



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 11:53 AM EDT

PDB ID : 9LU2 / pdb\_00009lu2  
Title : Crystal structure of Pseudoalteromonas sp. L11-2 tryptophan halogenase putative  
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Deposited on : 2025-02-07  
Resolution : 2.98 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](mailto: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>.

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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

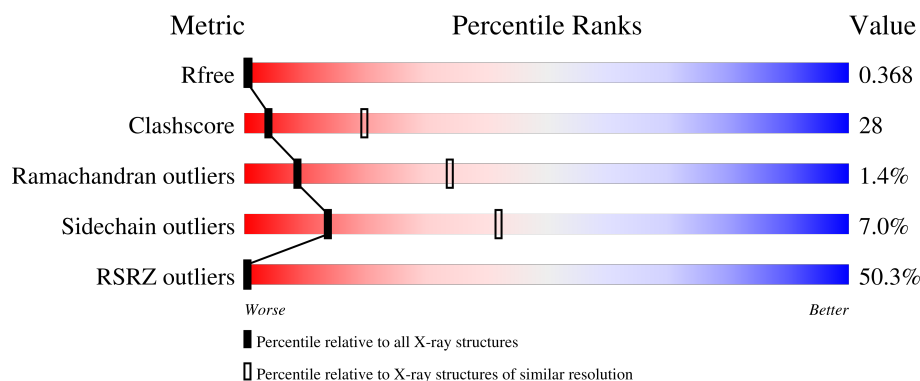
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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  $\geq 3$ , 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	514	<div> <div>46%</div> <div>53% 34% 5% 6%</div> </div>
1	B	514	<div> <div>49%</div> <div>49% 40% 7%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7679 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.

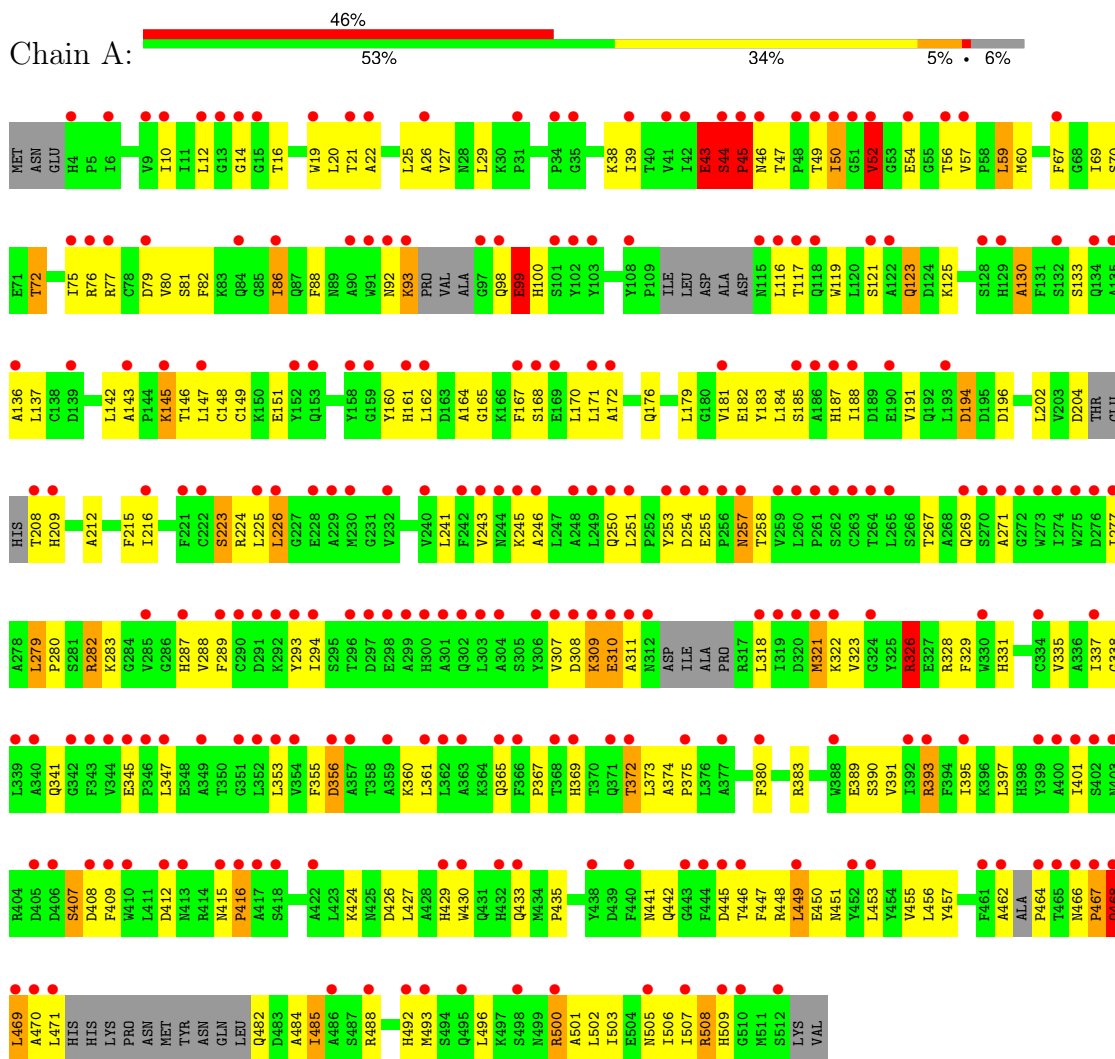
- Molecule 1 is a protein called L11-2 tryptophan halogenase putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3801	2424	653	707	17			
1	B	493	Total	C	N	O	S	0	0	0
			3878	2473	663	725	17			

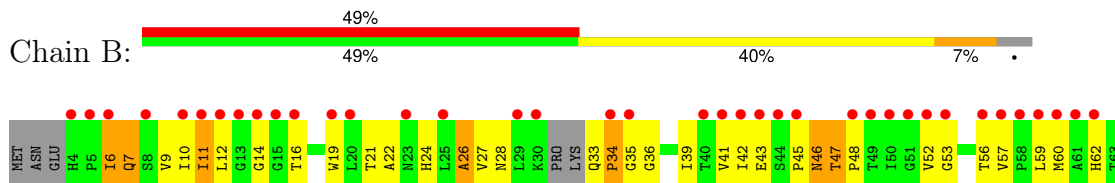
### 3 Residue-property plots [i](#)

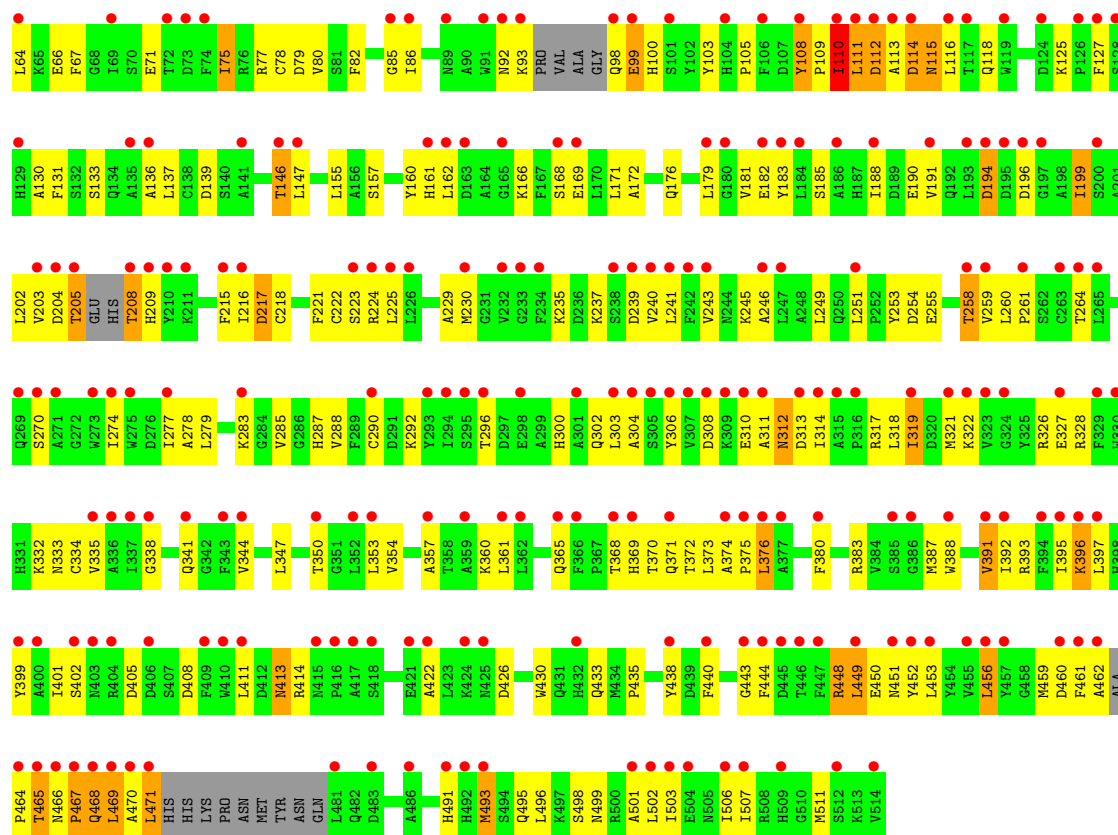
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L11-2 tryptophan halogenase putative



- Molecule 1: L11-2 tryptophan halogenase putative





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.90Å 63.16Å 214.08Å 90.00° 99.81° 90.00°	Depositor
Resolution (Å)	47.91 – 2.98 47.91 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.91-2.98) 98.0 (47.91-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.01Å)	Xtriage
Refinement program	REFMAC refmac5	Depositor
R, $R_{free}$	0.322 , 0.365 0.335 , 0.368	Depositor DCC
$R_{free}$ test set	1158 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.66	3/3898 (0.1%)	1.32	41/5288 (0.8%)
1	B	0.66	3/3976 (0.1%)	1.27	30/5397 (0.6%)
All	All	0.66	6/7874 (0.1%)	1.29	71/10685 (0.7%)

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	5
1	B	0	5
All	All	0	10

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	PRO	N-CD	9.89	1.61	1.47
1	A	321	MET	SD-CE	-6.32	1.63	1.79
1	A	407	SER	C-N	-6.25	1.24	1.33
1	B	199	ILE	CG1-CD1	-6.18	1.27	1.51
1	B	75	ILE	CG1-CD1	-5.65	1.29	1.51

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	GLN	N-CA-C	24.32	137.79	111.28
1	B	46	ASN	N-CA-C	-21.75	74.92	109.72
1	B	34	PRO	CB-CA-C	-21.52	76.06	111.56
1	A	321	MET	CB-CA-C	-18.17	74.27	110.42
1	B	469	LEU	N-CA-C	16.99	135.30	111.52

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	407	SER	Mainchain
1	A	500	ARG	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	3801	0	3668	207	2
1	B	3878	0	3748	223	3
All	All	7679	0	7416	424	3

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 28.

The worst 5 of 424 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:108:TYR:HE1	1:B:448:ARG:NH2	1.27	1.32
1:B:108:TYR:CE1	1:B:448:ARG:NH2	2.15	1.14
1:B:369:HIS:CE1	1:B:371:GLN:HB3	1.90	1.07
1:A:449:LEU:O	1:A:453:LEU:HB2	1.53	1.07
1:B:217:ASP:OD2	1:B:223:SER:OG	1.72	1.06

All (3) 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:47:THR:CG2	1:B:311:ALA:CB[1_455]	1.69	0.51
1:B:98:GLN:NE2	1:B:182:GLU:OE1[1_565]	1.70	0.50
1:A:47:THR:CG2	1:B:312:ASN:N[1_455]	2.03	0.17



## 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	469/514 (91%)	423 (90%)	43 (9%)	3 (1%)	21	53
1	B	481/514 (94%)	431 (90%)	40 (8%)	10 (2%)	5	25
All	All	950/1028 (92%)	854 (90%)	83 (9%)	13 (1%)	9	34

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	B	115	ASN
1	B	114	ASP
1	B	312	ASN
1	B	467	PRO

### 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	403/430 (94%)	370 (92%)	33 (8%)	10	35
1	B	412/430 (96%)	388 (94%)	24 (6%)	18	49
All	All	815/860 (95%)	758 (93%)	57 (7%)	14	42

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	HIS

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Mol	Chain	Res	Type
1	B	456	LEU
1	B	33	GLN
1	B	405	ASP
1	B	314	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	HIS
1	B	178	ASN
1	B	442	GLN
1	B	176	GLN
1	B	300	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	483/514 (93%)	2.13	239 (49%) 0 0	35, 46, 61, 74	0
1	B	493/514 (95%)	2.21	252 (51%) 0 0	30, 46, 63, 78	0
All	All	976/1028 (94%)	2.17	491 (50%) 0 0	30, 46, 63, 78	0

The worst 5 of 491 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	ALA	8.5
1	A	462	ALA	6.8
1	A	147	LEU	6.7
1	A	309	LYS	6.5
1	B	50	ILE	6.1

### 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.