Table 6. Coulomb, van der Waals and total non-bonded interaction energies between RBD and GRP78 for three replicas.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coulomb energy (kJ/mol) | Van der Waals energy(kJ/mol) | Total non-bonded energy (kJ/mol) |
| replica-1 | -100 ± 3 | -155 ± 12 | -255 ± 15 |
| replica-2 | -235 ± 21 | -163 ± 9 | -398 ± 30 |
| replica-3 | -83 ± 7 | -111 ± 5 | -194 ± 12 |