



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:23 PM GMT

PDB ID : 1TIB
Title : CONFORMATIONAL LABILITY OF LIPASES OBSERVED IN THE ABSENCE OF AN OIL-WATER INTERFACE: CRYSTALLOGRAPHIC STUDIES OF ENZYMES FROM THE FUNGI HUMICOLA LANUGINOSA AND RHIZOPUS DELEMAR
Authors : Derewenda, U.; Swenson, L.; Wei, Y.; Derewenda, Z.S.
Deposited on : 1993-12-06
Resolution : 1.84 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

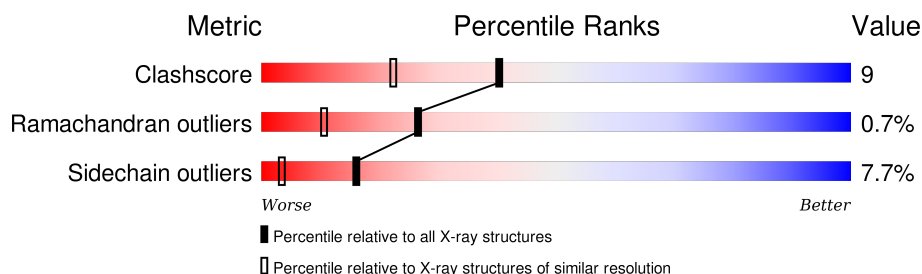
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (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. 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.

Note EDS was not executed.

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

2 Entry composition

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	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

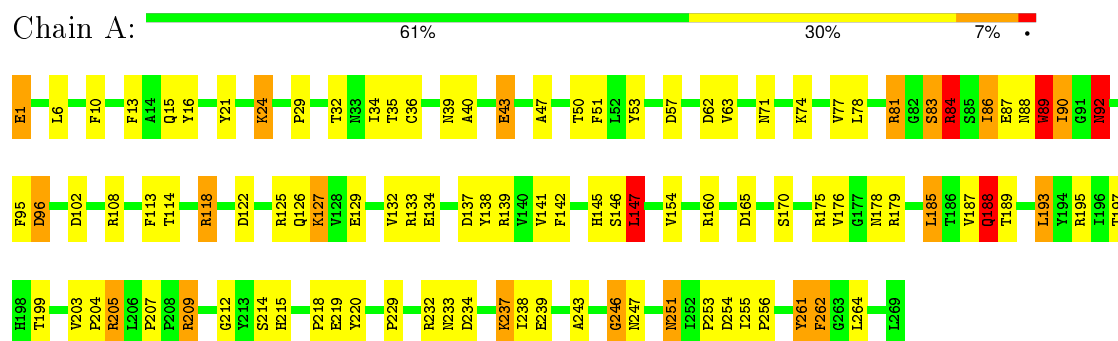
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	356	Total	O	0	0
			356	356		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: LIPASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.17Å 51.99Å 45.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 1.84	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-1.84)	Depositor
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 (Å 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	Bond lengths		Bond angles	
		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	Z	Observed(Å)	Ideal(Å)
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

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	187	VAL	CA-CB-CG2	12.54	129.72	110.90
1	A	179	ARG	NE-CZ-NH1	-12.49	114.05	120.30
1	A	232	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	127	LYS	CB-CG-CD	-11.79	80.96	111.60
1	A	209	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	89	TRP	CA-CB-CG	11.36	135.28	113.70
1	A	127	LYS	CB-CA-C	10.62	131.64	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LYS	N-CA-CB	-10.41	91.86	110.60
1	A	187	VAL	CB-CA-C	9.66	129.75	111.40
1	A	147	LEU	CB-CG-CD2	-9.63	94.62	111.00
1	A	160	ARG	NE-CZ-NH1	-9.51	115.54	120.30
1	A	262	PHE	C-N-CA	9.40	142.05	122.30
1	A	108	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	81	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	A	53	TYR	CB-CG-CD2	8.77	126.26	121.00
1	A	108	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	A	62	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	195	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	108	ARG	CD-NE-CZ	8.40	135.36	123.60
1	A	102	ASP	CB-CG-OD1	8.24	125.71	118.30
1	A	125	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	A	187	VAL	CG1-CB-CG2	-8.11	97.92	110.90
1	A	122	ASP	CB-CG-OD2	8.06	125.55	118.30
1	A	137	ASP	CB-CG-OD1	8.06	125.55	118.30
1	A	142	PHE	CB-CG-CD1	7.92	126.34	120.80
1	A	234	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	137	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	138	TYR	CB-CG-CD1	7.78	125.67	121.00
1	A	179	ARG	NH1-CZ-NH2	7.74	127.92	119.40
1	A	139	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	232	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	188	GLN	CA-CB-CG	7.52	129.95	113.40
1	A	197	THR	CA-CB-CG2	7.46	122.84	112.40
1	A	138	TYR	CB-CG-CD2	-7.39	116.56	121.00
1	A	89	TRP	CA-C-O	-7.36	104.64	120.10
1	A	89	TRP	CA-C-N	7.30	133.27	117.20
1	A	195	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	A	147	LEU	CA-CB-CG	7.19	131.84	115.30
1	A	203	VAL	CG1-CB-CG2	7.19	122.41	110.90
1	A	195	ARG	NH1-CZ-NH2	-7.16	111.52	119.40
1	A	142	PHE	CB-CG-CD2	-7.15	115.79	120.80
1	A	262	PHE	O-C-N	-7.15	111.05	123.20
1	A	84	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
1	A	209	ARG	CD-NE-CZ	6.94	133.31	123.60
1	A	83	SER	N-CA-CB	-6.89	100.16	110.50
1	A	254	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	A	90	ILE	CB-CA-C	6.70	124.99	111.60
1	A	84	ARG	CG-CD-NE	6.60	125.66	111.80
1	A	90	ILE	CA-C-N	6.55	129.31	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LYS	CG-CD-CE	-6.51	92.37	111.90
1	A	254	ASP	N-CA-CB	-6.50	98.90	110.60
1	A	203	VAL	CA-CB-CG2	-6.47	101.19	110.90
1	A	84	ARG	CB-CA-C	6.46	123.31	110.40
1	A	13	PHE	CB-CG-CD1	6.45	125.31	120.80
1	A	187	VAL	CA-CB-CG1	-6.44	101.24	110.90
1	A	84	ARG	CA-CB-CG	6.37	127.41	113.40
1	A	53	TYR	CA-CB-CG	6.36	125.47	113.40
1	A	133	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	57	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	134	GLU	CB-CA-C	-6.20	98.00	110.40
1	A	21	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	A	35	THR	CA-CB-CG2	6.11	120.95	112.40
1	A	219	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	141	VAL	CA-CB-CG2	6.06	119.99	110.90
1	A	47	ALA	O-C-N	-6.01	113.08	122.70
1	A	86	ILE	CB-CA-C	-5.96	99.67	111.60
1	A	86	ILE	CA-C-N	5.96	130.32	117.20
1	A	125	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	77	VAL	O-C-N	5.78	131.95	122.70
1	A	134	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	A	215	HIS	CA-CB-CG	5.73	123.33	113.60
1	A	88	ASN	N-CA-CB	-5.71	100.32	110.60
1	A	92	ASN	OD1-CG-ND2	-5.64	108.94	121.90
1	A	43	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	A	16	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	126	GLN	CA-C-O	5.62	131.90	120.10
1	A	113	PHE	CB-CG-CD2	-5.61	116.87	120.80
1	A	165	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	229	PRO	O-C-N	5.57	131.62	122.70
1	A	176	VAL	CA-CB-CG2	5.55	119.22	110.90
1	A	205	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	92	ASN	N-CA-CB	5.48	120.47	110.60
1	A	243	ALA	CB-CA-C	5.47	118.30	110.10
1	A	84	ARG	CD-NE-CZ	5.44	131.22	123.60
1	A	63	VAL	CA-CB-CG2	5.44	119.06	110.90
1	A	170	SER	O-C-N	-5.41	114.05	122.70
1	A	122	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	126	GLN	O-C-N	-5.37	114.12	122.70
1	A	214	SER	CB-CA-C	5.35	120.27	110.10
1	A	50	THR	CA-CB-CG2	5.34	119.88	112.40
1	A	175	ARG	CG-CD-NE	-5.32	100.62	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLN	C-N-CA	5.32	134.99	121.70
1	A	16	TYR	CB-CG-CD1	5.30	124.18	121.00
1	A	90	ILE	C-N-CA	5.29	133.42	122.30
1	A	145	HIS	CA-CB-CG	5.29	122.59	113.60
1	A	83	SER	CB-CA-C	5.29	120.14	110.10
1	A	146	SER	N-CA-CB	-5.28	102.58	110.50
1	A	89	TRP	N-CA-C	-5.23	96.87	111.00
1	A	96	ASP	N-CA-CB	5.22	120.00	110.60
1	A	246	GLY	N-CA-C	-5.22	100.04	113.10
1	A	53	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	43	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	A	256	PRO	O-C-N	-5.20	114.38	122.70
1	A	185	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	10	PHE	CB-CG-CD1	5.13	124.39	120.80
1	A	132	VAL	O-C-N	-5.11	114.52	122.70
1	A	219	GLU	CG-CD-OE1	5.11	128.52	118.30
1	A	13	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	261	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	189	THR	CA-CB-OG1	-5.04	98.42	109.00
1	A	205	ARG	CG-CD-NE	-5.04	101.22	111.80
1	A	129	GLU	CG-CD-OE2	-5.04	108.23	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ARG	Sidechain
1	A	84	ARG	Sidechain
1	A	89	TRP	Mainchain

5.2 Too-close contacts ⓘ

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.

All (35) 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: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
1:A:15:GLN:HE22	1:A:43:GLU:H	1.35	0.73
1:A:71:ASN:O	1:A:74:LYS:HE2	1.89	0.72
1:A:188:GLN:HE22	1:A:193:LEU:H	1.39	0.71
1:A:237:LYS:HE2	1:A:239:GLU:OE2	1.92	0.69
1:A:237:LYS:NZ	2:A:502:HOH:O	2.27	0.67
1:A:188:GLN:NE2	1:A:193:LEU:H	1.94	0.65
1:A:89:TRP:HE3	1:A:92:ASN:HD22	1.45	0.65
1:A:205:ARG:NH2	1:A:251:ASN:HD21	1.85	0.64
1:A:15:GLN:NE2	1:A:43:GLU:H	2.03	0.55
1:A:86:ILE:HD12	1:A:87:GLU:HG3	1.90	0.54
1:A:220:TYR:CE1	1:A:237:LYS:HG3	2.43	0.52
1:A:24:LYS:HG2	2:A:318:HOH:O	2.12	0.50
1:A:84:ARG:HG2	2:A:447:HOH:O	2.11	0.50
1:A:207:PRO:HG3	2:A:564:HOH:O	2.12	0.49
1:A:178:ASN:HA	1:A:212:GLY:O	2.13	0.47
1:A:204:PRO:HB2	1:A:247:ASN:ND2	2.30	0.47
1:A:261:TYR:O	1:A:262:PHE:HB2	2.16	0.46
1:A:238:ILE:HD13	1:A:246:GLY:HA3	1.99	0.44
1:A:36:CYS:HB3	1:A:40:ALA:HB3	1.99	0.44
1:A:218:PRO:HD3	2:A:465:HOH:O	2.18	0.43
1:A:147:LEU:HB2	2:A:490:HOH:O	2.18	0.43
1:A:114:THR:O	1:A:118:ARG:HG3	2.19	0.42
1:A:86:ILE:HD13	1:A:255:ILE:HG23	2.02	0.42
1:A:127:LYS:HG2	2:A:450:HOH:O	2.19	0.41
1:A:29:PRO:HG2	1:A:32:THR:HG21	2.01	0.41
1:A:209:ARG:HG3	2:A:282:HOH:O	2.20	0.41
1:A:209:ARG:HB3	1:A:209:ARG:HE	1.65	0.41
1:A:188:GLN:HA	2:A:368:HOH:O	2.20	0.41
1:A:34:ILE:HG12	1:A:51:PHE:CZ	2.55	0.40
1:A:39:ASN:HA	2:A:543:HOH:O	2.20	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	267/269 (99%)	255 (96%)	10 (4%)	2 (1%)	26	10

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%)	16	3

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	6	LEU
1	A	78	LEU
1	A	83	SER
1	A	84	ARG
1	A	90	ILE
1	A	95	PHE
1	A	96	ASP
1	A	147	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	154	VAL
1	A	185	LEU
1	A	188	GLN
1	A	193	LEU
1	A	237	LYS
1	A	251	ASN
1	A	253	PRO
1	A	264	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	25	ASN
1	A	33	ASN
1	A	71	ASN
1	A	92	ASN
1	A	135	HIS
1	A	188	GLN
1	A	247	ASN
1	A	251	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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.