



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:23 PM GMT

PDB ID : 1ORD
Title : CRYSTALLOGRAPHIC STRUCTURE OF A PLP-DEPENDENT ORNITHINE DECARBOXYLASE FROM LACTOBACILLUS 30A TO 3.1 ANGSTROMS RESOLUTION
Authors : Hackert, M.L.; Momany, C.; Ernst, S.; Ghosh, R.
Deposited on : 1995-02-08
Resolution : 3.00 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
<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

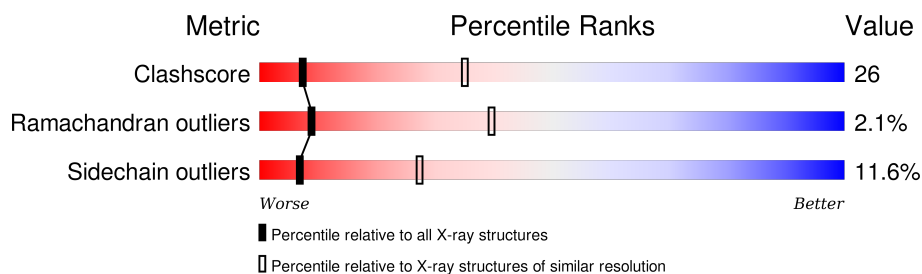
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. 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	730	
1	B	730	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14561 atoms, of which 2752 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 ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	730	Total	C	H	N	O	S	0	0	0
			7105	3726	1269	982	1109	19			
1	B	730	Total	C	H	N	O	S	0	0	0
			7105	3726	1269	982	1109	19			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

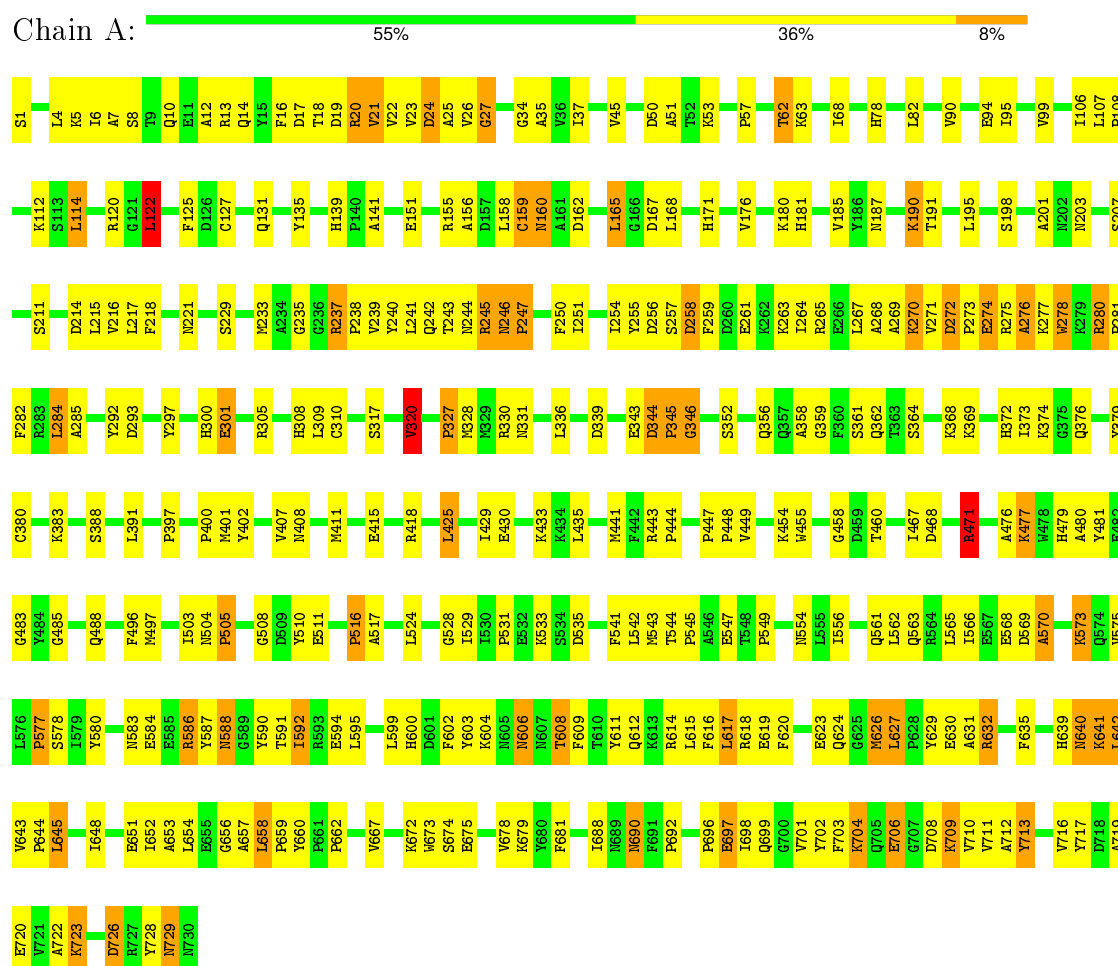
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	47	Total 141	H 94	O 47	0	0
3	B	60	Total 180	H 120	O 60	0	0

3 Residue-property plots

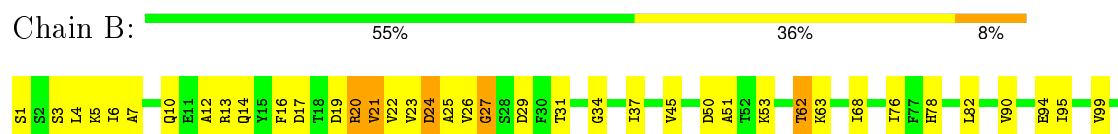
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ORNITHINE DECARBOXYLASE



• Molecule 1: ORNITHINE DECARBOXYLASE



K723					
	D726				
	N729				
	N730				
L642					
V643					
P644					
L645					
I648					
E651					
I652					
A653					
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A657					
L658					
P659					
Y660					
P661					
K672					
W673					
S674					
E675					
K679					
Y680					
P681					
L688					
N689					
N690					
F691					
P692					
A695					
P696					
E697					
I698					
Q699					
G700					
V701					
Y702					
F703					
E619					
K704					
G705					
E706					
G707					
D708					
K709					
V710					
V711					
A712					
Y713					
V716					
Y717					
D718					
A719					
E720					
V721					
A722					
Q574					
V575					
L576					
P577					
S578					
I579					
Y580					
N583					
E584					
E585					
R586					
Y587					
N588					
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Y603					
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E623					
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E630					
A631					
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K641					
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Y484					
G485					
Q488					
Y489					
Y490					
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I503					
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E511					
P516					
A517					
G528					
I529					
T530					
P531					
E532					
K533					
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I556					
Q561					
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R564					
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K374					
G375					
Q376					
Y379					
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S396					
P397					
F398					
Y399					
Q400					
M401					
V407					
M408					
L309					
E415					
Y510					
R418					
L425					
T428					
I429					
E430					
A431					
K432					
R433					
K434					
L435					
M441					
P447					
P448					
V449					
V450					
W455					
G458					
D459					
T460					
M465					
D468					
R471					
A476					
K477					
W478					
H479					
A480					
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R280					
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G283					
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A285					
Y292					
A299					
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Y303					
K304					
R305					
I306					
G307					
H308					
L309					
C310					
S317					
V320					
G321					
I326					
P327					
K328					
K329					
R330					
N331					
S332					
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L337					
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Q362					
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N228					
S229					
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G129					
A230					
M233					
A234					
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K263					
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R265					
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A269					
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D271					
D272					
P273					
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W278					
E103					
P108					
K112					
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Y117					
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L122					
C127					
P128					
G129					
H130			</		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	195.60 Å 195.60 Å 97.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.219 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14561	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: PLP

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	0.75	0/5985	0.88	7/8118 (0.1%)
1	B	0.78	0/5985	0.89	9/8118 (0.1%)
All	All	0.77	0/11970	0.88	16/16236 (0.1%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-7.66	93.96	113.10
1	B	27	GLY	N-CA-C	-7.24	95.01	113.10
1	B	239	VAL	N-CA-C	-6.45	93.60	111.00
1	A	122	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	471	ARG	NE-CZ-NH1	6.00	123.30	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	713	TYR	Sidechain
1	B	713	TYR	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	5836	1269	5623	295	0
1	B	5836	1269	5623	307	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
3	A	47	94	0	5	0
3	B	60	120	0	3	0
All	All	11809	2752	11260	589	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 26.

The worst 5 of 589 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:269:ALA:HA	1:B:275:ARG:NH2	1.83	0.92
1:B:612:GLN:HA	1:B:615:LEU:HD12	1.57	0.86
1:B:273:PRO:O	1:B:277:LYS:HB2	1.74	0.86
1:B:20:ARG:HA	1:B:20:ARG:HE	1.39	0.85
1:B:269:ALA:HA	1:B:275:ARG:CZ	2.06	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	728/730 (100%)	642 (88%)	70 (10%)	16 (2%)	8	38
1	B	728/730 (100%)	643 (88%)	70 (10%)	15 (2%)	9	40
All	All	1456/1460 (100%)	1285 (88%)	140 (10%)	31 (2%)	9	40

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ALA
1	A	339	ASP
1	A	376	GLN
1	B	339	ASP
1	B	376	GLN

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	617/617 (100%)	544 (88%)	73 (12%)	6	26
1	B	617/617 (100%)	547 (89%)	70 (11%)	7	28
All	All	1234/1234 (100%)	1091 (88%)	143 (12%)	7	27

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	659	PRO
1	B	50	ASP
1	B	641	LYS
1	A	675	GLU
1	A	728	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	B	187	ASN
1	B	607	ASN
1	B	101	ASN
1	B	202	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](#)

2 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	PLP	A	731	1	15,15,16	1.83	3 (20%)	21,22,23	1.88	7 (33%)
2	PLP	B	731	1	15,15,16	2.11	6 (40%)	21,22,23	1.50	3 (14%)

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	PLP	A	731	1	-	0/6/6/8	0/1/1/1
2	PLP	B	731	1	-	0/6/6/8	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	731	PLP	P-O2P	-2.25	1.46	1.54
2	B	731	PLP	P-O3P	-2.11	1.47	1.54
2	B	731	PLP	O3-C3	2.43	1.42	1.37
2	B	731	PLP	P-O4P	2.78	1.69	1.60
2	A	731	PLP	C2-N1	3.08	1.40	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	731	PLP	C5A-C5-C4	-3.39	117.16	121.65
2	A	731	PLP	O4P-P-O1P	-2.96	99.60	107.14
2	B	731	PLP	C2A-C2-C3	-2.77	117.70	121.04
2	A	731	PLP	C2A-C2-C3	-2.77	117.70	121.04
2	B	731	PLP	C5A-C5-C4	-2.33	118.56	121.65

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.