



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:59 AM UTC

PDB ID : 4WL3 / pdb\_00004wl3  
Title : Crystal structure determination of Bile Salt Hydrolase from *Enterococcus faecalis*  
Authors : Ramasamy, S.; Chand, D.; Suresh, C.G.  
Deposited on : 2014-10-06  
Resolution : 2.01 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

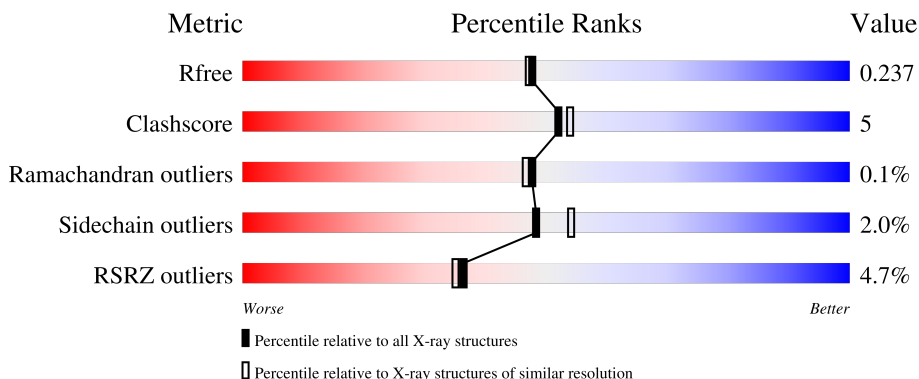
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

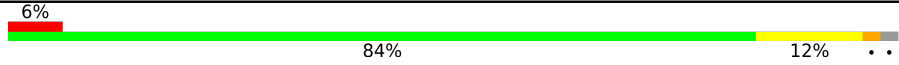


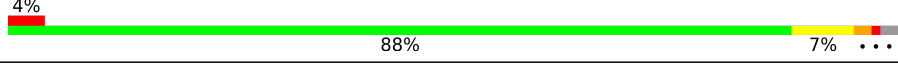
The reported resolution of this entry is 2.01 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	331	 6% 84% 12% ..
1	B	331	 3% 85% 10% ..
1	C	331	 5% 88% 8% ..
1	D	331	 4% 88% 7% ...

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10507 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 Bile salt hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2597	1658	420	510	9	0	0	0
1	B	323	2597	1658	420	510	9	0	0	0
1	C	323	2597	1658	420	510	9	0	0	0
1	D	323	2597	1658	420	510	9	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	LEU	-	expression tag	UNP C7CXJ5
A	326	GLU	-	expression tag	UNP C7CXJ5
A	327	HIS	-	expression tag	UNP C7CXJ5
A	328	HIS	-	expression tag	UNP C7CXJ5
A	329	HIS	-	expression tag	UNP C7CXJ5
A	330	HIS	-	expression tag	UNP C7CXJ5
A	331	HIS	-	expression tag	UNP C7CXJ5
A	332	HIS	-	expression tag	UNP C7CXJ5
B	325	LEU	-	expression tag	UNP C7CXJ5
B	326	GLU	-	expression tag	UNP C7CXJ5
B	327	HIS	-	expression tag	UNP C7CXJ5
B	328	HIS	-	expression tag	UNP C7CXJ5
B	329	HIS	-	expression tag	UNP C7CXJ5
B	330	HIS	-	expression tag	UNP C7CXJ5
B	331	HIS	-	expression tag	UNP C7CXJ5
B	332	HIS	-	expression tag	UNP C7CXJ5
C	325	LEU	-	expression tag	UNP C7CXJ5
C	326	GLU	-	expression tag	UNP C7CXJ5
C	327	HIS	-	expression tag	UNP C7CXJ5
C	328	HIS	-	expression tag	UNP C7CXJ5
C	329	HIS	-	expression tag	UNP C7CXJ5

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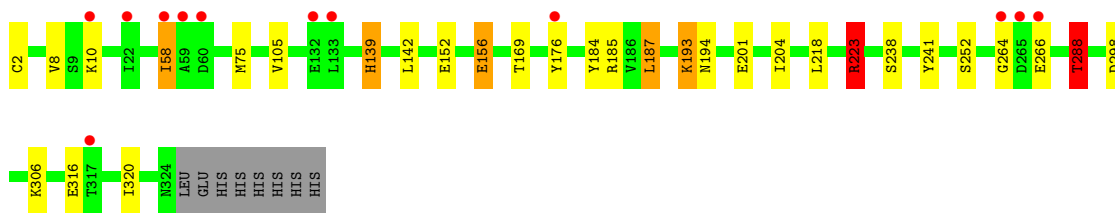
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Chain	Residue	Modelled	Actual	Comment	Reference
C	330	HIS	-	expression tag	UNP C7CXJ5
C	331	HIS	-	expression tag	UNP C7CXJ5
C	332	HIS	-	expression tag	UNP C7CXJ5
D	325	LEU	-	expression tag	UNP C7CXJ5
D	326	GLU	-	expression tag	UNP C7CXJ5
D	327	HIS	-	expression tag	UNP C7CXJ5
D	328	HIS	-	expression tag	UNP C7CXJ5
D	329	HIS	-	expression tag	UNP C7CXJ5
D	330	HIS	-	expression tag	UNP C7CXJ5
D	331	HIS	-	expression tag	UNP C7CXJ5
D	332	HIS	-	expression tag	UNP C7CXJ5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	30	Total O 30 30	0	0
2	C	32	Total O 32 32	0	0
2	D	23	Total O 23 23	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.20Å 131.62Å 86.72Å 90.00° 94.48° 90.00°	Depositor
Resolution (Å)	41.07 – 2.01 41.07 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.3 (41.07-2.01) 95.3 (41.07-2.01)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.205 , 0.235 0.212 , 0.237	Depositor DCC
$R_{free}$ test set	4645 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtrriage
Anisotropy	0.016	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 30.1	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	0.92	EDS
Total number of atoms	10507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	1.24	5/2656 (0.2%)	1.06	7/3601 (0.2%)
1	B	1.18	4/2656 (0.2%)	1.10	12/3601 (0.3%)
1	C	1.18	4/2656 (0.2%)	1.06	5/3601 (0.1%)
1	D	1.18	2/2656 (0.1%)	1.07	6/3601 (0.2%)
All	All	1.20	15/10624 (0.1%)	1.07	30/14404 (0.2%)

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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLY	N-CA	7.83	1.57	1.45
1	A	102	ILE	CA-CB	7.60	1.58	1.54
1	D	223	ARG	CD-NE	-7.22	1.36	1.46
1	C	223	ARG	CD-NE	-6.55	1.37	1.46
1	A	135	LEU	N-CA	5.98	1.53	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	ARG	NE-CZ-NH2	-11.52	108.83	119.20
1	D	223	ARG	NE-CZ-NH2	-11.20	109.12	119.20
1	C	223	ARG	NE-CZ-NH1	9.60	131.10	121.50
1	D	288	THR	N-CA-CB	-9.04	97.06	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	ARG	CD-NE-CZ	8.73	136.62	124.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ILE	Peptide
1	B	57	GLY	Peptide
1	D	223	ARG	Sidechain

## 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	2597	0	2504	37	1
1	B	2597	0	2504	34	0
1	C	2597	0	2504	19	1
1	D	2597	0	2504	33	0
2	A	34	0	0	0	1
2	B	30	0	0	0	0
2	C	32	0	0	0	1
2	D	23	0	0	0	0
All	All	10507	0	10016	103	2

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.

The worst 5 of 103 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:218:LEU:O	1:A:223:ARG:NH1	1.66	1.26
1:A:207:ARG:NH1	1:B:21:GLU:OE2	1.98	0.96
1:D:75:MET:HE1	1:D:105:VAL:HB	1.59	0.84
1:A:75:MET:HE1	1:A:105:VAL:CG1	2.07	0.83
1:D:75:MET:HE1	1:D:105:VAL:CG1	2.08	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:405:HOH:O	2:C:401:HOH:O[1_655]	1.24	0.96
1:A:24:TYR:OH	1:C:20:TYR:OH[1_655]	2.15	0.05

## 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	321/331 (97%)	308 (96%)	13 (4%)	0	100	100
1	B	321/331 (97%)	309 (96%)	11 (3%)	1 (0%)	36	35
1	C	321/331 (97%)	314 (98%)	7 (2%)	0	100	100
1	D	321/331 (97%)	306 (95%)	15 (5%)	0	100	100
All	All	1284/1324 (97%)	1237 (96%)	46 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ASP

### 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	290/298 (97%)	285 (98%)	5 (2%)	53	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	290/298 (97%)	286 (99%)	4 (1%)	59	66
1	C	290/298 (97%)	283 (98%)	7 (2%)	43	47
1	D	290/298 (97%)	283 (98%)	7 (2%)	43	47
All	All	1160/1192 (97%)	1137 (98%)	23 (2%)	48	54

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	201	GLU
1	D	139	HIS
1	D	58	ILE
1	D	156	GLU
1	B	139	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	GLN
1	C	324	ASN
1	D	183	ASN
1	D	139	HIS
1	B	25	ASN

### 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	323/331 (97%)	0.16	20 (6%) 26 25	9, 16, 38, 120	0
1	B	323/331 (97%)	-0.06	11 (3%) 48 47	10, 15, 31, 68	0
1	C	323/331 (97%)	0.03	18 (5%) 30 29	10, 15, 32, 63	0
1	D	323/331 (97%)	0.01	12 (3%) 45 44	10, 16, 34, 61	0
All	All	1292/1324 (97%)	0.04	61 (4%) 36 35	9, 16, 34, 120	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	PHE	10.4
1	A	133	LEU	8.5
1	D	59	ALA	8.3
1	A	128	ASN	7.8
1	A	134	PRO	7.6

### 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 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.