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Polarizable multipolar electrostatics for cholesterol

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Abstract

FFLUX is a novel force field under development for biomolecular modelling, and is based on topological atoms and the machine learning method kriging. Successful kriging models have been obtained for realistic electrostatics of amino acids, small peptides, and some carbohydrates but here, for the first time, we construct kriging models for a sizeable ligand of great importance, which is cholesterol. Cholesterol's mean total (internal) electrostatic energy prediction error amounts to 3.9 kJmol^{-1} , which pleasingly falls below the threshold of 1 kcalmol^{-1} often cited for accurate biomolecular modelling. We present a detailed analysis of the error distributions.

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