ELBA-1.0

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	
ϵ_{CC}, ϵ_{PP}	6.0 kJ/mol	1.434 kcal/mol	
ϵ_{GG}, ϵ_{EE}	4.0 kJ/mol	0.956 kcal/mol	
ϵ_{AA}, ϵ_{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	
$\alpha_{0_{CPG}}$, $\alpha_{0_{APG}}$	115°	115°	2.01 rad
$\alpha_{0_{PGE}}$	160°	160°	2.79 rad
$\alpha_{0_{GET}}$, $\alpha_{0_{ETT}}$, $\alpha_{0_{TTT}}^{saturated}$	180°	180°	3.14 rad
$\alpha_{0_{TTT}}^{cis-unsaturated}$	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	131 amu Å^2	1000 amu Å^2
I_W	1 amu nm^2	36 amu Å^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, $\epsilon_{WP}, \epsilon_{WG}, \epsilon_{WE}$, ϵ_{AW}, ϵ_{AP}, ϵ_{AG}, ϵ_{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. Within the same lipid molecule, nonbonded interactions between bonded pairs are zero (1-2 LJ and electrostatic 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 dipole orientation-restraining potential is c. Masses and principal moments of inertia are identified by m and I, respectively.