Table 5. The number of salt bridges formed between each region of the native/oxidized RBD and ACE2. Values are obtained by dividing the total number of salt bridges 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 | - | - | 0.80 ± 0.06 | - | 0.32 ± 0.08 |
| Oxidized | - | - | 0.89 ± 0.06 | - | - |