***Table 1.*** *Number of H bonds formed between RBD and each chain of SARS-CoV-2 S protein (chains A, B and C), along with the total H bonds. Values are averaged over the last 100 ns of MD simulation, representing bonds present in more than 10% of the frames.*

|  |  |  |  |
| --- | --- | --- | --- |
|  | | Native | Oxidized |
| RBD | chain A | 5.42 ± 0.26 | 5.43 ± 0.24 |
| chain B | 4.64 ± 0.30 | 5.12 ± 0.46 |
| chain C | 0.79 ± 0.11 | 0.64 ± 0.12 |
| total | 10.85 ± 0.41 | 11.19 ± 0.53 |