



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:03 PM UTC

PDB ID : 4KDE / pdb_00004kde
Title : Crystal Structure of the Apo Form of Thermus thermophilus Malate Dehydrogenase
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Deposited on : 2013-04-25
Resolution : 1.80 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

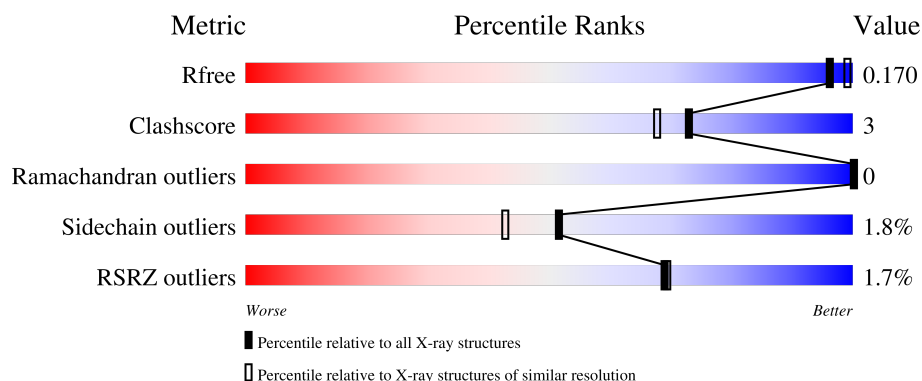
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 ≥ 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	341	% 89% 9% .
1	B	341	2% 90% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5875 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2521	1597	445	466	13			
1	B	329	Total	C	N	O	S	0	0	0
			2508	1588	443	464	13			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	ARG	-	expression tag	UNP P10584
A	329	LYS	-	expression tag	UNP P10584
A	330	LEU	-	expression tag	UNP P10584
A	331	ALA	-	expression tag	UNP P10584
A	332	ALA	-	expression tag	UNP P10584
A	333	ALA	-	expression tag	UNP P10584
A	334	LEU	-	expression tag	UNP P10584
A	335	GLU	-	expression tag	UNP P10584
A	336	HIS	-	expression tag	UNP P10584
A	337	HIS	-	expression tag	UNP P10584
A	338	HIS	-	expression tag	UNP P10584
A	339	HIS	-	expression tag	UNP P10584
A	340	HIS	-	expression tag	UNP P10584
A	341	HIS	-	expression tag	UNP P10584
B	328	ARG	-	expression tag	UNP P10584
B	329	LYS	-	expression tag	UNP P10584
B	330	LEU	-	expression tag	UNP P10584
B	331	ALA	-	expression tag	UNP P10584
B	332	ALA	-	expression tag	UNP P10584
B	333	ALA	-	expression tag	UNP P10584
B	334	LEU	-	expression tag	UNP P10584
B	335	GLU	-	expression tag	UNP P10584
B	336	HIS	-	expression tag	UNP P10584
B	337	HIS	-	expression tag	UNP P10584
B	338	HIS	-	expression tag	UNP P10584

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Chain	Residue	Modelled	Actual	Comment	Reference
B	339	HIS	-	expression tag	UNP P10584
B	340	HIS	-	expression tag	UNP P10584
B	341	HIS	-	expression tag	UNP P10584

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	449	Total 449	O 449	0	0
2	B	397	Total 397	O 397	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.17Å 86.01Å 118.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.86 – 1.80 27.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.86-1.80) 97.8 (27.86-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.144 , 0.170 0.144 , 0.170	Depositor DCC
R_{free} test set	2000 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

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	0.41	0/2565	0.71	0/3472
1	B	0.39	0/2552	0.71	0/3454
All	All	0.40	0/5117	0.71	0/6926

There are no bond length outliers.

There are no bond angle outliers.

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	2521	0	2569	17	0
1	B	2508	0	2553	15	0
2	A	449	0	0	6	0
2	B	397	0	0	8	0
All	All	5875	0	5122	32	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 3.

All (32) 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:308:GLU:OE1	2:B:731:HOH:O	1.90	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:OD2	2:A:794:HOH:O	1.97	0.81
1:B:191:MET:HE1	1:B:222:VAL:HG12	1.67	0.75
1:B:4:PRO:HG3	2:B:689:HOH:O	1.93	0.67
1:A:176:ASP:OD1	2:A:795:HOH:O	2.12	0.66
1:A:19:SER:O	2:A:784:HOH:O	2.15	0.63
1:B:131:ASN:ND2	2:B:736:HOH:O	2.04	0.60
1:A:265:ALA:HA	1:A:281:SER:HA	1.85	0.57
1:A:127:LEU:HD11	1:A:155:MET:HB2	1.90	0.54
1:B:265:ALA:HA	1:B:281:SER:HA	1.90	0.54
1:B:6:ARG:NE	2:B:742:HOH:O	2.14	0.52
1:A:188:SER:O	1:A:191:MET:HG2	2.10	0.50
1:A:318:MET:HE2	1:A:330:LEU:HD22	1.94	0.50
1:B:127:LEU:HD11	1:B:155:MET:HB2	1.94	0.49
1:A:264:MET:SD	1:A:284:VAL:HG21	2.53	0.49
1:A:114:ARG:NH2	2:A:800:HOH:O	2.48	0.47
1:B:187:HIS:HD2	2:B:736:HOH:O	1.98	0.47
1:A:145:PRO:HA	2:A:791:HOH:O	2.15	0.46
1:B:1:MET:HE3	1:B:1:MET:HB2	1.74	0.45
1:A:156:THR:HG21	1:A:281:SER:HB2	1.99	0.44
1:B:186:ASN:O	1:B:191:MET:HB3	2.18	0.44
1:B:295:GLU:O	2:B:794:HOH:O	2.21	0.43
1:A:96:MET:HE2	1:A:96:MET:HB3	1.90	0.43
1:B:150:ARG:HG3	1:B:291:TYR:OH	2.18	0.43
1:A:193:PRO:HG2	1:A:219:ILE:HG12	2.00	0.43
1:B:15:GLN:HG2	2:B:757:HOH:O	2.18	0.42
1:B:207:GLU:OE2	2:B:758:HOH:O	2.21	0.42
1:A:301:GLU:CD	1:A:304:ARG:HH21	2.27	0.42
1:A:93:LYS:HB3	1:A:96:MET:SD	2.60	0.42
1:B:156:THR:HG21	1:B:281:SER:HB2	2.00	0.42
1:A:122:LYS:HA	1:A:122:LYS:HD3	1.84	0.41
1:A:51:GLU:HG3	2:A:775:HOH:O	2.21	0.41

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	329/341 (96%)	328 (100%)	1 (0%)	0	100	100
1	B	327/341 (96%)	326 (100%)	1 (0%)	0	100	100
All	All	656/682 (96%)	654 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	255/263 (97%)	250 (98%)	5 (2%)	48	38
1	B	254/263 (97%)	250 (98%)	4 (2%)	55	47
All	All	509/526 (97%)	500 (98%)	9 (2%)	51	43

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	98	ARG
1	A	101	LEU
1	A	102	LEU
1	A	141	TYR
1	B	1	MET
1	B	45	GLN
1	B	141	TYR
1	B	191	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	300	ASN
1	B	320	GLN

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 oligosaccharides 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, 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	331/341 (97%)	-0.59	4 (1%) 76 77	7, 13, 32, 67	0
1	B	329/341 (96%)	-0.39	7 (2%) 63 64	7, 17, 43, 74	0
All	All	660/682 (96%)	-0.49	11 (1%) 69 69	7, 14, 39, 74	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ARG	3.9
1	B	94	ALA	3.8
1	A	145	PRO	3.5
1	B	145	PRO	3.5
1	B	95	GLY	3.3
1	B	150	ARG	2.4
1	B	99	ARG	2.3
1	A	96	MET	2.1
1	B	96	MET	2.1
1	A	92	ARG	2.1
1	B	92	ARG	2.1

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 oligosaccharides 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.