

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 2, 2023 – 10:56 PM EDT

PDB ID	:	6P3J
Title	:	Crystal structure of LigU
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Deposited on		
Resolution	:	2.02  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 (i) 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 (1)) were used in the production of this report:

:	FAILED
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber $(2001)$
:	Parkinson et al. (1996)
:	2.35.1
	: : : :

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.02 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5380 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	353	Total	С	Ν	Ο	$\mathbf{S}$	0	5	0
	I A	000	2575	1605	445	505	20			
1	В	352	Total	С	Ν	0	S	0	ე	0
	ГБ		2569	1598	455	496	20	0	2	0

• Molecule 1 is a protein called (4E)-oxalomesaconate Delta-isomerase.

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	LEU	-	expression tag	UNP Q0KJL4
А	359	GLU	-	expression tag	UNP Q0KJL4
А	360	HIS	-	expression tag	UNP Q0KJL4
А	361	HIS	-	expression tag	UNP Q0KJL4
А	362	HIS	-	expression tag	UNP Q0KJL4
А	363	HIS	-	expression tag	UNP Q0KJL4
А	364	HIS	-	expression tag	UNP Q0KJL4
А	365	HIS	-	expression tag	UNP Q0KJL4
В	358	LEU	-	expression tag	UNP Q0KJL4
В	359	GLU	-	expression tag	UNP Q0KJL4
В	360	HIS	-	expression tag	UNP Q0KJL4
В	361	HIS	-	expression tag	UNP Q0KJL4
В	362	HIS	-	expression tag	UNP Q0KJL4
В	363	HIS	-	expression tag	UNP Q0KJL4
В	364	HIS	-	expression tag	UNP Q0KJL4
В	365	HIS	-	expression tag	UNP Q0KJL4

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	5	Total Cl 5 5	0	0
2	В	4	Total Cl 4 4	0	0





• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	2	Total Ca 2 2	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	В	1	Total N 1	Na 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	120	Total O   120 120	0	0
5	В	104	Total O 104 104	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.





# 3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	62.78Å 67.36Å 161.07Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	41.99 - 2.02	Depositor	
% Data completeness	97.9 (41.99-2.02)	Depositor	
(in resolution range)		Depositor	
R <sub>merge</sub>	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.30 (at 2.01 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.15.2_3472	Depositor	
$R, R_{free}$	0.186 , $0.212$	Depositor	
Wilson B-factor $(Å^2)$	44.3	Xtriage	
Anisotropy	0.293	Xtriage	
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5380	wwPDB-VP	
Average B, all atoms $(Å^2)$	61.0	wwPDB-VP	

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

## 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers (i)

There are no such residues in this entry.

# 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

## 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

## 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

