**Supplementary material**

# Targeting the cell wall of Mycobacterium tuberculosis: A molecular modelling investigation of the interaction of imipenem and meropenem with *L*,*D*-transpeptidase 2

José Rogério A. Silva,[1] William R. Bishai,[2,] Thavendran Govender,[3] Gyanu Lamichhane,[3] Glenn E. M. Maguire,[4] Hendrik G. Kruger,[4] Jeronimo Lameira[1] and Cláudio N. Alves[1,*]

[1]*Laboratório de Planejamento e Desenvolvimento de Fármacos, Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, CP 11101, 66075-110, Belém, PA, Brazil.*

[2]*Department of Medicine, Division of Infectious Diseases, Johns Hopkins University School of Medicine, Baltimore, MD 21205, USA.*

[3]*Center for Tuberculosis Research, Division of Infectious Diseases, Johns Hopkins University School of Medicine, Baltimore, MD 21205, USA.*

[4]*Catalysis and Peptide Research Unit, School of Health Sciences, University of KwaZulu-Natal, Durban 4001, South Africa.*

Cláudio N. Alves, nahum_ufpa@yahoo.com.br

Supplementary figures that were mentioned in the text of the main paper are presented here. Note that the figure number corresponds to the data presented (and discussion) with the same number in the main paper.

The Cartesian coordinates of the calculated complexes are available in PDB format.

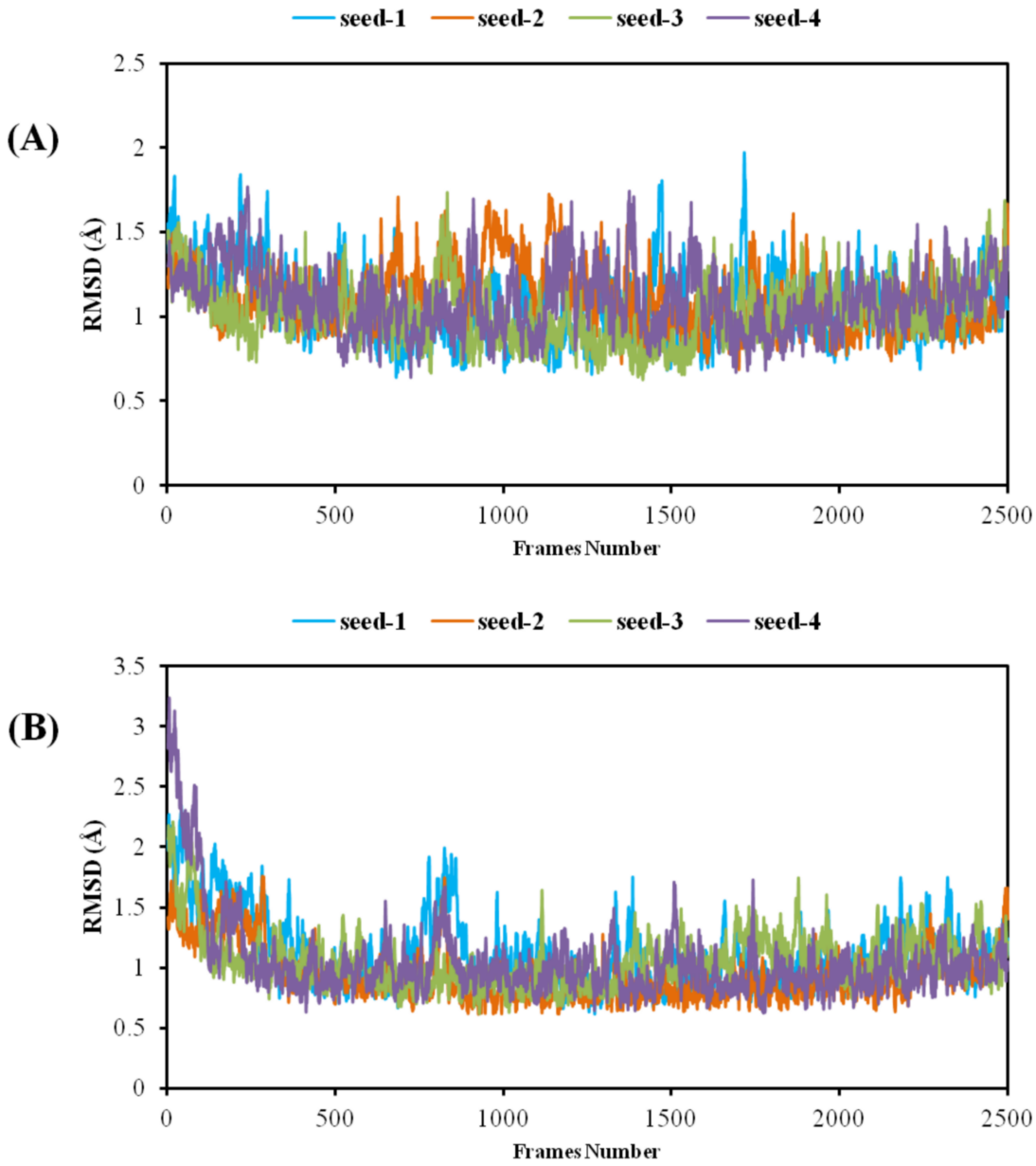


**Figure S1**. The RMSD plots for the imipenem (A) and meropenem (B) complexes from random seed, and starting from different sets of atomic coordinates and velocities.

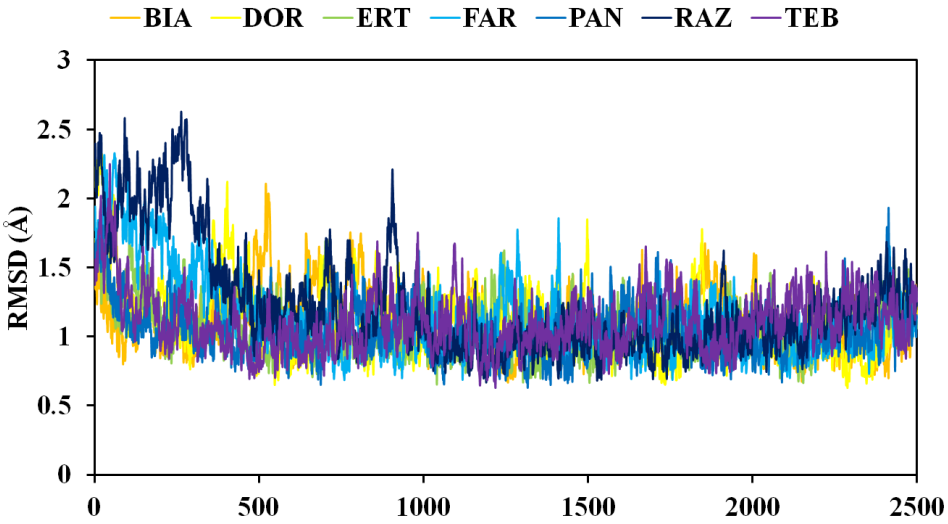


**Figure S4**. The time evolution of the root mean square deviation (RMSD) of the remaining inhibitor/$Ldt_{Mt2}$ complexes during 25 ns of MD simulations. (Refer to Figure 2 of the main paper for the inhibitor structures).

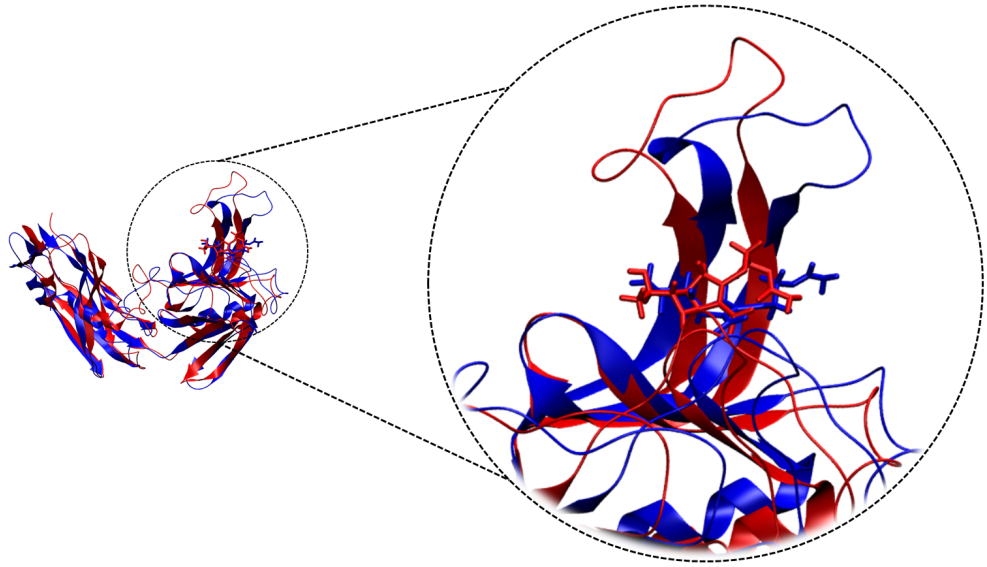

**Figure S6**. 3D structures for imipenem/ex-LdtMt2 complex in open (red) and closed conformations (blue) overlapped highlighting the β-hairpin flap region. The RMSD value found between these conformations is 3.40 Å.

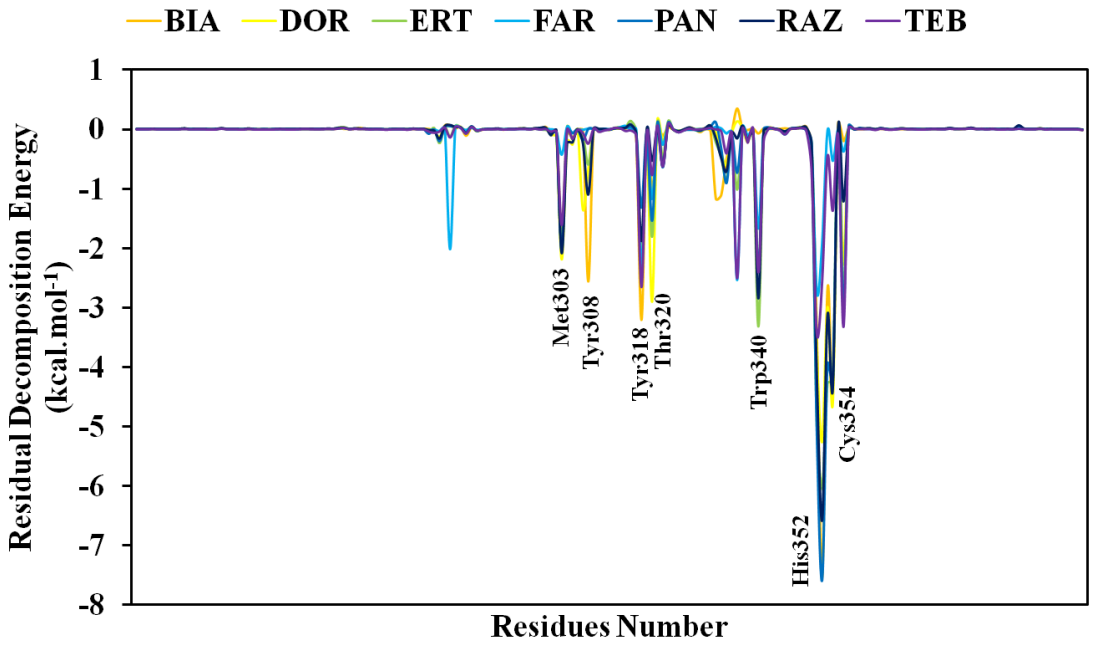


**Figure S8**. Average binding free energy decomposition per residue for inhibitor/Ldt$_{Mt2}$ complexes obtained by MM/GBSA approach. (Refer to Figure 2 of the main paper for the inhibitor structures).