



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 02:49 pm BST

PDB ID : 3ZPX
Title : USTILAGO MAYDIS LIPASE UM03410, SHORT FORM WITHOUT FLAP
Authors : Palm, G.J.; Hinrichs, W.
Deposited on : 2013-03-04
Resolution : 1.99 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

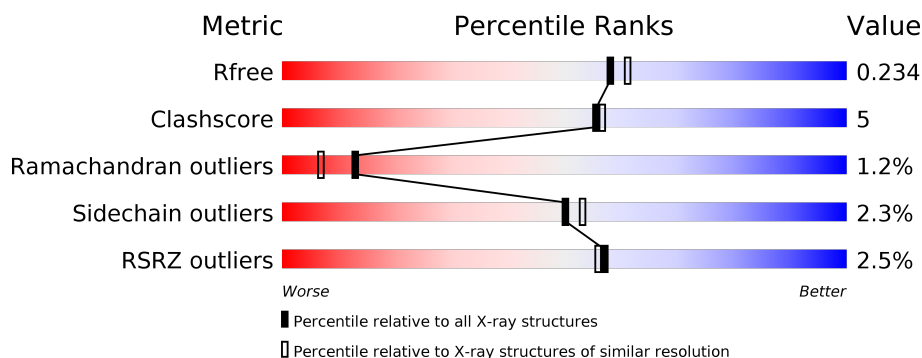
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 $\leq 5\%$. 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	458	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 77%, yellow 7%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 77% 7% 16% </div> </div>
1	B	458	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 75%, yellow 7%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 3% 75% 7% 16% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6314 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	383	Total	C	N	O	S	0	2	1
			2956	1899	491	560	6			
1	B	383	Total	C	N	O	S	0	10	1
			3011	1930	499	576	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	442	ALA	-	expression tag	UNP Q4P903
A	443	ALA	-	expression tag	UNP Q4P903
A	444	ALA	-	expression tag	UNP Q4P903
A	445	SER	-	expression tag	UNP Q4P903
A	446	PHE	-	expression tag	UNP Q4P903
A	447	LEU	-	expression tag	UNP Q4P903
A	448	GLU	-	expression tag	UNP Q4P903
A	449	GLN	-	expression tag	UNP Q4P903
A	450	LYS	-	expression tag	UNP Q4P903
A	451	LEU	-	expression tag	UNP Q4P903
A	452	ILE	-	expression tag	UNP Q4P903
A	453	SER	-	expression tag	UNP Q4P903
A	454	GLU	-	expression tag	UNP Q4P903
A	455	GLU	-	expression tag	UNP Q4P903
A	456	ASP	-	expression tag	UNP Q4P903
A	457	LEU	-	expression tag	UNP Q4P903
A	458	ASN	-	expression tag	UNP Q4P903
A	459	SER	-	expression tag	UNP Q4P903
A	460	ALA	-	expression tag	UNP Q4P903
A	461	VAL	-	expression tag	UNP Q4P903
A	462	ASP	-	expression tag	UNP Q4P903
A	463	HIS	-	expression tag	UNP Q4P903
A	464	HIS	-	expression tag	UNP Q4P903
A	465	HIS	-	expression tag	UNP Q4P903
A	466	HIS	-	expression tag	UNP Q4P903

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	HIS	-	expression tag	UNP Q4P903
A	468	HIS	-	expression tag	UNP Q4P903
B	442	ALA	-	expression tag	UNP Q4P903
B	443	ALA	-	expression tag	UNP Q4P903
B	444	ALA	-	expression tag	UNP Q4P903
B	445	SER	-	expression tag	UNP Q4P903
B	446	PHE	-	expression tag	UNP Q4P903
B	447	LEU	-	expression tag	UNP Q4P903
B	448	GLU	-	expression tag	UNP Q4P903
B	449	GLN	-	expression tag	UNP Q4P903
B	450	LYS	-	expression tag	UNP Q4P903
B	451	LEU	-	expression tag	UNP Q4P903
B	452	ILE	-	expression tag	UNP Q4P903
B	453	SER	-	expression tag	UNP Q4P903
B	454	GLU	-	expression tag	UNP Q4P903
B	455	GLU	-	expression tag	UNP Q4P903
B	456	ASP	-	expression tag	UNP Q4P903
B	457	LEU	-	expression tag	UNP Q4P903
B	458	ASN	-	expression tag	UNP Q4P903
B	459	SER	-	expression tag	UNP Q4P903
B	460	ALA	-	expression tag	UNP Q4P903
B	461	VAL	-	expression tag	UNP Q4P903
B	462	ASP	-	expression tag	UNP Q4P903
B	463	HIS	-	expression tag	UNP Q4P903
B	464	HIS	-	expression tag	UNP Q4P903
B	465	HIS	-	expression tag	UNP Q4P903
B	466	HIS	-	expression tag	UNP Q4P903
B	467	HIS	-	expression tag	UNP Q4P903
B	468	HIS	-	expression tag	UNP Q4P903

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	158	Total	O	0	0
			158	158		

- Molecule 1: LIPASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.75Å 100.15Å 129.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 1.99 39.57 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.57-1.99) 95.6 (39.57-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.235 0.184 , 0.234	Depositor DCC
R_{free} test set	2373 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6314	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PEG, EDO

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	0.45	0/3043	0.60	0/4150
1	B	0.44	1/3097 (0.0%)	0.59	0/4225
All	All	0.45	1/6140 (0.0%)	0.60	0/8375

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	GLY	C-N	-5.17	1.23	1.33

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	A	2956	0	2868	25	0
1	B	3011	0	2916	43	0
2	A	7	0	10	0	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
4	B	13	0	18	0	0
5	A	161	0	0	3	0
5	B	158	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6314	0	5824	60	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 5.

The worst 5 of 60 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:111[B]:LEU:O	1:B:112[B]:ASP:HB2	1.51	1.07
1:B:291[B]:ASN:O	1:B:292[B]:ASP:HB2	1.54	1.05
1:B:293[B]:THR:HG23	1:B:294[B]:ASN:N	1.76	0.97
1:B:293[B]:THR:HG23	1:B:294[B]:ASN:H	1.26	0.96
1:B:292[B]:ASP:O	1:B:293[B]:THR:HG22	1.71	0.89

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	383/458 (84%)	369 (96%)	12 (3%)	2 (0%)	29	23
1	B	391/458 (85%)	365 (93%)	14 (4%)	12 (3%)	4	1
All	All	774/916 (84%)	734 (95%)	26 (3%)	14 (2%)	13	3

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	LEU
1	B	112[A]	ASP
1	B	112[B]	ASP
1	B	291[A]	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	291[B]	ASN

5.3.2 Protein sidechains ⓘ

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	308/362 (85%)	302 (98%)	6 (2%)	57	61
1	B	315/362 (87%)	305 (97%)	10 (3%)	39	38
All	All	623/724 (86%)	607 (97%)	16 (3%)	50	48

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	ARG
1	B	98	GLN
1	B	293[A]	THR
1	B	49	SER
1	B	293[B]	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	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

4 ligands are 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	PEG	A	1401	-	6,6,6	0.43	0	5,5,5	0.37	0
4	PG4	B	1402	-	12,12,12	0.60	0	11,11,11	0.62	0
3	EDO	B	1401	-	3,3,3	0.59	0	2,2,2	0.24	0
3	EDO	A	1402	-	3,3,3	0.54	0	2,2,2	0.05	0

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	PEG	A	1401	-	-	0/4/4/4	-
4	PG4	B	1402	-	-	8/10/10/10	-
3	EDO	B	1401	-	-	1/1/1/1	-
3	EDO	A	1402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1402	PG4	O3-C5-C6-O4
4	B	1402	PG4	O2-C3-C4-O3
4	B	1402	PG4	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1402	PG4	O4-C7-C8-O5
3	B	1401	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	EDO	1	0

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, 95th 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 ²)	Q<0.9
1	A	383/458 (83%)	-0.00	6 (1%) 72 70	14, 25, 43, 64	0
1	B	383/458 (83%)	0.11	13 (3%) 45 44	12, 24, 44, 60	0
All	All	766/916 (83%)	0.05	19 (2%) 57 56	12, 24, 44, 64	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111[A]	LEU	6.5
1	B	294[A]	ASN	4.0
1	B	293[A]	THR	3.8
1	B	291[A]	ASN	3.8
1	A	49	SER	3.6

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	A	1401	7/7	0.84	0.15	37,49,58,60	0
4	PG4	B	1402	13/13	0.85	0.18	35,40,46,46	0
3	EDO	B	1401	4/4	0.87	0.15	32,40,41,45	0
3	EDO	A	1402	4/4	0.87	0.19	37,47,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.