



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 1EAA / pdb_00001eaa
Title : ATOMIC STRUCTURE OF THE CUBIC CORE OF THE PYRUVATE DE-HYDROGENASE MULTIENZYME COMPLEX
Authors : Mattevi, A.; Hol, W.G.J.
Deposited on : 1992-12-16
Resolution : 2.60 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
Xtrriage (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

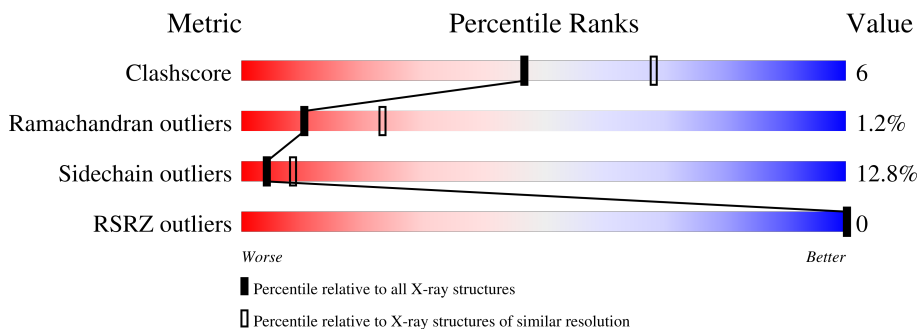
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	243	 70% 23% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1849 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 DIHYDROLIPOYL-TRANSACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1812	1168	310	327	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	LYS	GLU	conflict	UNP P10802

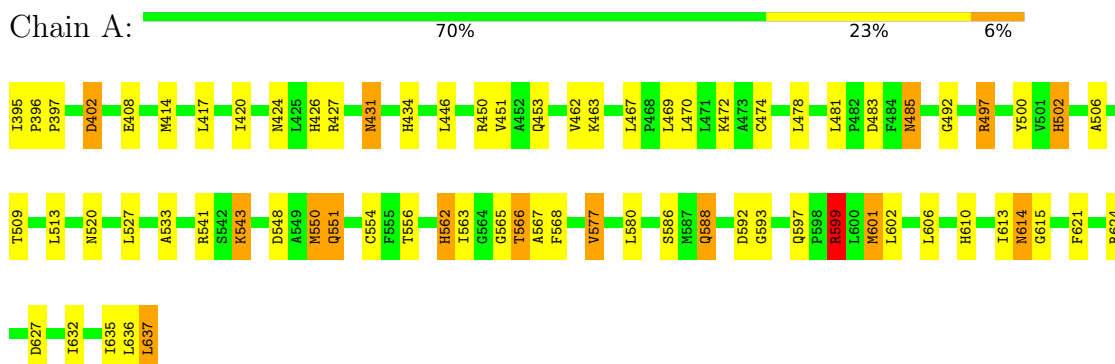
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	37	37	37	0	0

3 Residue-property plots [i](#)

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: DIHYDROLIPOYL-TRANSACETYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.77Å 224.77Å 224.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 10.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 70.2 (10.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.01 (at 2.65Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1849	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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 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	1.24	6/1849 (0.3%)	1.96	45/2519 (1.8%)

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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	562	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	502	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	610	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	434	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	502	HIS	CG-ND1	-5.10	1.32	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	ILE	N-CA-C	-13.58	100.89	111.62
1	A	577	VAL	N-CA-CB	-12.49	97.46	112.33
1	A	614	ASN	OD1-CG-ND2	-9.03	113.57	122.60
1	A	402	ASP	CA-CB-CG	8.93	121.53	112.60
1	A	497	ARG	CA-CB-CG	-8.77	96.56	114.10
1	A	577	VAL	CB-CA-C	8.56	119.86	110.62
1	A	592	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	627	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	565	GLY	CA-C-O	7.51	127.41	122.23
1	A	566	THR	N-CA-CB	-7.37	99.70	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	A	474	CYS	CA-C-O	-6.88	113.13	120.42
1	A	562	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	A	548	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	606	LEU	CA-C-O	-6.06	114.09	120.58
1	A	566	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	485	ASN	N-CA-C	-6.02	103.31	111.55
1	A	502	HIS	CA-CB-CG	6.01	119.81	113.80
1	A	568	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	420	ILE	N-CA-C	-5.97	104.69	110.42
1	A	614	ASN	CB-CG-ND2	5.95	125.32	116.40
1	A	551	GLN	CA-CB-CG	-5.79	102.52	114.10
1	A	481	LEU	CA-C-N	5.68	125.35	119.56
1	A	481	LEU	C-N-CA	5.68	125.35	119.56
1	A	424	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	541	ARG	CA-CB-CG	-5.52	103.06	114.10
1	A	599	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	396	PRO	N-CA-C	-5.46	104.04	110.70
1	A	551	GLN	N-CA-C	5.43	118.41	109.72
1	A	588	GLN	CG-CD-NE2	5.42	124.54	116.40
1	A	601	MET	CG-SD-CE	-5.39	89.03	100.90
1	A	483	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	509	THR	CA-C-N	5.30	124.94	119.05
1	A	509	THR	C-N-CA	5.30	124.94	119.05
1	A	602	LEU	O-C-N	-5.30	116.47	121.35
1	A	566	THR	OG1-CB-CG2	5.28	119.86	109.30
1	A	637	LEU	CA-CB-CG	5.28	134.78	116.30
1	A	424	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	621	PHE	CA-C-O	-5.26	115.29	120.82
1	A	533	ALA	N-CA-C	-5.25	105.45	111.07
1	A	593	GLY	N-CA-C	-5.21	108.49	114.69
1	A	463	LYS	O-C-N	-5.20	117.39	123.27
1	A	556	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	453	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	434	HIS	CA-CB-CG	5.04	118.83	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	500	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	1812	0	1855	21	2
2	A	37	0	0	2	0
All	All	1849	0	1855	21	2

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 6.

All (21) 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:586:SER:HB2	1:A:588:GLN:HE21	1.59	0.66
1:A:506:ALA:HB1	1:A:513:LEU:HD11	1.86	0.57
1:A:450:ARG:HG3	1:A:469:LEU:HD11	1.88	0.56
1:A:502:HIS:HD2	1:A:520:ASN:H	1.53	0.55
1:A:599:ARG:HB2	1:A:601:MET:HE3	1.90	0.54
1:A:462:VAL:HG21	1:A:527:LEU:HD22	1.93	0.51
1:A:502:HIS:CD2	1:A:520:ASN:H	2.30	0.48
1:A:562:HIS:H	1:A:562:HIS:CD2	2.32	0.47
1:A:550:MET:HE2	1:A:550:MET:HB2	1.81	0.46
1:A:614:ASN:HB3	2:A:650:HOH:O	2.16	0.45
1:A:599:ARG:CB	1:A:601:MET:HE3	2.48	0.44
1:A:462:VAL:CG2	1:A:527:LEU:HD22	2.47	0.44
1:A:632:ILE:O	1:A:635:ILE:HB	2.19	0.43
1:A:485:ASN:OD1	1:A:554:CYS:HB3	2.19	0.42
1:A:624:ARG:HA	1:A:624:ARG:HD2	1.81	0.42
1:A:599:ARG:HA	1:A:599:ARG:HD2	1.94	0.42
1:A:450:ARG:HG3	1:A:469:LEU:CD1	2.49	0.41
1:A:427:ARG:O	1:A:431:ASN:HB2	2.20	0.41
1:A:635:ILE:HD13	1:A:635:ILE:HG21	1.79	0.40
1:A:632:ILE:CD1	1:A:635:ILE:HD12	2.51	0.40
1:A:615:GLY:HA3	2:A:663:HOH:O	2.20	0.40

All (2) 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)
1:A:402:ASP:OD1	1:A:402:ASP:OD1[28_555]	0.50	1.70
1:A:402:ASP:CG	1:A:402:ASP:OD1[28_555]	1.65	0.55

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	241/243 (99%)	228 (95%)	10 (4%)	3 (1%)	10 23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	LYS
1	A	567	ALA
1	A	492	GLY

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	187/195 (96%)	163 (87%)	24 (13%)	4 8

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ILE
1	A	397	PRO

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Mol	Chain	Res	Type
1	A	408	GLU
1	A	414	MET
1	A	417	LEU
1	A	431	ASN
1	A	446	LEU
1	A	451	VAL
1	A	467	LEU
1	A	470	LEU
1	A	472	LYS
1	A	478	LEU
1	A	497	ARG
1	A	543	LYS
1	A	550	MET
1	A	551	GLN
1	A	566	THR
1	A	577	VAL
1	A	580	LEU
1	A	597	GLN
1	A	599	ARG
1	A	613	ILE
1	A	636	LEU
1	A	637	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	453	GLN
1	A	502	HIS
1	A	551	GLN
1	A	588	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	243/243 (100%)	-0.75	0 100 100	2, 17, 52, 67	0

There are no RSRZ outliers to report.

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.