|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Run** | **Energy (kJ/mol)** | **Protein-peptide distance (nm)** | **Number of Hydrogen Bonds** | **RMSD (nm)** | **Binding energies (kJ/mol)** |
| **Mean** | **SD** | **Mean** | **SD** | **Mean** | **SD** | **Mean** | **SD** | **Mean** | **SD** |
| 1 | -510162 | 1093 | 1.93 | 0.05 | 5.54 | 1.48 | 0.23 | 0.04 | -102.5 | 9.6 |
| 2 | -510194 | 1084 | 1.89 | 0.05 | 4.99 | 1.74 | 0.28 | 0.04 | -117.8 | 9.2 |
| 3 | -510179 | 1090 | 1.87 | 0.06 | 4.62 | 1.32 | 0.26 | 0.04 | -102.9 | 9.7 |
| **Mean** | **-510178** |  | **1.90** |  | **5.05** |  | **0.26** |  | **-107.7** |  |