



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 11:04 AM JST

PDB ID : 6IZ9  
Title : Crystal structure of the apo form of a beta-transaminase from *Mesorhizobium* sp. strain LUK  
Authors : Park, H.H.; Kwon, S.  
Deposited on : 2018-12-19  
Resolution : 2.20 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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

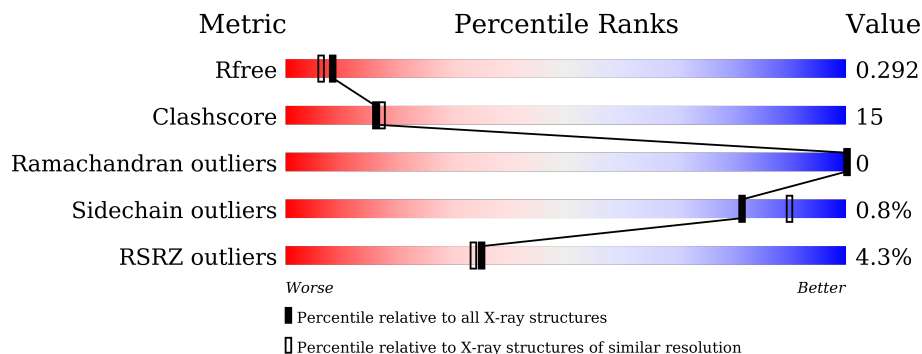
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	470	 4% 63% 23% 14%
1	B	470	 3% 63% 23% 14%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6060 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 Beta-transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	2855	1785	507	550	13	0	0	0
1	B	402	2826	1785	489	539	13	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A3EYF7
A	-12	ALA	-	expression tag	UNP A3EYF7
A	-11	SER	-	expression tag	UNP A3EYF7
A	-10	MET	-	expression tag	UNP A3EYF7
A	-9	THR	-	expression tag	UNP A3EYF7
A	-8	GLY	-	expression tag	UNP A3EYF7
A	-7	GLY	-	expression tag	UNP A3EYF7
A	-6	GLN	-	expression tag	UNP A3EYF7
A	-5	GLN	-	expression tag	UNP A3EYF7
A	-4	MET	-	expression tag	UNP A3EYF7
A	-3	GLY	-	expression tag	UNP A3EYF7
A	-2	ARG	-	expression tag	UNP A3EYF7
A	-1	GLY	-	expression tag	UNP A3EYF7
A	0	SER	-	expression tag	UNP A3EYF7
A	446	ALA	-	expression tag	UNP A3EYF7
A	447	ALA	-	expression tag	UNP A3EYF7
A	448	ALA	-	expression tag	UNP A3EYF7
A	449	LEU	-	expression tag	UNP A3EYF7
A	450	GLU	-	expression tag	UNP A3EYF7
A	451	HIS	-	expression tag	UNP A3EYF7
A	452	HIS	-	expression tag	UNP A3EYF7
A	453	HIS	-	expression tag	UNP A3EYF7
A	454	HIS	-	expression tag	UNP A3EYF7
A	455	HIS	-	expression tag	UNP A3EYF7
A	456	HIS	-	expression tag	UNP A3EYF7

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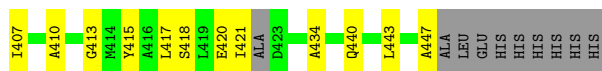
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP A3EYF7
B	-12	ALA	-	expression tag	UNP A3EYF7
B	-11	SER	-	expression tag	UNP A3EYF7
B	-10	MET	-	expression tag	UNP A3EYF7
B	-9	THR	-	expression tag	UNP A3EYF7
B	-8	GLY	-	expression tag	UNP A3EYF7
B	-7	GLY	-	expression tag	UNP A3EYF7
B	-6	GLN	-	expression tag	UNP A3EYF7
B	-5	GLN	-	expression tag	UNP A3EYF7
B	-4	MET	-	expression tag	UNP A3EYF7
B	-3	GLY	-	expression tag	UNP A3EYF7
B	-2	ARG	-	expression tag	UNP A3EYF7
B	-1	GLY	-	expression tag	UNP A3EYF7
B	0	SER	-	expression tag	UNP A3EYF7
B	446	ALA	-	expression tag	UNP A3EYF7
B	447	ALA	-	expression tag	UNP A3EYF7
B	448	ALA	-	expression tag	UNP A3EYF7
B	449	LEU	-	expression tag	UNP A3EYF7
B	450	GLU	-	expression tag	UNP A3EYF7
B	451	HIS	-	expression tag	UNP A3EYF7
B	452	HIS	-	expression tag	UNP A3EYF7
B	453	HIS	-	expression tag	UNP A3EYF7
B	454	HIS	-	expression tag	UNP A3EYF7
B	455	HIS	-	expression tag	UNP A3EYF7
B	456	HIS	-	expression tag	UNP A3EYF7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	185	Total O 185 185	0	0
2	B	194	Total O 194 194	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.40Å 62.40Å 171.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.22 – 2.20 39.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.22-2.20) 100.0 (39.22-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.241 , 0.291 0.241 , 0.292	Depositor DCC
$R_{free}$ test set	1860 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l 0.467 for h,-h-k,-l 0.027 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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 [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	0.28	0/2900	0.50	0/3939
1	B	0.29	0/2872	0.49	0/3895
All	All	0.29	0/5772	0.50	0/7834

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	2855	0	2688	91	0
1	B	2826	0	2651	74	0
2	A	185	0	0	11	0
2	B	194	0	0	4	0
All	All	6060	0	5339	160	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 15.

The worst 5 of 160 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:319:ILE:HD12	1:A:320:LEU:H	1.14	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:HD12	1:A:320:LEU:N	1.82	0.93
1:A:176:LEU:HD12	1:A:188:ALA:HB2	1.64	0.79
1:B:150:LEU:HD11	1:B:176:LEU:HD21	1.67	0.76
1:A:117:THR:HA	1:A:317:ASN:HD21	1.51	0.74

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	398/470 (85%)	387 (97%)	11 (3%)	0	100	100
1	B	392/470 (83%)	381 (97%)	11 (3%)	0	100	100
All	All	790/940 (84%)	768 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	262/346 (76%)	260 (99%)	2 (1%)	81	90
1	B	261/346 (75%)	259 (99%)	2 (1%)	81	90
All	All	523/692 (76%)	519 (99%)	4 (1%)	81	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	414	MET
1	B	286	MET
1	B	348	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	326	HIS

### 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 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, 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	406/470 (86%)	0.21	19 (4%) 31 30	16, 23, 33, 50	0
1	B	402/470 (85%)	0.18	16 (3%) 38 36	14, 23, 33, 46	0
All	All	808/940 (85%)	0.19	35 (4%) 35 33	14, 23, 33, 50	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	THR	4.4
1	B	376	PHE	4.2
1	A	387	VAL	3.5
1	A	398	PHE	3.4
1	A	183	HIS	3.4

### 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 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.