

Symbol	BRAHMS units	LAMMPS units	Other units
σ_{CC}, σ_{PP}	0.52 nm	5.2 Å	
σ_{GG}, σ_{EE}	0.46 nm	4.6 Å	
σ_{AA}, σ_{TT}	0.45 nm	4.5 Å	
σ_{WW}	0.30 nm	3.0 Å	
$\epsilon_{CC}, \epsilon_{PP}$	6.0 kJ/mol	1.434 kcal/mol	
$\epsilon_{GG}, \epsilon_{EE}$	4.0 kJ/mol	0.956 kcal/mol	
$\epsilon_{AA}, \epsilon_{TT}$	3.5 kJ/mol	0.837 kcal/mol	
ϵ_{WW}	1 kJ/mol	0.239 kcal/mol	
ϵ_{WW}^{tot}	$1.95 \epsilon_{WW}$	0.466 kcal/mol	
ϵ_{WP}	$1.8\sqrt{\epsilon_{WW} \epsilon_{PP}}$	1.054 kcal/mol	
ϵ_{WG}	$1.2\sqrt{\epsilon_{WW} \epsilon_{GG}}$	0.574 kcal/mol	
ϵ_{WE}	$1.6\sqrt{\epsilon_{WW} \epsilon_{EE}}$	0.765 kcal/mol	
ϵ_{AW}	$1.5\sqrt{\epsilon_{AA} \epsilon_{WW}}$	0.671 kcal/mol	
ϵ_{AP}	$2.5\sqrt{\epsilon_{AA} \epsilon_{PP}}$	2.738 kcal/mol	
ϵ_{AG}	$1.5\sqrt{\epsilon_{AA} \epsilon_{GG}}$	1.341 kcal/mol	
ϵ_{AE}	$2.5\sqrt{\epsilon_{AA} \epsilon_{EE}}$	2.236 kcal/mol	
Q_C, Q_A	+0.7 e	+0.7 e	1.12×10^{-19} C
Q_P	-0.7 e	-0.7 e	-1.12×10^{-19} C
μ_G	1.6 D	0.333 e Å	
μ_E	2 D	0.416 e Å	
μ_W	2.3 D	0.479 e Å	
k	1260 kJ/(mol nm ²)	3.011 kcal/(mol Å ²)	
w	30 kJ/mol	2*3.585 kcal/mol	
c	10 kJ/mol	2*1.195 kcal/mol	
$\alpha_{0CPG}, \alpha_{0APG}$	115°	115°	2.01 rad
α_{0PGE}	160°	160°	2.79 rad
$\alpha_{0GET}, \alpha_{0ETT}, \alpha_{0TTT}^{saturated}$	180°	180°	3.14 rad
$\alpha_{0TTT}^{cis-unsaturated}$	120°	120°	2.09 rad
m_C, m_P	90 amu	90 g/mol	14.9×10^{-23} g
m_G, m_E	62 amu	62 g/mol	10.3×10^{-23} g
m_T, m_A	42 amu	42 g/mol	7.0×10^{-23} g
m_W	40 amu	40 g/mol	6.6×10^{-23} g
$I_{G,E}$	10 amu nm ²		1000 amu Å ²
I_W	1 amu nm ²		100 amu Å ²

Subscripts C, A, P, G, E, T and W stand for the site types *choline, amine, phosphate, glycerol, ester, tail* and *water*, respectively. Lennard-Jones cross-terms are calculated by the standard Lorentz-Berthelot rule except for increased ϵ terms representing hydrogen bonding; in particular, $\epsilon_{WP}, \epsilon_{WG}, \epsilon_{WE}, \epsilon_{AW}, \epsilon_{AP}, \epsilon_{AG}, \epsilon_{AE}$ are set as reported in the table. Charges and dipoles are identified by Q and μ ; cross terms are obtained via standard electrostatic formulae. Nonbonded interactions between bonded pairs are zero (in technical jargon: 1-2 LJ and Coul interactions are excluded). The rigidity of the Hooke harmonic potential is identified by k ; reference lengths are set to $0.9 \sigma_{ij}$. The rigidity of the angle potential is identified by w . The rigidity of the orientation-restraining potential is c . Masses and principal moments of inertia are identified by m and I , respectively.