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B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S.

Swaminathan, and M. Karplus, CHARMM: A Program for Macromolecular Energy, Minimization, and Dynamics Calculations, *J. Comp. Chem.*, 4, 187-217

(1983); and B. R. Brooks, C. L. Brooks III, A. D. MacKerell, Jr., L.

Nilsson, R. J. Petrella, B. Roux, Y. Won, M. Karplus, et al., CHARMM: The

Biomolecular Simulation Program, *J. Comput. Chem.*, 30, 1545-1614 (2009).

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