	47 39
All	All	1038/1228 (84%)	1023 (99%)	13 (1%)	2 (0%)	47 39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL

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Mol	Chain	Res	Type
1	B	173	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/502 (87%)	417 (95%)	21 (5%)	25	10
1	B	438/502 (87%)	415 (95%)	23 (5%)	22	9
All	All	876/1004 (87%)	832 (95%)	44 (5%)	24	9

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	558	LYS
1	B	197	LEU
1	B	529	ARG
1	A	559	THR
1	B	149	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	B	285	GLN
1	B	330	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	536/614 (87%)	0.29	35 (6%) 18 25	14, 23, 50, 76	0
1	B	534/614 (86%)	0.10	22 (4%) 37 44	13, 22, 44, 78	0
All	All	1070/1228 (87%)	0.20	57 (5%) 26 33	13, 23, 47, 78	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	LEU	8.7
1	A	564	LYS	7.3
1	B	330	GLN	6.7
1	A	550	LEU	6.6
1	A	561	ASP	6.6

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.