-----CUSTOM IMPLEMENTATION-----Real: -41.939546567266156 -119.5635334904723 Self: Recip: 1.590877271736388 Electrostatic: -159.9122027860021 -----LAMMPS-----Electrostatic: -159.9123532955388 -----MADELUNG------Electrostatic: -158.987671863514 _____ -----CUSTOM IMPLEMENTATION------Total lattice: -159.9122027860021 -----GULP------Total lattice: -159.91346321