Supporting Information on "Replica-exchange umbrella sampling combined with Gaussian accelerated molecular dynamics for free-energy calculation of biomolecules"

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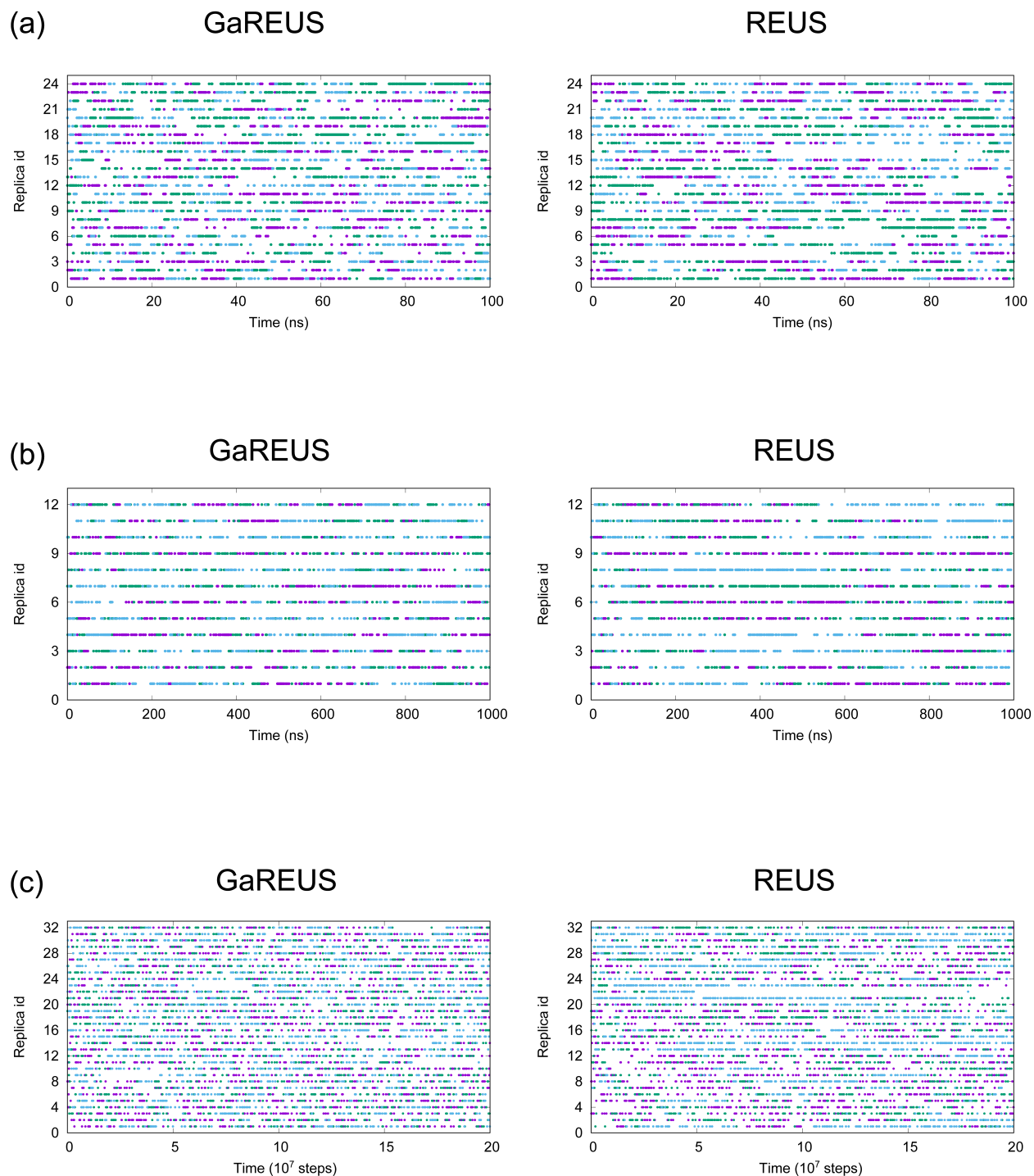
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Figure S1. Time series of replica exchanges of parameters in GaREUS and REUS simulations. (a) Bi9. The midpoint values of ω angles -15˚ (purple), 90˚ (green), and -150˚. (b) Chignolin. The midpoint values ξ_i = 19 Å (purple), 11 Å (green), and 7 Å (cyan). (c) AdK. The midpoint values ξ_i = 30 Å (purple), 24.5 Å (green), and 20.5 Å (cyan).
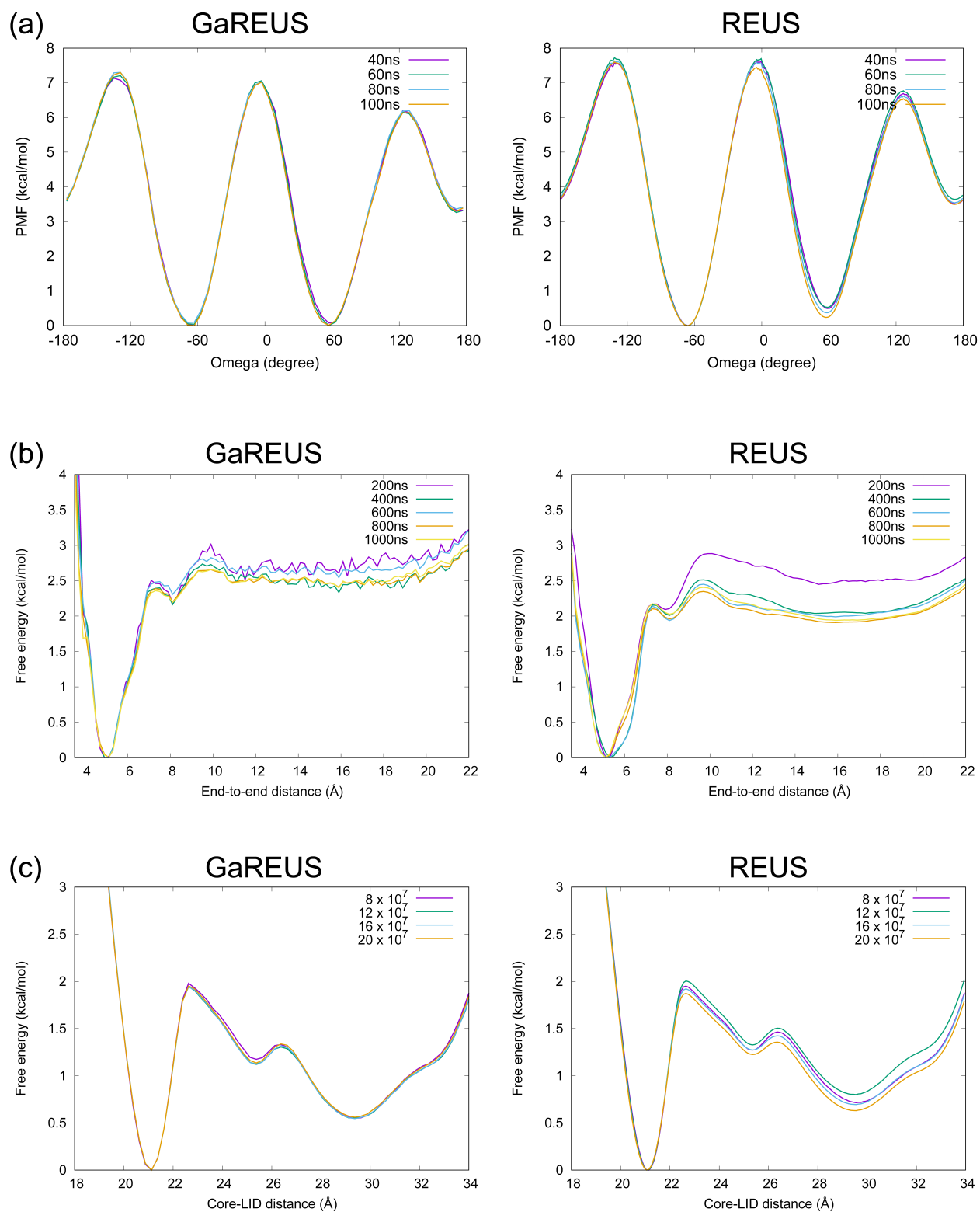
Figure S2. Free-energy landscapes of GaREUS and REUS along the CV for (a) Bi9, (b) chignolin, and (c) AdK.

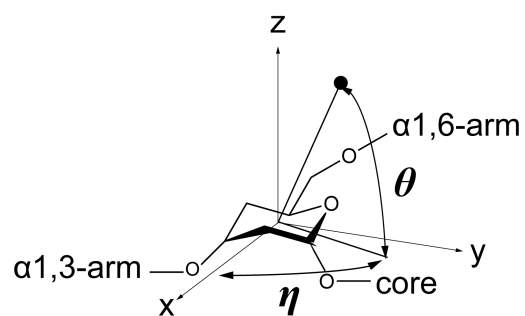Figure S3. Definition of the spherical coordinate. The angle η represents swing motion of the α1,6-arm around the z (polar) axis, while the angle θ represents up down motion with respect to the xy-plane.