Table S9. Contribution of each energy component.

Energy component	E_{Coulomb}	$E_{\text{FACTS,GB}}$	$E_{\text{FACTS,SA}}$	$E_{\phi/\psi}$	E_{χ}	E_{Hbond}	$E_{\text{atom-pair}}$
Weight[1)]	0.16	0.16	0.05	1.2	1.0	4.0	12.0
Contribution (%)[2)]	7.6	9.6	6.8	19.9	10.0	7.9	38.1

1) Energy weight used for each component

2) Contribution is defined as the standard deviation of each energy term for the training set decoy conformations averaged over training loop target multiplied by the energy weight. These values are then normalized.