Table 2. Coulomb, van der Waals and total non-bonded interaction energies between RBD and ACE2 for the native and oxidized complexes.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Coulomb energy (kJ/mol) | Van der Waals energy (kJ/mol) | Total energy (kJ/mol) |
| Native | -325 ± 15 | -229 ± 7 | -554 ± 21 |
| Oxidized | -409 ± 4 | -300 ± 17 | -709 ± 14 |