

(Supporting Information)

**Molecular Insights into the Differential Dynamics of SARS-CoV-2 Variants of
Concern**

Nabanita Mandal^a, Aditya K. Padhi^b and Soumya Lipsa Rath^{a*}

^aNational Institute of Technology, Warangal, Telangana, 506004, India

^bLaboratory for Structural Bioinformatics, Center for Biosystems Dynamics Research, RIKEN, 1-7-22 Suehiro, Tsurumi, Yokohama, Kanagawa 230-0045, Japan.

* Corresponding Author Email: slrath@nitw.ac.in

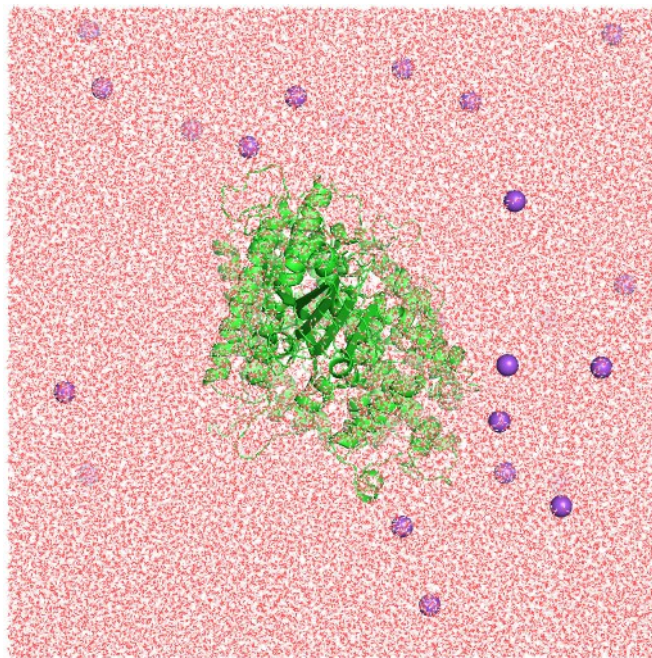


Figure S1. The WT RBD/ACE2 complex showing the surrounding water box with TIP3P water molecules and neutralizing ions

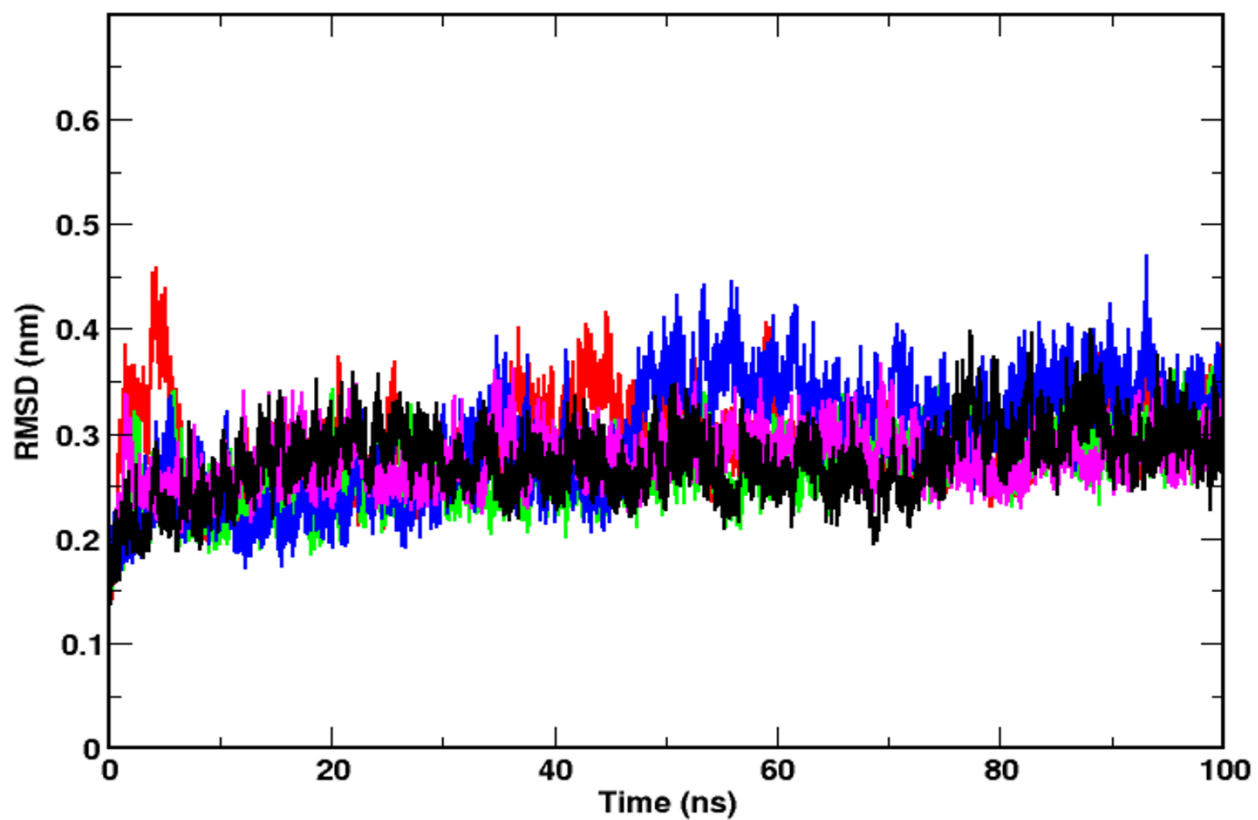
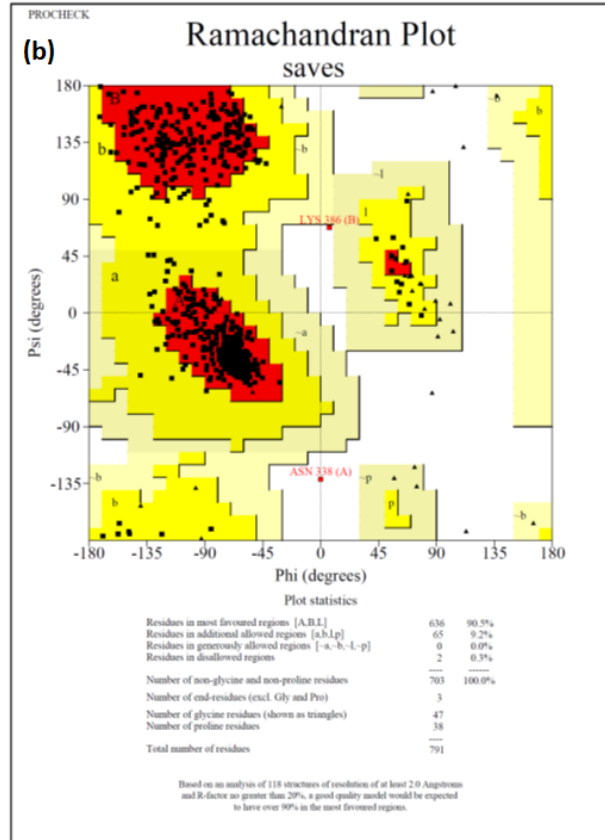
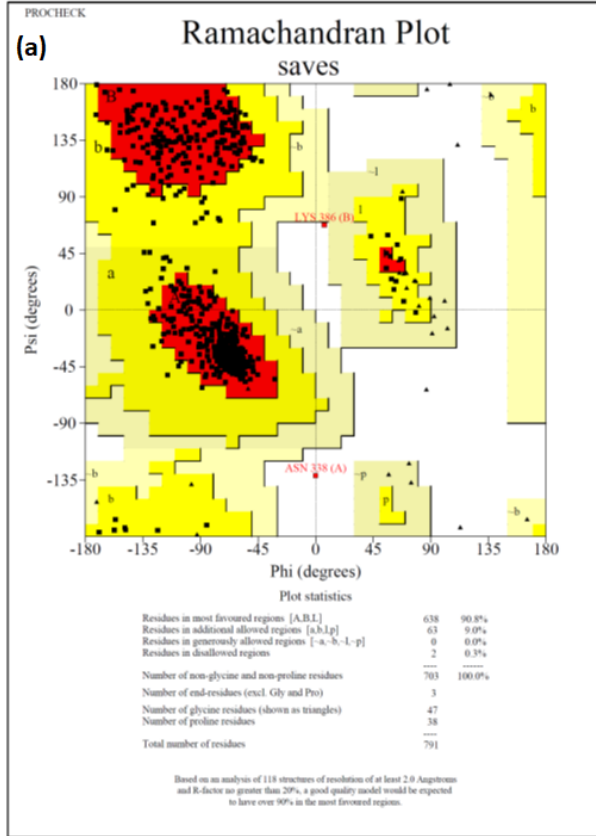
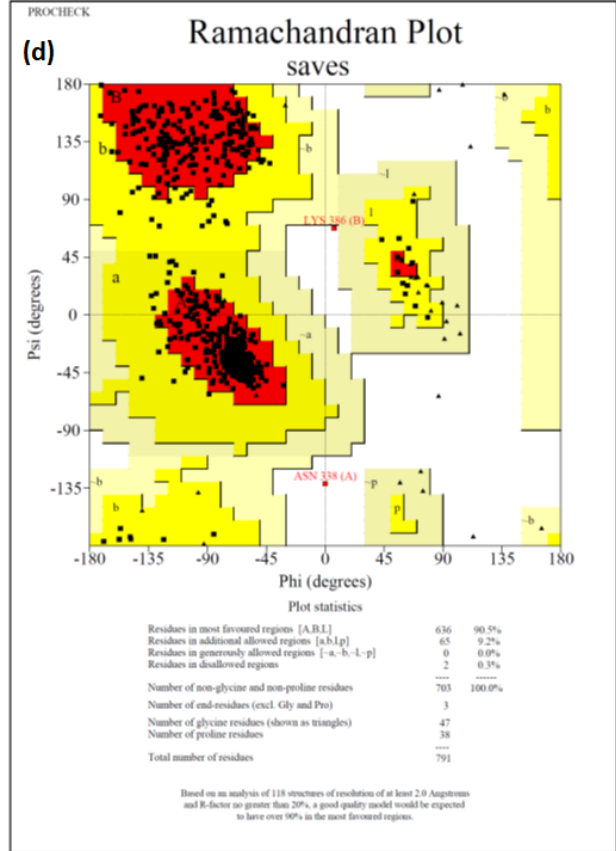
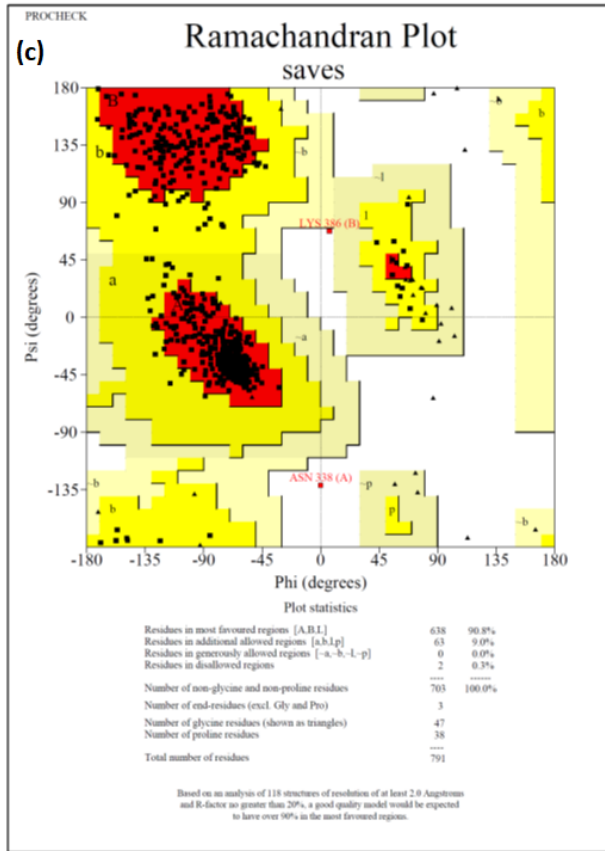


Figure S2. Time evolution of the protein RMSDs of the RBD/ACE2 protein complex in WT (black), Alpha (green), Beta (blue), Gamma (red), and Delta (magenta). The systems were found to be largely stable after 50ns.





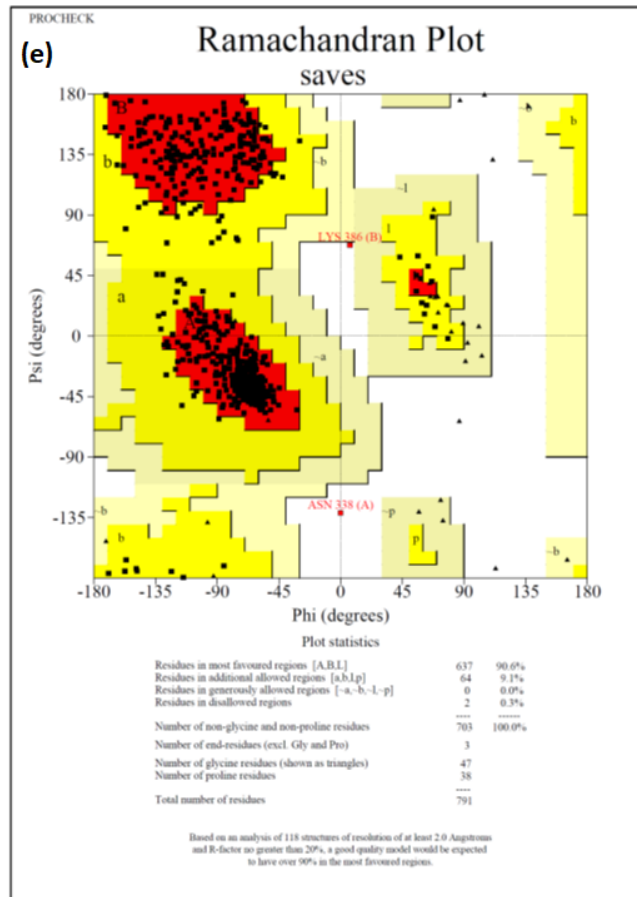


Figure S4. Ramachandran plot generated by PROCHECK analysis displaying the stereochemical properties of WT and the four models that were generated showing structural similarity. (a) WT (b) Gamma (c) Alpha (d) Beta and (e) Delta.

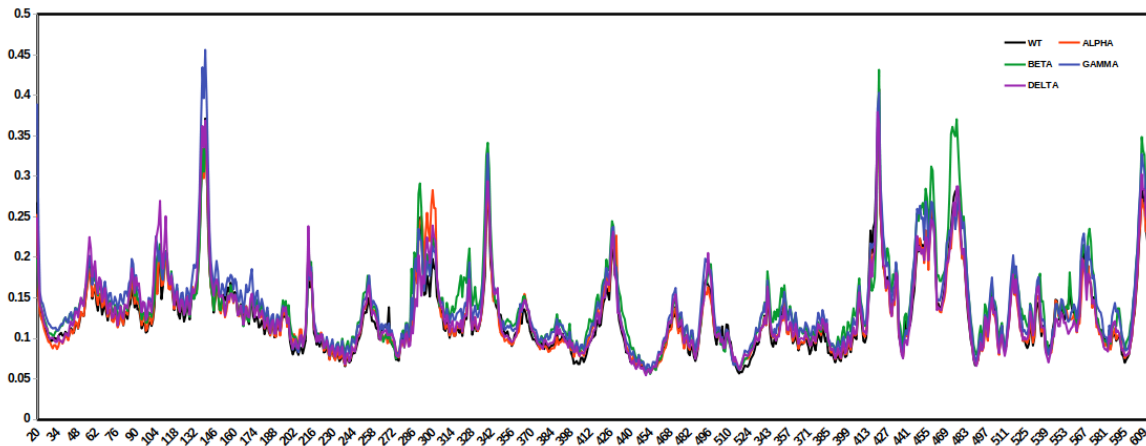


Figure S5. RMSF of CA atoms of the RBD/ACE2 complex for all the five systems under study.

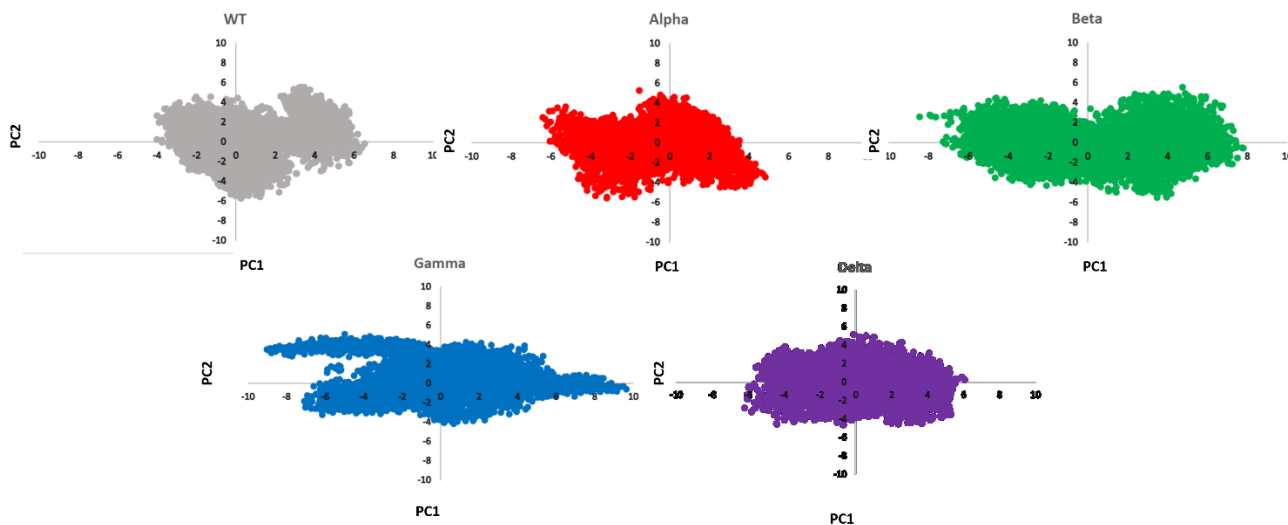


Figure S6. Distribution of simulated structures on the plane constituted by the first two principal components of ACE2 and RBD in WT (grey), Alpha (red), Beta (green), Gamma (blue), and Delta (magenta).

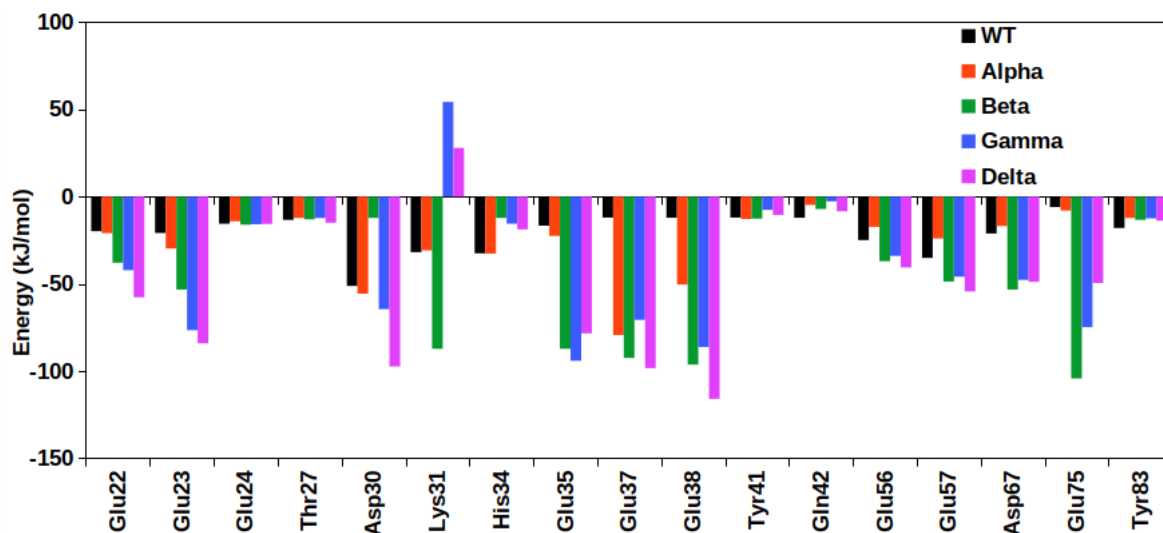


Figure S7. Residue level contribution of ACE2 towards the total interaction energy for all the five systems under study.

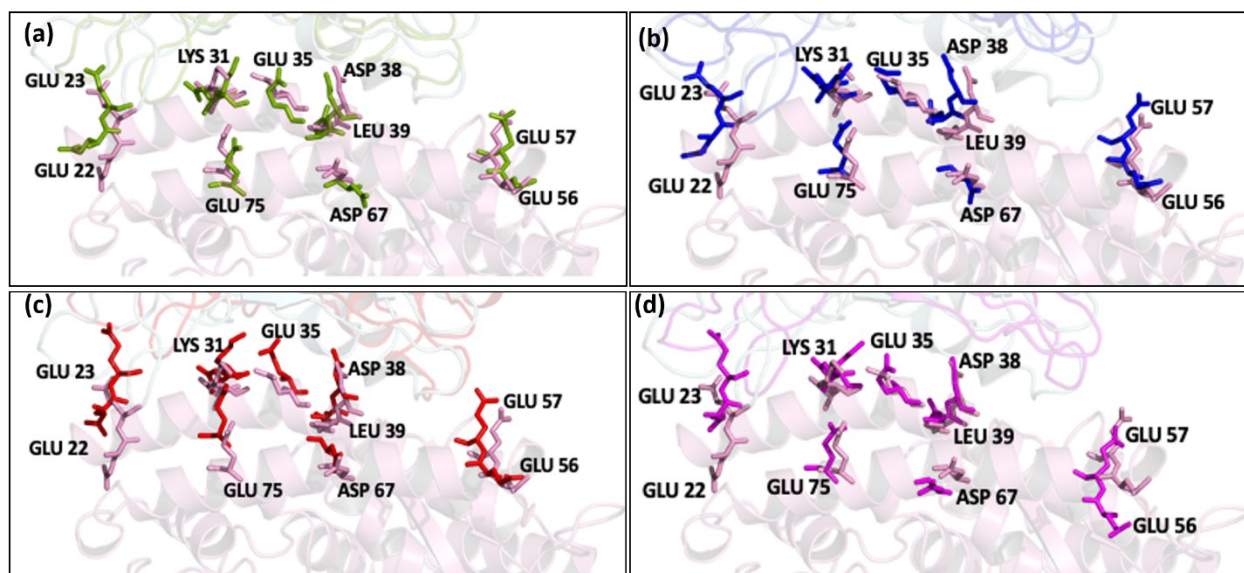


Figure S8. ACE2 interfacial residues that interact with RBD. Superimposed images of WT with (a) Alpha, (b) Beta (c) Gamma, and (d) Delta. Color scheme: WT (pink), Alpha (green), Beta (blue), Gamma (red) and Delta (magenta). The residues lie at a similar position in the ACE2 receptor.



Figure S9. Superimposed structure of RBD/ACE2 complex of time-averaged B.167.2 structure (shown in magenta) and cryo-EM (PDB ID:78VB) (shown in cyan) [21] showing similarity between the two with RMSD 1.7 Å.

Table S1. RMSD of the triplicates

System	Average RMSD from triplicates (nm)	Std Deviation
WT	0.27	0.03
Alpha	0.27	0.03
Beta	0.27	0.04
Gamma	0.26	0.04
Delta	0.25	0.02