

Characterization of a new glucose-tolerant GH1 β -glycosidase from *Aspergillus fumigatus* with transglycosylation activity

Lucas Matheus Soares Pereira¹, Aline Vianna Bernardi¹, Luis Eduardo Gerolamo¹, Wellington Ramos Pedersoli², Cláudia Batista Carraro², Roberto do Nascimento Silva², Sergio Akira Uyemura³ and Taísa Magnani Dinamarco^{1,3*}

¹Faculty of Philosophy, Sciences and Literature of Ribeirão Preto, Chemistry Department, University of São Paulo, Ribeirão Preto, São Paulo, Brazil. ²Ribeirão Preto Medical School, Department of Biochemistry and Immunology, University of São Paulo, Ribeirão Preto, São Paulo, Brazil, ³Faculty of Pharmaceutical Science, Department of Clinical, Toxicological and Bromatological Analysis, University of São Paulo, Ribeirão Preto, São Paulo, Brazil.

*Correspondence: author: tdinamarco@ffclrp.usp.br; Tel.: +55-16-3315-9121; Fax: +55-16-3315-9101

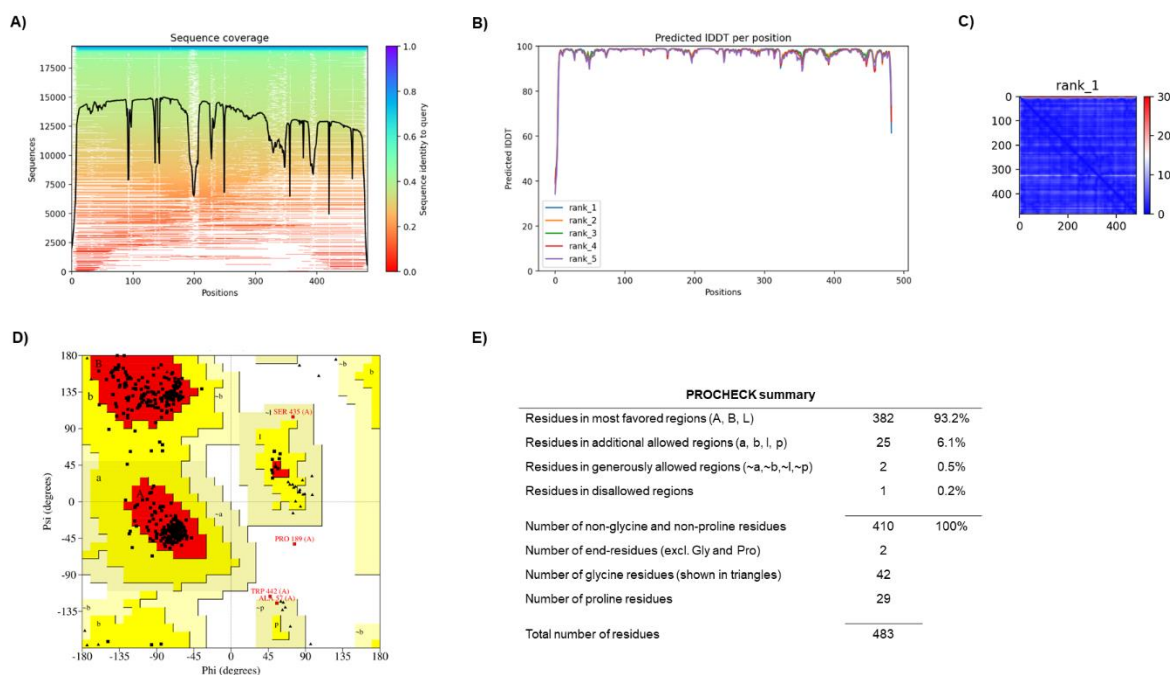


Figure S1: Prediction and validation of AfBgl1.3 tridimensional structure.

A) Sequence coverage from the alignments made for structure prediction. **B)** pLDDT for each model predicted, showing the confidence metric per residue. For the model used in this study, confidence values were pLDDT = 97.4, pTM=0.953. **C)** PAE (Predicted Alignment Error) plot for the model used in the study, showing the high model quality. **D)** Ramachandran plot and **(E)** PROCHECK summary. It

is possible to notice that 93.2% of residues are located in the most favored regions, indicating a good quality model (>90%). Considering the unusuality measurement, G-factors were 0.35 (dihedrals), -0.23 (covalent), and 0.13 (overall), indicating that the model can be used for the proposed objective in this article, although some energy minimization may be needed for molecular simulation studies