

# Binding mechanism of SARS-CoV-2 spike protein with human ACE2 receptor

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## Supplementary Material

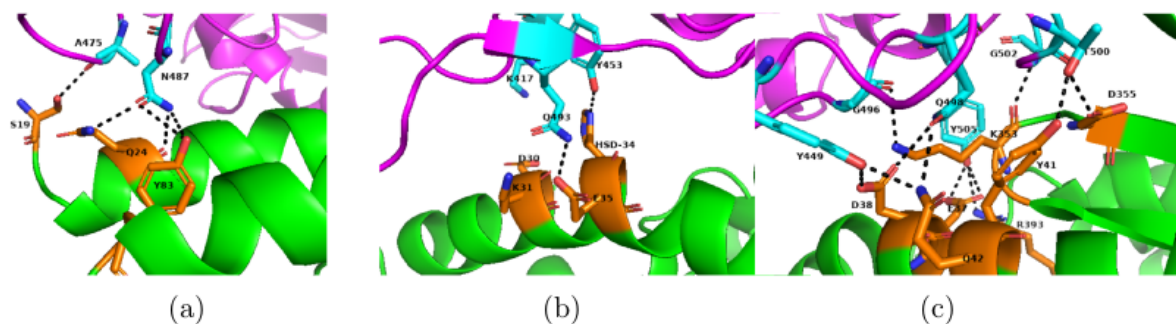


Figure S1: Details of hydrogen bondings at the three key contact sites on binding interface between SARS-CoV-2 CTD and hACE2 receptor. hACE2 receptor is shown in green and SARS-CoV-2 CTD is shown in magenta color. The contact residues which can form potential hydrogen bonds are shown as sticks & labelled by 1 residue letter (for 624<sup>th</sup> frame).

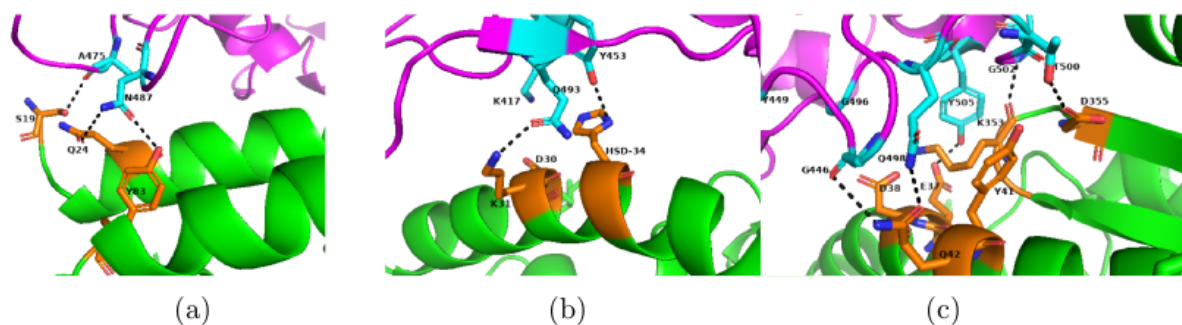


Figure S2: Details of hydrogen bondings at the three key contact sites on binding interface between SARS-CoV-2 CTD and hACE2 receptor. hACE2 receptor is shown in green and SARS-CoV-2 CTD is shown in magenta color. The contact residues which can form potential hydrogen bonds are shown as sticks & labelled by 1 residue letter (for 1249<sup>th</sup> frame).

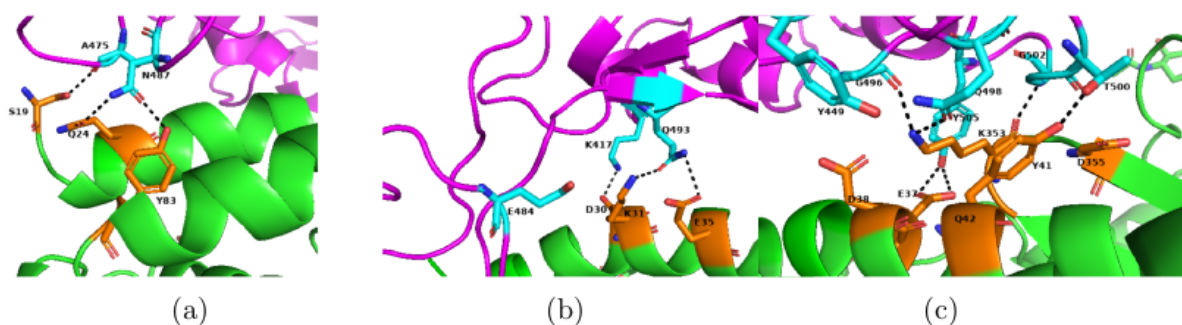


Figure S3: Details of hydrogen bondings at the three key contact sites on binding interface between SARS-CoV-2 CTD and hACE2 receptor. hACE2 receptor is shown in green and SARS-CoV-2 CTD is shown in magenta color. The contact residues which can form potential hydrogen bonds are shown as sticks & labelled by 1 residue letter (for 1874<sup>th</sup> frame).

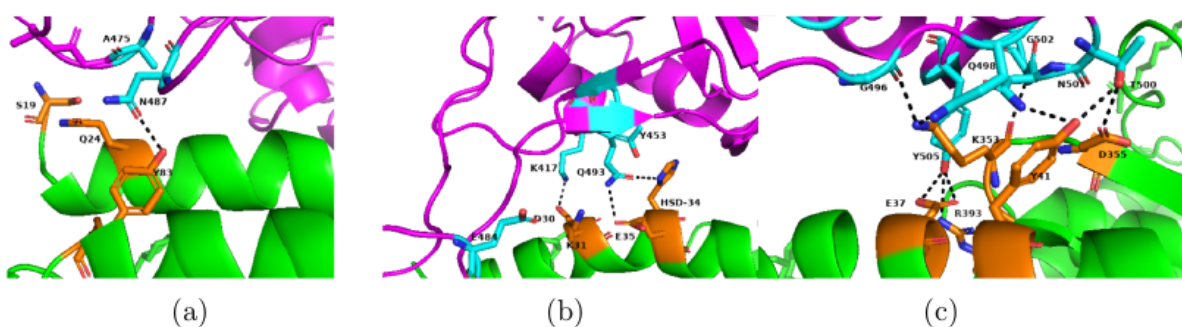


Figure S4: Details of hydrogen bondings at the three key contact sites on binding interface between SARS-CoV-2 CTD and hACE2 receptor. hACE2 receptor is shown in green and SARS-CoV-2 CTD is shown in magenta color. The contact residues which can form potential hydrogen bonds are shown as sticks & labelled by 1 residue letter (for 2449<sup>th</sup> frame).

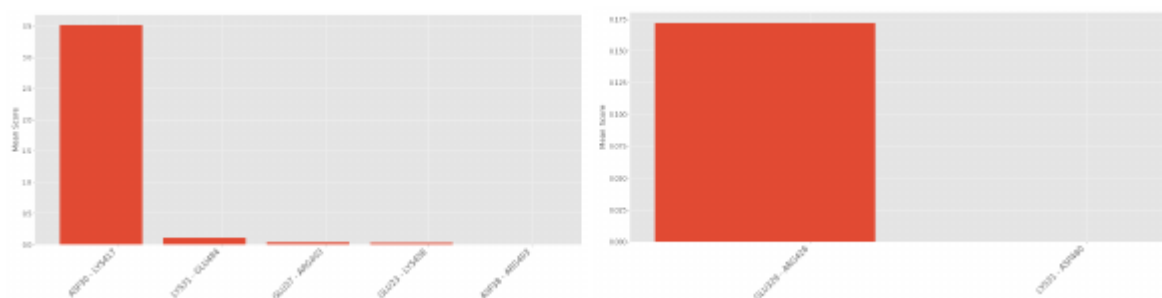


Figure S5: Salt-bridges (Mean contact score) for SARS-CoV-2 CTD/hACE2 (left) & SARS-CoV RBD/hACE2.

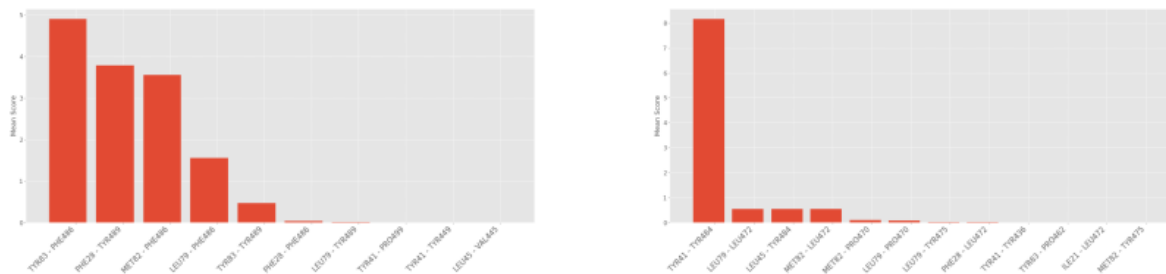


Figure S6: Hydrophobic interaction (mean contact score) for SARS-CoV-2 CTD/hACE2 (left) & SARS-CoV RBD/hACE2 (right) .

Table S1: Significant hydrogen bonds formed at the interface between SARS-CoV-2-CTD/hACE2 and SARS-CoV RBD/hACE2.

SARS-CoV-2 CTD	hACE2	SARS-CoV RBD
A475	S19	D463
N487	Q24	N473, Y475
K417	D30	Y442
Q493	K31	T476, N479
Y453, S494	H34	Y442
Q493	E35	-
Y505	E37	-
Q498, Y449	D38	Y436
T500	Y41	T486
Q498, Y449	Q42	Y436
N487	Y83	N475
G502, G496	K353	G488
T500	G355	T486
-	CARA-BMAN3	VAL404