



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:13 AM GMT

PDB ID : 3LAD  
Title : REFINED CRYSTAL STRUCTURE OF LIPOAMIDE DEHYDROGENASE  
FROM AZOTOBACTER VINELANDII AT 2.2 ANGSTROMS RESOLU-  
TION. A COMPARISON WITH THE STRUCTURE OF GLUTATHIONE  
REDUCTASE  
Authors : Mattevi, A.; Schierbeek, A.J.; Hol, W.G.J.  
Deposited on : 1991-12-11  
Resolution : 2.20 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](mailto: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.

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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)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
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

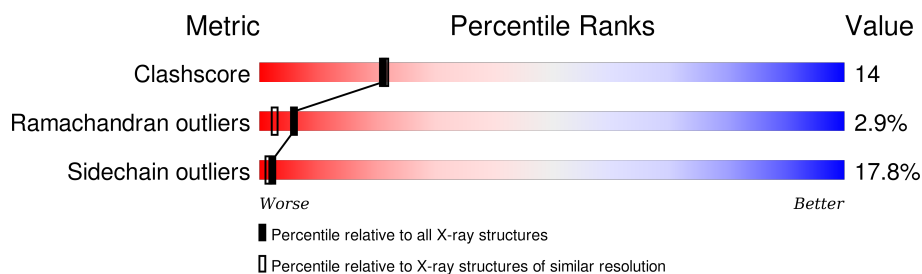
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 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	476	 55% 32% 9% ..
1	B	476	 63% 28% 7% ..

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7411 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3427	2174	585	657	11			
1	B	472	Total	C	N	O	S	0	0	0
			3427	2174	585	657	11			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

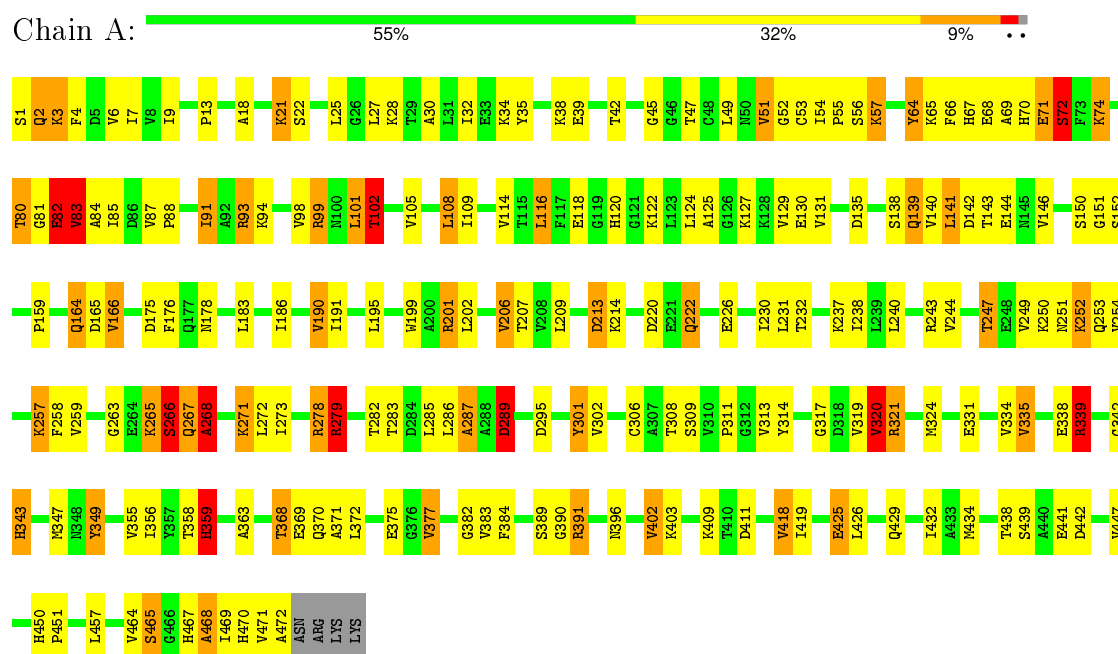
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total 212	O 212	0	0
3	B	239	Total 239	O 239	0	0

### 3 Residue-property plots

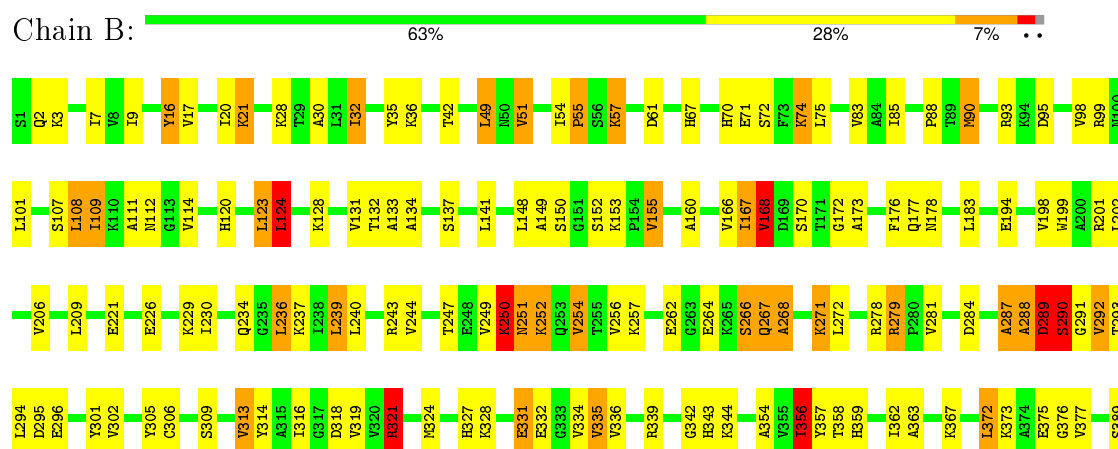
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



K390	K391	A394	A395	A396	D407	D411	R412	V413	V416	H417	V418	I419	V427	K428	Q429	D442	L443	M446	V447	L453	S454	E459	S465	G466	H467	V471	H472	ASN	ARG	LYS	LYS
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## 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, $\alpha$ , $\beta$ , $\gamma$	64.13Å 83.86Å 191.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	GROMOS, TNT, X-PLOR	Depositor
R, $R_{free}$	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 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: FAD

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	0.98	3/3478 (0.1%)	1.77	60/4717 (1.3%)
1	B	0.97	3/3478 (0.1%)	1.77	65/4717 (1.4%)
All	All	0.98	6/6956 (0.1%)	1.77	125/9434 (1.3%)

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	2
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	ALA	N-CA	13.46	1.73	1.46
1	A	418	VAL	CA-CB	6.65	1.68	1.54
1	A	84	ALA	N-CA	6.52	1.59	1.46
1	B	356	ILE	CA-CB	6.17	1.69	1.54
1	B	266	SER	CA-CB	-5.55	1.44	1.52

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	278	ARG	NE-CZ-NH2	-11.57	114.51	120.30
1	B	278	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	A	321	ARG	NE-CZ-NH2	-11.01	114.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ARG	NE-CZ-NH2	-10.93	114.83	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	HIS	Peptide
1	A	64	TYR	Sidechain
1	B	267	GLN	Mainchain
1	B	359	HIS	Peptide

## 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	3427	0	3501	127	0
1	B	3427	0	3501	81	0
2	A	53	0	31	3	0
2	B	53	0	30	1	0
3	A	212	0	0	14	0
3	B	239	0	0	4	0
All	All	7411	0	7063	201	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 14.

The worst 5 of 201 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:468:ALA:CA	1:A:468:ALA:N	1.73	1.46
1:A:70:HIS:CD2	1:A:83:VAL:HG12	1.59	1.38
1:A:70:HIS:CD2	1:A:83:VAL:CG1	2.25	1.19
1:A:70:HIS:HD2	1:A:83:VAL:CG1	1.54	1.19
1:A:176:PHE:CE1	1:A:271:LYS:HE3	1.83	1.13

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	470/476 (99%)	419 (89%)	37 (8%)	14 (3%)	5	2
1	B	470/476 (99%)	425 (90%)	32 (7%)	13 (3%)	6	3
All	All	940/952 (99%)	844 (90%)	69 (7%)	27 (3%)	6	2

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	3	LYS
1	A	190	VAL
1	B	251	ASN
1	B	289	ASP

### 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	352/359 (98%)	281 (80%)	71 (20%)	1	1
1	B	352/359 (98%)	298 (85%)	54 (15%)	3	2
All	All	704/718 (98%)	579 (82%)	125 (18%)	2	1

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	VAL

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Mol	Chain	Res	Type
1	A	441	GLU
1	B	356	ILE
1	A	358	THR
1	A	396	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	HIS
1	B	50	ASN
1	B	234	GLN
1	A	359	HIS
1	B	417	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](#)

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	FAD	A	480	-	48,58,58	1.80	7 (14%)	54,89,89	1.98	10 (18%)
2	FAD	B	480	-	48,58,58	1.56	7 (14%)	54,89,89	2.42	15 (27%)

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	FAD	A	480	-	-	0/30/50/50	0/6/6/6
2	FAD	B	480	-	-	0/30/50/50	0/6/6/6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	FAD	C1'-N10	-8.69	1.39	1.48
2	A	480	FAD	P-O5'	-3.90	1.41	1.59
2	B	480	FAD	C1'-C2'	-2.96	1.31	1.51
2	B	480	FAD	C6-C5X	-2.59	1.37	1.41
2	B	480	FAD	C10-N1	-2.50	1.31	1.35

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	N3A-C2A-N1A	-8.27	122.56	128.89
2	B	480	FAD	N3A-C2A-N1A	-6.06	124.25	128.89
2	B	480	FAD	C4X-C4-N3	-4.62	117.28	123.59
2	B	480	FAD	C2B-C1B-N9A	-4.14	107.96	114.29
2	A	480	FAD	C4X-C4-N3	-4.02	118.09	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	FAD	3	0
2	B	480	FAD	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 ⓘ

### 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.