



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 08:59 AM BST

PDB ID : 6M0D  
Title : Beijerinckia indica beta-fructosyltransferase  
Authors : Tonozuka, T.  
Deposited on : 2020-02-21  
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.

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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	:	<b>FAILED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

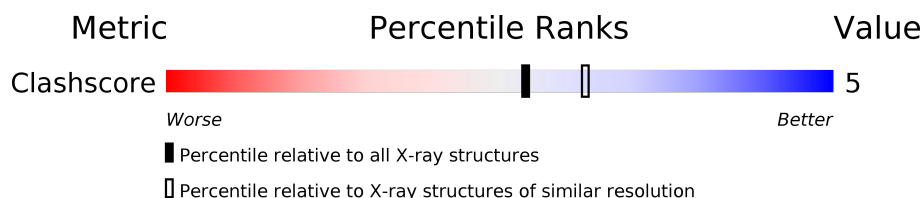
# 1 Overall quality at a glance

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))
Clashscore	141614	5594 (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 on 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	523	 80% 11% 9%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3761 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 Levansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3693	2353	634	698	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP B2IF78
A	-5	SER	-	expression tag	UNP B2IF78
A	-4	GLY	-	expression tag	UNP B2IF78
A	-3	MET	-	expression tag	UNP B2IF78
A	-2	LYS	-	expression tag	UNP B2IF78
A	-1	GLU	-	expression tag	UNP B2IF78
A	0	THR	-	expression tag	UNP B2IF78
A	1	ALA	-	expression tag	UNP B2IF78
A	2	ALA	-	expression tag	UNP B2IF78
A	3	ALA	-	expression tag	UNP B2IF78
A	4	LYS	-	expression tag	UNP B2IF78
A	5	PHE	-	expression tag	UNP B2IF78
A	6	GLU	-	expression tag	UNP B2IF78
A	7	ARG	-	expression tag	UNP B2IF78
A	8	GLN	-	expression tag	UNP B2IF78
A	9	HIS	-	expression tag	UNP B2IF78
A	10	MET	-	expression tag	UNP B2IF78
A	11	ASP	-	expression tag	UNP B2IF78
A	12	SER	-	expression tag	UNP B2IF78
A	13	PRO	-	expression tag	UNP B2IF78
A	14	ASP	-	expression tag	UNP B2IF78
A	15	LEU	-	expression tag	UNP B2IF78
A	16	GLY	-	expression tag	UNP B2IF78
A	17	THR	-	expression tag	UNP B2IF78
A	18	ASP	-	expression tag	UNP B2IF78
A	19	ASP	-	expression tag	UNP B2IF78
A	20	ASP	-	expression tag	UNP B2IF78

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ASP	-	expression tag	UNP B2IF78
A	22	LYS	-	expression tag	UNP B2IF78
A	23	ALA	-	expression tag	UNP B2IF78
A	24	MET	-	expression tag	UNP B2IF78
A	25	ALA	-	expression tag	UNP B2IF78
A	26	ASP	-	expression tag	UNP B2IF78
A	27	ILE	-	expression tag	UNP B2IF78
A	28	GLY	-	expression tag	UNP B2IF78
A	29	SER	-	expression tag	UNP B2IF78
A	?	-	GLY	deletion	UNP B2IF78
A	?	-	PRO	deletion	UNP B2IF78
A	?	-	TYR	deletion	UNP B2IF78
A	?	-	ALA	deletion	UNP B2IF78
A	?	-	ASP	deletion	UNP B2IF78
A	479	PRO	THR	conflict	UNP B2IF78
A	495	GLY	ARG	conflict	UNP B2IF78
A	?	-	LEU	deletion	UNP B2IF78
A	?	-	GLY	deletion	UNP B2IF78
A	?	-	GLN	deletion	UNP B2IF78
A	?	-	GLY	deletion	UNP B2IF78
A	?	-	ASN	deletion	UNP B2IF78
A	?	-	GLY	deletion	UNP B2IF78
A	?	-	HIS	deletion	UNP B2IF78
A	?	-	GLY	deletion	UNP B2IF78
A	?	-	VAL	deletion	UNP B2IF78
A	?	-	THR	deletion	UNP B2IF78
A	?	-	ASN	deletion	UNP B2IF78
A	?	-	GLY	deletion	UNP B2IF78
A	?	-	GLN	deletion	UNP B2IF78

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	66	Total O 66 66	0	0



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.89Å 80.90Å 92.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.30 – 2.20	Depositor
% Data completeness (in resolution range)	99.3 (44.30-2.20)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.222 , 0.266	Depositor
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.103	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.01% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.72	0/3811	0.88	0/5213

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	SER	Peptide

### 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	3693	0	3479	38	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	66	0	0	0	0
All	All	3761	0	3479	38	1

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 5.

The worst 5 of 38 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:111:GLN:H	1:A:518:ASN:ND2	1.72	0.88
1:A:353:THR:HG23	1:A:361:LYS:HD3	1.63	0.78
1:A:358:THR:OG1	1:A:359:GLN:OE1	2.09	0.70
1:A:175:VAL:HB	1:A:186:ASN:ND2	2.08	0.69
1:A:79:ASN:ND2	1:A:499:ILE:HG23	2.16	0.61

All (1) 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:70:SER:OG	1:A:171:ASP:OD2[3_454]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

Of 2 ligands modelled in this entry, 2 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.

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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