

# Full wwPDB X-ray Structure Validation Report (i)

### Feb 5, 2024 – 01:54 AM EST

PDB ID	:	1TIC
Title	:	CONFORMATIONAL LABILITY OF LIPASES OBSERVED IN THE AB-
		SENCE OF AN OIL-WATER INTERFACE: CRYSTALLOGRAPHIC STUD-
		IES OF ENZYMES FROM THE FUNGI HUMICOLA LANUGINOSA AND
		RHIZOPUS DELEMAR
Authors	:	Derewenda, U.; Swenson, L.; Green, R.; Joerger, R.; Haas, M.J.; Derewenda,
		Z.S.
Deposited on		
Resolution	:	2.60  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.60 Å.

141614

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		Percent	tile Ranks	Value	
	Clashscore		]	7	
	Worse	-		Better	
	Perc	entile relative to all X-ray structures			
	Perc	entile relative to X-ray structures of sin	milar resolution		
	Metric	Whole archive	Sin	nilar resolution	
	wiethic	$(\# {\rm Entries})$	(#Entries	, resolution $range(\text{\AA}))$	

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 >=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 <=5%

3518(2.60-2.60)

Note EDS was not executed.

Clashscore

Mol	Chain	Length	Quality of chain			
1	А	269	97%	•		
1	В	269	99%	•		



### $1 \mathrm{TIC}$

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 534 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.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	А	265	Total C   265 265	0	0	265
1	В	269	Total C   269 269	0	0	269

• Molecule 1 is a protein called LIPASE.



# 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. 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. 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.

Note EDS was not executed.

• Molecule 1: LIPASE

V3 P3 V2 P2

Chain A:	97%	••
SER ASP GLY GLY V209 V229 V229 L269 L269		
• Molecule 1: LIPASE		
Chain B:	99%	·



## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	C 1 21 1	Depositor	
Cell constants	92.77Å 128.86Å 78.35Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $135.82^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	7.50 - 2.60	Depositor	
% Data completeness	(Not available) (7.50-2.60)	Depositor	
(in resolution range)	(100 available) (1.50-2.00)	Depositor	
$R_{merge}$	(Not available)	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
Refinement program	PROLSQ	Depositor	
$R, R_{free}$	0.160 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	534	wwPDB-VP	
Average B, all atoms $(Å^2)$	15.0	wwPDB-VP	



# 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	А	265	0	0	2	0
1	В	269	0	0	2	0
All	All	534	0	0	4	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 7.

All (4) 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:33:VAL:CA	1:B:34:PRO:CA	2.90	0.49
1:A:249:VAL:CA	1:A:250:PRO:CA	2.91	0.49
1:A:209:VAL:CA	1:A:210:PRO:CA	2.93	0.47
1:B:249:VAL:CA	1:B:250:PRO:CA	2.99	0.41

There are no symmetry-related clashes.



## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 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 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

