***Table S3.*** *Number of H-bonds formed between residues (or glycans) of the RBD and chain B 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 B** | **Native** | **Oxidized** |
| Ser383-Asp985 | 0.27 ± 0.03 | 0.35 ± 0.08 |
| Ser383-Arg983 | 0.26 ± 0.02 | 0.30 ± 0.02 |
| Ser383-Glu988 | 0.41 ± 0.21 | 0.49 ± 0.14 |
| Glu465-Asn234 | 0.27 ± 0.18 | 0.42 ± 0.21 |
| Glu516-Tyr200 | 0.58 ± 0.06 | 0.41 ± 0.19 |
| Thr385-Asp985 | 0.47 ± 0.06 | 0.38 ± 0.08 |
| Arg319-Asp737 | 0.20 ± 0.19 | 0.29 ± 0.18 |
| Thr415-Tyr369 | 0 | 0.21 ± 0.10 |
| Tyr489-Asp364 | 0 | 0.20 ± 0.19 |
| Asp405-Ser375 | 0.16 ± 0.15 | 0.22 ± 0.21 |
| Arg403-Phe374 | 0.11 ± 0.08 | 0.19 ± 0.10 |
| Tyr505-Ser373 | 0.12 ± 0.10 | 0.19 ± 0.18 |
| Lys462-Asp198 | 0.27 ± 0.09 | 0.18 ± 0.17 |
| Asn460-N234B | 0.10 ± 0.05 | 0.18 ± 0.02 |
| Thr500-N343B | 0.13 ± 0.12 | 0.17 ± 0.10 |
| N331A-Pro225 | 0 | 0.17 ± 0.16 |
| Glu471-Lys113 | 0 | 0.17 ± 0.09 |
| Tyr453-Ala372 | 0.11 ± 0.10 | 0.13 ± 0.12 |
| Asn450-N343B | 0 | 0.12 ± 0.06 |
| Arg466-Gln115 | 0.12 ± 0.07 | 0.12 ± 0.06 |
| N331A-Gln173 | 0 | 0.11 ± 0.05 |
| Lys417-Asn370 | 0 | 0.11 ± 0.04 |
| Ser383-Arg983 | 0.26 ± 0.02 | 0 |
| Gln474-N234B | 0.20 ± 0.17 | 0 |
| Gly381-Arg983 | 0.26 ± 0.02 | 0 |
| Thr470-N165B | 0.20 ± 0.14 | 0 |
| Glu484-N165B | 0.15 ± 0.05 | 0 |
| Glu471-N165B | 0.13 ± 0.10 | 0 |
| Arg319-Gly755 | 0.14 ± 0.13 | 0 |
| Gly502-N343B | 0.11 ± 0.10 | 0 |