***Table S5.*** *Number of salt bridges formed between residues of the RBD and the remaining SARS-CoV-2 S trimer (i.e., chain A, B, and C) for the native and oxidized systems. The values represent the average number of salt bridges observed in the last 100 ns of MD simulations, normalized to the total number of frames with a prevalence exceeding 10% in all frames.*

|  |  |  |  |
| --- | --- | --- | --- |
|  | **RBD-remaining SARS-CoV-2 S trimer** | **Native** | **Oxidized** |
| **chain A** | Arg328-Asp578 | 1.00 ± 0.00 | 1.00 ± 0.00 |
| Lys535-Glu583 | 0.40 ± 0.02 | 0.29 ± 0.10 |
| Lys535-Glu554 | 0 | 0.65 ± 0.09 |
| **chain B** | Lys462-Asp198 | 0.49 ± 0.11 | 0.33 ± 0.30 |
| Arg319-Asp737 | 0.21 ± 0.21 | 0.41 ± 0.29 |
| Glu471-Lys113 | 0 | 0.37 ± 0.13 |
| **chain C** | Asp427-Lys986 | 0.18 ± 0.13 | 0.12 ± 0.06 |