

Article

Structural evidence of active site adaptability towards different sized substrates of aromatic amino acid aminotransferase from *Psychrobacter* sp. B6

Anna Bujacz ^{1,*}, Jędrzej Rum ¹, Maria Rutkiewicz ², Agnieszka J. Pietrzyk-Brzezinska ¹ and Grzegorz Bujacz ¹

¹ Institute of Molecular and Industrial Biotechnology, Lodz University of Technology, Stefanowskiego 4/10, 90-924 Lodz, Poland; jedrzej.rum@dokt.p.lodz.pl (J.R.); agnieszka.pietrzyk-brzezinska@p.lodz.pl (A.J.P.-B.); grzegorz.bujacz@p.lodz.pl (G.B.)

² Macromolecular Structure and Interaction, Max Delbrück Center for Molecular Medicine, Robert-Rössle-Straße 10, 13125 Berlin, Germany; maria.rutkiewicz@mdc-berlin.de

* Correspondence: anna.bujacz@p.lodz.pl

For both subunits A and B of *PsyArAT*/FOH dimer (Figure S1A,B) volume differences are not big but noticeable (Table 1). In *PsyArAT*/YOH volume of the active pocket of monomer A (Figure S1C) is bigger than in monomer B (Figure S1D). For the *PsyArAT*/WOH differences between active site volume are the most visible. Only one monomer of each dimer bound the ligand. The volume of active pocket of monomers A and C with bound inhibitor is much smaller (Figure S1E) in comparison to empty subunits (monomers B and D) (Figure S1F). *PsyArAT*/DOH crystallized as monomer in asymmetric unit and its active site (Figure S1G) is the smallest, especially comparing to the native *PsyArAT* (PDB ID: 4RKC) (Figure S1H).

Citation: Bujacz, A.; Rum, J.; Rutkiewicz, M.; Pietrzyk-Brzezinska, A.J.; Bujacz, G. Structural Evidence of Active Site Adaptability Towards Different Sized Substrates of Aromatic Amino Acid Aminotransferase from *Psychrobacter* sp. B6. *Materials* **2021**, *14*, 3351. <https://doi.org/10.3390/ma14123351>

Academic Editor(s): Shouke Yan

Received: 06 May 2021

Accepted: 09 June 2021

Published: 17 June 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).

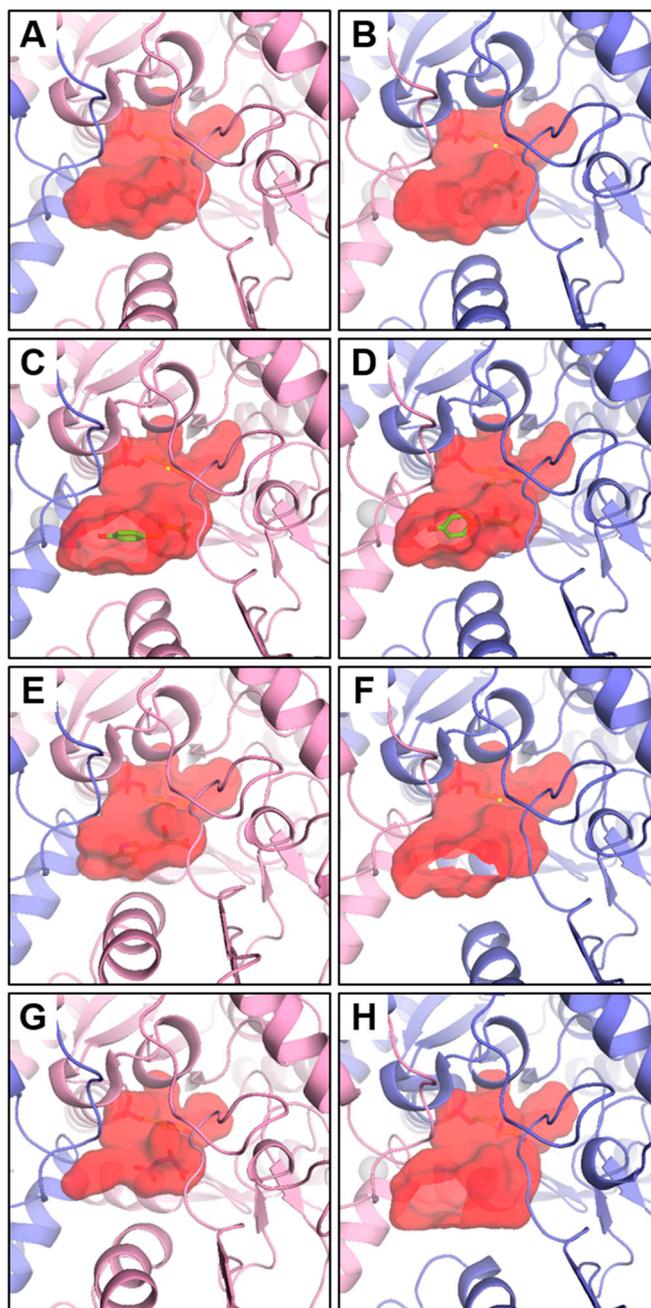


Figure S1. Graphical volume representations of *PsyArAT* active sites. (A, B) *PsyArAT*/FOH monomer A and B, respectively; (C, D) *PsyArAT*/YOH monomer A and B, respectively; (E, F) *PsyArAT*/WOH - monomer A and B, respectively; (G) *PsyArAT*/DOH monomer; (H) *PsyArAT* (PDB ID: 4RKC) monomer B.