

Supplementary information for

Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2

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Table S1. Composition of membrane of the viral membrane taken from reference (1).

Lipid Type	Outer leaflet	Inner leaflet
DPPC	48	46
POPC	72	69
DPPE	144	138
POPE	216	207
DPPS	48	46
POPS	72	69
PSM	240	230
CHOL	360	345

Table S2. Glycan composition at each site in this study. Taken with permission from reference 1.

Site	Composition and Type	Sequence	Alternative Sequence(s)
N61 N122 N603 N709 N717 N801 N1074	HexNAc(2)Hex(5) High-Mannose		
N234	HexNAc(2)Hex(8) High-Mannose		
N657	HexNAc(3)Hex(6) Hybrid		
N149 N331 N343 N616 N1134	HexNAc(4)Hex(3) Fuc(1) Complex		
N1158 ^a	HexNAc(4)Hex(4) Complex		
N1098 ^a	HexNAc(4)Hex(4) Fuc(1)NeuAc(1) Complex		
N165 ^a	HexNAc(4)Hex(5) Fuc(3)NeuAc(1) Complex		
N282	HexNAc(5)Hex(3) Fuc(1) Complex		
N17 ^b	HexNAc(5)Hex(4) Fuc(1) Complex		
N1173	HexNAc(6)Hex(3) Fuc(1) Complex		
N74 ^c	HexNAc(6)Hex(4) Fuc(1)NeuAc(1) Complex		
N1194 ^d	HexNAc(6)Hex(5) Fuc(1) NeuAc(1) Complex		
T323	O-glycan		

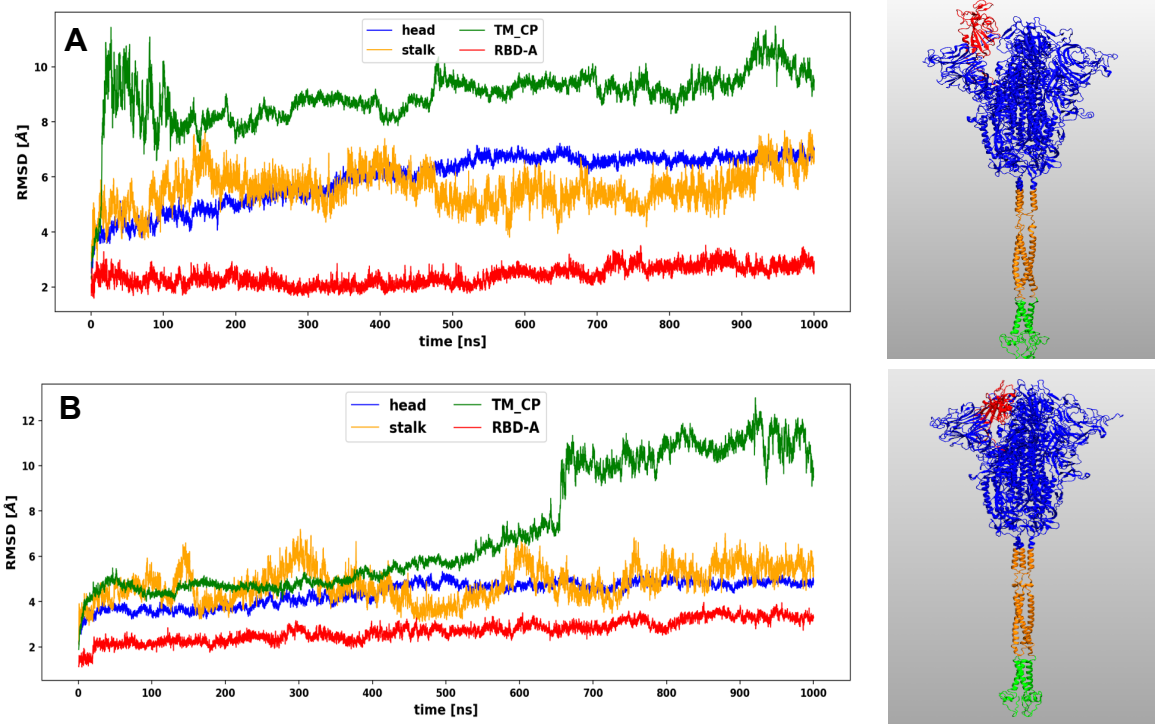


Figure S1. RMSD of different regions in the spike protein for A) open and B) closed states

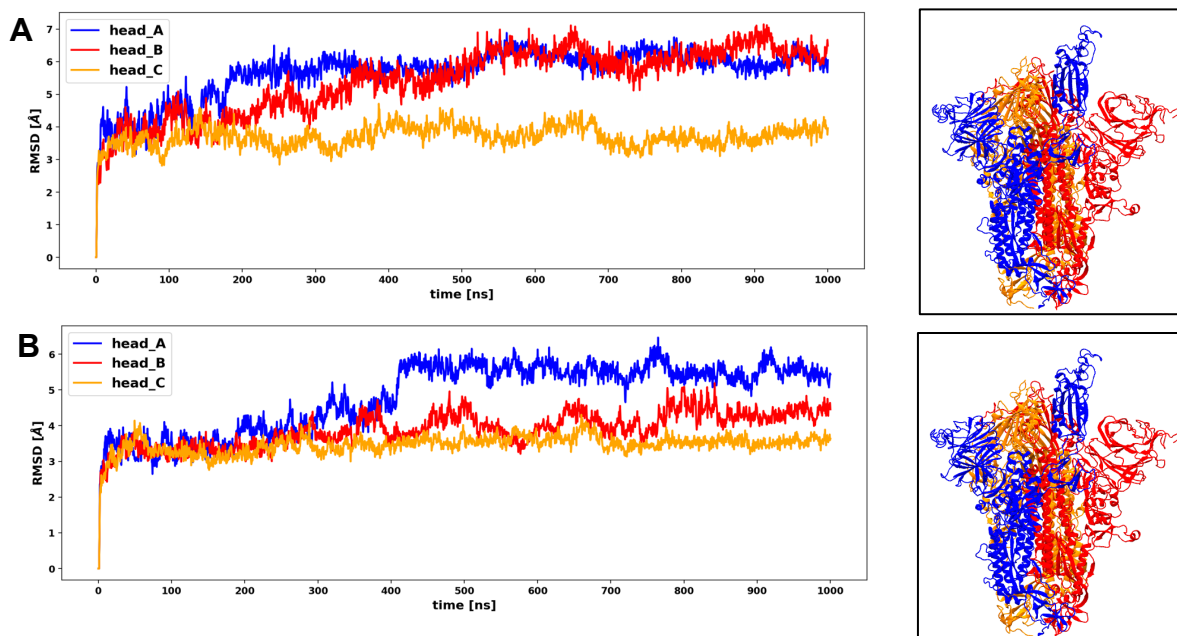


Figure S2. RMSD of different monomers in spike trimer for A) open and B) closed conformations

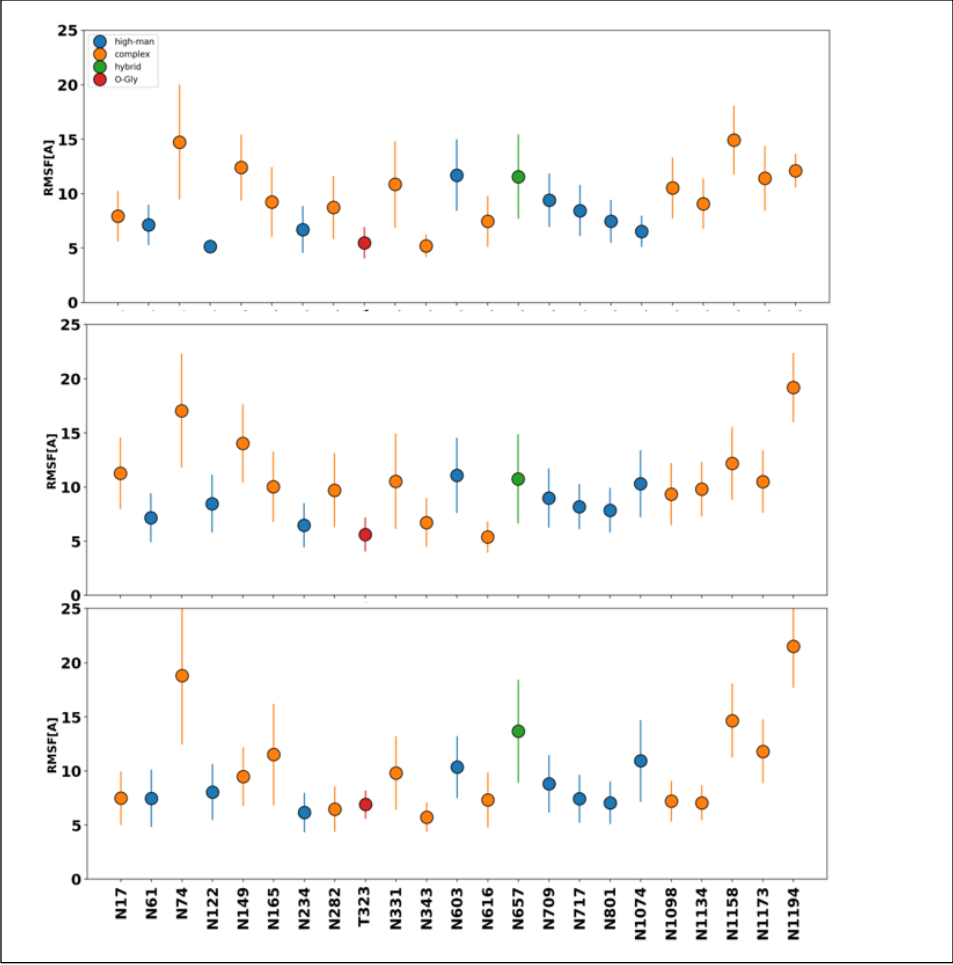


Figure S3. Glycan RMSF for closed state and from top to bottom for chain A, B and C.

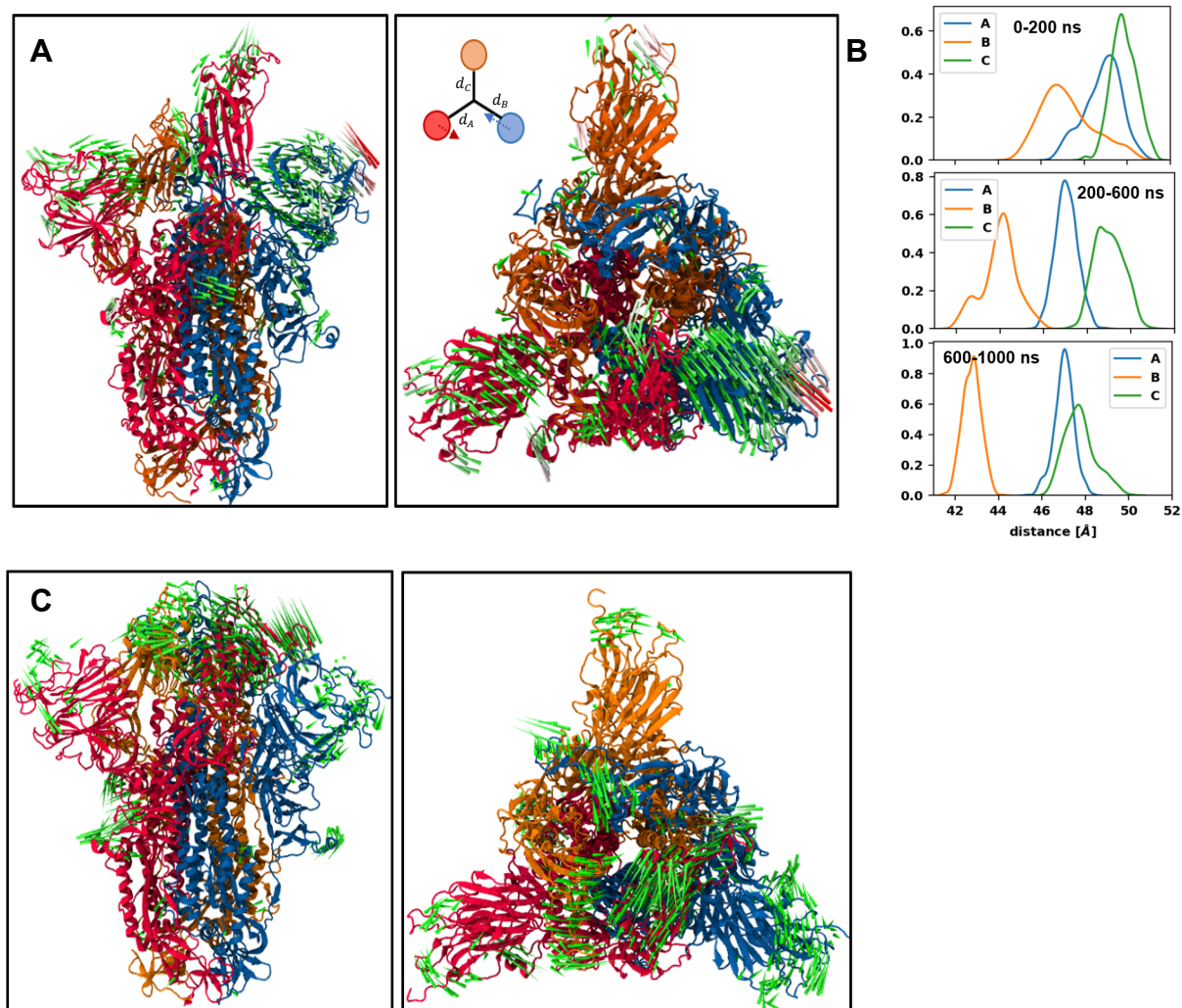


Figure S4. A) porcupine plot of first principal component (PC1) for RBD-up state B) distribution of distance between center of mass of NTD of each monomer in open state from the center of apex. From top to bottom corresponds to 0-200 ns, 200-600ns and 600-1000ns of trajectory C) porcupine plot of (PC1) for the closed state.

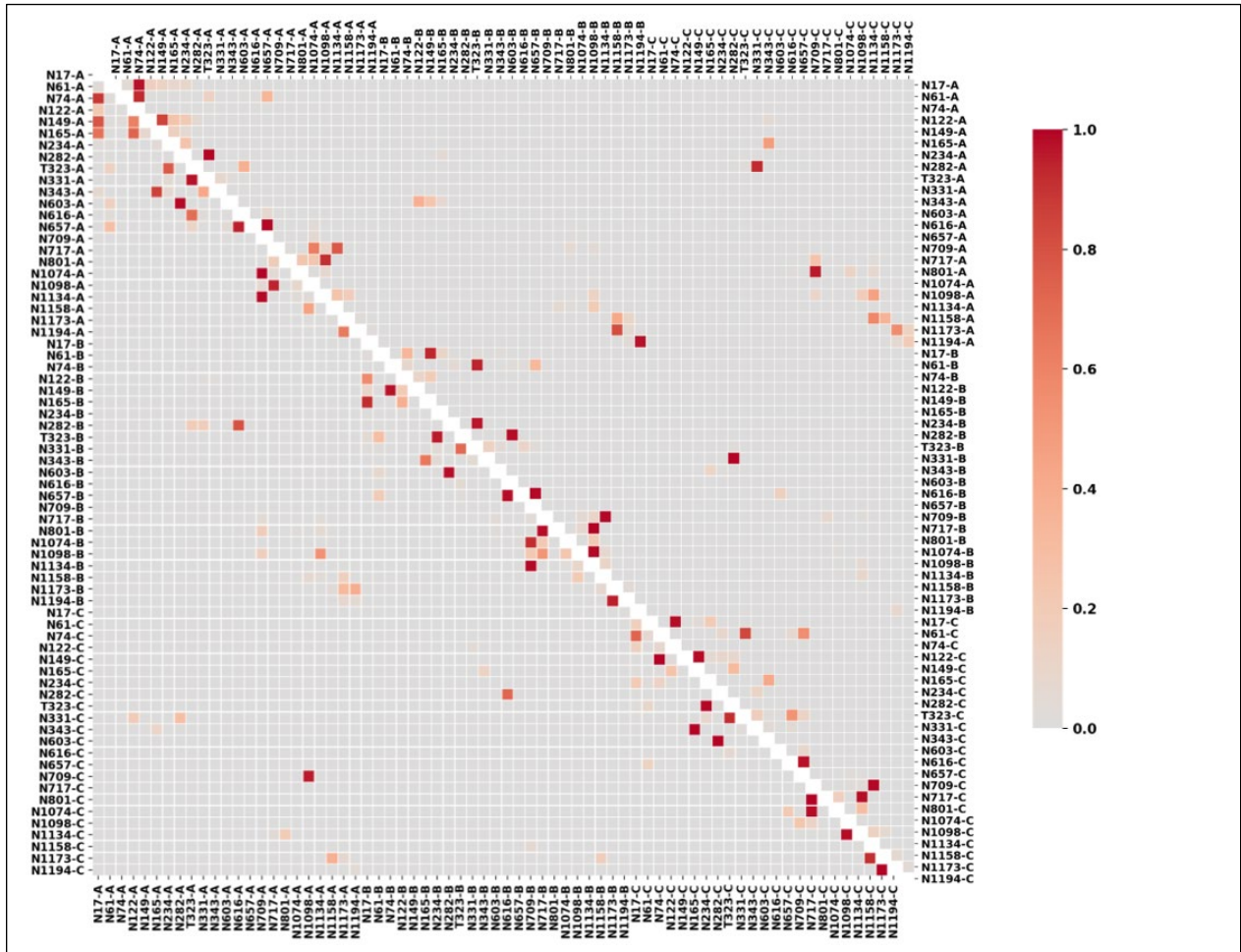


Figure S5. Adjacency matrix of glycan-glycan interactions for RBD-up and RBD-down states. Lower triangle represents the adjacency matrix for RBD-down state using the whole simulation and upper triangle is for RBD-up state using the whole simulation.

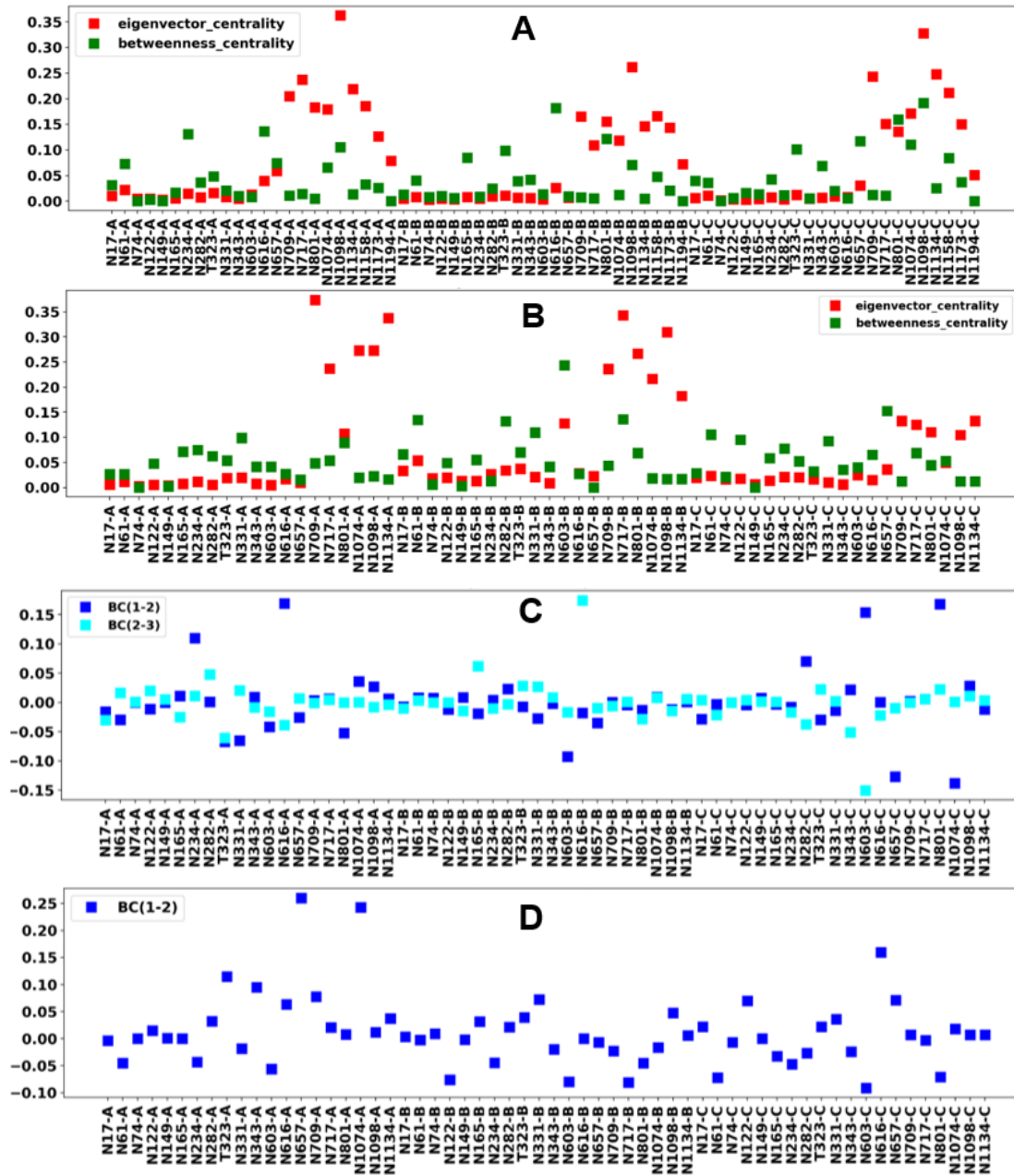


Figure S6. A) network centralities for the head region in open state of spike and the total simulation time B) network centralities for the head in closed state and total simulation time. C) change in betweenness centrality of open state between first (0-200 ns) and second (200-600 ns) BC(1-2) and second and third (600 – 1000 ns) BC(2-3). D) change in betweenness centrality of closed state from 0-500 ns to 500-1000 ns.

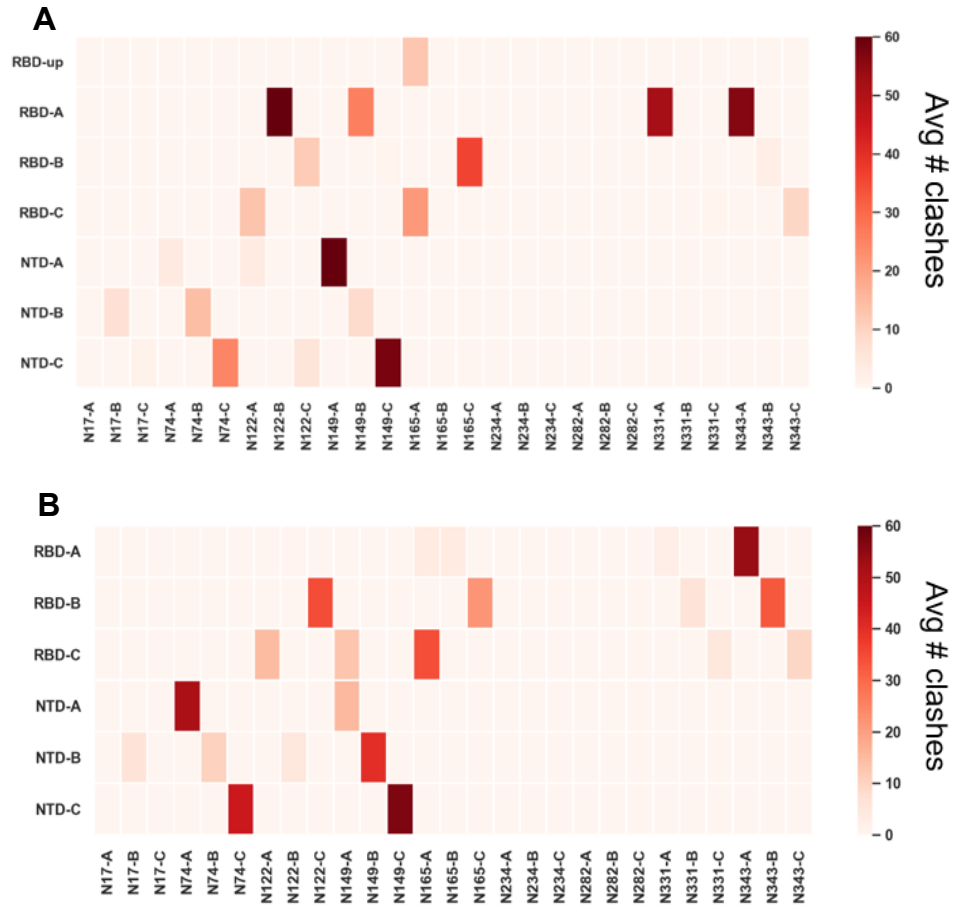


Figure S7. Avg number of clashes of each glycan with the overlaid antibody in A) open and B) closed states of the spike

References:

1. H. Woo *et al.*, Modeling and Simulation of a Fully-glycosylated Full-length SARS-CoV-2 Spike Protein in a Viral Membrane. *bioRxiv* (2020).