



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2023 – 06:42 AM EDT

PDB ID : 3B9N  
Title : Crystal structure of long-chain alkane monooxygenase (LadA)  
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Deposited on : 2007-11-06  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

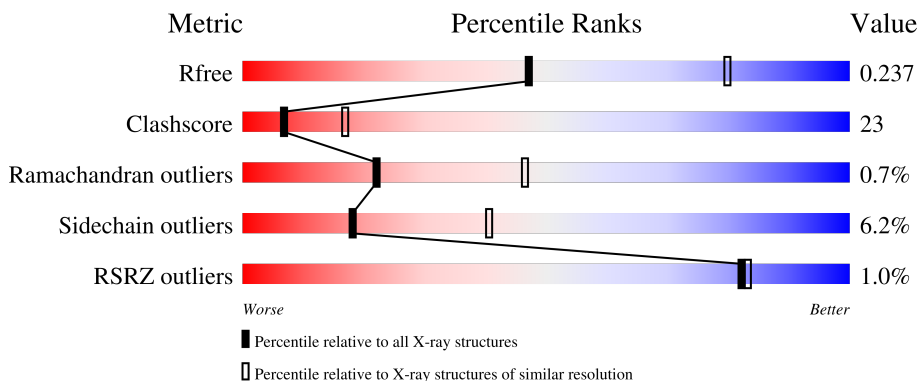
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	440	57% 38% . .
1	B	440	2% 56% 38% . .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7369 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 Alkane monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3513	2243	609	647	14	0	0	0
1	B	434	3520	2248	609	648	15	0	0	0

- Molecule 2 is water.

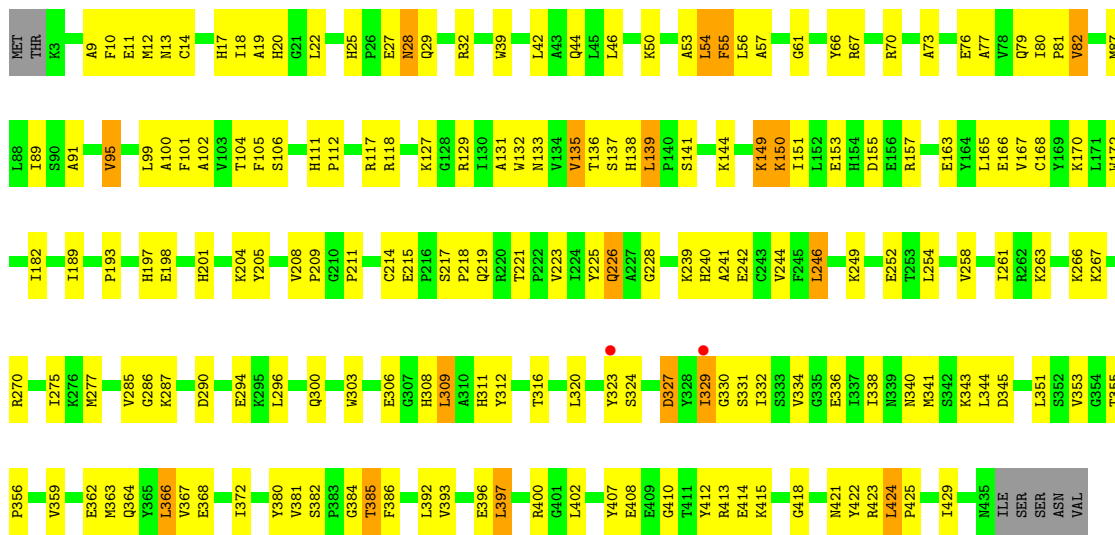
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	172	172	172	0	0
2	B	164	164	164	0	0

### 3 Residue-property plots

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

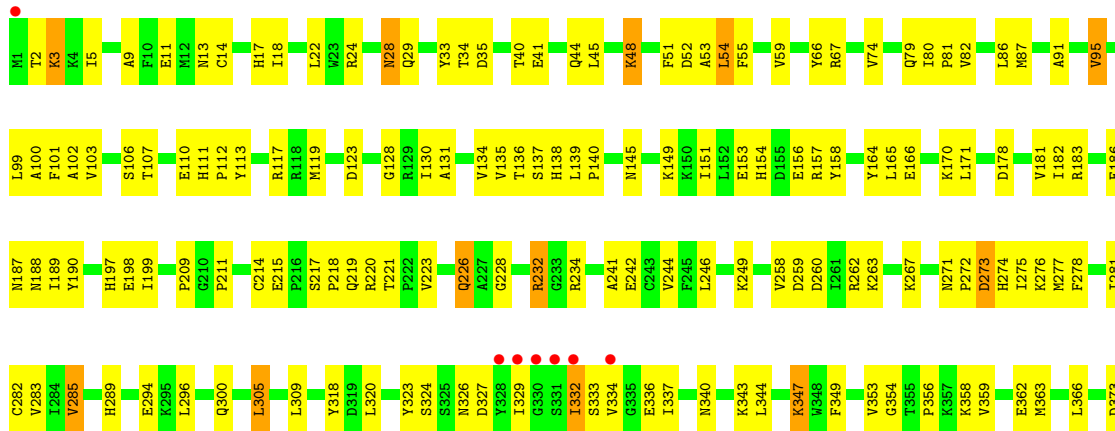
- Molecule 1: Alkane monooxygenase

Chain A:



- Molecule 1: Alkane monooxygenase

Chain B:



G374	F375	Q379	Y380	V381	S382	F383	T385	F386	I390	E391	L392	V393	V394	P395	F396	L397	V405	D406	E409	G410	R413	E414	K415	G418	N421	Y422	R423	L424	H428	I429	A430	R434	ASN	ILE	SER	SER	ASN	ASN	VAL
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.50Å 77.50Å 323.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.86 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 70.9 (48.86-2.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.30 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.183 , 0.249 0.184 , 0.237	Depositor DCC
$R_{free}$ test set	2160 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtrriage
Anisotropy	0.846	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4297e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.37	0/3606	0.62	1/4877 (0.0%)
1	B	0.36	0/3613	0.61	0/4886
All	All	0.37	0/7219	0.62	1/9763 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	THR	N-CA-C	-5.49	96.17	111.00

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	3513	0	3410	168	0
1	B	3520	0	3423	162	0
2	A	172	0	0	10	0
2	B	164	0	0	11	0
All	All	7369	0	6833	322	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 23.

The worst 5 of 322 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:332:ILE:HD11	1:B:336:GLU:HB2	1.48	0.95
1:B:45:LEU:HD12	1:B:48:LYS:HE3	1.45	0.95
1:A:422:TYR:HD1	1:A:423:ARG:HG3	1.40	0.87
1:A:53:ALA:HB2	1:A:100:ALA:HB3	1.59	0.84
1:A:380:TYR:H	1:A:385:THR:HG21	1.46	0.81

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	431/440 (98%)	403 (94%)	25 (6%)	3 (1%)	22	46
1	B	432/440 (98%)	400 (93%)	29 (7%)	3 (1%)	22	46
All	All	863/880 (98%)	803 (93%)	54 (6%)	6 (1%)	22	46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	SER
1	B	149	LYS
1	A	139	LEU
1	A	329	ILE
1	B	424	LEU

### 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	372/379 (98%)	352 (95%)	20 (5%)	22	47
1	B	373/379 (98%)	347 (93%)	26 (7%)	15	35
All	All	745/758 (98%)	699 (94%)	46 (6%)	18	40

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	HIS
1	B	285	VAL
1	B	153	GLU
1	B	232	ARG
1	B	326	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	GLN
1	B	274	HIS
1	B	379	GLN
1	A	154	HIS
1	A	138	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 monosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	433/440 (98%)	-0.40	2 (0%) 91 92	20, 32, 54, 71	0
1	B	434/440 (98%)	-0.32	7 (1%) 72 74	19, 34, 58, 78	0
All	All	867/880 (98%)	-0.36	9 (1%) 82 83	19, 34, 56, 78	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	4.1
1	A	329	ILE	3.5
1	B	330	GLY	3.3
1	B	331	SER	3.3
1	B	334	VAL	2.9

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.