

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

May 27, 2020 – 02:19 am BST

PDB ID : 1TIB

Title : CONFORMATIONAL LABILITY OF LIPASES OBSERVED IN THE AB-

SENCE OF AN OIL-WATER INTERFACE: CRYSTALLOGRAPHIC STUDIES OF ENZYMES FROM THE FUNGI HUMICOLA LANUGINOSA AND

RHIZOPUS DELEMAR

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Deposited on : 1993-12-06

Resolution : 1.84 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Xtriage (Phenix) : NOT EXECUTED 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)

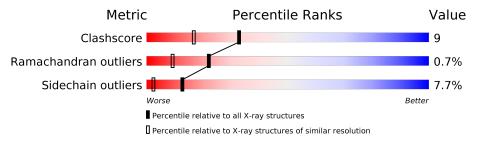
Validation Pipeline (wwPDB-VP) : 2.11

# 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 1.84 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar  resolution} \\ (\#{\rm Entries,  resolution  range(\AA)}) \end{array}$
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of cha	iin	
1	A	269	61%	30%	7% •



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2427 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 LIPASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	269	Total 2071	C 1303	N 359	O 403	S 6	0	0	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	356	Total O 356 356	0	0

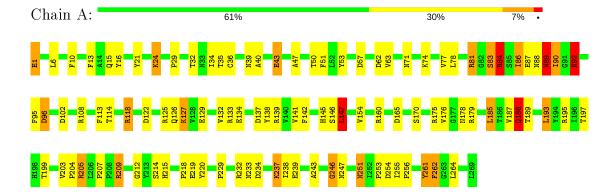


# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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





# 4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	103.17Å 51.99Å 45.73Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	7.50 - 1.84	Depositor
% Data completeness	(Not available) (7.50-1.84)	Depositor
(in resolution range)	, , , , , , , , , , , , , , , , , , ,	Беровног
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
$R, R_{free}$	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2427	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	28.0	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).

Mol	Chain	Boı	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	1.24	$4/2121 \ (0.2\%)$	2.69	117/2887 (4.1%)	

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	3

#### All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	A	127	LYS	CD-CE	20.74	2.03	1.51
1	A	24	LYS	CD-CE	9.15	1.74	1.51
1	A	127	LYS	CB-CG	6.12	1.69	1.52
1	A	209	ARG	CD-NE	5.34	1.55	1.46

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	84	ARG	NE-CZ-NH1	52.11	146.35	120.30
1	A	84	ARG	NE-CZ-NH2	-42.01	99.29	120.30
1	A	118	ARG	CD-NE-CZ	37.45	176.03	123.60
1	A	209	ARG	NE-CZ-NH1	17.29	128.94	120.30
1	A	89	TRP	N-CA-CB	14.05	135.90	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	84	ARG	Sidechain
1	A	89	TRP	Mainchain

### 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	2071	0	1965	35	0
2	A	356	0	0	10	0
All	All	2427	0	1965	35	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 9.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:A:127:LYS:CE	1:A:127:LYS:CD	2.03	1.36
1:A:205:ARG:HH22	1:A:251:ASN:HD21	1.02	0.93
1:A:1:GLU:HG2	1:A:233:ASN:HA	1.61	0.83
1:A:205:ARG:HH22	1:A:251:ASN:ND2	1.82	0.75
1:A:127:LYS:CG	1:A:127:LYS:CE	2.67	0.73

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.



Mo	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	267/269 (99%)	255 (96%)	10 (4%)	2 (1%)	22 9

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	THR
1	A	92	ASN

#### 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	$220/220 \; (100\%)$	203 (92%)	17 (8%)	13 2

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
1	A	147	LEU
1	A	237	LYS
1	A	95	PHE
1	A	251	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	$\mathbf{Type}$
1	A	92	ASN
1	A	251	ASN
1	A	188	GLN
1	A	33	ASN
1	A	135	HIS

#### 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 carbohydrates 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.

