Erratum: "Density of states simulations of proteins" [J. Chem. Phys. 118, 4285 (2003)]

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We have detected an error in the message passing component of our code used to perform the calculations presented in the paper entitled "Density of states simulations of proteins." This led to incorrect numerical results in our computations, with the reported transitions being artificially sharp and shifted towards lower temperatures. The density-of-states simulation scheme proposed in the article, however, and the conclusions of our work remain unchanged. All of the calculations presented in Ref. 1 have been repeated with the correct code and compiler. The new results are given in Figs. 4–8 which should replace the corresponding old figures of Ref. 1. The specific heat for the case of peptides in vacuum (not shown) did not show any distinct transition. In fact, for the particular case of deca-alanine, we find nonhelical conformations having energy comparable to that of the native state. In general, the transitions from the unfolded to folded state are now spread over a larger temperature range.

[1] N. Rathore, T. A. Knotts, and J. J. de Pablo, J. Chem. Phys. **118**, 4285 (2003).

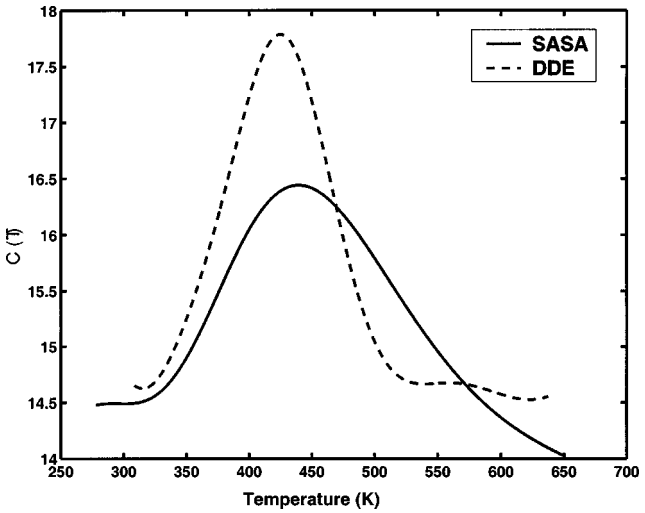

FIG. 5. Dimensionless specific heat per unit residue, $C(T)$, as a function of temperature for Met-enkephalin.

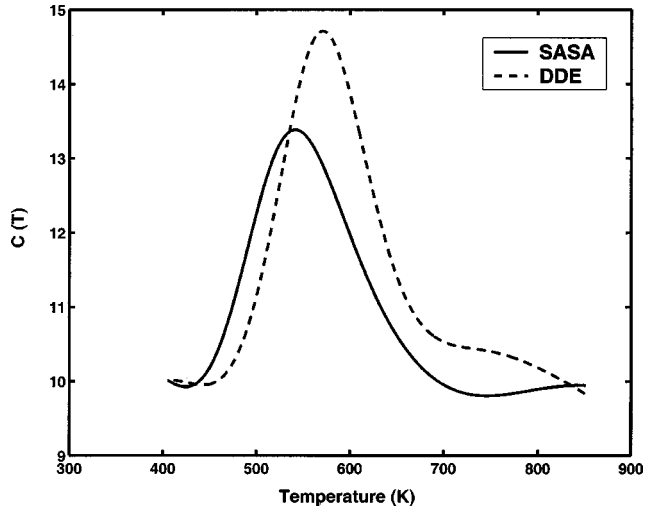

FIG. 4. Dimensionless specific heat per unit residue, $C(T)$, as a function of temperature for deca-alanine.

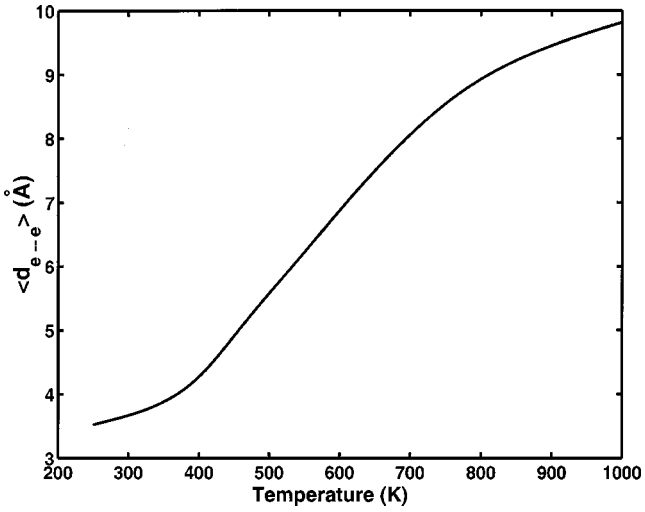

FIG. 6. Average end-to-end distance $\langle d_{e-e} \rangle$ as a function of temperature for Met-enkephalin in a distance dependent dielectric (DDE).

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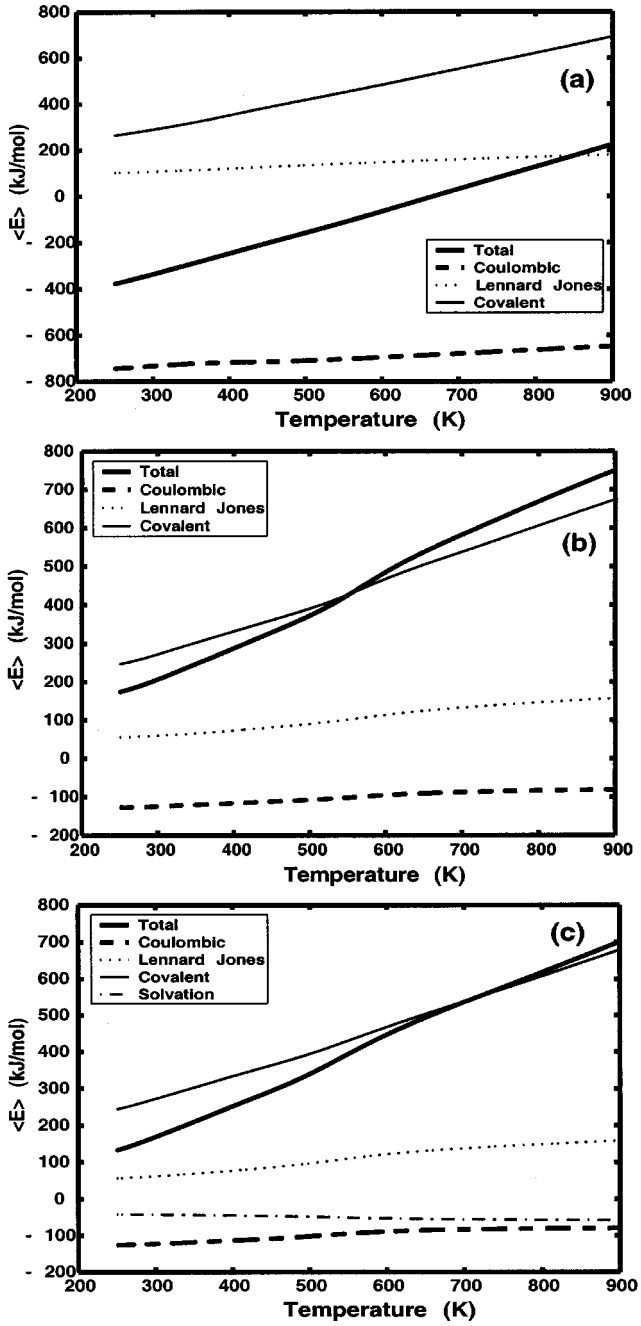

FIG. 7. Temperature dependence of the average energies (total, covalent, Lennard-Jones, Coulombic, and solvation) for deca-alanine in three different environments: (a) vacuum (VAC), (b) distance dependent dielectric (DDE), and (c) implicit solvent (SASA).

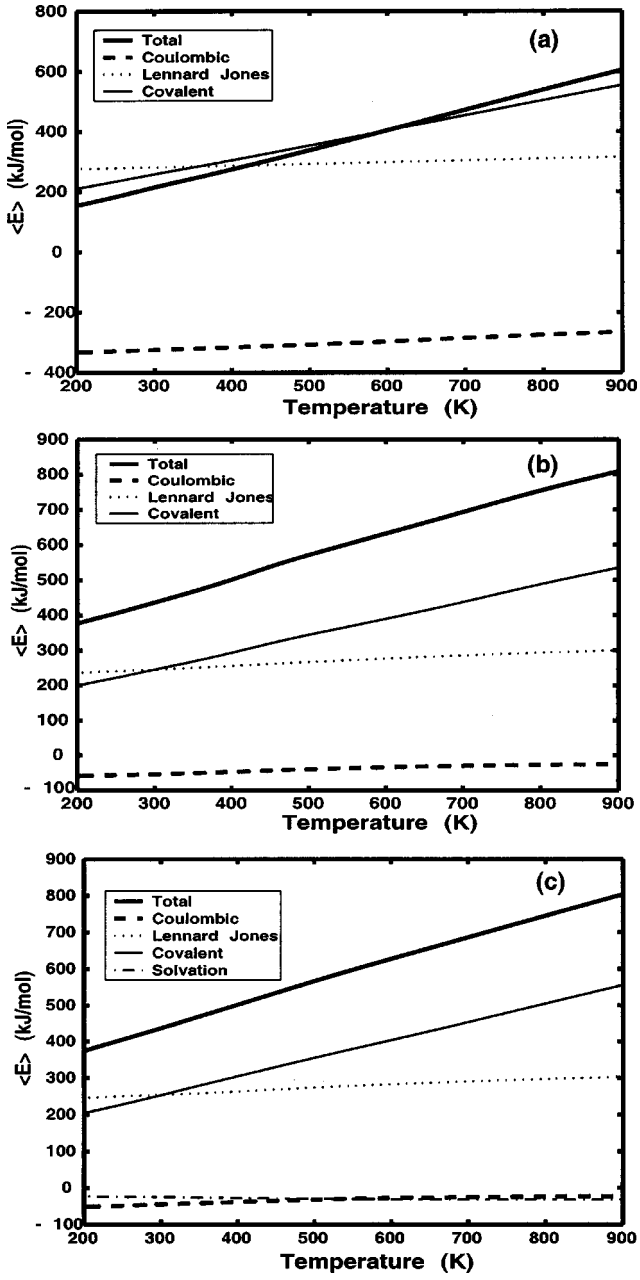

FIG. 8. Temperature dependence of the average energies (total, covalent, Lennard-Jones, Coulombic, and solvation) for Met-enkephalin in three different environments: (a) vacuum (VAC), (b) distance dependent dielectric (DDE), and (c) implicit solvent (SASA).