

Making it rain: cloud-based molecular simulations for everyone

Pablo R. Arantes,^{*,†,⊥} Marcelo D. Polêto,^{*,‡} Conrado Pedebos,^{*,¶,§} and Rodrigo Ligabue-Braun^{*,||}

[†]*Department of Bioengineering, University of California, Riverside, CA 92521, United States*

[‡]*Department of Biochemistry, Virginia Tech, Blacksburg, VA 24061, United States*

[¶]*School of Chemistry, University of Southampton, Highfield Campus, Southampton SO17 1BJ, United Kingdom*

[§]*Present Address: Department of Biochemistry, University of Oxford, Oxford OX1 3QU, United Kingdom*

^{||}*Department of Pharmacosciences, Federal University of Health Sciences of Proto Alegre (UFCSPA), Porto Alegre 90050-170, RS, Brazil.*

[⊥]*Corresponding author*

E-mail: pabloa@ucr.edu; mdpoleto@vt.edu; conrado.pedebos@bioch.ox.ac.uk;
rodrigolb@ufcspa.edu.br

Supporting Information

List of Figures

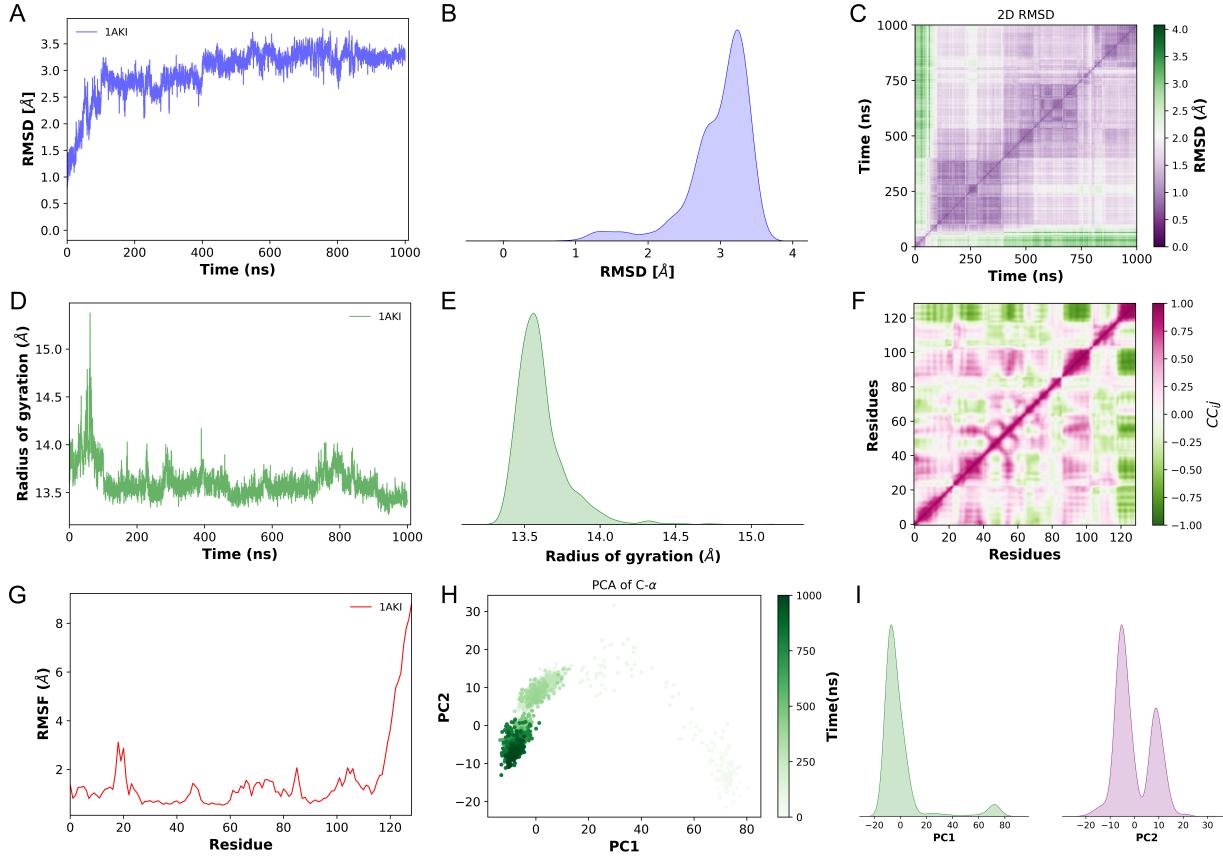


Figure S 1: Structural analyses of MD simulations using PyTraj embedded in the notebooks: RMSD values over time (A), its distribution (B) and a 2D RMSD plot (C); radius of gyration over time (D) and its distribution (E); Cross-correlation analysis (F); RMSF per residue (G); Principal Component Analysis (H) and its eigenvector distribution (I).