Table 5. Non-bonded interaction energies between amino acid residues of region IV of RBD and ACE2 for the native and oxidized complexes. The residues with non-bonded energy absolute values of less than 10 kJ/mol for native and oxidized complexes are not shown here.

|  |  |  |
| --- | --- | --- |
| Interaction | native (kJ/mol) | oxidized (kJ/mol) |
| Glu484-ACE2 | -54.8 ± 10.6 | -1.4 ± 0.4 |
| Phe486-ACE2 | -30.1 ± 0.6 | -11.8 ± 6.5 |
| Asn487-ACE2 | -42.5 ± 1.5 | -19.3 ± 4.5 |
| Cys488-ACE2 | -1.7 ± 0.1 | -58.8 ± 21.4 |