Initial geometries of model compounds

Interaction Parameter Optimization

Partial Atomic Charges

VDW Parameters

Internal Parameter Optimization

Bonds

Angles

Torsions

Improps, Urey-Bradley

Crystal and solution condensed phase MD simulations

Parameter Optimization Complete
Figure 3, continued
Figure 3, continued
Figure 4

(A) Energy (kcal/mol) vs. Gamma (degrees)

(B) Probability vs. Gamma (degrees)
Figure 9

A: Graph showing energy (kcal/mol) against Epsilon (degrees).
B: Graph showing energy (kcal/mol) against Epsilon (degrees).
C: Graph showing probability against Epsilon (degrees).
D: Graph showing probability against Epsilon (degrees).
Figure 10
Figure 11

A

B
Figure 16

![Graph showing energy (kcal/mol) vs. H-O2'-C2'-C3' dihedral (degrees). The graph has a peak at approximately 120 degrees, with energy values ranging from 0 to 16 kcal/mol. The data points are marked with crosses, and the curve represents the trend of energy with dihedral angle.]
Figure 17

A

B

C

Energy (kcal/mol)

Energy (kcal/mol)

Probability

Pseudorotation angle (degrees)

0 60 120 180 240 300 360