Molecular dynamics simulation study of the interaction between human angiotensin converting enzyme 2 and spike protein receptor binding domain of the SARS-CoV-2 B.1.617 variant

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SUPPLEMENTARY MATERIALS

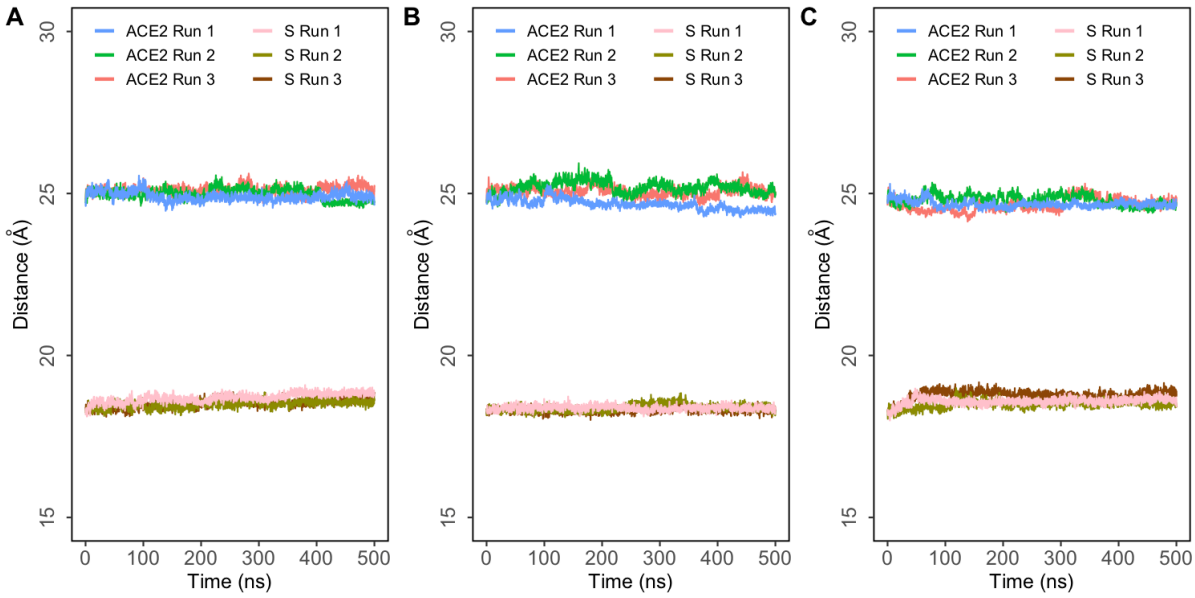

Figure S1. Radius of gyration (Rg) of human ACE2 (hACE2) and spike (S) protein of SARS-CoV-2 receptor-binding domain (RBD) from three 500 ns simulations of **(A)** E484Q+L452R; **(B)** E484Q; **(C)** L452R.

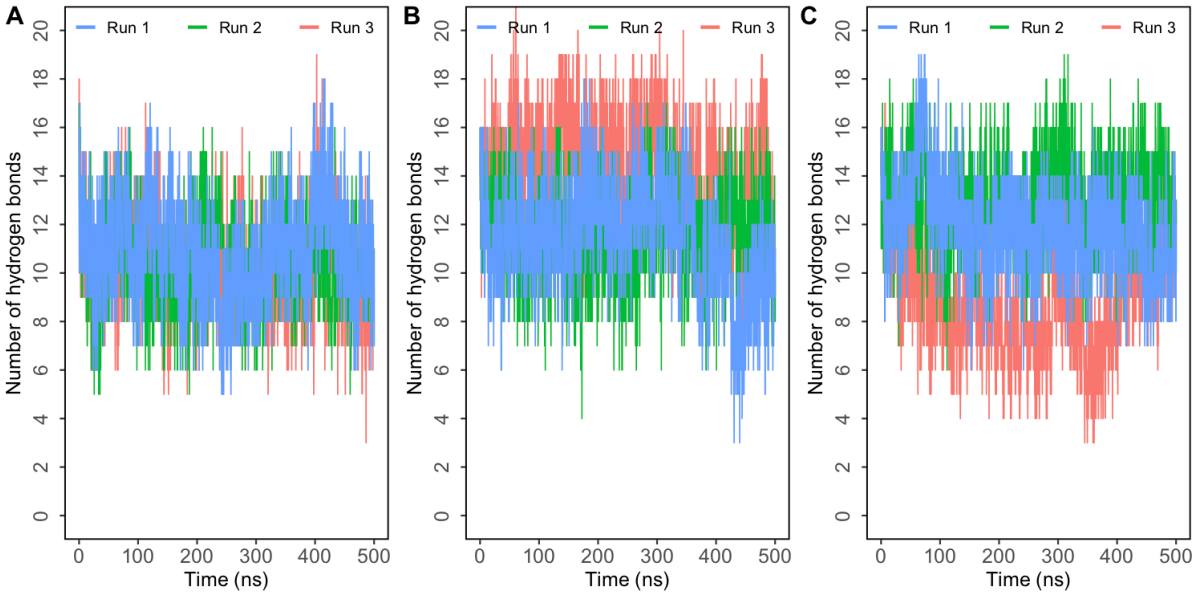

Figure S2. Hydrogen bonds between of human ACE2 (hACE2) and spike (S) protein of SARS-CoV-2 receptor-binding domain (RBD) from three 500 ns simulations of **(A)** E484Q+L452R; **(B)** E484Q; **(C)** L452R.