



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2022 – 01:09 am BST

PDB ID : 7ZMC  
Title : Ketosynthase domain of module 4 from *Brevibacillus Brevis* orphan BGC11  
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Deposited on : 2022-04-19  
Resolution : 3.10 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](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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.30  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.30

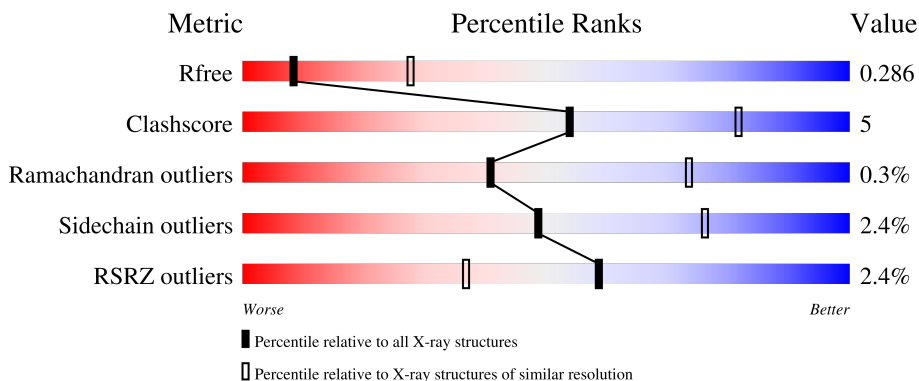
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of 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	635	 2% 74% 10% 16%
1	B	635	 2% 73% 11% 15%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16679 atoms, of which 8300 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 Putative polyketide synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	532	8270	2632	4116	722	785	15	0	0	0
1	B	539	8409	2679	4184	737	794	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1586	GLY	-	expression tag	UNP C0ZGQ6
A	2220	ALA	-	expression tag	UNP C0ZGQ6
B	1586	GLY	-	expression tag	UNP C0ZGQ6
B	2220	ALA	-	expression tag	UNP C0ZGQ6



THR  
ALA  
GLY  
GLU  
PRO  
ALA  
TYR  
LEU  
HIS  
PRO  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.56Å 191.79Å 293.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.10 48.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.97-3.10) 85.7 (48.97-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.49 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.263 , 0.288 0.263 , 0.286	Depositor DCC
$R_{free}$ test set	1913 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtrriage
Anisotropy	0.654	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	0.27	0/4239	0.53	0/5738
1	B	0.27	0/4313	0.53	0/5835
All	All	0.27	0/8552	0.53	0/11573

There are no bond length outliers.

There are no bond angle outliers.

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	4154	4116	4111	39	0
1	B	4225	4184	4177	49	0
All	All	8379	8300	8288	88	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 5.

All (88) 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:1852:TYR:OH	1:B:2186:SER:OG	1.92	0.87
1:A:1686:CYS:O	1:A:1690:THR:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1765:MET:O	1:A:1768:SER:OG	2.03	0.77
1:B:1765:MET:SD	1:B:2018:GLY:N	2.58	0.76
1:A:1721:GLU:N	1:A:1721:GLU:OE1	2.20	0.74
1:A:2170:ILE:HD12	1:A:2170:ILE:O	1.89	0.72
1:B:1721:GLU:OE1	1:B:1721:GLU:N	2.23	0.72
1:B:1596:ILE:HG23	1:B:1836:VAL:HG13	1.74	0.70
1:A:1599:ILE:HG22	1:A:1836:VAL:HG22	1.78	0.65
1:A:1771:THR:HG22	1:A:1860:ILE:HD12	1.78	0.64
1:A:1679:GLN:NE2	1:A:1719:TYR:O	2.32	0.62
1:A:1897:TYR:O	1:A:1898:ILE:HD12	1.99	0.62
1:B:2064:ARG:NH1	1:B:2189:ALA:O	2.34	0.60
1:A:2064:ARG:NH1	1:A:2189:ALA:O	2.32	0.60
1:B:2074:LEU:HD13	1:B:2082:ILE:HD11	1.84	0.59
1:A:1992:TRP:O	1:A:2008:ARG:NH1	2.34	0.59
1:A:1894:THR:HG22	1:A:2006:TYR:CD2	2.39	0.57
1:B:2150:ASP:O	1:B:2153:ILE:HG13	2.06	0.56
1:A:1895:VAL:HG11	1:A:1898:ILE:HD11	1.85	0.56
1:A:1683:PHE:O	1:A:1687:VAL:HG23	2.06	0.56
1:B:2049:VAL:HG12	1:B:2165:TRP:CH2	2.42	0.54
1:A:1762:VAL:HG11	1:A:1775:LEU:CD1	2.36	0.54
1:B:1764:THR:O	1:B:1768:SER:OG	2.25	0.54
1:A:1609:ILE:HD11	1:A:1952:THR:HG21	1.91	0.53
1:B:1676:MET:O	1:B:1681:ARG:NH2	2.40	0.53
1:B:1977:ASP:OD2	1:B:1979:SER:OG	2.27	0.53
1:A:1596:ILE:HG23	1:A:1836:VAL:HG13	1.90	0.53
1:A:1895:VAL:HG11	1:A:1898:ILE:CD1	2.39	0.53
1:B:2124:LEU:O	1:B:2124:LEU:HD23	2.09	0.52
1:B:1898:ILE:O	1:B:1898:ILE:HG23	2.09	0.52
1:B:1766:CYS:O	1:B:1768:SER:N	2.43	0.52
1:A:2074:LEU:HD13	1:A:2082:ILE:HD11	1.91	0.51
1:A:2135:THR:O	1:A:2138:VAL:HG12	2.11	0.51
1:B:1722:TYR:HE2	1:B:2199:LEU:HD12	1.75	0.51
1:A:1762:VAL:HG11	1:A:1775:LEU:HD12	1.93	0.51
1:B:1764:THR:OG1	1:B:1768:SER:N	2.44	0.50
1:B:2066:LEU:HD21	1:B:2115:LEU:HD22	1.93	0.49
1:B:2096:ARG:HB3	1:B:2165:TRP:CZ3	2.48	0.48
1:A:2081:GLU:HB2	1:A:2185:ILE:HD11	1.96	0.47
1:B:1630:ARG:NH1	1:B:1831:GLU:OE2	2.46	0.47
1:A:2074:LEU:CD1	1:A:2082:ILE:HD11	2.44	0.47
1:A:1787:VAL:HG12	1:A:1788:ALA:N	2.30	0.46
1:A:1898:ILE:O	1:A:1898:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2066:LEU:HD21	1:B:2115:LEU:CD2	2.45	0.46
1:B:2066:LEU:HD12	1:B:2067:SER:N	2.30	0.46
1:B:1925:LYS:N	1:B:1925:LYS:HD3	2.31	0.46
1:B:2094:GLU:OE1	1:B:2094:GLU:N	2.49	0.46
1:A:1767:SER:OG	1:A:1771:THR:HG23	2.17	0.45
1:B:1945:ALA:O	1:B:1948:ILE:HG22	2.16	0.45
1:A:2094:GLU:OE1	1:A:2094:GLU:N	2.50	0.45
1:B:2023:HIS:O	1:B:2024:LEU:HD23	2.17	0.45
1:A:1866:THR:OG1	1:A:1868:GLY:O	2.34	0.45
1:A:1877:GLN:O	1:A:1880:VAL:HG12	2.18	0.44
1:B:1892:PRO:HA	1:B:1895:VAL:HG23	2.00	0.44
1:A:1679:GLN:CD	1:A:1719:TYR:O	2.55	0.44
1:A:1690:THR:HG21	1:A:1835:ALA:HB3	1.99	0.44
1:A:1711:VAL:HG22	1:A:1787:VAL:HB	1.99	0.44
1:A:1769:SER:HB2	1:A:1944:SER:O	2.18	0.44
1:B:1714:TYR:O	1:B:1790:ALA:HA	2.19	0.43
1:A:1766:CYS:O	1:A:1768:SER:N	2.52	0.43
1:B:2139:PHE:CD2	1:B:2145:LEU:HD21	2.53	0.43
1:B:1596:ILE:HG23	1:B:1836:VAL:CG1	2.46	0.43
1:B:1629:ASP:N	1:B:1629:ASP:OD1	2.50	0.42
1:B:2101:VAL:HG21	1:B:2107:LEU:HB2	2.01	0.42
1:A:1942:GLY:H	1:A:1946:ALA:HB2	1.85	0.42
1:B:1907:LEU:C	1:B:1907:LEU:HD23	2.39	0.42
1:B:2004:ARG:HG2	1:B:2005:GLU:N	2.35	0.42
1:B:2157:LYS:CE	1:B:2157:LYS:HA	2.49	0.42
1:B:1773:ILE:HD11	1:B:1948:ILE:HD12	2.02	0.42
1:B:2035:ARG:O	1:B:2035:ARG:HD3	2.20	0.42
1:B:2063:GLN:OE1	1:B:2115:LEU:HD21	2.20	0.42
1:A:1881:ILE:HD13	1:A:1916:LEU:HG	2.02	0.42
1:B:1714:TYR:CD1	1:B:1776:ALA:HB2	2.54	0.41
1:B:1830:GLY:O	1:B:1942:GLY:HA2	2.21	0.41
1:B:1898:ILE:O	1:B:1898:ILE:CG2	2.68	0.41
1:B:1722:TYR:CE2	1:B:2199:LEU:HD12	2.54	0.41
1:B:1909:ASP:N	1:B:1910:PRO:CD	2.84	0.41
1:A:1909:ASP:N	1:A:1910:PRO:CD	2.84	0.41
1:A:2130:LYS:H	1:A:2130:LYS:HD2	1.85	0.41
1:B:1592:LEU:O	1:B:1856:LYS:HA	2.21	0.41
1:B:1942:GLY:H	1:B:1946:ALA:HB2	1.85	0.41
1:A:1864:GLY:O	1:A:1866:THR:HG23	2.21	0.40
1:B:2063:GLN:O	1:B:2066:LEU:HG	2.22	0.40
1:B:1719:TYR:CD1	1:B:1719:TYR:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1917:THR:HG23	1:B:1982:PRO:HD3	2.03	0.40
1:B:1691:ILE:HG22	1:B:1696:TYR:O	2.21	0.40
1:A:2034:HIS:O	1:A:2035:ARG:HG2	2.21	0.40
1:B:1942:GLY:O	1:B:1943:GLU:HB2	2.21	0.40

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	522/635 (82%)	486 (93%)	35 (7%)	1 (0%)	47	79
1	B	527/635 (83%)	490 (93%)	35 (7%)	2 (0%)	34	69
All	All	1049/1270 (83%)	976 (93%)	70 (7%)	3 (0%)	41	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1765	MET
1	A	1943	GLU
1	B	1767	SER

### 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	441/516 (86%)	432 (98%)	9 (2%)	55	80
1	B	447/516 (87%)	435 (97%)	12 (3%)	44	74
All	All	888/1032 (86%)	867 (98%)	21 (2%)	49	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1608	ASN
1	A	1720	GLU
1	A	1766	CYS
1	A	1785	CYS
1	A	1951	LEU
1	A	2066	LEU
1	A	2113	TYR
1	A	2130	LYS
1	A	2177	TYR
1	B	1719	TYR
1	B	1720	GLU
1	B	1765	MET
1	B	1766	CYS
1	B	1785	CYS
1	B	1925	LYS
1	B	2035	ARG
1	B	2056	ASP
1	B	2102	LYS
1	B	2113	TYR
1	B	2157	LYS
1	B	2181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

### 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, 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	532/635 (83%)	0.12	13 (2%) 59 37	83, 119, 185, 247	0
1	B	539/635 (84%)	0.19	13 (2%) 59 37	83, 117, 185, 239	0
All	All	1071/1270 (84%)	0.16	26 (2%) 59 37	83, 118, 185, 247	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1974	PRO	4.9
1	A	2036	PRO	4.6
1	B	1722	TYR	3.4
1	B	2034	HIS	3.2
1	B	2200	PRO	3.1
1	B	1702	GLY	3.0
1	A	1976	ILE	2.9
1	A	1975	ASN	2.8
1	A	1627	PRO	2.5
1	A	1719	TYR	2.5
1	A	2178	GLY	2.5
1	A	1972	LEU	2.5
1	B	1999	ILE	2.4
1	A	1973	ASN	2.4
1	A	2034	HIS	2.3
1	B	1767	SER	2.3
1	B	1724	LEU	2.3
1	B	1764	THR	2.2
1	A	1702	GLY	2.2
1	A	1626	ILE	2.1
1	A	1971	THR	2.1
1	B	1897	TYR	2.1
1	B	1769	SER	2.1
1	B	1944	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2079	LEU	2.0
1	B	2000	ASP	2.0

## 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 monosaccharides 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.