

In Silico Analysis of a GH3 β -glucosidase from *Microcystis aeruginosa* CACIAM 03

Gustavo Marques Serra ^{1,*}, Andrei Santos Siqueira ², Fábio Alberto de Molfetta ³,
Agenor Valadares Santos ¹ and Luciana Pereira Xavier ^{1,*}

¹ Laboratório de Biotecnologia de Enzimas e Biotransformações, Instituto de Ciências Biológicas, Universidade Federal do Pará-UFPA, Belém 66075-110, Brazil; avsantos@ufpa.br

² Laboratório de Tecnologia Biomolecular, Instituto de Ciências Biológicas, Universidade Federal do Pará-UFPA, Belém 66075-110, Brazil; andrei.siqueira@icb.ufpa.br

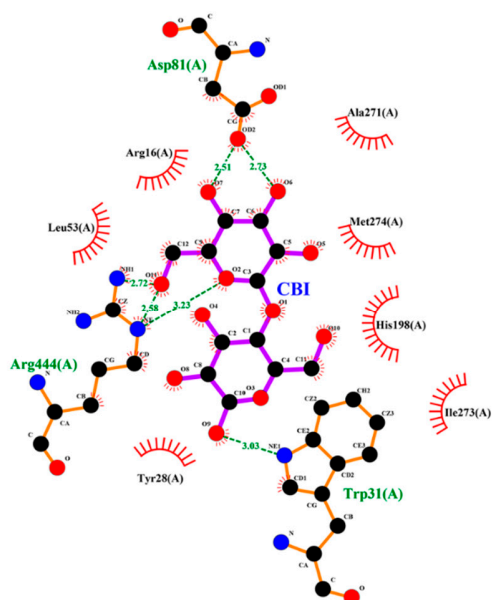
³ Laboratório de Modelagem Molecular, Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará-UFPA, Belém 66075-10, Brazil; fabioam@ufpa.br

* Correspondence: gustavo.serra@icb.ufpa.br (G.M.S.); lpxavier@ufpa.br (L.P.X.); Tel.: +55-91-98182-3213 (G.M.S.); +55-91-99294-4213 (L.P.X.)

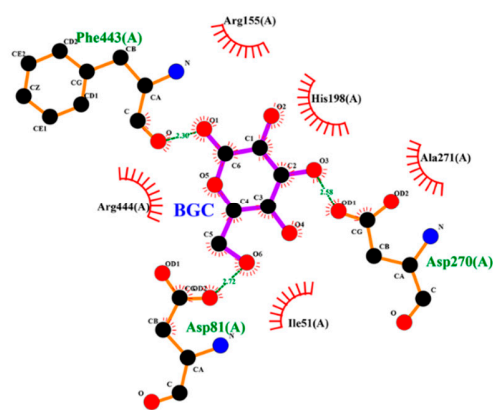
Supplementary Material

Table S1. Validation of three-dimensional structure of MaBgl3 using MolProbity, Verify3D and ERRAT.

Ramachandran plot (%)			Verify 3D score (%)	ERRAT score (%)	RMSD (Å)
Favorable Regions	Allowed Regions	Disallowed Regions			
95.19	4.81	0.0	97.32	89.08	0.087



(a)



(b)

Figure S1. Hydrogen interactions were obtained with PoseView server. (a) CBI and (b) BGC.

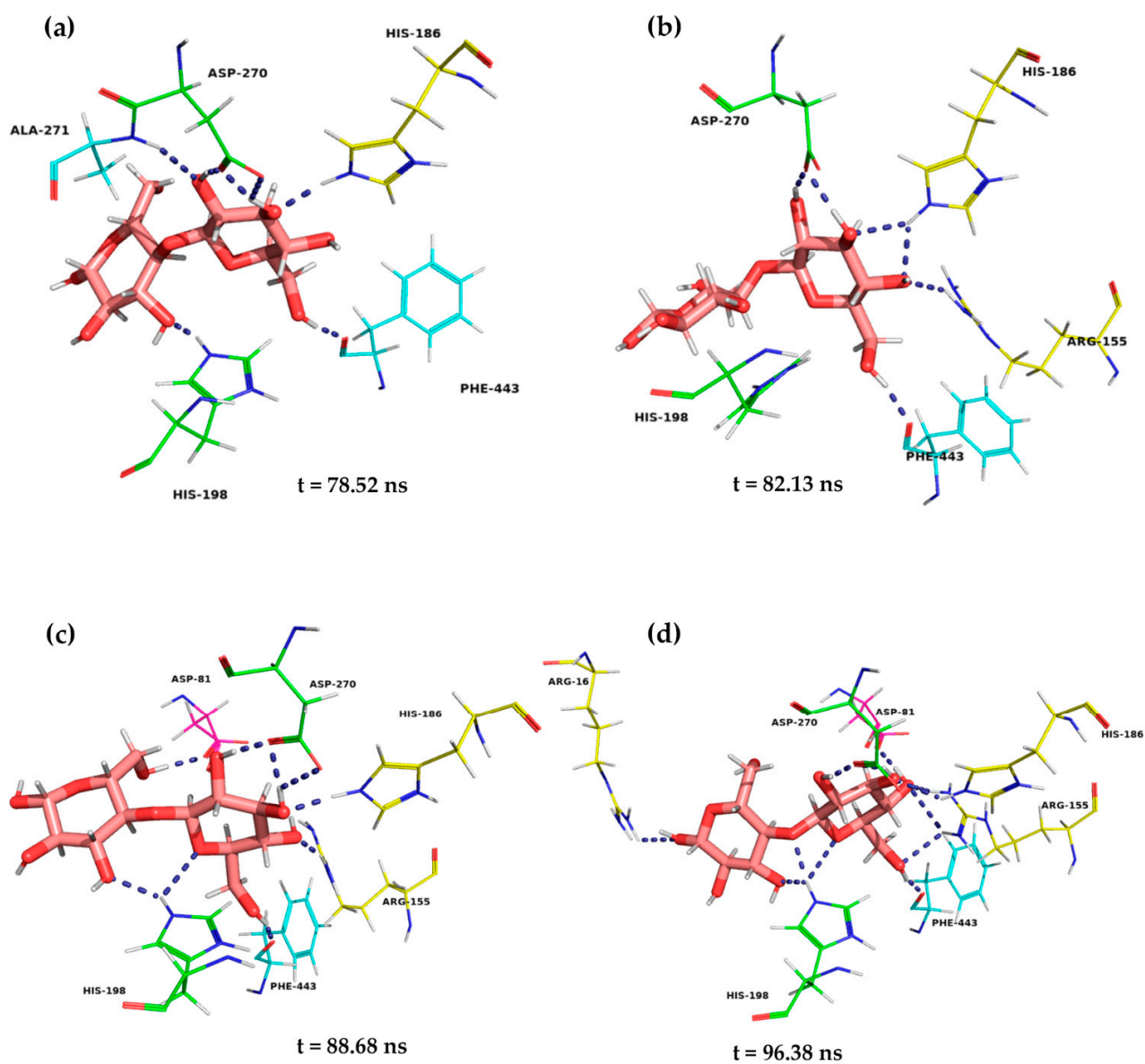


Figure S2. Stick representation of CBI at time (a) 78.52 ns, (b) 82.13 ns, (c) 88.68 ns and (d) 96.38 ns. Hydrogen bonds interactions are in dashed blue lines.

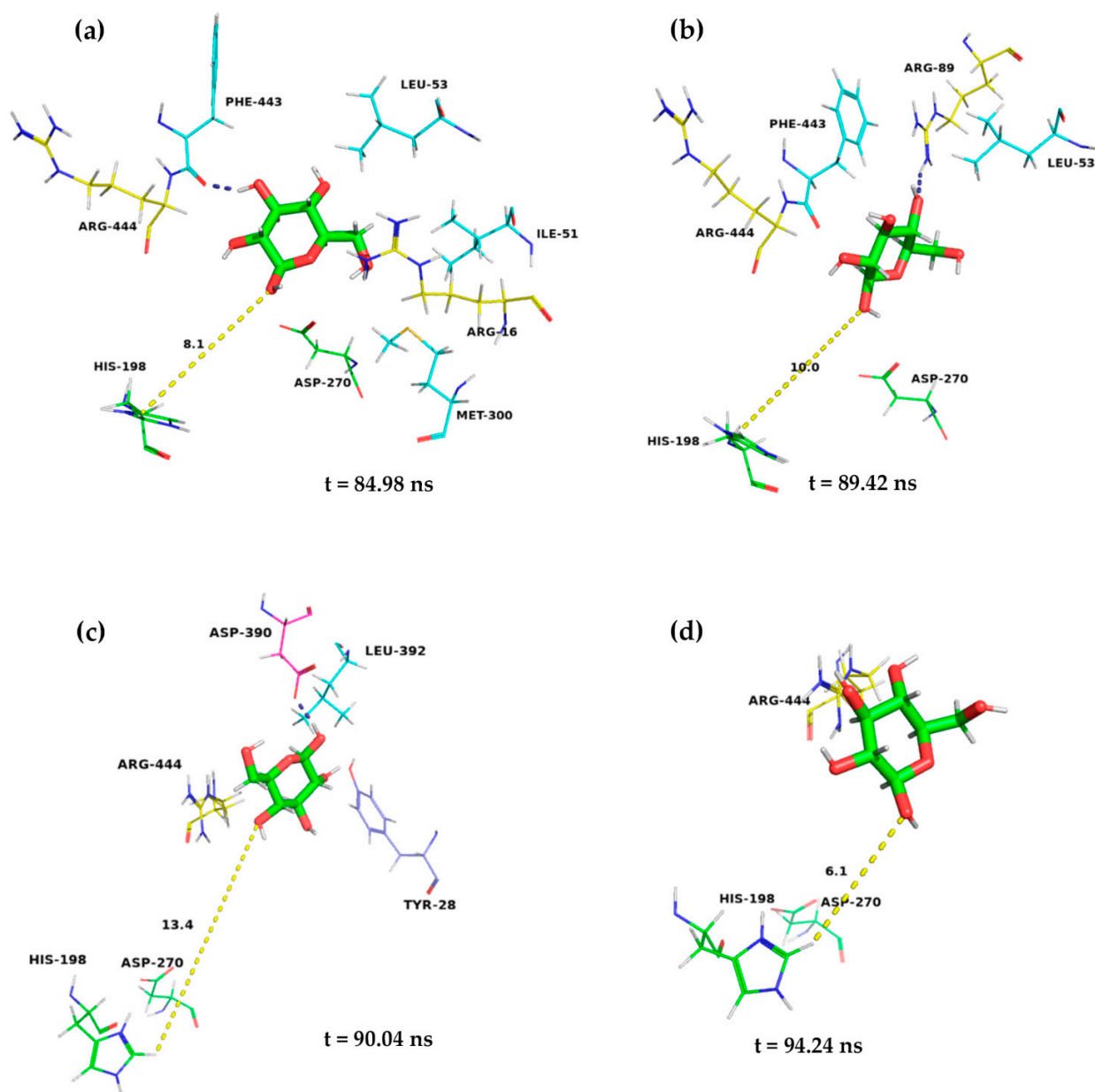


Figure S3. Stick representation of BGC at time (a) 84.98 ns, (b) 89.42 ns, (c) 90.04 ns and (d) 94.24 ns. Hydrogen bonds interactions are in dashed blue lines and distance measures are in yellow dashed lines.

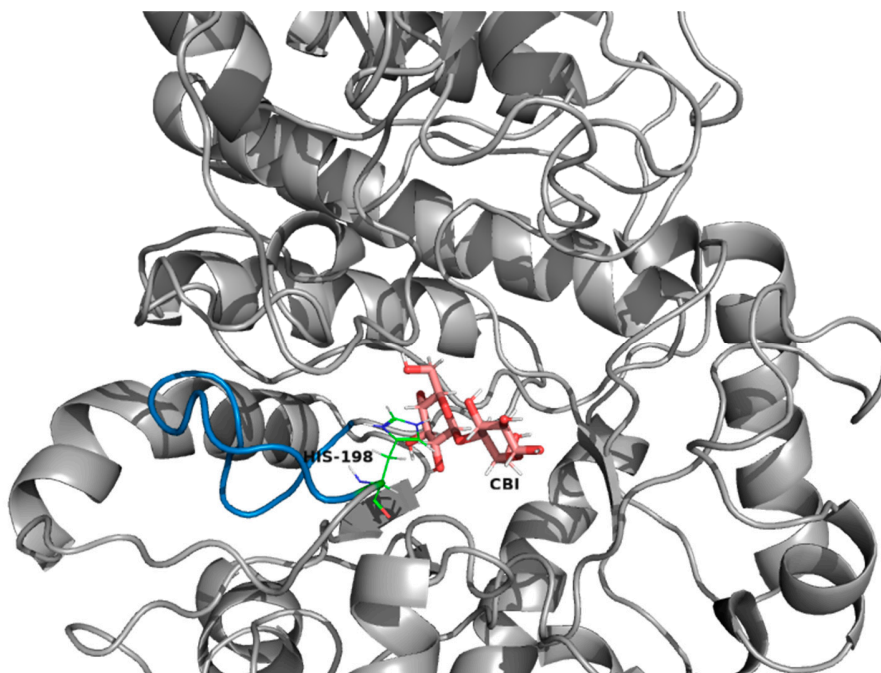


Figure S4. MaBgl3 final pose of trajectory. General acid/base catalyst His198 is present in the loop of the enzyme active site and the substrate CBI.