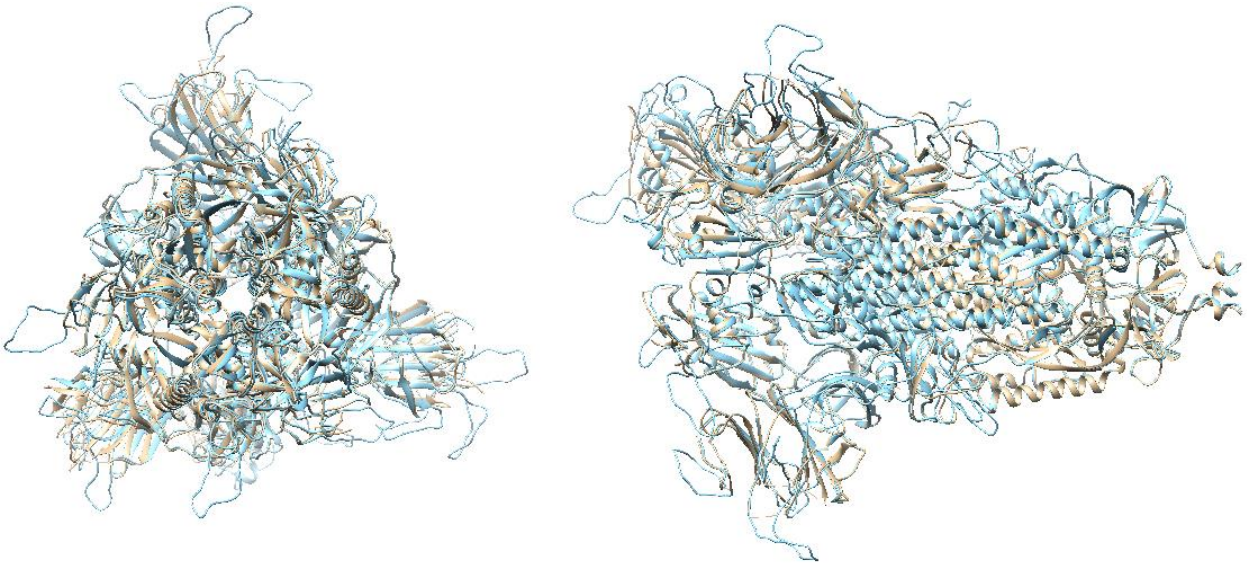
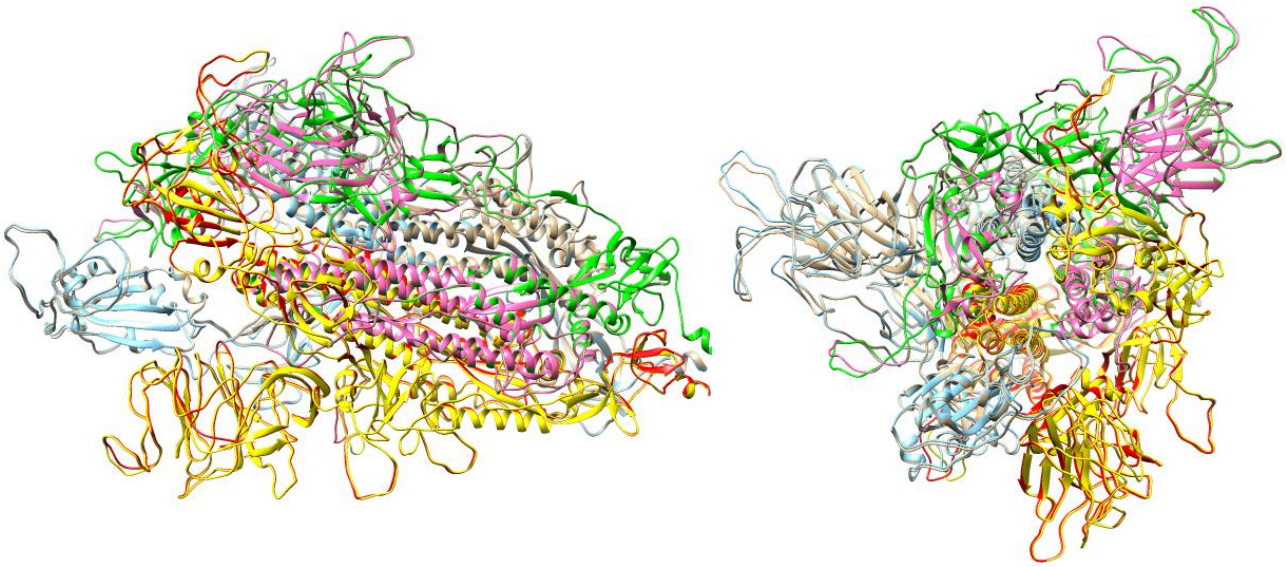
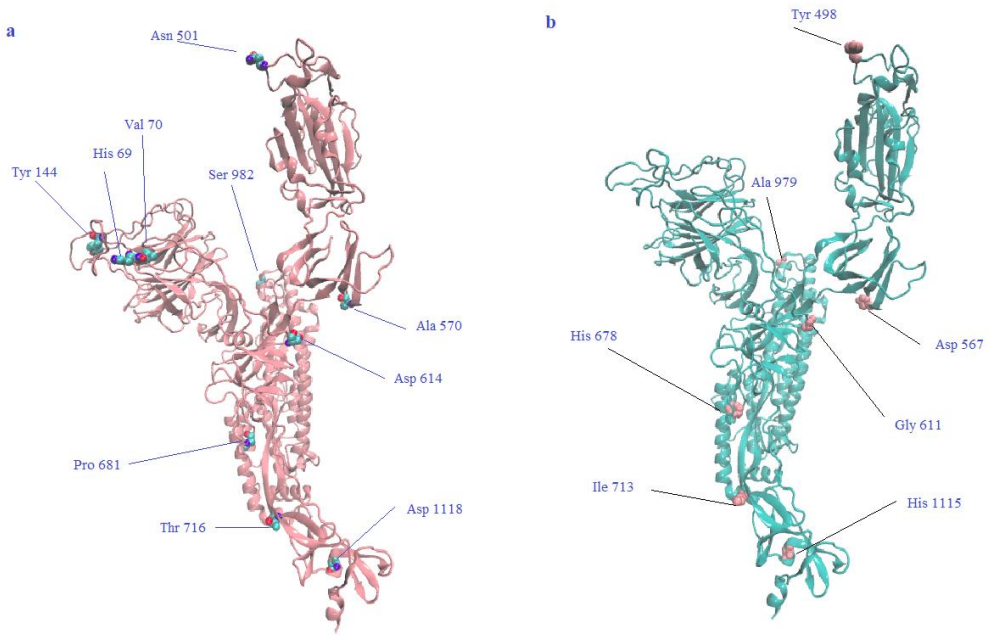
Appendix 1



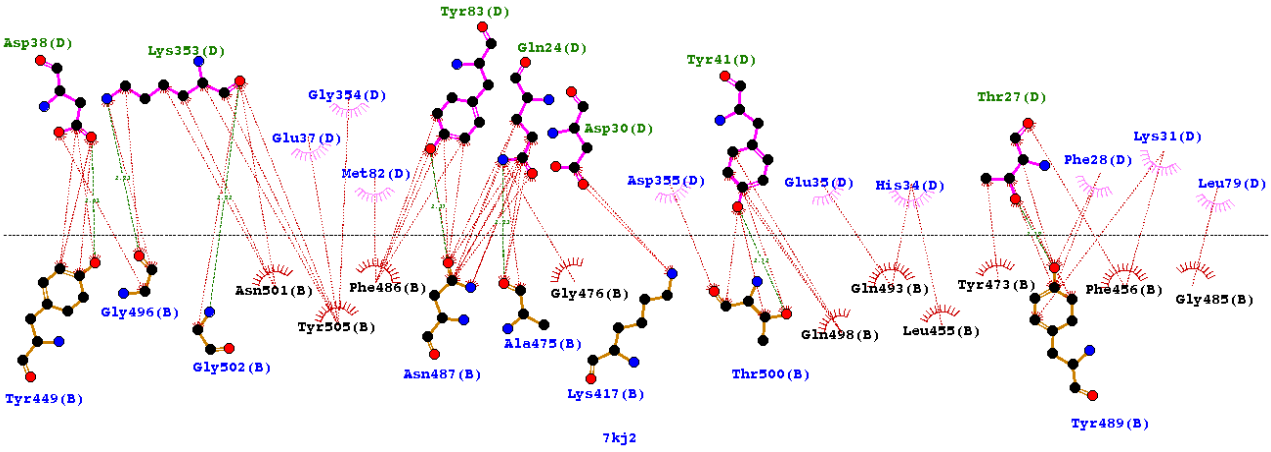
Appendix 1a. Chain A, B and C of spike of SARSCoV-2 (7kj2) are golden, and for model structure of the complete 3D structure of spike protein are blue.



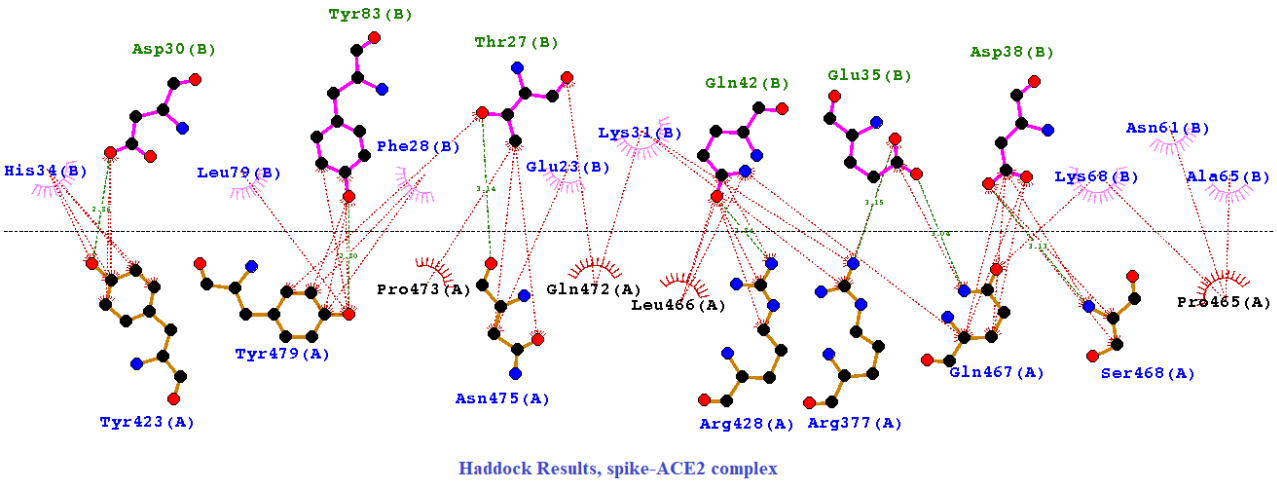
Appendix 1b. Chain A, B and C of non-mutated spike are blue, red and pink, respectively and for UK SARS-CoV-2 spike protein are golden, yellow and green, respectively.



Appendix 1c. Chain A of wild type spike protein (a) and UK SARS-CoV-2 spike protein (b).

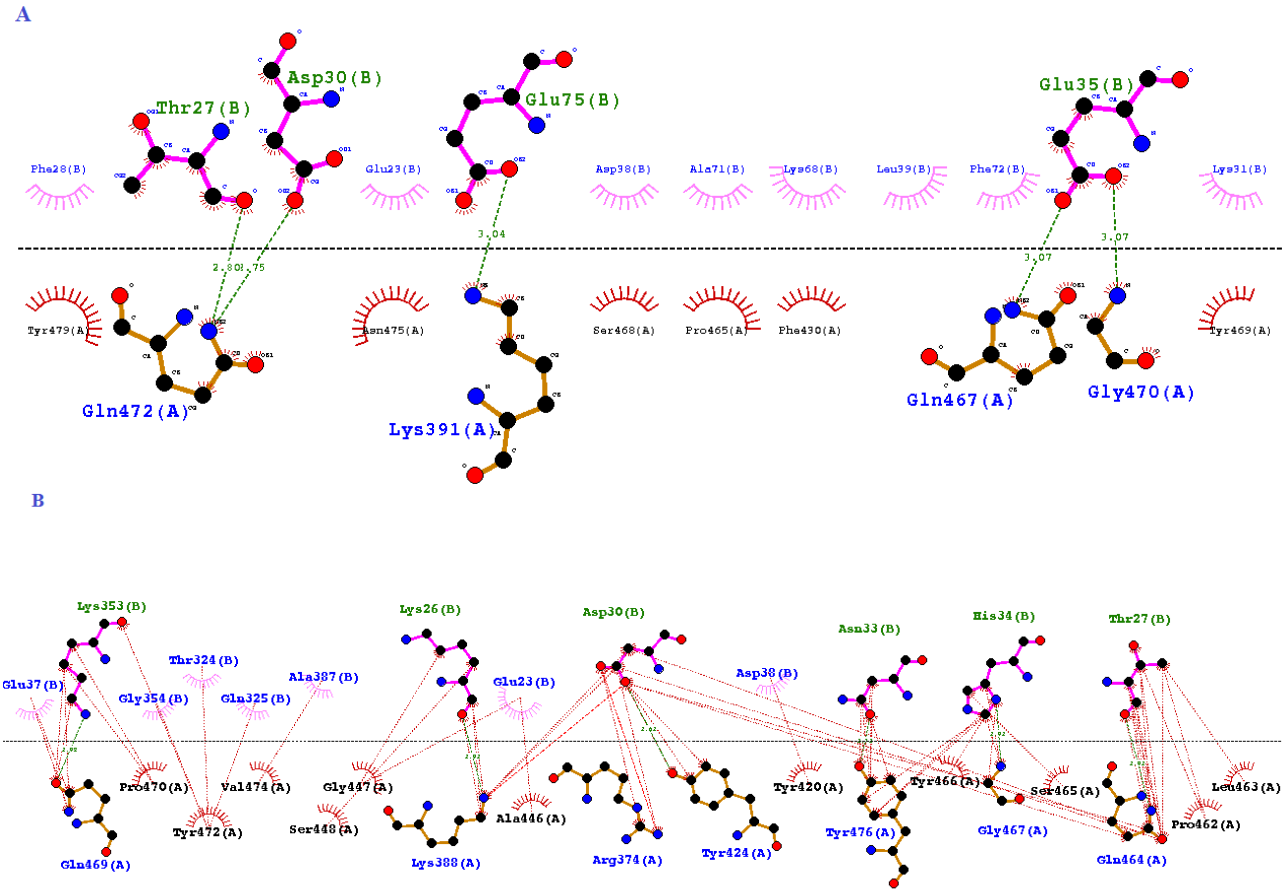


Appendix 1d. Residues involved in spike-ACE2 interaction in 7kj2 structure using ligplot software (B: B chain of spike protein and D: ACE2).

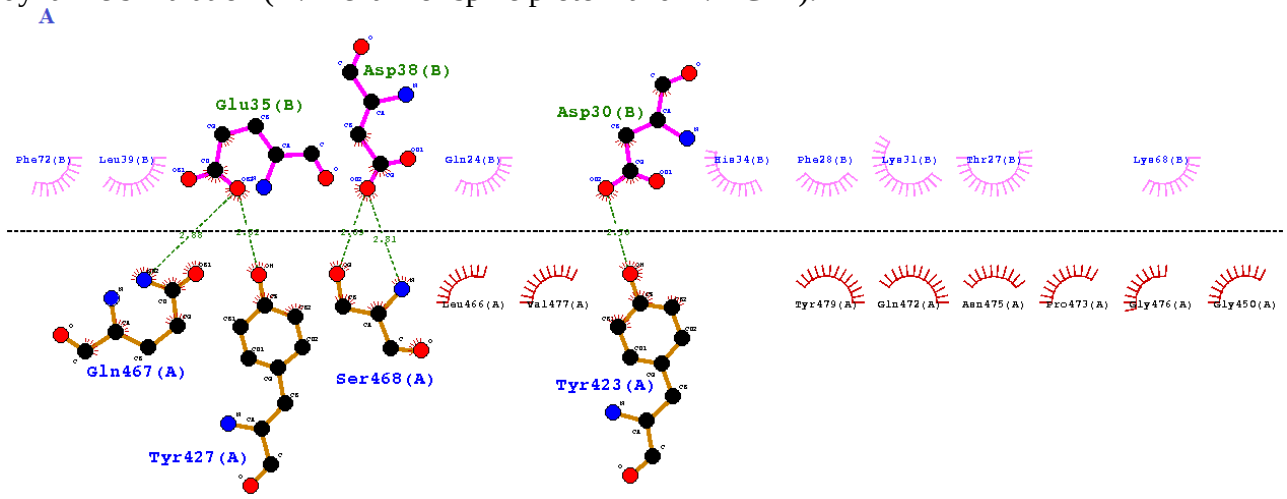


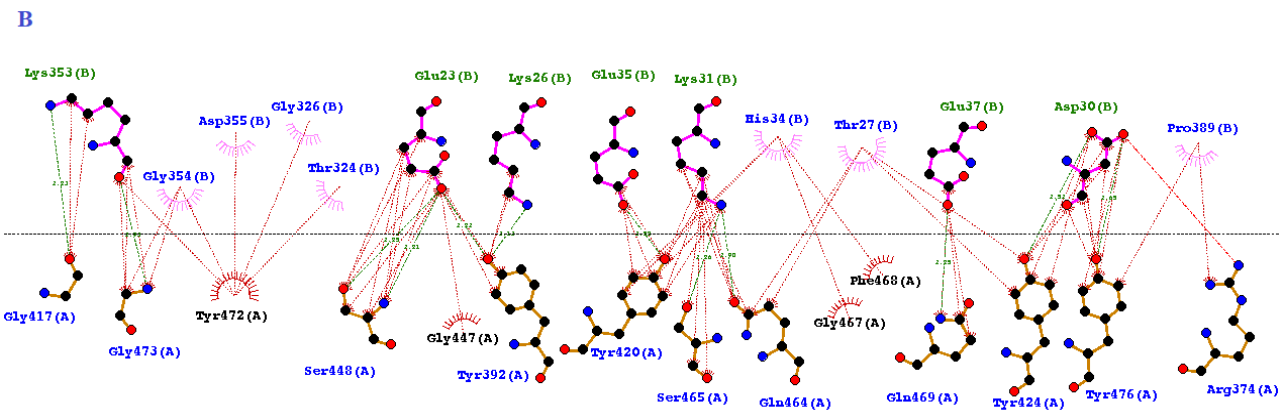
Appendix 1e. Residues involved in spike-ACE2 interaction in wild-type form of haddock results using ligplot software (A: A chain of spike protein and B: ACE2).

Appendix 2
Residues involved in interactions between SARS-CoV-2 spike protein and ACE2 protein were examined in each 10ns of the molecular dynamic simulation results in wild-type (A) and mutated (B) SARS-CoV-2 spike-ACE2 complex

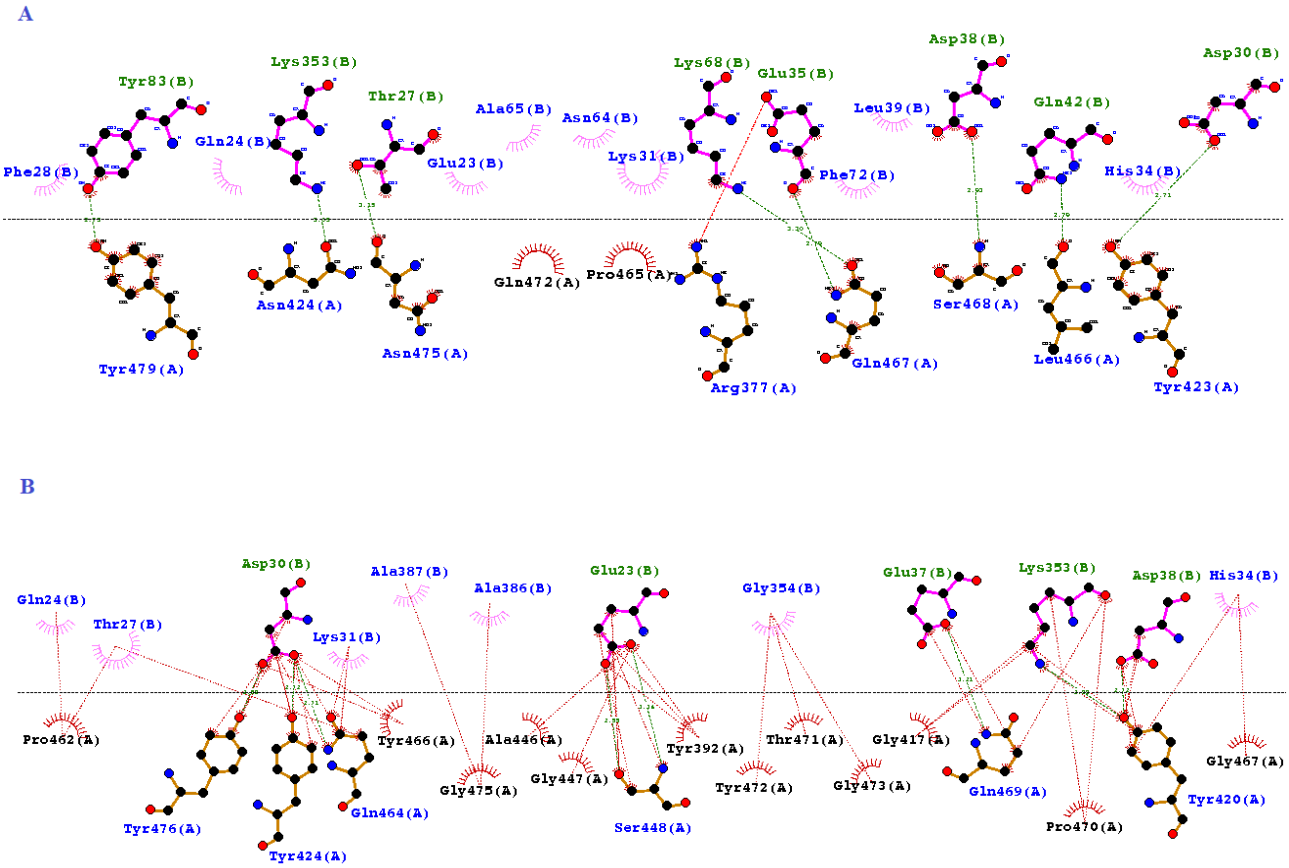


Appendix 2A. Residues involved in interactions between spike and ACE2 in 10ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).



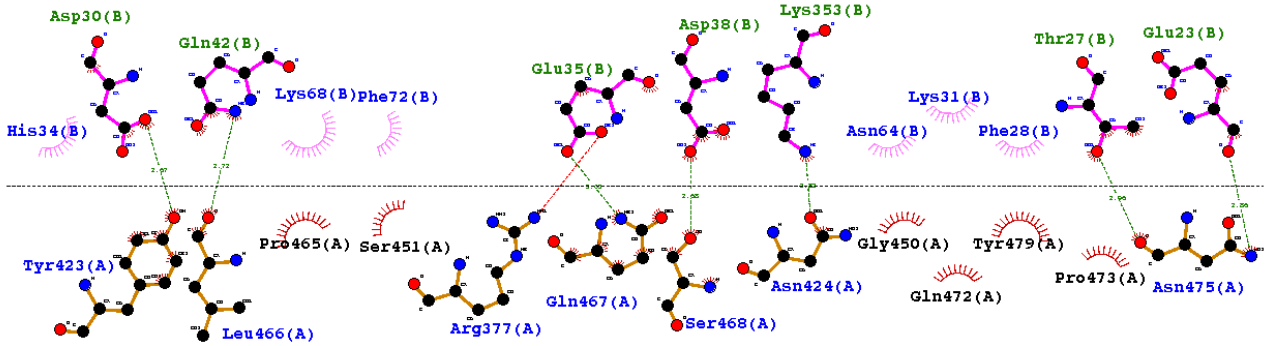


Appendix 2B. Residues involved in interactions between spike and ACE2 in 20ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).

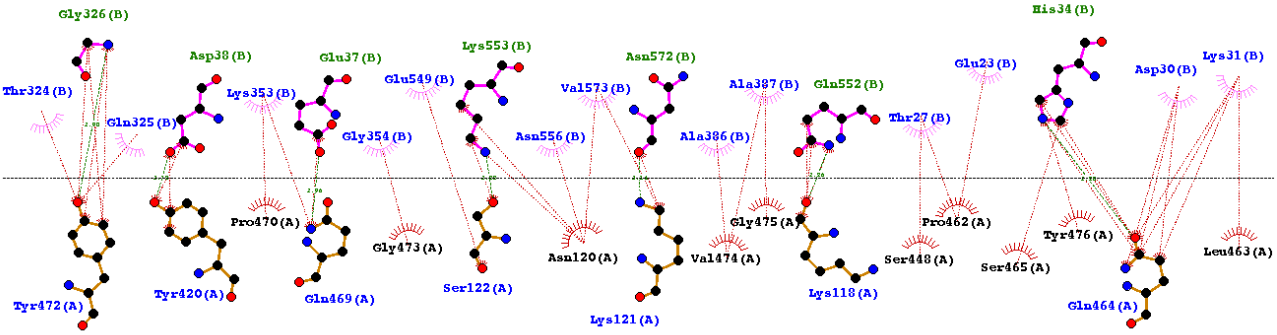


Appendix 2C. Residues involved in interactions between spike and ACE2 in 30ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).

A

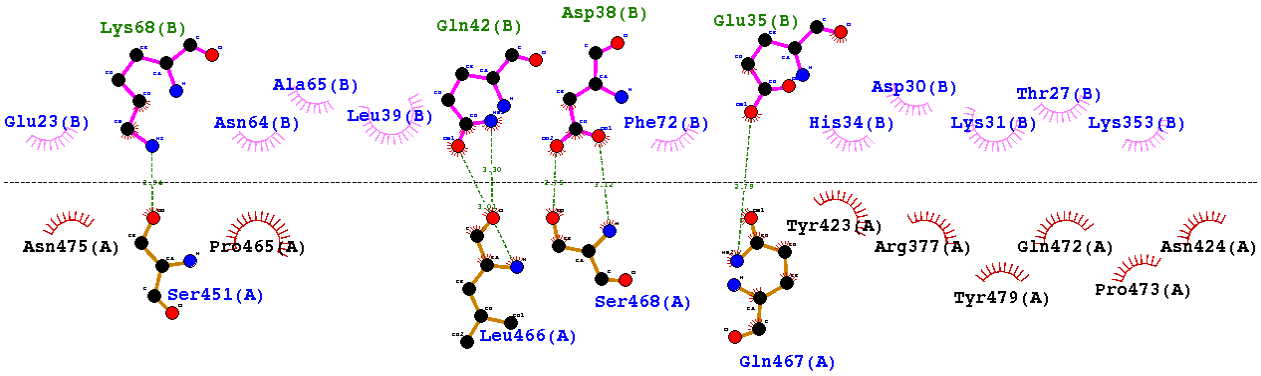


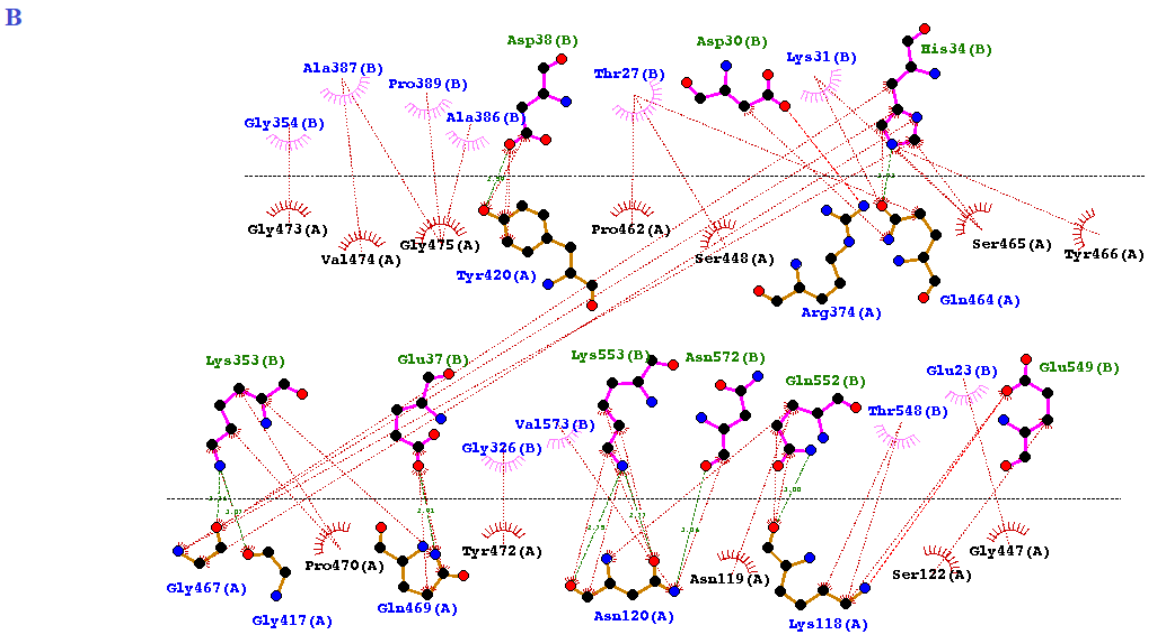
B



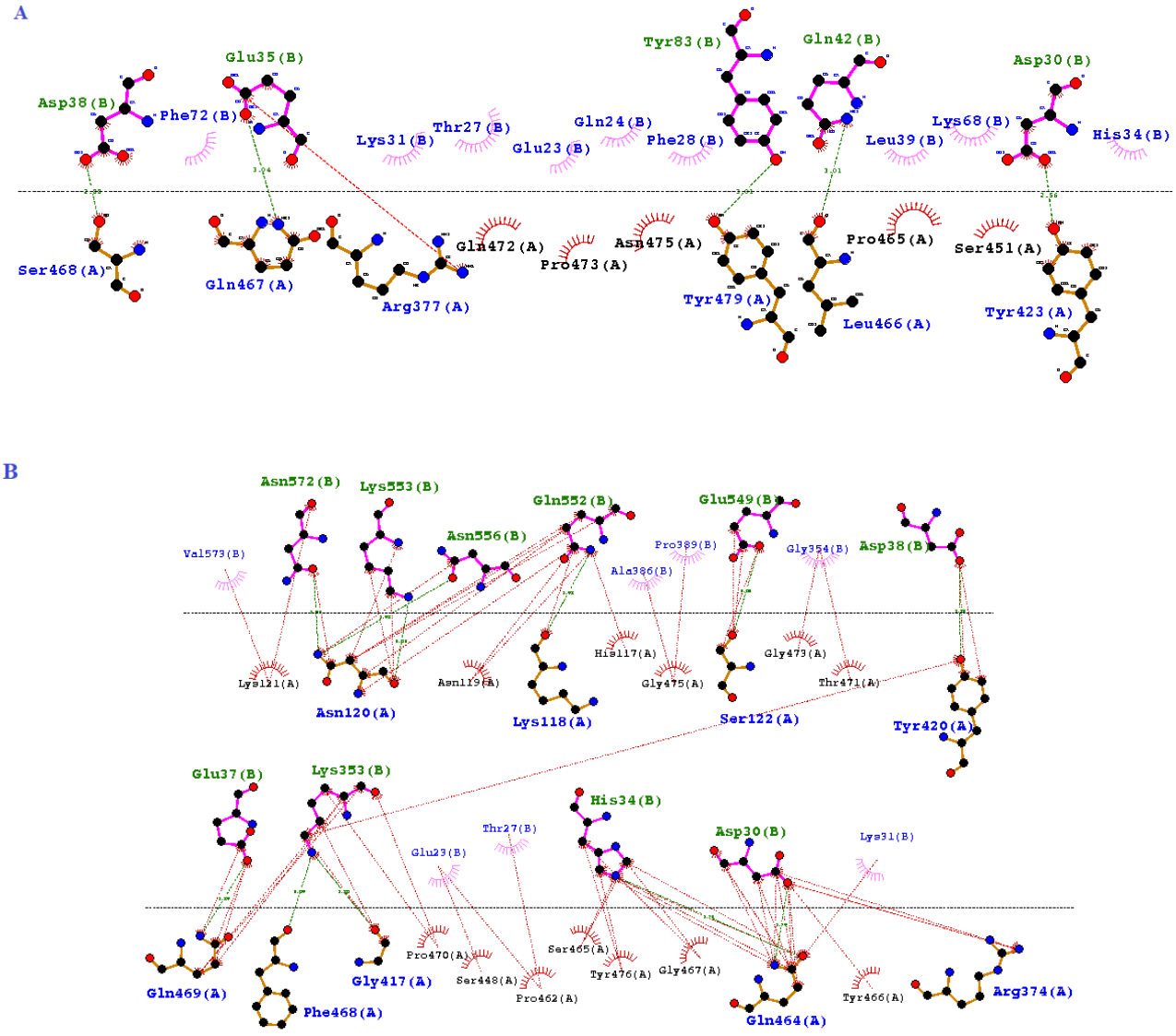
Appendix 2D. Residues involved in interactions between spike and ACE2 in 40ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).

A

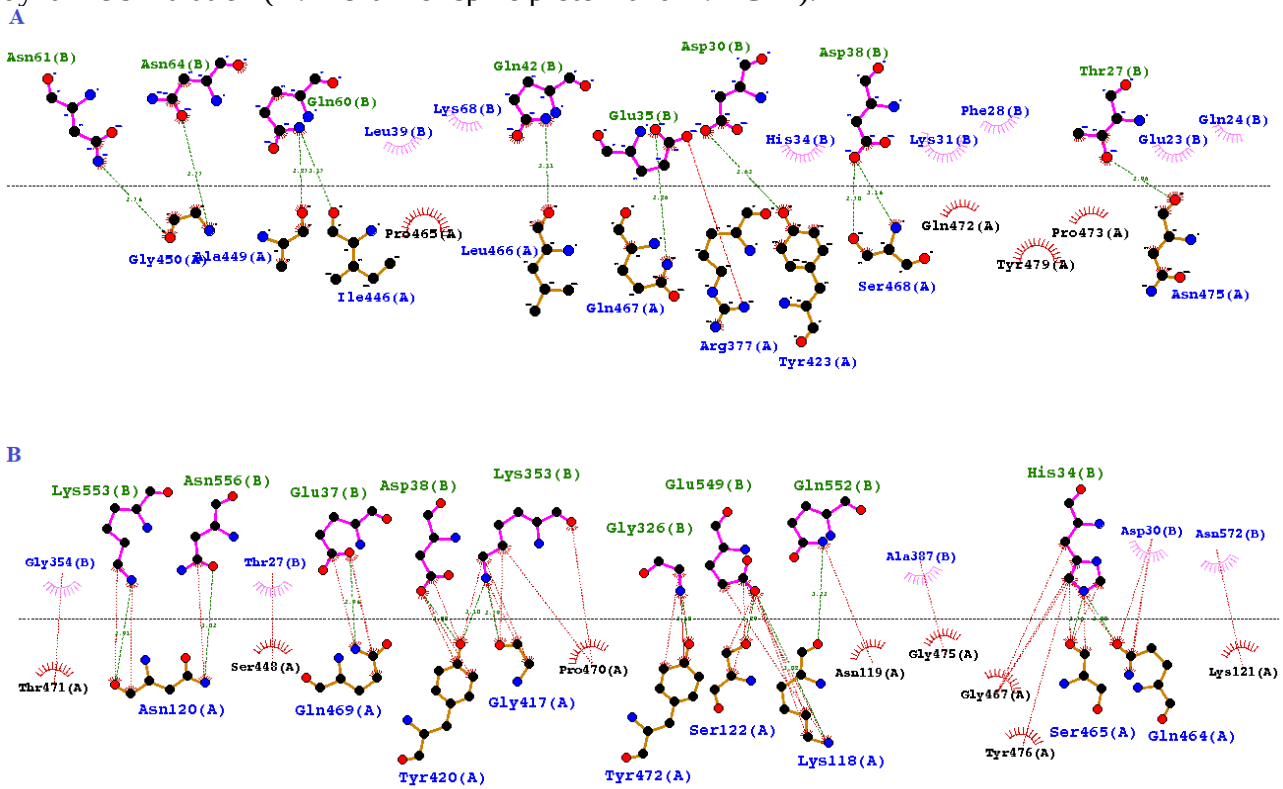




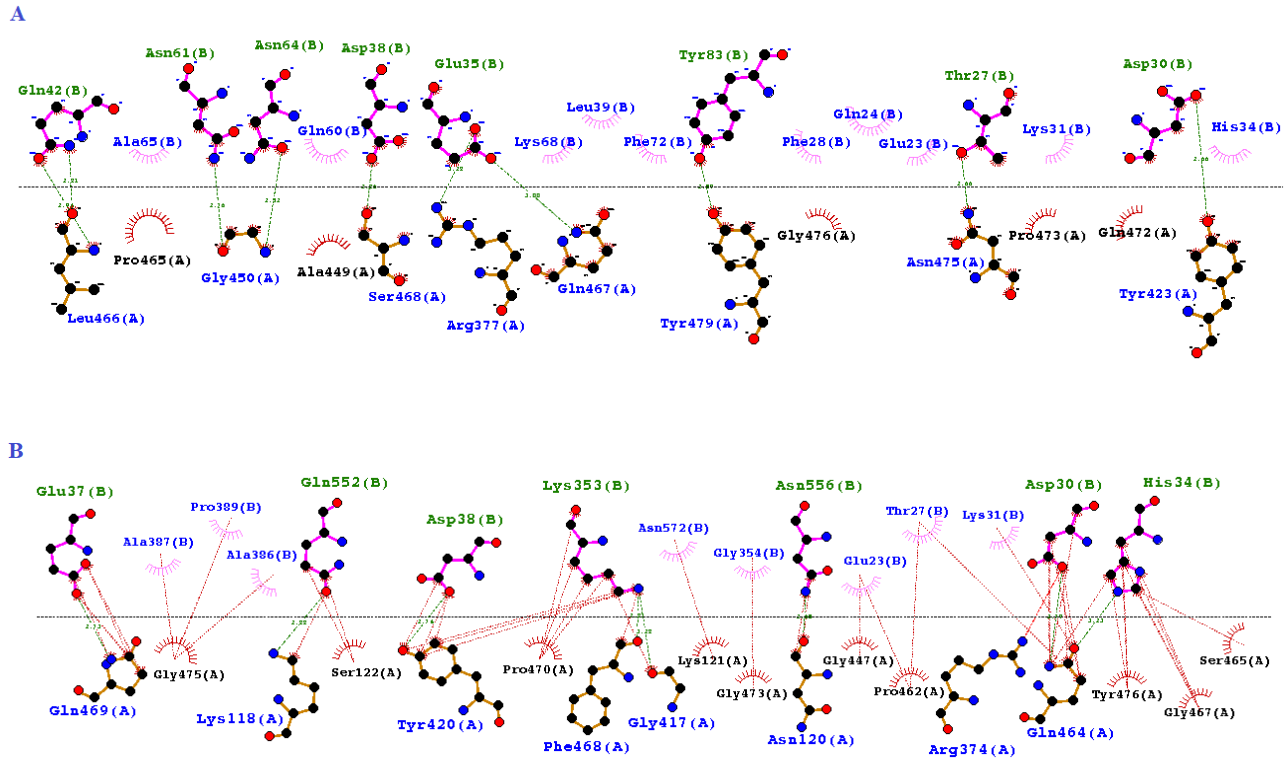
Appendix 2E. Residues involved in interactions between spike and ACE2 in 50ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).



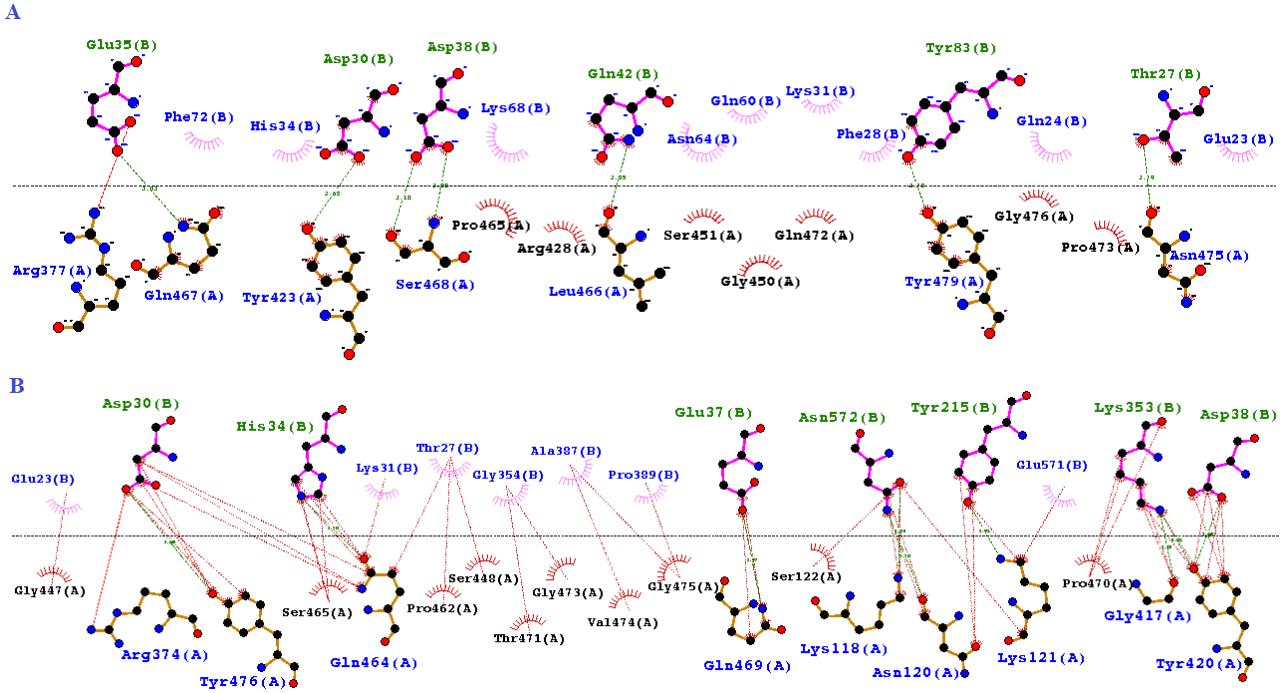
Appendix 2F. Residues involved in interactions between spike and ACE2 in 60ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).



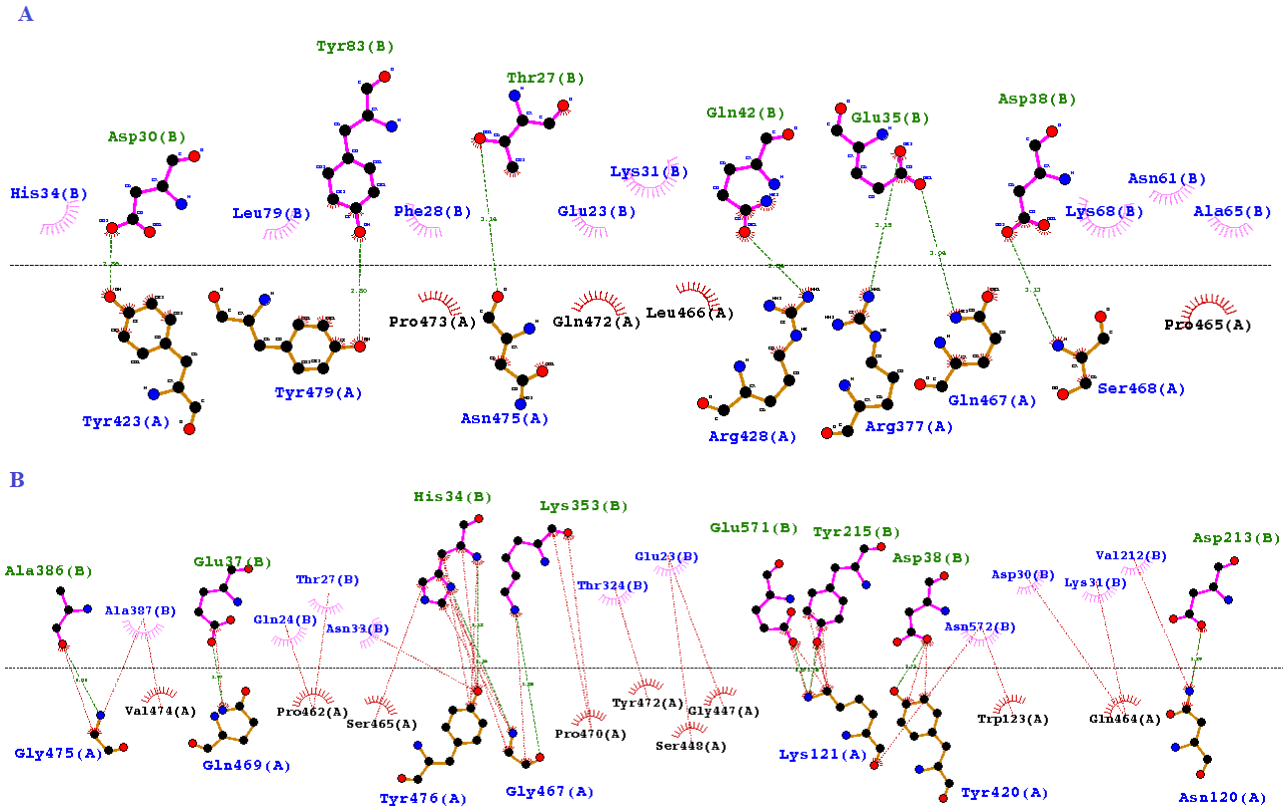
Appendix 2G. Residues involved in interactions between spike and ACE2 in 70ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).



Appendix 2H. Residues involved in interactions between spike and ACE2 in 80ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).

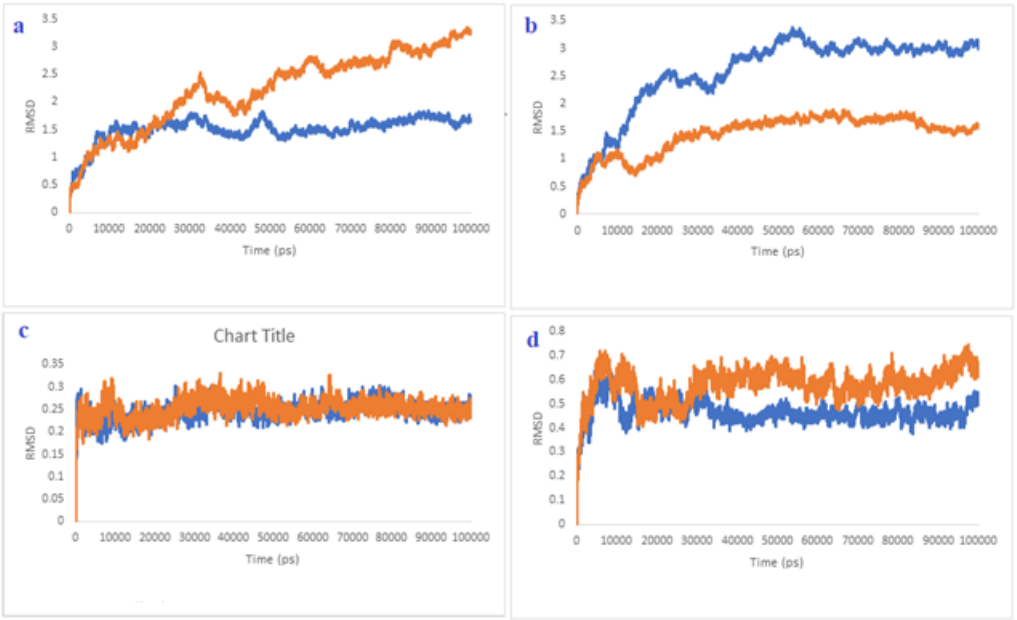


Appendix 2I. Residues involved in interactions between spike and ACE2 in 90ns of the molecular dynamic simulation (A: A chain of spike protein and B: ACE2).

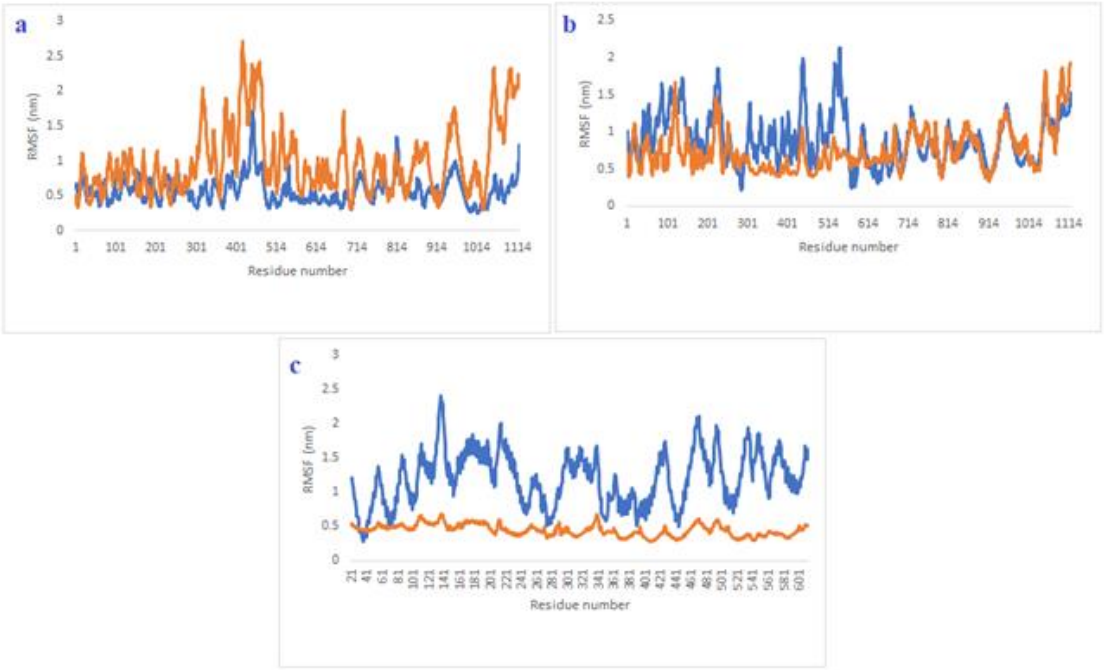


Appendix 2J. Residues involved in interactions between spike and ACE2 in 100ns of the molecular dynamic simulation(A: A chain of spike protein and B: ACE2).

Appendix 3.
RMSD of the backbone Cα atoms for monomeric wild-type spike (blue) and for monomeric mutant spike protein (orange) of SARS-CoV-2 (a), wild type spike-ACE2 complex (blue) and mutant spike-ACE2 complex (b), ACE2 in wild type spike-ACE2 complex (blue) and ACE2 in mutant spike-ACE2 complex (orange) (c) and active site of wild type spike (blue) and active site of mutant spike in spike-ACE2 complex (orange) (d).



Appendix 4. RMSF of the backbone Cα atoms of wild-type spike and mutant spike (a), spike in wild type spike-ACE2 complex and mutant spike-ACE2 complex (b), and ACE2 in in wild type spike-ACE2 complex and mutant spike-ACE2 complex (c).


a
RMSF (nm)
Residue number
b
RMSF (nm)
Residue number
c
RMSF (nm)
Residue number