Table 4. The number of H-bonds formed between each region of the native/oxidized RBD and ACE2. Values are obtained by dividing the total number of H-bonds to the total number of MD frames (with the abundance of more than 10% in all frames), using the last 100 ns of MD simulation.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | region Ⅰ-ACE2 | region II\*-ACE2 | region II&III-ACE2 | region III\*-ACE2 | region IV-ACE2 |
| Native | - | - | 0.50 ± 0.01 | 0.85 ± 0.09 | 0.53 ± 0.05 |
| Oxidized | - | - | 0.38 ± 0.05 | 1.29 ± 0.10 | - |