



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2022 – 02:12 PM JST

PDB ID : 7ERU
Title : Crystal structure of L-histidine decarboxylase (C57S mutant) from *Photobacterium phosphoreum*
Authors : Oda, Y.; Nakata, K.; Yamaguchi, H.; Kashiwagi, T.; Miyano, H.; Mizukoshi, T.
Deposited on : 2021-05-07
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

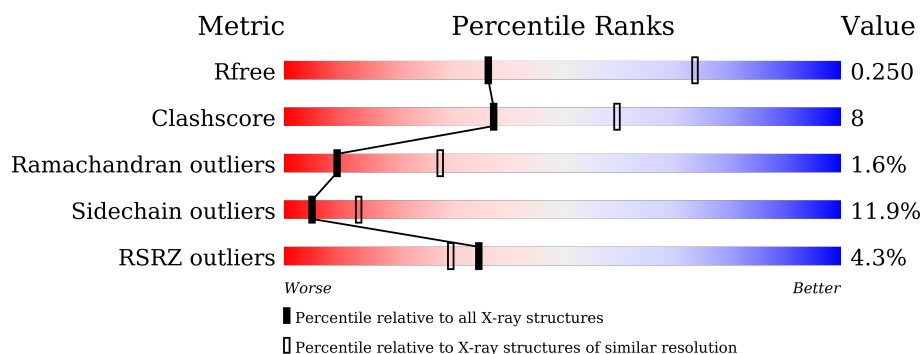
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	373	<div> <div>4%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2965 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	P	S	0	0	0
			2965	1886	495	566	1	17			

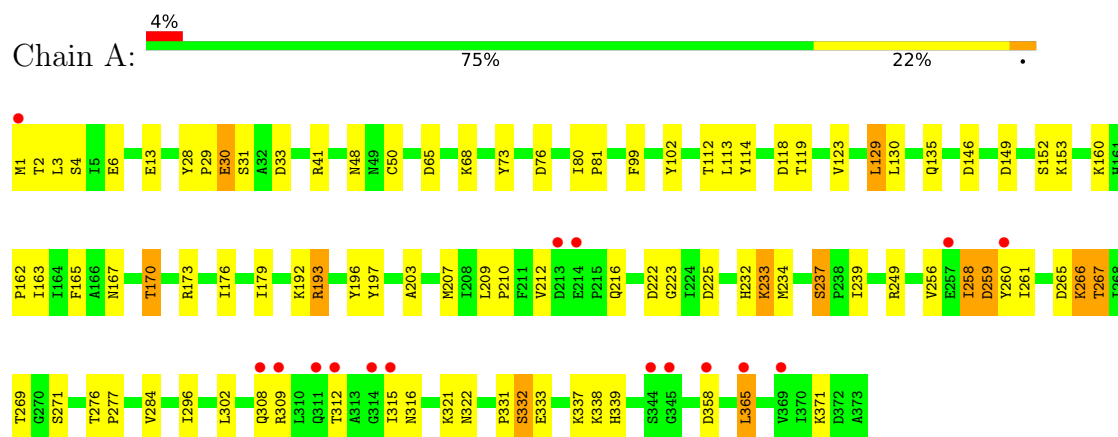
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	CYS	engineered mutation	UNP Q1JU62

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: Histidine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	111.43Å 111.43Å 126.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.13 – 2.85 45.09 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.13-2.85) 100.0 (45.09-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.248 0.190 , 0.250	Depositor DCC
R_{free} test set	567 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2965	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: LLP

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	0.71	0/3010	0.87	0/4076

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 [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	2965	0	2868	45	0
All	All	2965	0	2868	45	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 8.

All (45) 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:265:ASP:OD2	1:A:267:THR:HB	1.90	0.71
1:A:237:SER:OG	1:A:239:ILE:O	2.14	0.64
1:A:48:ASN:HD21	1:A:271:SER:HB2	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD12	1:A:163:ILE:HG22	1.83	0.60
1:A:129:LEU:HB3	1:A:130:LEU:HD23	1.84	0.60
1:A:276:THR:OG1	1:A:277:PRO:HD3	2.03	0.57
1:A:48:ASN:ND2	1:A:271:SER:HB2	2.19	0.57
1:A:258:ILE:HG22	1:A:261:ILE:O	2.04	0.57
1:A:216:GLN:N	1:A:216:GLN:OE1	2.40	0.54
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.07	0.54
1:A:256:VAL:HG23	1:A:266:LYS:HE2	1.90	0.54
1:A:114:TYR:CD1	1:A:135:GLN:HB3	2.44	0.53
1:A:130:LEU:HD23	1:A:130:LEU:N	2.23	0.52
1:A:6:GLU:OE2	1:A:6:GLU:N	2.40	0.52
1:A:170:THR:HG22	1:A:173:ARG:H	1.74	0.51
1:A:339:HIS:CG	1:A:365:LEU:CD2	2.94	0.51
1:A:258:ILE:HG23	1:A:259:ASP:N	2.27	0.49
1:A:119:THR:HG23	1:A:167:ASN:HD21	1.78	0.48
1:A:203:ALA:HB1	1:A:233:LLP:HE3	1.96	0.48
1:A:216:GLN:OE1	1:A:322:ASN:ND2	2.47	0.47
1:A:114:TYR:CE1	1:A:135:GLN:HB3	2.49	0.47
1:A:207:MET:O	1:A:296:ILE:HD11	2.15	0.47
1:A:232:HIS:H	1:A:232:HIS:CD2	2.31	0.46
1:A:80:ILE:HG13	1:A:81:PRO:HD2	1.98	0.45
1:A:339:HIS:CD2	1:A:365:LEU:HD22	2.52	0.45
1:A:193:ARG:NH1	1:A:223:GLY:O	2.50	0.45
1:A:73:TYR:CG	1:A:284:VAL:CG1	3.00	0.44
1:A:99:PHE:O	1:A:102:TYR:HB3	2.17	0.44
1:A:50:CYS:HB2	1:A:271:SER:HA	2.00	0.43
1:A:48:ASN:OD1	1:A:271:SER:HB2	2.18	0.43
1:A:73:TYR:CG	1:A:284:VAL:HG11	2.54	0.43
1:A:33:ASP:O	1:A:33:ASP:CG	2.58	0.42
1:A:28:TYR:HB3	1:A:29:PRO:CD	2.50	0.42
1:A:209:LEU:N	1:A:210:PRO:CD	2.83	0.42
1:A:339:HIS:CG	1:A:365:LEU:HD22	2.54	0.42
1:A:197:TYR:HA	1:A:225:ASP:OD2	2.20	0.41
1:A:30:GLU:HA	1:A:233:LLP:HA	2.02	0.41
1:A:197:TYR:CE1	1:A:225:ASP:HB3	2.55	0.41
1:A:123:VAL:CG2	1:A:165:PHE:CZ	3.03	0.41
1:A:162:PRO:O	1:A:196:TYR:HB2	2.21	0.41
1:A:176:ILE:HD12	1:A:216:GLN:NE2	2.36	0.41
1:A:3:LEU:HD23	1:A:3:LEU:HA	1.96	0.40
1:A:179:ILE:HD11	1:A:222:ASP:HB3	2.02	0.40
1:A:73:TYR:CD1	1:A:284:VAL:HG13	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:O	1:A:153:LYS:HG3	2.22	0.40

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	370/373 (99%)	333 (90%)	31 (8%)	6 (2%)	9	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	259	ASP
1	A	332	SER
1	A	260	TYR
1	A	146	ASP
1	A	331	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	319/319 (100%)	281 (88%)	38 (12%)	5	13

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	13	GLU
1	A	30	GLU
1	A	31	SER
1	A	41	ARG
1	A	65	ASP
1	A	68	LYS
1	A	76	ASP
1	A	112	THR
1	A	118	ASP
1	A	129	LEU
1	A	152	SER
1	A	160	LYS
1	A	170	THR
1	A	192	LYS
1	A	193	ARG
1	A	212	VAL
1	A	234	MET
1	A	237	SER
1	A	249	ARG
1	A	258	ILE
1	A	266	LYS
1	A	267	THR
1	A	269	THR
1	A	302	LEU
1	A	309	ARG
1	A	312	THR
1	A	315	ILE
1	A	316	ASN
1	A	321	LYS
1	A	332	SER
1	A	333	GLU
1	A	337	LYS
1	A	338	LYS
1	A	358	ASP
1	A	365	LEU
1	A	371	LYS

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	22	GLN
1	A	91	ASN
1	A	167	ASN
1	A	232	HIS
1	A	349	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	LLP	A	233	1	23,24,25	0.47	0	25,32,34	0.81	1 (4%)

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
1	LLP	A	233	1	-	10/16/17/19	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LLP	OP4-P-OP1	-2.81	98.61	106.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	233	LLP	C4-C4'-NZ-CE
1	A	233	LLP	C5'-OP4-P-OP2
1	A	233	LLP	C5'-OP4-P-OP3
1	A	233	LLP	N-CA-CB-CG
1	A	233	LLP	C-CA-CB-CG
1	A	233	LLP	CG-CD-CE-NZ
1	A	233	LLP	CA-CB-CG-CD
1	A	233	LLP	CE-CD-CG-CB
1	A	233	LLP	C5'-OP4-P-OP1
1	A	233	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	233	LLP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	372/373 (99%)	-0.10	16 (4%) 35 30	27, 52, 121, 173	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	TYR	5.0
1	A	257	GLU	4.2
1	A	315	ILE	3.5
1	A	314	GLY	3.3
1	A	312	THR	3.2
1	A	369	VAL	2.9
1	A	1	MET	2.8
1	A	358	ASP	2.7
1	A	344	SER	2.6
1	A	365	LEU	2.6
1	A	308	GLN	2.6
1	A	214	GLU	2.5
1	A	311	GLN	2.4
1	A	213	ASP	2.4
1	A	345	GLY	2.3
1	A	309	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	233	24/25	0.98	0.17	31,41,47,62	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.