



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:49 AM UTC

PDB ID : 1IBV / pdb_00001ibv
Title : STRUCTURE OF THE D53,54N MUTANT OF HISTIDINE DECARBOXY-
LASE BOUND WITH HISTIDINE METHYL ESTER AT-170 C
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Deposited on : 2001-03-29
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

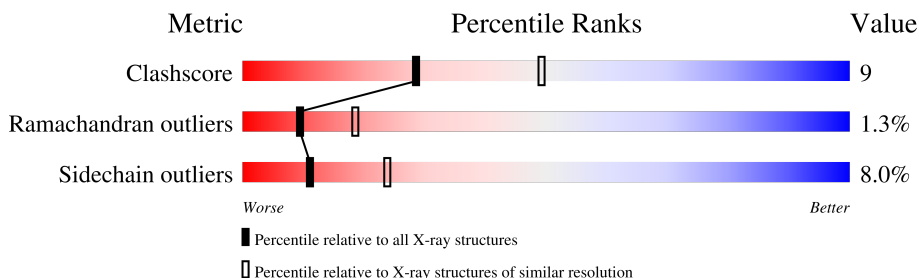
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	81	78% 17% 5%
1	C	81	75% 20% 5%
1	E	81	79% 15% 6%
2	B	229	70% 26% . .
2	D	229	72% 24% .
2	F	229	73% 23% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7332 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 HISTIDINE DECARBOXYLASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	0	0	0
			621	384	109	126	2			
1	C	81	Total	C	N	O	S	0	0	0
			621	384	109	126	2			
1	E	81	Total	C	N	O	S	0	0	0
			621	384	109	126	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASN	ASP	engineered mutation	UNP P00862
A	54	ASN	ASP	engineered mutation	UNP P00862
C	53	ASN	ASP	engineered mutation	UNP P00862
C	54	ASN	ASP	engineered mutation	UNP P00862
E	53	ASN	ASP	engineered mutation	UNP P00862
E	54	ASN	ASP	engineered mutation	UNP P00862

- Molecule 2 is a protein called Histidine decarboxylase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1775	1127	286	351	11			
2	D	229	Total	C	N	O	S	0	0	0
			1775	1127	286	351	11			
2	F	229	Total	C	N	O	S	0	0	0
			1775	1127	286	351	11			

There are 3 discrepancies between the modelled and reference sequences:

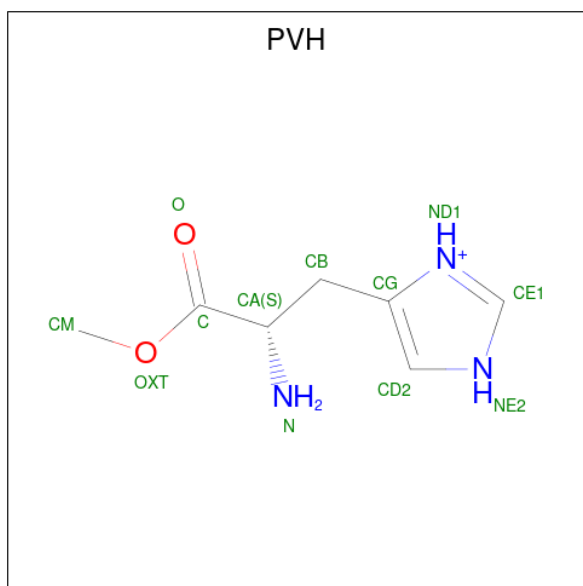
Chain	Residue	Modelled	Actual	Comment	Reference
B	483	PYR	SER	conflict	UNP P00862
D	483	PYR	SER	conflict	UNP P00862

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Chain	Residue	Modelled	Actual	Comment	Reference
F	483	PYR	SER	conflict	UNP P00862

- Molecule 3 is HISTIDINE-METHYL-ESTER (CCD ID: PVH) (formula: $C_7H_{12}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	7	3	2		
3	D	1	Total	C	N	O	0	0
			12	7	3	2		
3	F	1	Total	C	N	O	0	0
			12	7	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	13	Total	O	0	0
			13	13		
4	C	17	Total	O	0	0
			17	17		
4	D	17	Total	O	0	0
			17	17		
4	E	26	Total	O	0	0
			26	26		
4	F	21	Total	O	0	0
			21	21		

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. 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: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain A: 



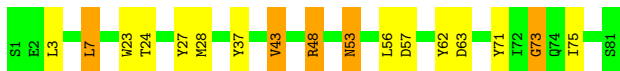
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain C: 



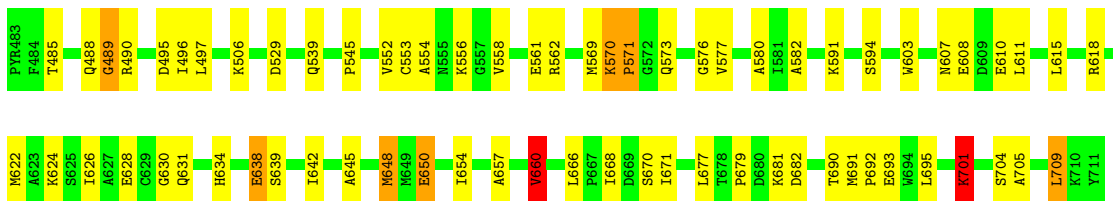
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain E: 



- Molecule 2: Histidine decarboxylase alpha chain

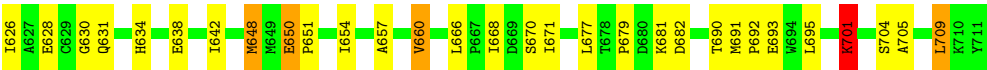
Chain B: 



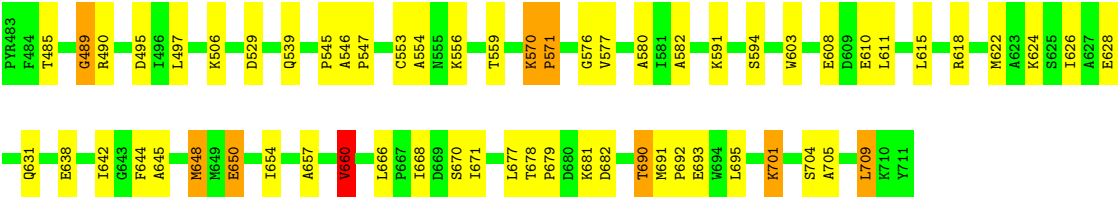
- Molecule 2: Histidine decarboxylase alpha chain

Chain D: 





● Molecule 2: Histidine decarboxylase alpha chain



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.27Å 115.48Å 206.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.243 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7332	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PVH, 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	0.47	0/629	0.97	2/848 (0.2%)
1	C	0.43	0/629	0.98	3/848 (0.4%)
1	E	0.46	0/629	0.98	2/848 (0.2%)
2	B	0.46	0/1816	0.95	11/2463 (0.4%)
2	D	0.47	0/1816	0.97	10/2463 (0.4%)
2	F	0.47	0/1816	0.96	9/2463 (0.4%)
All	All	0.47	0/7335	0.96	37/9933 (0.4%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	489	GLY	N-CA-C	8.53	123.59	111.14
2	F	489	GLY	N-CA-C	8.45	123.47	111.14
2	D	489	GLY	N-CA-C	7.84	122.59	111.14
2	F	666	LEU	N-CA-C	7.47	119.06	109.72
2	B	666	LEU	N-CA-C	7.43	119.14	109.93

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	621	0	615	13	0
1	C	621	0	615	13	0
1	E	621	0	615	11	0
2	B	1775	0	1704	40	0
2	D	1775	0	1704	35	0
2	F	1775	0	1704	33	0
3	B	12	0	7	0	0
3	D	12	0	7	0	0
3	F	12	0	7	1	0
4	A	14	0	0	0	0
4	B	13	0	0	1	0
4	C	17	0	0	0	0
4	D	17	0	0	0	0
4	E	26	0	0	0	0
4	F	21	0	0	1	0
All	All	7332	0	6978	125	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 9.

The worst 5 of 125 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:603:TRP:HZ2	2:D:610:GLU:HG3	1.39	0.87
2:F:603:TRP:HZ2	2:F:610:GLU:HG3	1.39	0.87
1:A:75:ILE:HD11	2:B:545:PRO:HB2	1.59	0.85
1:E:75:ILE:HD11	2:F:545:PRO:HB2	1.60	0.83
2:B:603:TRP:HZ2	2:B:610:GLU:HG3	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	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	18
1	C	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	18
1	E	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	9	18
2	B	227/229 (99%)	213 (94%)	11 (5%)	3 (1%)	9	18
2	D	227/229 (99%)	211 (93%)	13 (6%)	3 (1%)	9	18
2	F	227/229 (99%)	212 (93%)	12 (5%)	3 (1%)	9	18
All	All	918/930 (99%)	850 (93%)	56 (6%)	12 (1%)	9	18

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	571	PRO
2	D	571	PRO
2	F	571	PRO
2	F	705	ALA
2	B	705	ALA

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	66/66 (100%)	61 (92%)	5 (8%)	12	26
1	C	66/66 (100%)	61 (92%)	5 (8%)	12	26
1	E	66/66 (100%)	61 (92%)	5 (8%)	12	26
2	B	188/188 (100%)	173 (92%)	15 (8%)	11	24
2	D	188/188 (100%)	173 (92%)	15 (8%)	11	24
2	F	188/188 (100%)	172 (92%)	16 (8%)	10	22
All	All	762/762 (100%)	701 (92%)	61 (8%)	11	24

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	556	LYS

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Mol	Chain	Res	Type
2	F	650	GLU
2	D	660	VAL
2	F	648	MET
2	F	701	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	528	GLN
2	F	565	ASN
2	F	631	GLN
2	F	607	ASN
1	C	8	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PVH	F	801	2	12,12,12	0.65	0	15,15,15	1.91	4 (26%)
3	PVH	B	801	2	12,12,12	0.63	0	15,15,15	1.84	3 (20%)
3	PVH	D	801	2	12,12,12	0.69	0	15,15,15	1.84	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PVH	F	801	2	-	3/10/10/10	0/1/1/1
3	PVH	B	801	2	-	4/10/10/10	0/1/1/1
3	PVH	D	801	2	-	4/10/10/10	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	801	PVH	OXT-C-CA	4.50	122.95	111.50
3	B	801	PVH	OXT-C-CA	4.36	122.60	111.50
3	D	801	PVH	OXT-C-CA	4.30	122.44	111.50
3	B	801	PVH	OXT-C-O	-3.45	117.14	123.85
3	F	801	PVH	OXT-C-O	-3.30	117.43	123.85

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	PVH	CA-C-OXT-CM
3	F	801	PVH	CA-C-OXT-CM
3	B	801	PVH	O-C-OXT-CM
3	D	801	PVH	O-C-OXT-CM
3	F	801	PVH	O-C-OXT-CM

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	PVH	1	0

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.