## Calculating Potential energy of a system of water molecules

The electrostatic, vanderwaal and total energy were calculated using the code. The outputs for the code are:

electrostatic energy: -5159.430611238769 Vanderwaal energy: 599.7631387966753 Total energy: -4559.667472442094

electrostatic energy and vanderwaal energy was calculated for  $^{432}\mathrm{C}_2$  pairs of water molecules. It wasnt calculated for intramolecular atoms.