|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Interactions#** | **Atom Type1** | **Atom Type 2** | **Emin (kcal/mol)** | **Rmin (Å)** | **E (kcal/mol)** | **R (Å)** |
| Potassium-Water  | POT  | OT | -0.015033 |  4.211 | -17.800 | 2.67 |
| Potassium-Carbonyl  | POT | O | -0.455556 | 3.044 | -26.000 | 2.48 |
| Water-Carbonyl | OT | O |  -0.338333 | 3.200 | -8.950 | 1.71 |

#**E** and **R** are the minimized energy and distance for ion-water, ion-carbonyl and water-carbonyl interactions in the CHARMM36m-NBFIX force field, with Lennard-Jones (LJ) parameters **Emin** and **Rmin**. Consistent with a AMBER-like force field, note that the ion-protein interaction has the most negative minimized energy.