



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 05:16 PM EDT

PDB ID : 9BWK / pdb\_00009bwk  
Title : Crystal structure of polyketoacyl-CoA thiolase from Burkholderia sp.  
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Deposited on : 2024-05-21  
Resolution : 2.20 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 : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

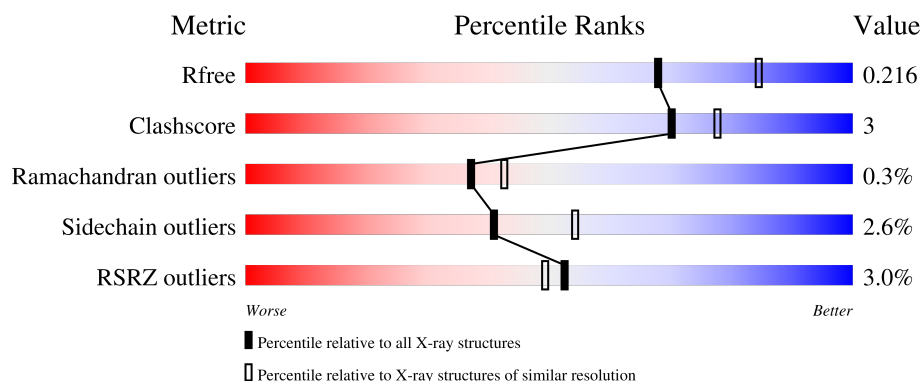
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	399	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	399	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11636 atoms, of which 5780 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	394	Total	C	H	N	O	S	0	0	0
			5754	1787	2892	516	545	14			
1	B	393	Total	C	H	N	O	S	0	0	0
			5745	1784	2888	515	544	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0AAC9EFY7
A	2	HIS	-	expression tag	UNP A0AAC9EFY7
A	79	ASN	ASP	conflict	UNP A0AAC9EFY7
B	1	GLY	-	expression tag	UNP A0AAC9EFY7
B	2	HIS	-	expression tag	UNP A0AAC9EFY7
B	79	ASN	ASP	conflict	UNP A0AAC9EFY7

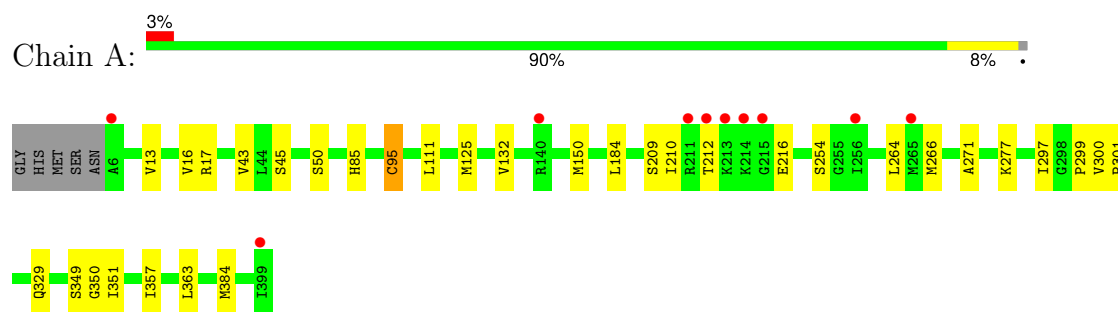
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	37	Total	O	0	0
			37	37		

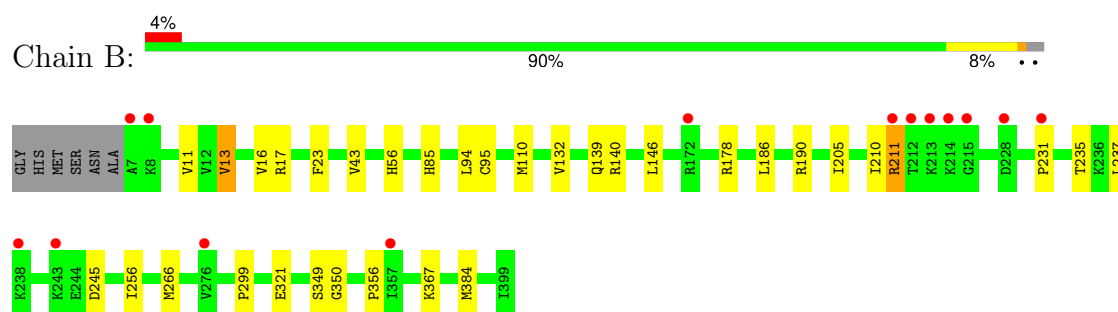
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.48Å 130.48Å 122.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 2.20 39.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (39.09-2.20) 92.7 (39.09-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, $R_{free}$	0.174 , 0.216 0.174 , 0.216	Depositor DCC
$R_{free}$ test set	1855 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.63	0/2905	0.79	0/3937
1	B	0.50	0/2900	0.68	0/3930
All	All	0.57	0/5805	0.74	0/7867

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	356	PRO	Peptide

### 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	2862	2892	2892	21	0
1	B	2857	2888	2887	18	0
2	A	100	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	0	0	0	0
All	All	5856	5780	5779	38	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.

All (38) 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:A:95:CYS:O	1:A:384:MET:HE2	1.90	0.72
1:B:132:VAL:HG22	1:B:146:LEU:HD12	1.71	0.70
1:B:13:VAL:HG11	1:B:266:MET:HE3	1.76	0.67
1:A:125:MET:HE3	1:A:150:MET:CG	2.26	0.66
1:B:16:VAL:HG12	1:B:43:VAL:HG13	1.77	0.65
1:A:266:MET:CE	1:A:271:ALA:HA	2.29	0.62
1:A:125:MET:HE3	1:A:150:MET:HG3	1.84	0.60
1:A:266:MET:HE1	1:A:271:ALA:HA	1.83	0.59
1:B:94:LEU:HD22	1:B:94:LEU:N	2.20	0.56
1:B:186:LEU:HD11	1:B:190:ARG:CZ	2.37	0.55
1:B:186:LEU:HD13	1:B:190:ARG:HG3	1.89	0.54
1:A:17:ARG:HD2	1:A:363:LEU:HG	1.90	0.54
1:A:266:MET:CE	1:A:271:ALA:CA	2.86	0.54
1:A:266:MET:HE2	1:A:271:ALA:CA	2.39	0.53
1:A:277:LYS:N	1:A:277:LYS:HD3	2.23	0.53
1:A:266:MET:CE	1:A:271:ALA:N	2.75	0.50
1:A:111:LEU:HD22	1:B:110:MET:HE2	1.94	0.49
1:A:125:MET:HE3	1:A:150:MET:HG2	1.95	0.49
1:B:231:PRO:O	1:B:235:THR:HG23	2.13	0.47
1:A:184:LEU:C	1:A:184:LEU:HD23	2.39	0.47
1:A:16:VAL:HG12	1:A:43:VAL:HG13	1.98	0.46
1:B:178:ARG:NH2	1:B:237:LEU:O	2.45	0.45
1:A:349:SER:OG	1:A:350:GLY:N	2.51	0.44
1:B:17:ARG:O	1:B:205:ILE:HA	2.17	0.44
1:A:254:SER:HA	1:A:351:ILE:HA	2.00	0.44
1:B:210:ILE:O	1:B:211:ARG:C	2.61	0.43
1:A:209:SER:OG	1:A:216:GLU:HG3	2.19	0.43
1:B:16:VAL:HG12	1:B:43:VAL:CG1	2.46	0.43
1:A:299:PRO:HG3	1:A:384:MET:C	2.44	0.42
1:A:300:VAL:HB	1:A:301:PRO:HD3	2.01	0.42
1:B:299:PRO:HG3	1:B:384:MET:C	2.44	0.42
1:B:139:GLN:O	1:B:140:ARG:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLU:OE1	1:B:367:LYS:NZ	2.52	0.41
1:A:210:ILE:O	1:A:212:THR:HG23	2.21	0.41
1:B:349:SER:OG	1:B:350:GLY:N	2.53	0.41
1:B:23:PHE:HB2	1:B:256:ILE:HD12	2.03	0.41
1:B:210:ILE:O	1:B:210:ILE:HG13	2.21	0.40
1:A:266:MET:HE2	1:A:271:ALA:HA	1.98	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	392/399 (98%)	379 (97%)	12 (3%)	1 (0%)	37	42
1	B	391/399 (98%)	377 (96%)	13 (3%)	1 (0%)	37	42
All	All	783/798 (98%)	756 (97%)	25 (3%)	2 (0%)	37	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	ILE
1	B	211	ARG

### 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	288/292 (99%)	279 (97%)	9 (3%)	35	47
1	B	288/292 (99%)	282 (98%)	6 (2%)	48	63
All	All	576/584 (99%)	561 (97%)	15 (3%)	41	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	45	SER
1	A	50	SER
1	A	85	HIS
1	A	95	CYS
1	A	132	VAL
1	A	264	LEU
1	A	297	ILE
1	A	329	GLN
1	B	11	VAL
1	B	13	VAL
1	B	56	HIS
1	B	85	HIS
1	B	95	CYS
1	B	245	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	159	GLN
1	B	159	GLN
1	B	274	GLN

### 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 oligosaccharides 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	394/399 (98%)	-0.41	10 (2%)	58 55	42, 56, 90, 159	0
1	B	393/399 (98%)	0.01	14 (3%)	46 43	47, 74, 116, 157	0
All	All	787/798 (98%)	-0.20	24 (3%)	52 49	42, 62, 110, 159	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	4.5
1	B	7	ALA	3.9
1	A	211	ARG	3.1
1	B	214	LYS	3.1
1	B	276	VAL	3.1
1	A	214	LYS	3.1
1	B	212	THR	3.1
1	B	211	ARG	3.0
1	A	213	LYS	3.0
1	B	215	GLY	2.9
1	A	265	MET	2.9
1	B	238	LYS	2.8
1	B	228	ASP	2.6
1	B	213	LYS	2.6
1	A	212	THR	2.6
1	A	256	ILE	2.4
1	B	172	ARG	2.4
1	B	231	PRO	2.4
1	A	399	ILE	2.3
1	B	357	ILE	2.3
1	B	243	LYS	2.1
1	B	8	LYS	2.1
1	A	140	ARG	2.0
1	A	215	GLY	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 oligosaccharides 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.