Table 3. Total non-bonded interaction energy between regions of the RBD (i.e., Ⅰ, Ⅱ\*, Ⅱ&Ⅲ, Ⅲ\*, and Ⅳ) and ACE2 for the native and oxidized complexes.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | region I-ACE2 (kJ/mol) | region Ⅱ\*-ACE2 (kJ/mol) | region Ⅱ&Ⅲ-ACE2 (kJ/mol) | region Ⅲ\*-ACE2 (kJ/mol) | region Ⅳ-ACE2 (kJ/mol) |
| native | < 10-2 | < 10-2 | -84 ± 7 | -339 ± 14 | -130 ± 9 |
| oxidized | < 10-2 | < 10-2 | -94 ± 2 | -502 ± 15 | -113 ± 9 |