The following form of the classical force field relating the potential energy $U^{tot}(\mathbf{r})$ to atomic coordinates $\mathbf{r}$ for the ensemble of atoms has been chosen. It is split into non-bonded $U^{NB}(\mathbf{r})$ and bonded contributions as given by eq. 1,

$$U^{tot}(\mathbf{r}) = U^{NB}(\mathbf{r}) + \sum_{bends} U^{BEND}(\theta_{ijk}) + \sum_{dihedrals} U^{DIHEDRAL}(\phi_{ijkl}) + \sum_{\substack{improper\\dihedrals}} U^{IMP}(\phi_{ijkl}^{imp}), \qquad (1)$$

where the sums are over each bond, bend, dihedral and improper dihedral in the system. The contributions to the potential energy due to bonds, bends, dihedrals and out-of-plane bending (improper dihedrals) are

$$U^{BEND}(\theta_{ijk}) = \frac{1}{2} k_{\alpha\beta\gamma}^{BEND}(\theta_{ijk} - \theta_{ijk}^0)^2 \qquad (2)$$

$$U^{DIHEDRAL}(\phi_{ijkl}) = \sum_n \frac{1}{2} k_{\alpha\beta\gamma\delta,n}^{DIHEDRAL}[1 - \cos(n\phi_{ijkl})] \qquad (3)$$

$$U^{IMP}(\phi_{ijkl}^{imp}) = \frac{1}{2} k_{\alpha\beta\gamma\delta}^{IMP}(\phi_{ijkl}^{imp})^2 \qquad (4)$$

where θ_{ijk} and θ_{ijk}^0 are the instantaneous and equilibrium bending angles for atoms i, j and k; ϕ_{ijkl} is the dihedral angle for atoms i, j, k and l; and ϕ_{ijkl}^{imp} is the out-of-plane bending angle for an sp^2 center at atom j. The strength of these interactions is characterized by the corresponding force constants $k_{\alpha\beta\gamma}^{BEND}$, $k_{\alpha\beta\gamma\delta,n}^{DIHEDRAL}$, and $k_{\alpha\beta\gamma\delta}^{IMP}$, respectively. The subscripts α, β, γ, and δ denote atom type for atoms i, j, k, and l, respectively.

The nonbonded energy $U^{NB}(\mathbf{r})$ consists of the sum of two-body repulsion and dispersion energy terms $U^{RD}(\mathbf{r})$, the energy due to interactions of fixed charges $U^{coul}(\mathbf{r})$, and the polarization energy $U^{pol}(\mathbf{r})$ arising from the interaction between induced dipoles with fixed charges and other induced dipoles:

$$U^{NB}(\mathbf{r}) = U^{RD}(\mathbf{r}) + U^{coul}(\mathbf{r}) + U^{pol}(\mathbf{r}) =$$

$$\sum_{i>j}\left(A_{\alpha\beta}\exp(-B_{\alpha\beta}r_{ij}) - C_{\alpha\beta}r_{ij}^{-6} + D\left(\frac{12}{B_{\alpha\beta}r_{ij}}\right)^{12}\right) + \sum_{i>j}\left(\frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}\right) - 0.5\sum_i \vec{\mu}_i \vec{E}_i^0. \qquad (5)$$

where $\vec{\mu}_i = \alpha_i \vec{E}_i^{tot}$ is an induced dipole at force center i, α_i is the isotropic atomic polarizability, $\vec{E}_i^{tot}$ is the total electrostatic field at the atomic site i due to permanent charges q_j and induced dipoles $\vec{\mu}_j$, ε_0 is the dielectric permittivity of vacuum, $\vec{E}_i^0$ is the electric field due to fixed charges only, and $A_{\alpha\beta}$ and $B_{\alpha\beta}$ are the repulsion parameters and $C_{\alpha\beta}$ is the dispersion parameter for interaction between atoms i and j with atom types α and β. The term $D\left(\frac{12}{B_{\alpha\beta}r_{ij}}\right)^{12}$, with $D = 5 \cdot 10^{-5}$ kcal/mol for all pair interactions, is essentially zero at typical nonbonded atomic separations, but becomes the dominant term at $r_{ij} < 1$ Å, ensuring that $U^{RD}(\mathbf{r})$ is repulsive at distances much smaller than the size of

an atom. Intramolecular nonbonded interactions are included for atoms separated by three or more covalent bonds. We used Thole screening (a_T=0.4) that smears induced dipoles in order to prevent the so-called "polarization catastrophe" from occurring. The interaction between an induced dipole and a partial charge separated by 3 bonds was scaled by 0.8.