



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 02:34 AM UTC

PDB ID : 1PYA / pdb_00001pya
Title : REFINED STRUCTURE OF THE PYRUVOYL-DEPENDENT HISTIDINE
DECARBOXYLASE FROM LACTOBACILLUS 30A
Authors : Gallagher, T.; Rozwarski, D.A.; Ernst, S.R.; Hackert, M.L.
Deposited on : 1992-12-18
Resolution : 2.50 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

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
Mogul : 2022.3.0, CSD as543be (2022)
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

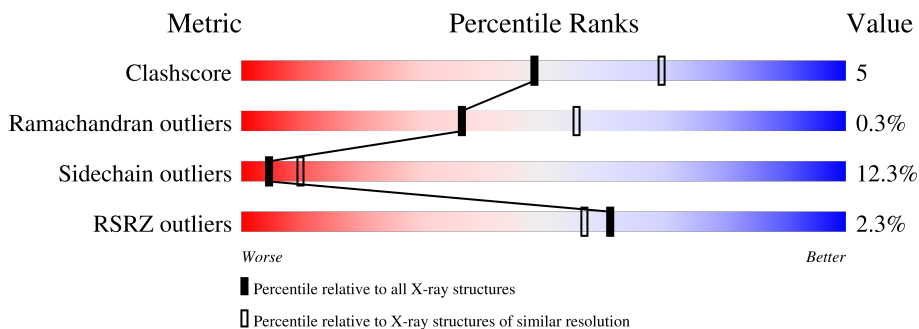
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	81	
1	C	81	
1	E	81	
2	B	229	
2	D	229	
2	F	229	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10140 atoms, of which 2478 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 PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	81	770	384	149	107	128	2	0	0	0
1	C	81	770	384	149	107	128	2	0	0	0
1	E	81	770	384	149	107	128	2	0	0	0

- Molecule 2 is a protein called PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	229	2139	1127	363	286	352	11	0	0	0
2	D	229	2139	1127	363	286	352	11	0	0	0
2	F	229	2139	1127	363	286	352	11	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	H O		
3	A	54	162	108 54	0	0
3	B	106	318	212 106	0	0
3	C	61	183	122 61	0	0
3	D	92	276	184 92	0	0
3	E	58	174	116 58	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	F	100	300	200	100	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: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain A: 



- Molecule 1: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain C: 




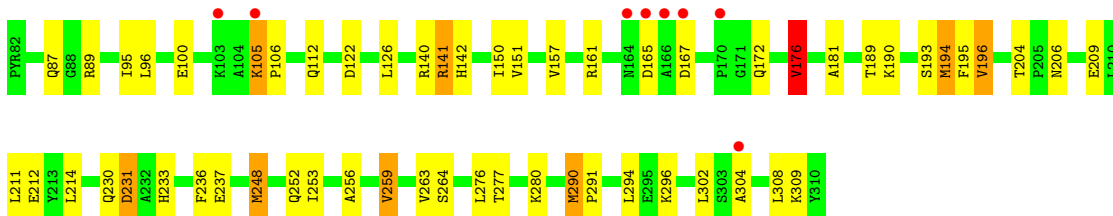
- Molecule 1: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain E: 




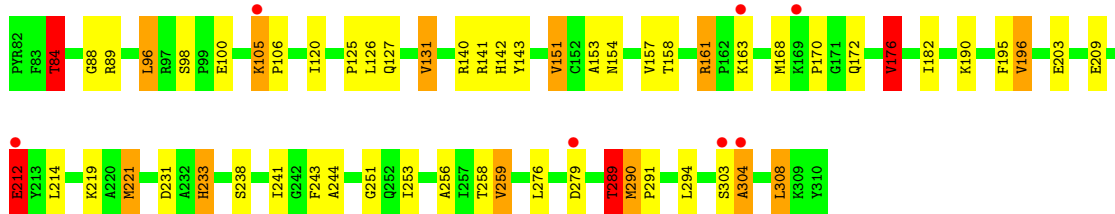
- Molecule 2: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain B: 



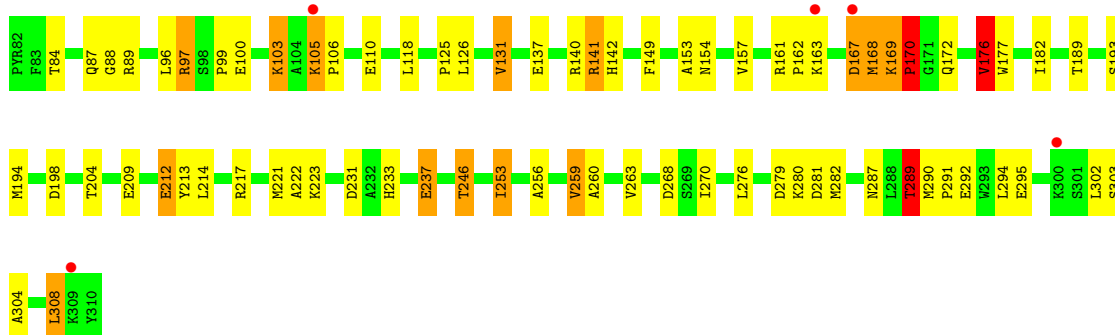
● Molecule 2: PYRUVYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain D:  3% 75% 18% 5%



● Molecule 2: PYRUVYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain F:  2% 67% 25% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	221.70Å 221.70Å 107.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 156.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 99.5 (156.77-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.150 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYR

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	0.92	0/629	1.75	13/848 (1.5%)
1	C	0.88	0/629	1.81	15/848 (1.8%)
1	E	0.89	0/629	1.77	14/848 (1.7%)
2	B	0.96	4/1816 (0.2%)	1.70	21/2463 (0.9%)
2	D	0.96	7/1816 (0.4%)	1.72	26/2463 (1.1%)
2	F	0.96	5/1816 (0.3%)	1.70	36/2463 (1.5%)
All	All	0.94	16/7335 (0.2%)	1.73	125/9933 (1.3%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	131	VAL	CA-CB	7.93	1.65	1.54
2	B	259	VAL	CA-CB	7.68	1.65	1.54
2	B	233	HIS	CD2-NE2	-7.11	1.30	1.37
2	F	259	VAL	CA-CB	7.11	1.64	1.54
2	D	131	VAL	CA-CB	7.01	1.63	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	THR	N-CA-CB	-9.68	95.26	110.46
1	A	67	THR	N-CA-CB	-8.79	96.66	110.46
2	F	279	ASP	CA-CB-CG	8.59	121.19	112.60
2	F	268	ASP	CA-CB-CG	8.41	121.01	112.60
2	D	89	ARG	NE-CZ-NH2	-8.37	111.67	119.20

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	621	149	611	10	0
1	C	621	149	611	5	0
1	E	621	149	611	12	0
2	B	1776	363	1704	17	0
2	D	1776	363	1704	21	0
2	F	1776	363	1704	27	0
3	A	54	108	0	1	0
3	B	106	212	0	0	0
3	C	61	122	0	0	0
3	D	92	184	0	3	0
3	E	58	116	0	2	0
3	F	100	200	0	1	0
All	All	7662	2478	6945	77	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 5.

The worst 5 of 77 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)
2:D:105:LYS:NZ	2:D:106:PRO:O	1.89	1.06
2:B:112:GLN:HE22	2:B:236:PHE:H	1.24	0.82
2:D:289:THR:HG23	2:D:291:PRO:HD2	1.65	0.78
2:F:110:GLU:HG3	2:F:222:ALA:HB1	1.68	0.75
2:F:100:GLU:HB2	2:F:125:PRO:HB3	1.68	0.75

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	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
1	C	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
1	E	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
2	B	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
2	D	227/229 (99%)	219 (96%)	7 (3%)	1 (0%)	30	49
2	F	227/229 (99%)	218 (96%)	7 (3%)	2 (1%)	14	27
All	All	918/930 (99%)	879 (96%)	36 (4%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	304	ALA
2	D	304	ALA
2	F	170	PRO

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	66/66 (100%)	55 (83%)	11 (17%)	2	4
1	C	66/66 (100%)	62 (94%)	4 (6%)	17	35
1	E	66/66 (100%)	60 (91%)	6 (9%)	9	19
2	B	188/188 (100%)	163 (87%)	25 (13%)	4	8
2	D	188/188 (100%)	166 (88%)	22 (12%)	5	11
2	F	188/188 (100%)	162 (86%)	26 (14%)	3	7
All	All	762/762 (100%)	668 (88%)	94 (12%)	4	10

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	259	VAL
2	F	105	LYS
2	D	289	THR
1	E	50	LYS
2	F	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	69	ASN
2	D	127	GLN
2	F	287	ASN
2	D	233	HIS
1	E	35	ASN

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	81/81 (100%)	-0.39	0 100 100	8, 14, 21, 43	0
1	C	81/81 (100%)	-0.44	1 (1%) 76 73	8, 14, 24, 41	0
1	E	81/81 (100%)	-0.50	0 100 100	8, 13, 23, 44	0
2	B	228/229 (99%)	-0.15	8 (3%) 47 42	8, 18, 37, 54	0
2	D	228/229 (99%)	-0.17	7 (3%) 51 47	8, 18, 34, 47	0
2	F	228/229 (99%)	-0.25	5 (2%) 62 58	8, 16, 32, 51	0
All	All	927/930 (99%)	-0.26	21 (2%) 61 57	8, 16, 34, 54	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	167	ASP	3.3
2	F	105	LYS	3.1
2	D	304	ALA	3.1
2	D	105	LYS	3.1
2	B	170	PRO	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 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.