Table 4. Non-bonded interaction energies between amino acid residues of region III\* 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) |
| Tyr499-ACE2 | -10.3 ± 1.7 | -12.2 ± 3.3 |
| Leu455-ACE2 | -10.2 ±0.1 | -11.7 ± 0.6 |
| Phe456-ACE2 | -21.2 ± 0.2 | -19.3 ±1.2 |
| Lys458-ACE2 | -0.6 ± 0.7 | -13.5 ± 4.2 |
| Tyr473-ACE2 | -7.0 ± 0.3 | -11.7 ± 3.6 |
| Ala475-ACE2 | -30.3 ± 0.8 | -10.7 ± 1.2 |
| Gly476-ACE2 | -11.5 ± 0.7 | -10.1 ± 1.2 |
| Ser477-ACE2 | -4.9 ± 0.5 | -11.8 ± 2.1 |
| Pro479-ACE2 | -0.008 ± 0.001 | -11.9 ± 3.2 |
| Tyr489-ACE2 | -21.9 ± 0.2 | -25.1 ± 3.1 |
| Gln493-ACE2 | -29.9 ± 2.1 | -46.8 ± 6.1 |
| Gln496-ACE2 | -7.1 ± 0.8 | -22.3 ± 7.2 |
| Gln498-ACE2 | -13.8 ± 1.3 | -46.7 ± 13.1 |
| Thr500-ACE2 | -37.4 ± 7.7 | -44.6 ± 5.5 |
| Asn501-ACE2 | -53.9 ± 5.3 | -58.2 ±2.3 |
| Gly502-ACE2 | -20.2 ± 0.6 | -22.9 ± 0.7 |
| Tyr505-ACE2 | -34.2 ± 1.6 | -41.2 ± 7.2 |