



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:09 AM GMT

PDB ID : 2FX5
Title : Pseudomonas mendocina lipase
Authors : Bott, R.; Wu, S.
Deposited on : 2006-02-03
Resolution : 1.80 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

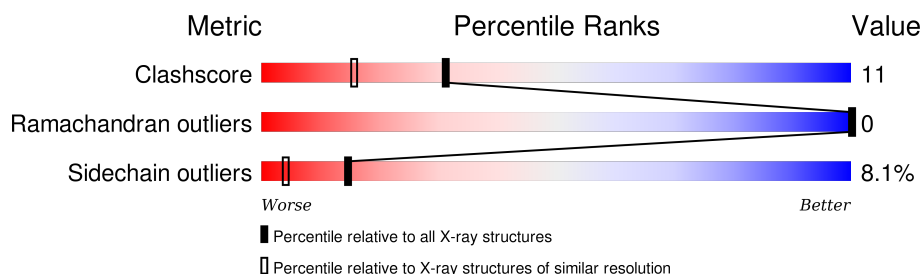
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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	258	 69% 21% 7% •

2 Entry composition [i](#)

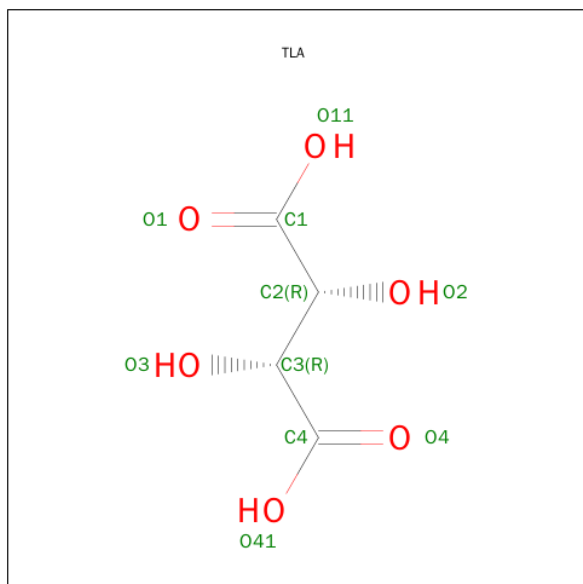
There are 3 unique types of molecules in this entry. The entry contains 2061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	258	1947	1214	358	366	9	0	0	0

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	4	6	0	0

- Molecule 3 is water.

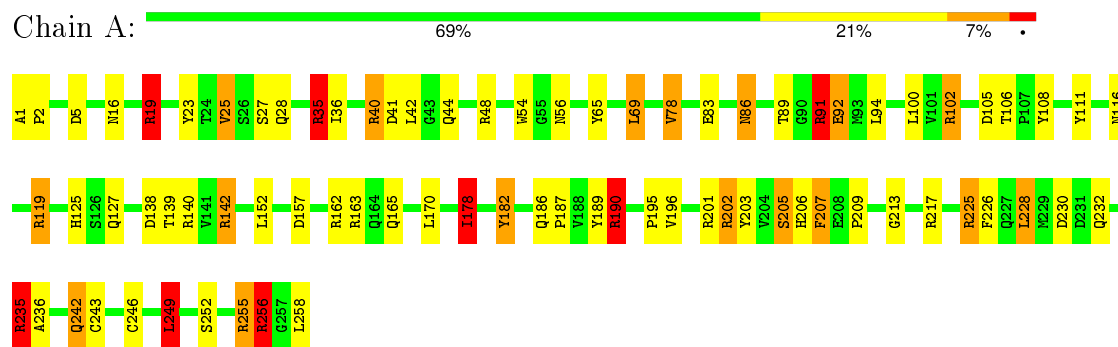
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	104	104	104	0	0

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 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	58.50Å 58.50Å 145.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2061	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLA

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	0.86	0/2003	2.17	71/2724 (2.6%)

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	7

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	NE-CZ-NH2	-28.93	105.84	120.30
1	A	256	ARG	NE-CZ-NH1	22.33	131.46	120.30
1	A	19	ARG	NE-CZ-NH2	-21.08	109.76	120.30
1	A	162	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	A	119	ARG	NE-CZ-NH2	12.77	126.68	120.30
1	A	35	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	A	163	ARG	CD-NE-CZ	11.55	139.77	123.60
1	A	217	ARG	NE-CZ-NH2	11.17	125.88	120.30
1	A	19	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	202	ARG	NE-CZ-NH1	10.59	125.60	120.30
1	A	91	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	A	235	ARG	CD-NE-CZ	10.46	138.24	123.60
1	A	225	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	203	TYR	CB-CG-CD1	-10.20	114.88	121.00
1	A	162	ARG	CD-NE-CZ	9.91	137.47	123.60
1	A	35	ARG	NE-CZ-NH1	-9.56	115.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH1	-9.34	115.63	120.30
1	A	142	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	255	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	A	48	ARG	CD-NE-CZ	8.84	135.97	123.60
1	A	23	TYR	O-C-N	8.77	136.72	122.70
1	A	255	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	41	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	201	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	157	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	A	256	ARG	CD-NE-CZ	8.07	134.90	123.60
1	A	182	TYR	CB-CG-CD1	7.69	125.61	121.00
1	A	25	VAL	N-CA-CB	-7.67	94.63	111.50
1	A	249	LEU	CB-CA-C	7.26	124.00	110.20
1	A	142	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	242	GLN	N-CA-CB	-7.17	97.70	110.60
1	A	201	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	111	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	48	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	91	ARG	CG-CD-NE	6.95	126.39	111.80
1	A	138	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	102	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	A	83	GLU	CA-CB-CG	6.38	127.44	113.40
1	A	106	THR	N-CA-CB	6.29	122.24	110.30
1	A	65	TYR	CB-CG-CD1	6.24	124.75	121.00
1	A	207	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	A	203	TYR	CB-CA-C	-6.17	98.06	110.40
1	A	78	VAL	N-CA-CB	6.11	124.95	111.50
1	A	182	TYR	CG-CD2-CE2	6.06	126.15	121.30
1	A	163	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	105	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	178	ILE	CA-CB-CG2	6.00	122.90	110.90
1	A	230	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	196	VAL	CB-CA-C	-5.99	100.02	111.40
1	A	189	TYR	CB-CG-CD1	-5.94	117.43	121.00
1	A	69	LEU	CB-CA-C	5.80	121.21	110.20
1	A	190	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	5	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	258	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	108	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	152	LEU	CA-C-N	5.68	127.56	116.20
1	A	91	ARG	CD-NE-CZ	5.67	131.53	123.60
1	A	162	ARG	NH1-CZ-NH2	-5.66	113.17	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	GLU	CG-CD-OE2	-5.57	107.15	118.30
1	A	41	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	A	78	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	A	252	SER	N-CA-CB	5.25	118.38	110.50
1	A	182	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	116	ASN	N-CA-CB	5.25	120.04	110.60
1	A	92	GLU	CG-CD-OE1	5.12	128.54	118.30
1	A	249	LEU	N-CA-CB	-5.10	100.19	110.40
1	A	86	ASN	CB-CG-OD1	-5.10	111.41	121.60
1	A	111	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	178	ILE	CB-CA-C	5.03	121.66	111.60
1	A	16	ASN	O-C-N	5.02	130.74	122.70
1	A	205	SER	O-C-N	5.00	130.71	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	19	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	255	ARG	Sidechain
1	A	256	ARG	Sidechain
1	A	35	ARG	Sidechain
1	A	40	ARG	Sidechain

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	1947	0	1846	41	1
2	A	10	0	3	0	0
3	A	104	0	0	7	0
All	All	2061	0	1849	41	1

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 11.

All (41) 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:91:ARG:NE	1:A:92:GLU:OE2	2.11	0.84
1:A:249:LEU:HD22	1:A:249:LEU:O	1.78	0.83
1:A:249:LEU:HD22	1:A:249:LEU:C	2.00	0.82
1:A:89:THR:OG1	1:A:91:ARG:HD2	1.81	0.81
1:A:182:TYR:HD2	1:A:186:GLN:NE2	1.83	0.76
1:A:165:GLN:OE1	3:A:359:HOH:O	2.02	0.76
1:A:190:ARG:NE	3:A:301:HOH:O	2.10	0.75
1:A:182:TYR:HD2	1:A:186:GLN:HE21	1.34	0.75
1:A:182:TYR:CD2	1:A:186:GLN:NE2	2.57	0.72
1:A:235:ARG:HH21	1:A:235:ARG:HG2	1.55	0.70
1:A:35:ARG:HD2	3:A:352:HOH:O	1.91	0.69
1:A:54:TRP:HE1	1:A:56:ASN:HD22	1.44	0.64
1:A:86:ASN:HD22	1:A:127:GLN:HE22	1.45	0.62
1:A:119:ARG:HD3	1:A:228:LEU:O	2.00	0.61
1:A:36:ILE:HD13	1:A:100:LEU:HD21	1.85	0.58
1:A:1:ALA:HA	1:A:2:PRO:C	2.22	0.58
1:A:243:CYS:O	1:A:246:CYS:HB2	2.04	0.55
1:A:178:ILE:HD11	3:A:300:HOH:O	2.06	0.55
1:A:249:LEU:CD2	1:A:249:LEU:O	2.52	0.53
1:A:142:ARG:HB2	3:A:283:HOH:O	2.08	0.53
1:A:236:ALA:O	1:A:243:CYS:HB2	2.09	0.52
1:A:249:LEU:CD2	1:A:249:LEU:C	2.75	0.52
1:A:205:SER:HB2	3:A:315:HOH:O	2.12	0.49
1:A:139:THR:HA	1:A:165:GLN:HG3	1.94	0.49
1:A:27:SER:HA	1:A:36:ILE:O	2.12	0.49
1:A:225:ARG:NH2	3:A:330:HOH:O	2.47	0.48
1:A:209:PRO:O	1:A:213:GLY:HA2	2.14	0.47
1:A:91:ARG:HD3	1:A:92:GLU:OE1	2.15	0.46
1:A:91:ARG:HD3	1:A:92:GLU:CD	2.36	0.46
1:A:178:ILE:HG12	1:A:206:HIS:CD2	2.50	0.46
1:A:19:ARG:HA	1:A:19:ARG:HD2	1.71	0.45
1:A:125:HIS:CD2	1:A:209:PRO:HG2	2.53	0.43
1:A:36:ILE:CD1	1:A:100:LEU:HD21	2.46	0.43
1:A:226:PHE:CE2	1:A:235:ARG:HD3	2.54	0.43
1:A:1:ALA:HB1	1:A:140:ARG:HG3	2.00	0.43
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.84	0.43
1:A:232:GLN:O	1:A:235:ARG:HB3	2.19	0.43
1:A:195:PRO:HA	1:A:256:ARG:O	2.19	0.42
1:A:142:ARG:HG2	1:A:142:ARG:NH1	2.35	0.42
1:A:182:TYR:CE2	1:A:186:GLN:NE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:N	1:A:187:PRO:CD	2.84	0.41

All (1) 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)
1:A:44:GLN:NE2	1:A:182:TYR:OH[8_566]	2.19	0.01

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	256/258 (99%)	251 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	198/198 (100%)	182 (92%)	16 (8%)	15	4

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	28	GLN
1	A	40	ARG
1	A	42	LEU
1	A	69	LEU
1	A	78	VAL
1	A	91	ARG
1	A	94	LEU
1	A	170	LEU
1	A	178	ILE
1	A	202	ARG
1	A	207	PHE
1	A	228	LEU
1	A	235	ARG
1	A	242	GLN
1	A	249	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	75	HIS
1	A	86	ASN
1	A	186	GLN
1	A	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TLA	A	259	-	3,9,9	5.67	1 (33%)	6,12,12	3.30	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	A	259	-	-	0/4/12/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	259	TLA	O3-C3	-9.78	1.22	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	259	TLA	C4-C3-C2	-3.92	105.31	113.35
2	A	259	TLA	C1-C2-C3	-3.66	105.85	113.35
2	A	259	TLA	O3-C3-C4	5.33	124.67	111.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.