***Table S2.*** *Number of H-bonds formed between residues (or glycans) of the RBD and chain A in the native and oxidized SARS-CoV-2 S trimer. Values represent the average count per MD frame over the last 100 ns of the simulation, where only bonds with a prevalence exceeding 10% in all frames are considered.*

|  |  |  |
| --- | --- | --- |
| **RBD-chain A** | **Native** | **Oxidized** |
| Arg328-Asp578 | 1.17 ± 0.17 | 1.33 ± 0.13 |
| Val539-Gly550 | 0.80 ± 0.04 | 0.80 ± 0.05 |
| Asn536-Leu552 | 0.40 ± 0.02 | 0.55 ± 0.05 |
| Phe541-Gly548 | 0.54 ± 0.04 | 0.47 ± 0.10 |
| Lys353-Glu554 | 0.49 ± 0.01 | 0.43 ± 0.04 |
| Arg328-Asn542 | 0.38 ± 0.01 | 0.33 ± 0.05 |
| Phe541-Thr547 | 0.20 ± 0.03 | 0.29 ± 0.10 |
| Asp389-Asn542 | 0.22 ± 0.04 | 0.27 ± 0.01 |
| Asn536-Thr553 | 0.11 ± 0.01 | 0.21 ± 0.06 |
| Phe329-Gln580 | 0.15 ± 0.04 | 0.19 ± 0.01 |
| Arg328-Asn544 | 0.14 ± 0.06 | 0.15 ± 0.10 |
| Lys535-Glu583 | 0.20 ± 0.09 | 0.15 ± 0.05 |
| Val320-Ser591 | 0.12 ± 0.06 | 0.13 ± 0.12 |
| His519-Phe562 | 0.13 ± 0.07 | 0.12 ± 0.08 |
| His519-Gln564 | 0.13 ± 0.04 | 0 |
| Ile326-Asn542 | 0.12 ± 0.04 | 0 |
| N331A-Arg577 | 0.12 ± 0.05 | 0 |