



# wwPDB X-ray Structure Validation Summary Report

Oct 3, 2023 – 05:25 AM EDT

PDB ID : 6O1J  
Title : Alpha-L-fucosidase AlfC fucosyltransferase mutant N243A  
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Deposited on : 2019-02-20  
Resolution : 2.00 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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.35.1

## 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 2.00 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

There are 3 unique types of molecules in this entry. The entry contains 21640 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 AlfC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	Total 2636	C 1685	N 433	O 505	S 13	0	0	0
1	B	324	Total 2600	C 1660	N 427	O 500	S 13	0	0	0
1	C	323	Total 2592	C 1655	N 426	O 499	S 12	0	0	0
1	D	324	Total 2602	C 1663	N 427	O 499	S 13	0	0	0
1	E	327	Total 2624	C 1678	N 431	O 503	S 12	0	0	0
1	F	323	Total 2593	C 1655	N 426	O 499	S 13	0	0	0
1	G	317	Total 2548	C 1628	N 419	O 489	S 12	0	0	0
1	H	323	Total 2596	C 1658	N 426	O 499	S 13	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

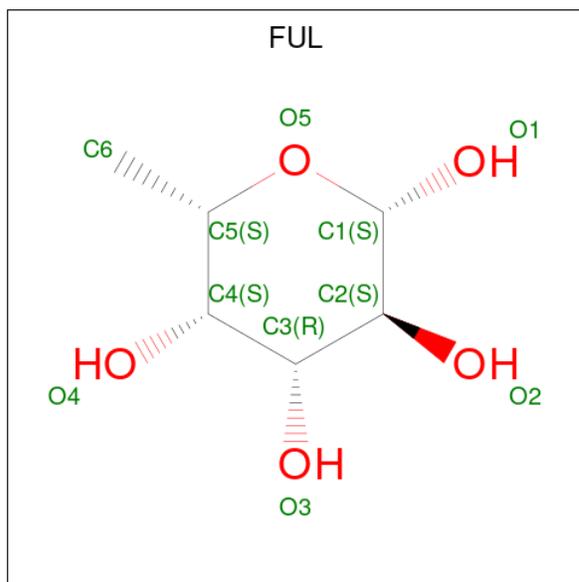
Chain	Residue	Modelled	Actual	Comment	Reference
A	243	ALA	ASN	engineered mutation	UNP K0NB39
A	345	LEU	-	expression tag	UNP K0NB39
B	243	ALA	ASN	engineered mutation	UNP K0NB39
B	345	LEU	-	expression tag	UNP K0NB39
C	243	ALA	ASN	engineered mutation	UNP K0NB39
C	345	LEU	-	expression tag	UNP K0NB39
D	243	ALA	ASN	engineered mutation	UNP K0NB39
D	345	LEU	-	expression tag	UNP K0NB39
E	243	ALA	ASN	engineered mutation	UNP K0NB39
E	345	LEU	-	expression tag	UNP K0NB39
F	243	ALA	ASN	engineered mutation	UNP K0NB39
F	345	LEU	-	expression tag	UNP K0NB39
G	243	ALA	ASN	engineered mutation	UNP K0NB39

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Chain	Residue	Modelled	Actual	Comment	Reference
G	345	LEU	-	expression tag	UNP K0NB39
H	243	ALA	ASN	engineered mutation	UNP K0NB39
H	345	LEU	-	expression tag	UNP K0NB39

- Molecule 2 is beta-L-fucopyranose (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 6 5	0	0
2	B	1	Total C O 11 6 5	0	0
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0
2	E	1	Total C O 11 6 5	0	0
2	F	1	Total C O 11 6 5	0	0
2	G	1	Total C O 11 6 5	0	0
2	H	1	Total C O 11 6 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0
3	B	120	Total 120	O 120	0	0
3	C	96	Total 96	O 96	0	0
3	D	95	Total 95	O 95	0	0
3	E	92	Total 92	O 92	0	0
3	F	99	Total 99	O 99	0	0
3	G	83	Total 83	O 83	0	0
3	H	60	Total 60	O 60	0	0

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

### 3 Data and refinement statistics i

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.30Å 259.92Å 80.35Å 90.00° 118.81° 90.00°	Depositor
Resolution (Å)	47.75 – 2.00	Depositor
% Data completeness (in resolution range)	91.3 (47.75-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.230 , 0.243	Depositor
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.363	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.088 for -h-l,k,h 0.088 for l,k,-h-l 0.088 for h,-k,-h-l 0.087 for -h-l,-k,l 0.356 for l,-k,h	Xtriage
Reported twinning fraction	0.645 for H, K, L 0.355 for -L, -K, -H	Depositor
Outliers	0 of 176954 reflections	Xtriage
Total number of atoms	21640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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.

## 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](#)

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### 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](#)

8 ligands are 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
2	FUL	B	401	-	11,11,11	1.51	1 (9%)	15,16,16	1.43	3 (20%)
2	FUL	C	401	-	11,11,11	1.34	1 (9%)	15,16,16	1.21	2 (13%)
2	FUL	A	401	-	11,11,11	1.39	1 (9%)	15,16,16	1.47	2 (13%)
2	FUL	H	401	-	11,11,11	1.25	1 (9%)	15,16,16	0.87	0
2	FUL	G	401	-	11,11,11	1.35	1 (9%)	15,16,16	0.78	0
2	FUL	F	401	-	11,11,11	1.39	1 (9%)	15,16,16	1.46	2 (13%)
2	FUL	E	401	-	11,11,11	1.31	1 (9%)	15,16,16	1.06	1 (6%)
2	FUL	D	401	-	11,11,11	1.45	1 (9%)	15,16,16	2.14	4 (26%)

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
2	FUL	B	401	-	-	-	0/1/1/1
2	FUL	C	401	-	-	-	0/1/1/1
2	FUL	A	401	-	-	-	0/1/1/1
2	FUL	H	401	-	-	-	0/1/1/1
2	FUL	G	401	-	-	-	0/1/1/1
2	FUL	F	401	-	-	-	0/1/1/1
2	FUL	E	401	-	-	-	0/1/1/1
2	FUL	D	401	-	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FUL	O5-C1	3.57	1.51	1.42
2	F	401	FUL	O5-C1	3.42	1.51	1.42
2	B	401	FUL	O5-C1	3.38	1.51	1.42
2	D	401	FUL	O5-C1	3.32	1.51	1.42
2	C	401	FUL	O5-C1	3.21	1.50	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FUL	O5-C5-C4	4.81	118.15	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FUL	C3-C4-C5	4.10	116.15	109.77
2	A	401	FUL	C3-C4-C5	3.70	115.54	109.77
2	F	401	FUL	C3-C4-C5	3.68	115.51	109.77
2	B	401	FUL	O5-C5-C4	2.83	114.60	109.52

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.