



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2020 – 08:50 PM BST

PDB ID : 6M6P  
Title : Structure of Marine bacterial laminarinase mutant E135A in complex with 1, 3-beta-cellobiosyl-glucose  
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Deposited on : 2020-03-16  
Resolution : 2.27 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 : **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) : 2.14.6

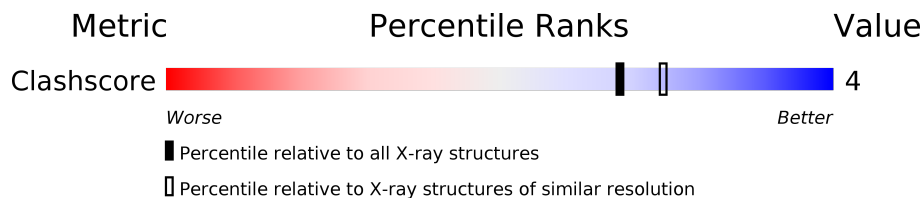
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 141614                      | 7711 (2.30-2.26)                                      |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2024 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 laminarinase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 231      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1857  | 1180 | 319 | 350 | 8 |         |         |       |

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-3)-alpha-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 2   | B     | 4        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 45    | 24 | 21 |         |         |       |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 121      | Total | O   | 0       | 0       |
|     |       |          | 121   | 121 |         |         |

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

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

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | C 2 2 21  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 67.00Å 95.64Å 72.99Å<br>90.00° 90.00° 90.00°                | Depositor |
| Resolution (Å)   | 43.90 – 2.27  | Depositor |
| % Data completeness<br>(in resolution range)             | 97.7 (43.90-2.27)   | Depositor |
| $R_{merge}$  | 0.11  | Depositor |
| $R_{sym}$  | (Not available)   | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 2.31 (at 2.27Å)   | Xtriage   |
| Refinement program                                       | REFMAC 5.8.0258   | Depositor |
| R, $R_{free}$  | 0.174 , 0.228   | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 33.0  | Xtriage   |
| Anisotropy   | 0.872   | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 2024  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 36.0  | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CA, BGC

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     | 0.63         | 0/1918      | 0.75        | 0/2614      |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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     | 1857  | 0        | 1717     | 12      | 1            |
| 2   | B     | 45    | 0        | 39       | 2       | 1            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 121   | 0        | 0        | 0       | 0            |
| All | All   | 2024  | 0        | 1756     | 14      | 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 4.

The worst 5 of 14 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:91:THR:HG22 | 1:A:217:PHE:HB2 | 1.70                     | 0.74              |
| 1:A:91:THR:HG23 | 1:A:95:LYS:O    | 1.91                     | 0.70              |
| 1:A:33:ASN:OD1  | 1:A:34:GLY:N    | 2.27                     | 0.64              |
| 2:B:3:BGC:O3    | 2:B:4:BGC:O5    | 2.23                     | 0.53              |
| 1:A:91:THR:CG2  | 1:A:95:LYS:O    | 2.58                     | 0.50              |

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:22:ASN:OD1 | 2:B:4:BGC:O2[6_555] | 1.98                     | 0.22              |

## 4.3 Torsion angles [i](#)

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

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

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

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

### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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](#)

4 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

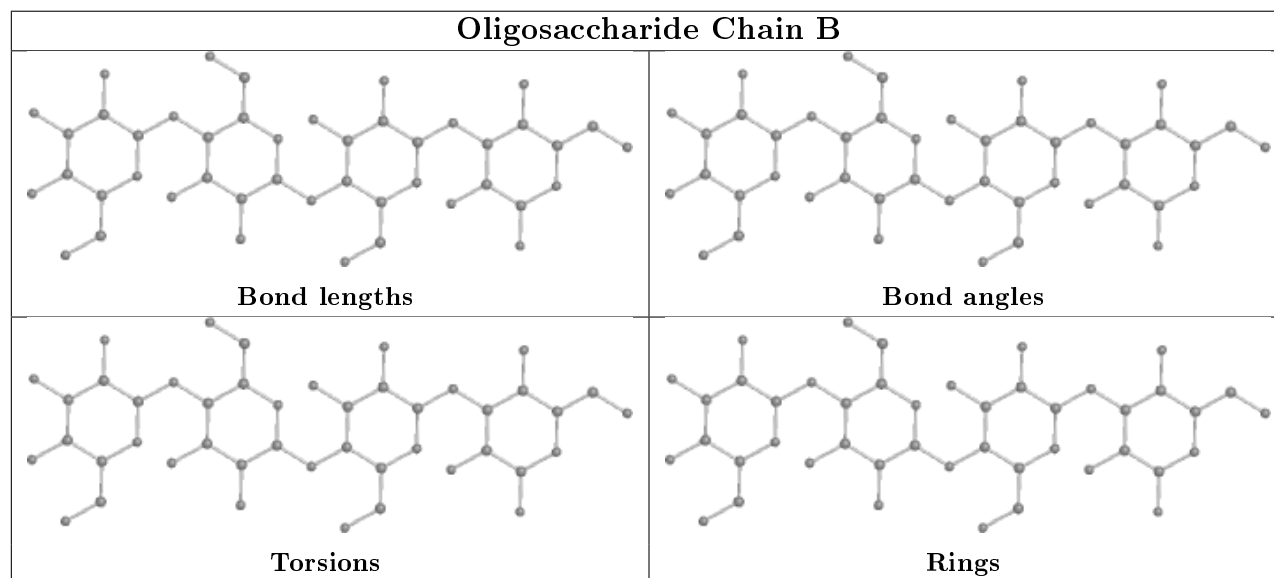
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 4.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 5.3 Carbohydrates ⓘ

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

### 5.4 Ligands ⓘ

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

### 5.5 Other polymers ⓘ

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