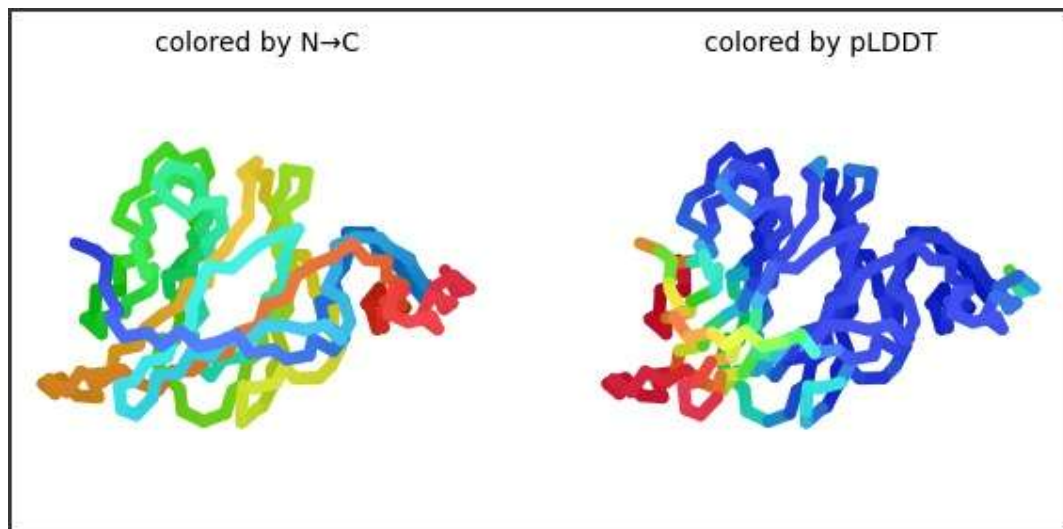
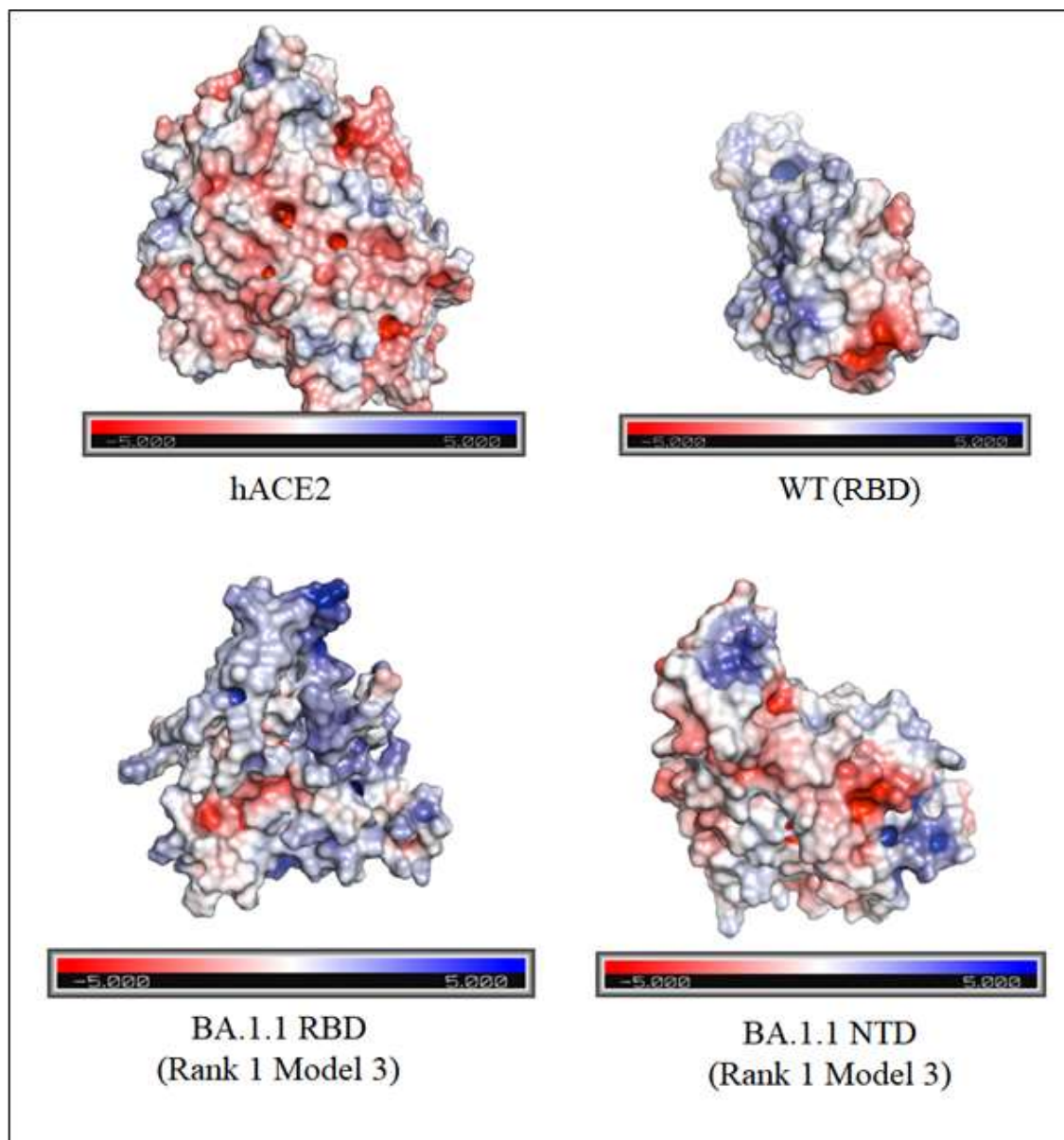


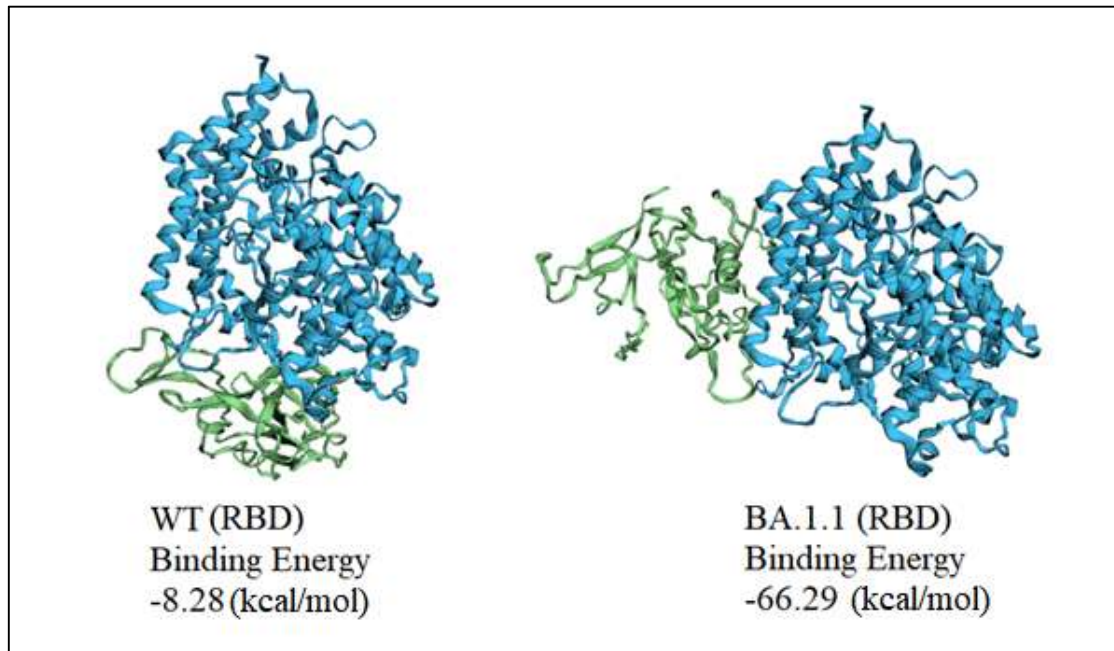
**Figure 2.1** – AlphaFold model prediction of the BA.1.1 Omicron Variant RBD structure (Model 3 Rank 1)



**Figure 2.2** – AlphaFold model prediction of the BA.1.1 Omicron Variant NTD structure (Model 3 Rank 1)



**Figure 3.0** – Comparison between the wild-type (WT), Omicron variants (BA.1.1) spike receptor-binding domains (RBD), N-Terminal Domain (NTD) and shown human ACE2. The protein surface is coloured according to the electrostatic potential show in top view. Colour scale ranges from  $-5 \text{ kT/e}$  (red) to  $+5 \text{ kT/e}$  (blue) as reported by the bar at the bottom of each model.



**Figure 4.0** - Docking between wild-type (WT)-RBD and Omicron BA.1.1-RBD with hACE2. Docking score are shown in MM/GBSA free energy decomposition analysis for binding free energy calculations at the top of each variant. hACE2, human angiotensin I-converting enzyme 2; RBD, receptor-binding domain.