



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:31 am BST

PDB ID : 1XAA  
Title : 3-ISOPROPYLMALATE DEHYDROGENASE, LOW TEMPERATURE  
(100K) STRUCTURE  
Authors : Nagata, C.; Moriyama, H.; Tanaka, N.  
Deposited on : 1995-11-09  
Resolution : 2.10 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](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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

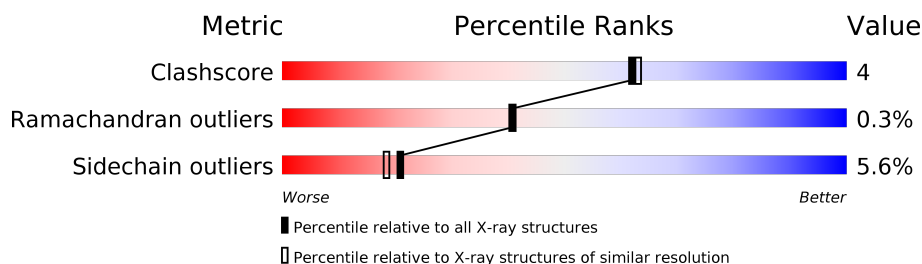
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4031 atoms, of which 1140 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 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	H	N	O	S	0	0	0
			3143	1654	548	452	483	6			

- Molecule 2 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	296	Total	H	O	0	0
			888	592	296		

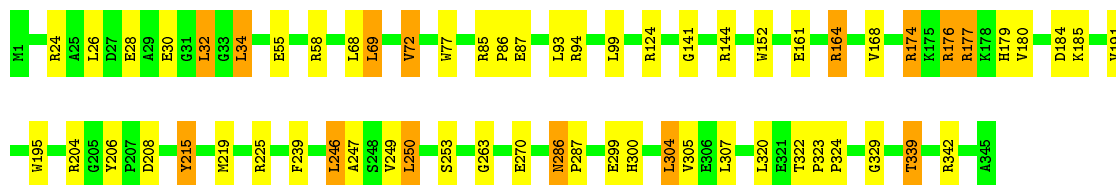
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain A:  82% 14%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.00 Å 77.00 Å 156.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.83	0/2650	1.49	35/3596 (1.0%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ARG	NE-CZ-NH1	11.79	126.19	120.30
1	A	174	ARG	NE-CZ-NH2	-11.29	114.66	120.30
1	A	176	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	A	177	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	A	176	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	A	177	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	24	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	195	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	A	77	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	A	152	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	A	191	VAL	CG1-CB-CG2	-7.39	99.07	110.90
1	A	124	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	152	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	77	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	152	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	A	219	MET	CG-SD-CE	-6.43	89.91	100.20
1	A	85	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	195	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	94	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	215	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	85	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	152	TRP	CB-CG-CD1	-5.76	119.52	127.00
1	A	72	VAL	N-CA-CB	-5.72	98.92	111.50
1	A	239	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	34	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	195	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	A	304	LEU	CA-CB-CG	5.51	127.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	77	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	A	225	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	152	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	A	225	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	94	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	124	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	180	VAL	CG1-CB-CG2	-5.05	102.82	110.90

There are no chirality outliers.

There are no planarity outliers.

## 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	2595	548	2633	23	2
2	A	296	592	0	1	3
All	All	2891	1140	2633	23	3

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 4.

All (23) 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:174:ARG:HD3	1:A:208:ASP:OD2	2.02	0.60
1:A:99:LEU:HA	1:A:263:GLY:HA3	1.83	0.59
1:A:247:ALA:HA	1:A:250:LEU:HD22	1.87	0.56
1:A:176:ARG:NH1	1:A:177:ARG:NH2	2.57	0.53
1:A:26:LEU:HD22	1:A:307:LEU:HD22	1.92	0.50
1:A:141:GLY:O	1:A:144:ARG:HD2	2.11	0.50
1:A:322:THR:OG1	1:A:339:THR:HG21	2.11	0.50
1:A:339:THR:HB	1:A:342:ARG:NH2	2.27	0.50
1:A:299:GLU:HG3	1:A:305:VAL:HG22	1.97	0.47
1:A:55:GLU:HA	1:A:58:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:O	1:A:179:HIS:HD2	1.99	0.46
1:A:69:LEU:HB3	1:A:270:GLU:HB3	1.98	0.46
1:A:30:GLU:HB3	1:A:32:LEU:HD13	1.98	0.45
1:A:323:PRO:HG2	1:A:329:GLY:HA3	1.99	0.44
1:A:246:LEU:O	1:A:249:VAL:HG22	2.17	0.44
1:A:323:PRO:HA	1:A:324:PRO:HD3	1.89	0.44
1:A:161:GLU:HA	1:A:164:ARG:HD3	2.00	0.44
1:A:300:HIS:HE1	2:A:514:HOH:O	2.00	0.44
1:A:72:VAL:HG13	1:A:86:PRO:HB3	1.99	0.44
1:A:185:LYS:HD2	1:A:185:LYS:HA	1.86	0.43
1:A:339:THR:HB	1:A:342:ARG:HH22	1.83	0.43
1:A:184:ASP:O	1:A:215:TYR:HA	2.21	0.41
1:A:286:ASN:HD22	1:A:287:PRO:HD2	1.85	0.40

All (3) 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)
2:A:585:HOH:H1	2:A:585:HOH:H1[6_554]	1.25	0.35
1:A:206:TYR:HH	2:A:537:HOH:H1[4_545]	1.34	0.26
1:A:206:TYR:HH	2:A:537:HOH:O[4_545]	1.59	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	343/345 (99%)	335 (98%)	7 (2%)	1 (0%)	41 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	SER



### 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	266 / 266 (100%)	251 (94%)	15 (6%)	21	18

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	32	LEU
1	A	34	LEU
1	A	68	LEU
1	A	69	LEU
1	A	87	GLU
1	A	93	LEU
1	A	164	ARG
1	A	168	VAL
1	A	246	LEU
1	A	250	LEU
1	A	286	ASN
1	A	304	LEU
1	A	320	LEU
1	A	339	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	HIS
1	A	286	ASN
1	A	300	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](#)

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.