Table S2. Number of H-bonds and salt bridges formed between residues of the native RBD and ACE2 proteins. The values are obtained by dividing the total number of H-bonds (or 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 the MD simulation.

|  |  |  |  |
| --- | --- | --- | --- |
| region of RBD | native RBD-ACE2 | number of H-bonds | number of salt bridges |
| II&III | Lys417-Asp30 | 0.50 ± 0.01 | 0.80 ± 0.06 |
| III\* | Gly502-Lys353 | 0.37 ± 0.03 | - |
| Thr500-Asp335 | 0.35 ± 0.09 | - |
| Ala475-Ser19 | 0.13 ± 0.03 | - |
| IV | Asn487-Tyr83 | 0.32 ± 0.02 | - |
| Glu484-Lys31 | 0.21 ± 0.05 | 0.32 ± 0.08 |