



# wwPDB X-ray Structure Validation Summary Report

Mar 10, 2026 – 07:53 AM UTC

PDB ID : 3IPL / pdb\_00003ipl  
Title : CRYSTAL STRUCTURE OF o-succinylbenzoic acid-CoA ligase FROM Staphylococcus aureus subsp. aureus Mu50  
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Deposited on : 2009-08-17  
Resolution : 2.30 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.

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 Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

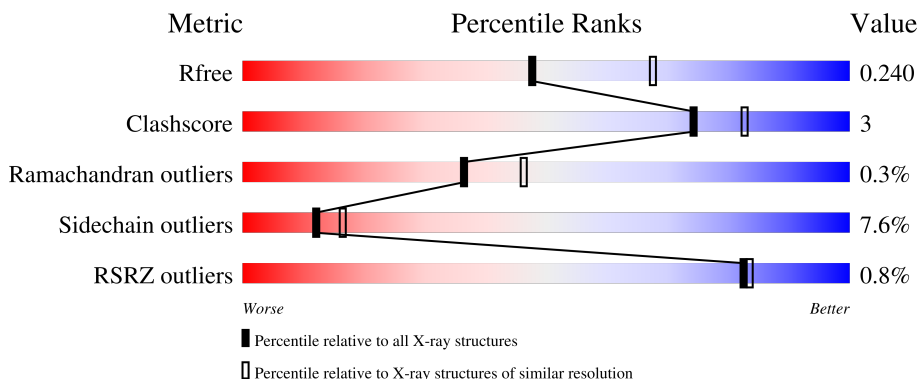
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	501	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 1%, green 99%, yellow 99%, orange 99%, grey 99%);"></div> <div style="margin-left: 10px;">%</div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>76%</span> <span>11%</span> <span>• 11%</span> </div>
1	B	501	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 1%, green 99%, yellow 99%, orange 99%, grey 99%);"></div> <div style="margin-left: 10px;">%</div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>75%</span> <span>12%</span> <span>• 11%</span> </div>
1	C	501	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, green 99%, yellow 99%, orange 99%, grey 99%);"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>62%</span> <span>7%</span> <span>• 29%</span> </div>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10478 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 2-succinylbenzoate--CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3588	2293	602	674	19	0	11	0
1	B	445	3600	2303	600	676	21	0	13	0
1	C	357	2873	1831	475	548	19	0	10	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P63526
A	1	LEU	-	expression tag	UNP P63526
A	492	GLU	-	expression tag	UNP P63526
A	493	GLY	-	expression tag	UNP P63526
A	494	HIS	-	expression tag	UNP P63526
A	495	HIS	-	expression tag	UNP P63526
A	496	HIS	-	expression tag	UNP P63526
A	497	HIS	-	expression tag	UNP P63526
A	498	HIS	-	expression tag	UNP P63526
A	499	HIS	-	expression tag	UNP P63526
B	0	SER	-	expression tag	UNP P63526
B	1	LEU	-	expression tag	UNP P63526
B	492	GLU	-	expression tag	UNP P63526
B	493	GLY	-	expression tag	UNP P63526
B	494	HIS	-	expression tag	UNP P63526
B	495	HIS	-	expression tag	UNP P63526
B	496	HIS	-	expression tag	UNP P63526
B	497	HIS	-	expression tag	UNP P63526
B	498	HIS	-	expression tag	UNP P63526
B	499	HIS	-	expression tag	UNP P63526
C	0	SER	-	expression tag	UNP P63526
C	1	LEU	-	expression tag	UNP P63526
C	492	GLU	-	expression tag	UNP P63526

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLY	-	expression tag	UNP P63526
C	494	HIS	-	expression tag	UNP P63526
C	495	HIS	-	expression tag	UNP P63526
C	496	HIS	-	expression tag	UNP P63526
C	497	HIS	-	expression tag	UNP P63526
C	498	HIS	-	expression tag	UNP P63526
C	499	HIS	-	expression tag	UNP P63526

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	162	Total 162	O 162	0	0
2	B	152	Total 152	O 152	0	0
2	C	103	Total 103	O 103	0	0



GLU	THR	VAL	VAL	ARG	ARG	VAL	ALA	PRO	LYS	ASP	LEU	ILE	ILE	SER	PRO	SER	SER	GLY	ALA	ASN	ILE	L154	GLU	ASN	ASN	ILE	D162	PRO	TYR	TYR	PRO	LYS	HIS	PHE	GLN	ILE	ILE	GLU	GLU	THR	VAL	ASP	THR	ALA	LYS	GLN	GLN	PHE	PRO	PRO	GLY	ILE	ILE	THR	ASP	ASP	ASP	TRP	THR	GLY	GLN	VAL	PRO	PRO	E348	LYS	L349	M350	LYS	I351	TYR	PHE	VAL	L361	SER	GLU	P363	SER	ASP	N376	ASP	ILE	I383	SER	LYS	LYS	V389	ALA
D393	ARG	ARG	ALA	TYR	LEU	ASP	LEU	ILE	ILE	LEU	GLY	GLY	ASN	ASN	ILE	TYR	PRO	LYS	HIS	PHE	GLN	ILE	ILE	GLU	GLU	THR	VAL	ASP	THR	ALA	LYS	GLN	GLN	PHE	PRO	PRO	GLY	ILE	ILE	THR	ASP	ASP	ASP	TRP	THR	GLY	GLN	VAL	PRO	PRO	E348	LYS	L349	M350	LYS	I351	TYR	PHE	VAL	L361	SER	GLU	P363	SER	ASP	N376	ASP	ILE	I383	SER	LYS	LYS	V389	ALA														
GLN	LEU	ILE	ALA	TYR	LEU	ASP	LEU	ILE	ILE	LEU	GLY	GLY	ASN	ASN	ILE	TYR	PRO	LYS	HIS	PHE	GLN	ILE	ILE	GLU	GLU	THR	VAL	ASP	THR	ALA	LYS	GLN	GLN	PHE	PRO	PRO	GLY	ILE	ILE	THR	ASP	ASP	ASP	TRP	THR	GLY	GLN	VAL	PRO	PRO	E348	LYS	L349	M350	LYS	I351	TYR	PHE	VAL	L361	SER	GLU	P363	SER	ASP	N376	ASP	ILE	I383	SER	LYS	LYS	V389	ALA														

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.51Å 65.42Å 114.96Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.0 (20.00-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.185 , 0.241 0.184 , 0.240	Depositor DCC
$R_{free}$ test set	1311 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.8	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	0.96	EDS
Total number of atoms	10478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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	0.59	1/3699 (0.0%)	0.90	4/5020 (0.1%)
1	B	0.61	0/3714	0.93	1/5038 (0.0%)
1	C	0.59	0/2958	0.95	3/4015 (0.1%)
All	All	0.60	1/10371 (0.0%)	0.93	8/14073 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	TYR	CA-C	-8.00	1.49	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	GLY	N-CA-C	7.27	118.91	111.56
1	C	101	LEU	CA-C-N	6.75	128.27	119.84
1	C	101	LEU	C-N-CA	6.75	128.27	119.84
1	C	327	VAL	N-CA-C	-5.59	107.33	113.43
1	A	392	TYR	CA-C-O	5.36	121.71	118.33

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	3588	0	3594	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3600	0	3603	23	0
1	C	2873	0	2858	17	0
2	A	162	0	0	2	0
2	B	152	0	0	0	0
2	C	103	0	0	1	0
All	All	10478	0	10055	63	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 63 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:208:VAL:HG13	1:A:233:VAL:HG22	1.46	0.98
1:A:208:VAL:CG1	1:A:233:VAL:HG22	2.11	0.81
1:B:167:MET:HE2	1:B:306:THR:HG23	1.64	0.79
1:A:149:SER:HB2	1:A:152:ASN:HD22	1.58	0.67
1:B:242:LEU:HD22	1:B:246:LYS:HE3	1.75	0.67

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	452/501 (90%)	437 (97%)	14 (3%)	1 (0%)	43 55
1	B	454/501 (91%)	441 (97%)	12 (3%)	1 (0%)	43 55
1	C	363/501 (72%)	351 (97%)	9 (2%)	3 (1%)	16 20
All	All	1269/1503 (84%)	1229 (97%)	35 (3%)	5 (0%)	36 38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	SER
1	B	310	SER
1	C	310[A]	SER
1	C	310[B]	SER
1	C	102	PRO

### 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	401/440 (91%)	371 (92%)	30 (8%)	12	17
1	B	403/440 (92%)	366 (91%)	37 (9%)	8	11
1	C	322/440 (73%)	301 (94%)	21 (6%)	15	22
All	All	1126/1320 (85%)	1038 (92%)	88 (8%)	12	16

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	351	ILE
1	C	80	LEU
1	B	366	LEU
1	B	457	LEU
1	C	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	29	ASN
1	C	45	GLN
1	A	333	ASN
1	A	266	GLN
1	C	88	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 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 [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	445/501 (88%)	-0.34	4 (0%) 81 82	20, 43, 76, 105	11 (2%)
1	B	445/501 (88%)	-0.25	5 (1%) 78 79	21, 42, 101, 127	13 (2%)
1	C	357/501 (71%)	-0.40	1 (0%) 90 90	21, 43, 77, 105	10 (2%)
All	All	1247/1503 (82%)	-0.33	10 (0%) 82 83	20, 43, 88, 127	34 (2%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	SER	3.7
1	C	1	LEU	3.0
1	A	150	PRO	2.8
1	B	118	PHE	2.8
1	A	153	ILE	2.7

### 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.