Published in final edited form as:

J Chem Theory Comput. 2017 January 10; 13(1): 392. doi:10.1021/acs.jctc.6b01188.

Correction to Variational Optimization of an All-Atom Implicit Solvent Force Field To Match Explicit Solvent Simulation Data

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In our original manuscript,¹ we stated that the following torsion correction was applied to the backbone angle ψ in EEF1-SB:

$$E_{\psi} = k_{\psi} (1 + \cos(\psi - \delta)) \quad (1)$$

We would like to clarify that in order to avoid applying the correction to the special cases of glycine and proline, we did not implement it directly on the ψ torsion angle N-C-CA-N, but to the angle ψ' (N-C-CA-CB), which, to a good approximation, is related to ψ by a constant phase offset. Thus the term implemented was:

$$E_{\psi'} = k_{\psi} (1 + \cos(\psi' - \delta')), \quad (2)$$

in which k_{ψ} has the value given in the manuscript, and $\delta' = -103^\circ$. This correction term was applied to the angles defined by the following atom types:

N	C	CT1	CT1
N	C	CT1	CT2
N	C	CT1	CT3
NH1	C	CT1	CT1
NH1	C	CT1	CT2
NH1	C	CT1	CT3

This includes all standard amino acids except for PRO, GLY, GLU, GLP and HSP.

To clarify the implementation, we have included the CHARMM force field files as supporting information with this correction.

References

1. Bottaro S, Lindorff-Larsen K, Best RB. *J Chem Theor Comput.* 2013; 9:5641–5652.