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Erratum: "Modeling the amide I bands of small peptides" [J. Chem. Phys. 125, 044312 (2006)]

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The description of the N- and C-site frequency shift maps was unclear and the two maps were interchanged in the supporting information.[1] To make this clear, the value of $\Delta\omega_N(-180, -180)$ is 0.40 cm^{-1} and the value of $\Delta\omega_C(-180, -180)$ is -13.41 cm^{-1} and the frequency of the N-site (defined in Figure 1) is, thus, lower than that of the C-site (defined in Figure 1) for the choice of Ramachandran angles. Furthermore, the transition charges in Table I (column 3) all have the wrong sign in the printed paper .

The charges used in the force field denoted GROMOS in the paper originate from the file ffG43a1.rtp provided with GROMACS.

The errors in the mappings pointed out above were only present in the paper and calculations performed and presented in the paper and later publications based on these maps were all correct.

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[1]T. L. C. Jansen, A. G. Dijkstra, T. M. Watson, J. D. Hirst, and J. Knoester, J. Chem. Phys. **125**, 044312 (2006).

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