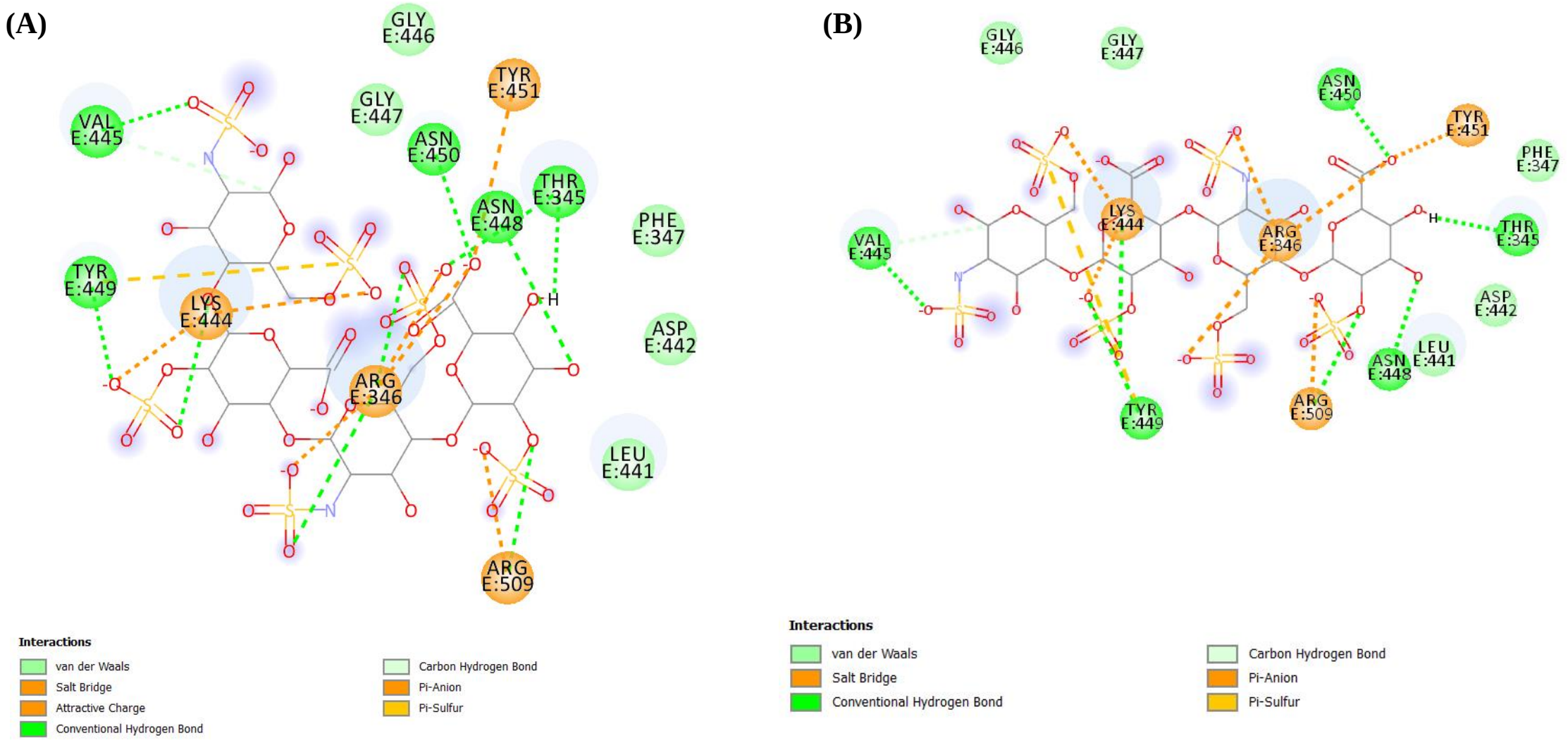
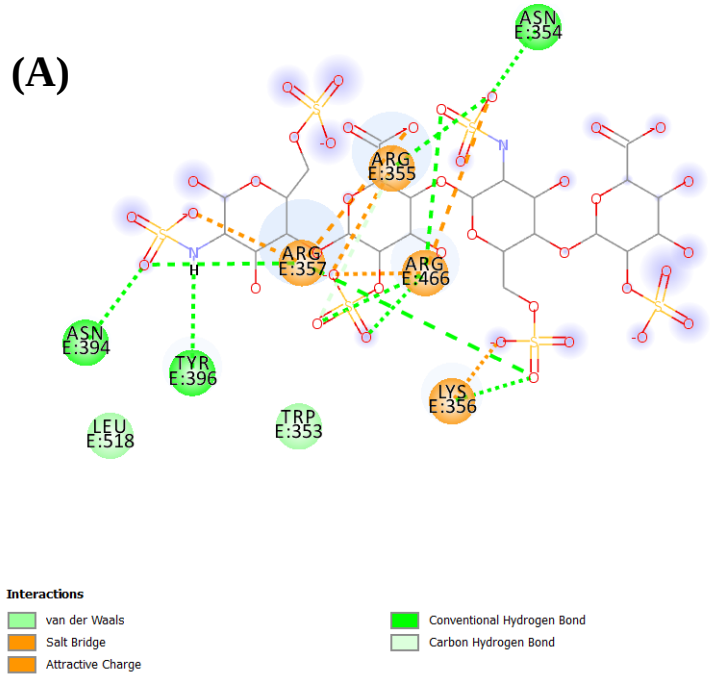
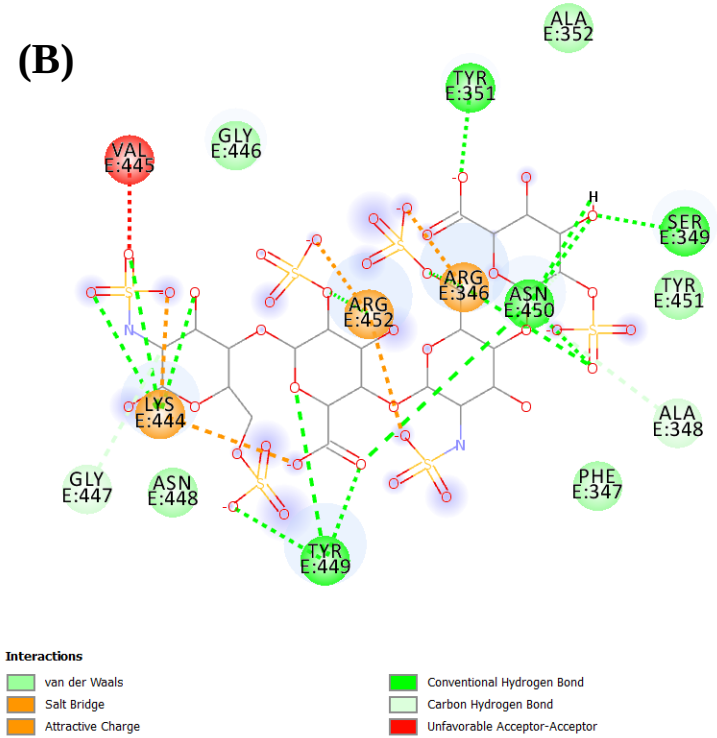


Supporting Information Figure S1. Molecular docking interactions of heparin to SARS-CoV-2 spike RBD mutants. The docked structures of Heparin-mutant RBD complexes were obtained from cluster 0 provided by Cluspro webserver. Two-dimensional (2D) diagrams of heparin-RBD interactions for (A) K417N, and (B) K417T. The protein residues and interactions are colored accordingly and provided in figure.


(A)
ASN E:354
ARG E:355
ARG E:357
ARG E:466
ASN E:394
TYR E:396
LYS E:356
LEU E:518
TRP E:353
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond


(B)
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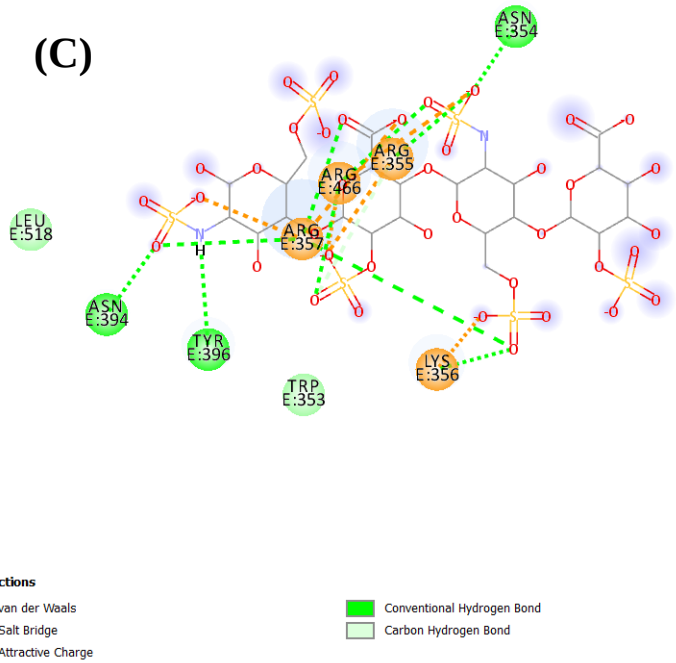
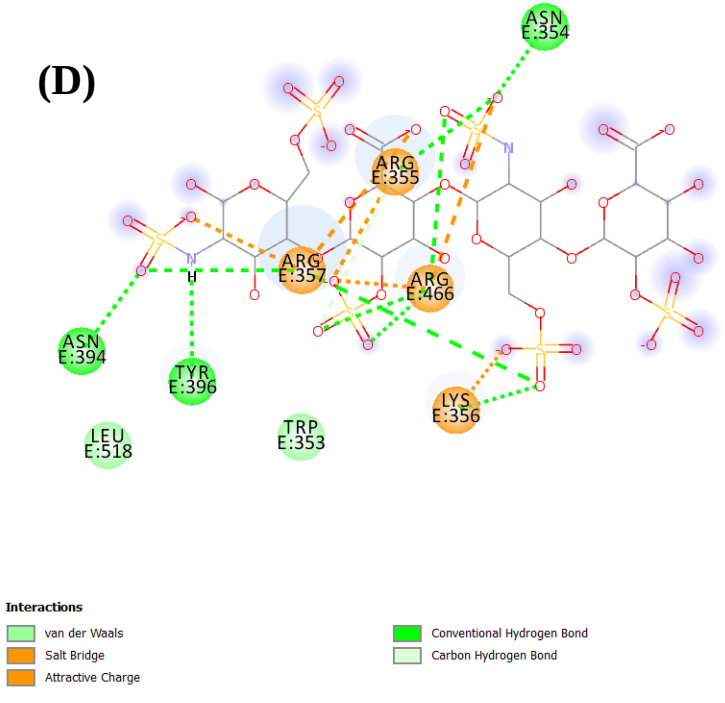
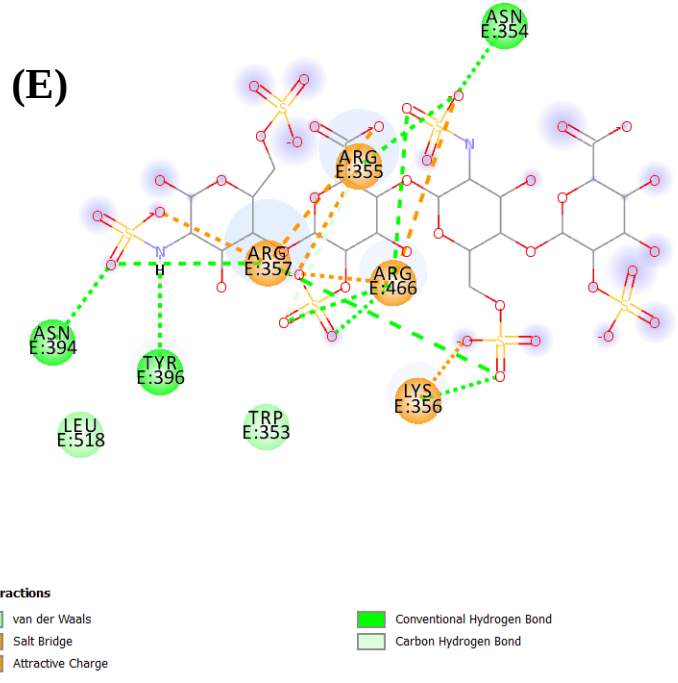
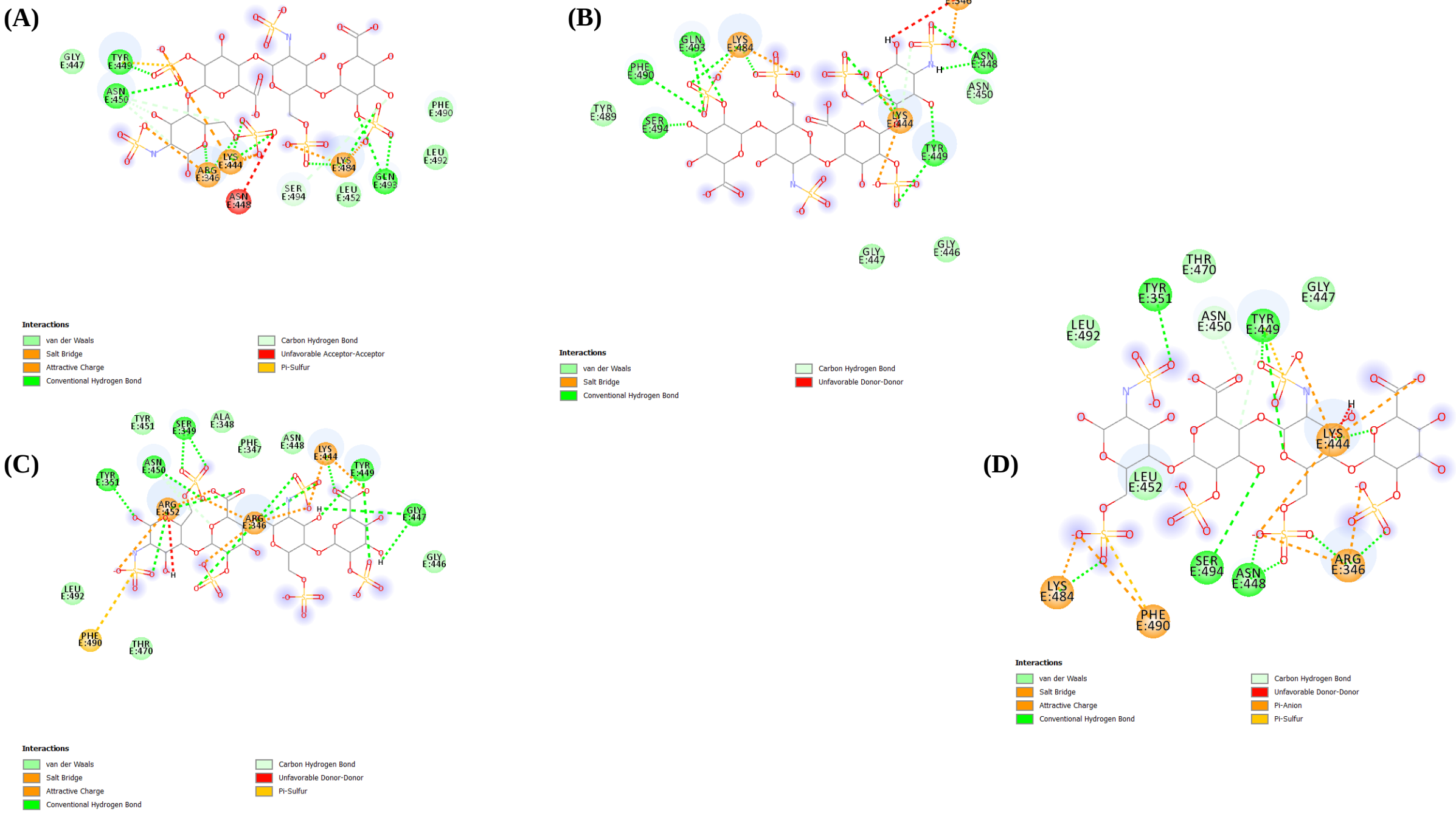
TYR E:351
GLY E:446
VAL E:445
SER E:349
TYR E:451
ARG E:346
ARG E:452
ASN E:450
LYS E:444
ALA E:348
GLY E:447
ASN E:448
PHE E:347
TYR E:449
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor


(C)
ASN E:354
ARG E:355
ARG E:466
LEU E:518
ARG E:357
ASN E:394
TYR E:396
LYS E:356
TRP E:353
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond

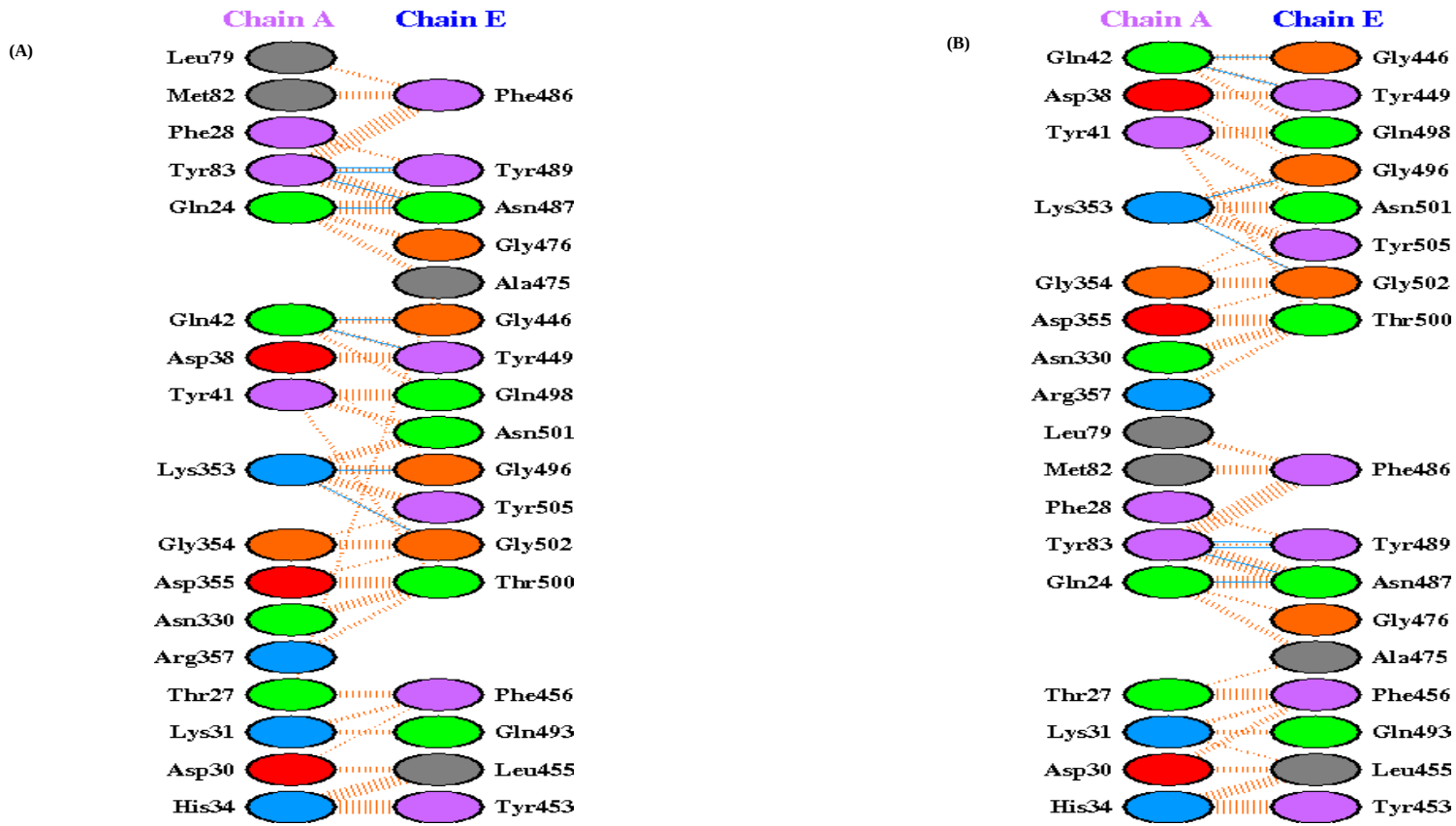

(D)
ASN E:354
ARG E:355
ARG E:357
ARG E:466
ASN E:394
TYR E:396
LYS E:356
LEU E:518
TRP E:353
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond


(E)
ASN E:354
ARG E:355
ARG E:357
ARG E:466
ASN E:394
TYR E:396
LYS E:356
LEU E:518
TRP E:353
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond


(A)
GLY E:447
TYR E:449
ASN E:450
PHE E:490
LEU E:492
LYS E:444
ARG E:346
LYS E:484
GLN E:493
SER E:494
LEU E:452
ASN E:448
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Sulfur
(B)
ARG E:346
GLN E:493
LYS E:484
ASN E:448
PHE E:490
ASN E:450
TYR E:489
SER E:494
LYS E:444
TYR E:449
GLY E:447
GLY E:446
Interactions
van der Waals
Salt Bridge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
(C)
TYR E:451
SER E:349
ALA E:348
PHE E:347
ASN E:448
LYS E:444
ASN E:450
TYR E:449
TYR E:351
ARG E:452
ARG E:346
GLY E:447
GLY E:446
LEU E:492
PHE E:490
THR E:470
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
Pi-Sulfur
(D)
THR E:470
TYR E:351
GLY E:447
LEU E:492
ASN E:450
TYR E:449
LYS E:444
LEU E:452
SER E:494
ARG E:346
ASN E:448
LYS E:484
PHE E:490
Interactions
van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Donor-Donor
Pi-Anion
Pi-Sulfur

Supporting Information Figure 2. Molecular docking interactions of heparin to SARS-CoV-2 RBD variants. The docked structures of Heparin-mutant RBD complexes obtained from cluster 1. Two-dimensional (2D) diagrams of heparin-mutant RBD interactions for (A) N501Y, (B) L452R, (C) E484Q, (D) K417N, and (E) K417T.

Supporting Information Figure 3. Molecular docking interactions of heparin to SARS-CoV-2 RBD variants. The docked structures of Heparin-mutant RBD complexes obtained from cluster 1. Two-dimensional (2D) diagrams of heparin-RBD interactions for (A) K417N-E484K-N501Y, (B) K417T-E484K-N501Y N501Y, (C) L452R-E484K, and (D) E484K. The protein residues and interactions are colored accordingly and provided in figure.



Supporting Information Figure 4. Molecular docking interactions of ACE2 to SARS-CoV-2 RBD variants in the presence of heparin. Two-dimensional (2D) diagrams of RBD/ACE2 interactions in the presence of heparin for (A) K417N, and (B) K417T.