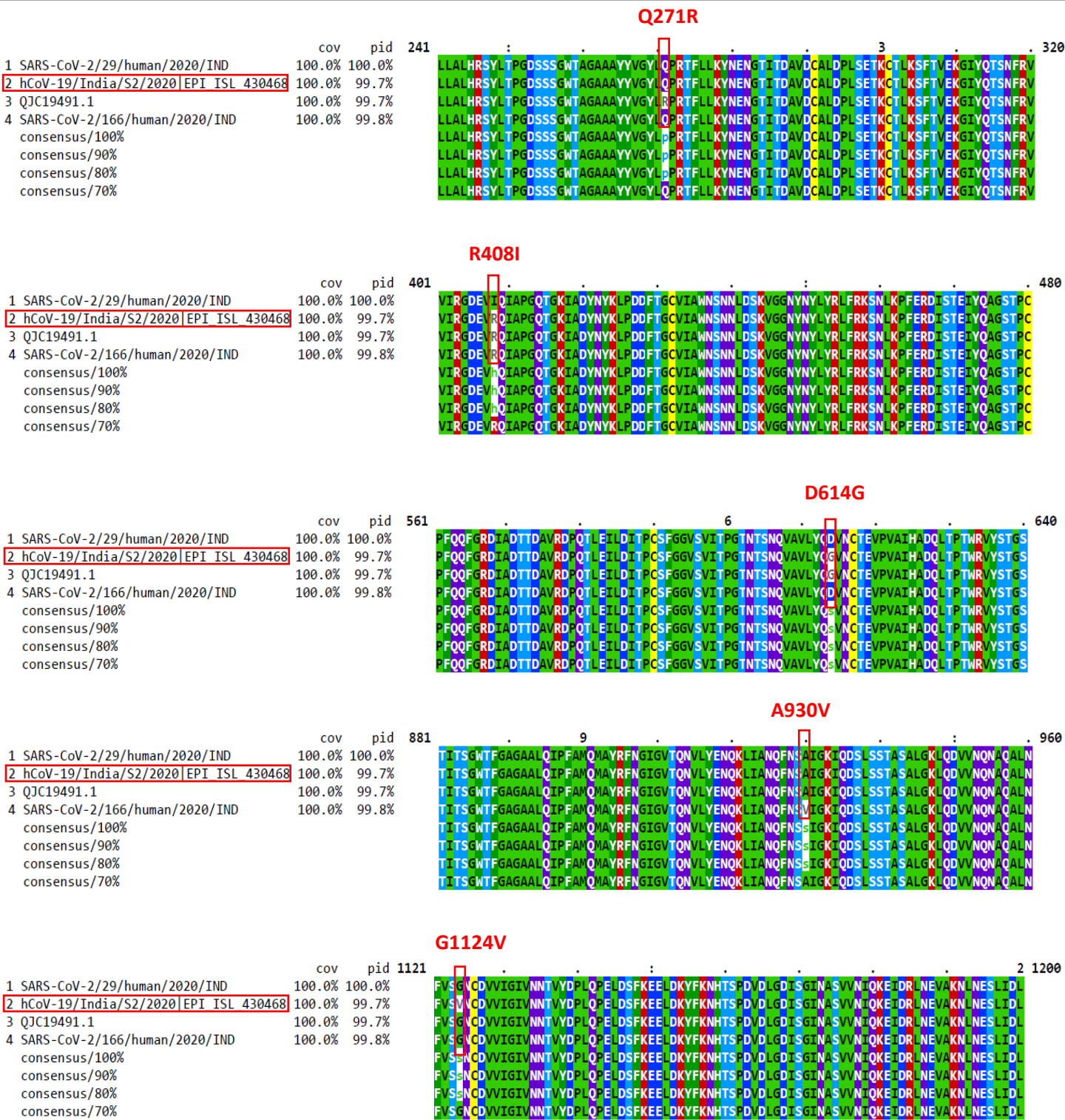


Virus Name	Accession Number	Region of Collection Within West Bengal
hCoV-19/India/S2/2020	EPI_ISL_430468	Kolkata
hCoV-19/India/S11/2020	EPI_ISL_430467	East Medinipur
hCoV-19/India/S5/2020	EPI_ISL_430465	Darjeeling
hCoV-19/India/S3/2020	EPI_ISL_430464	Kolkata
hCoV-19/India/S6/2020	EPI_ISL_430466	Tehatta

Figure 1: Table represents tabulation of accession numbers of the sequences from Kolkata used for the analyses with specific regions of sample collection



B

aa POSITIO N	Kolkata
271	Q
408	R
614	G
723	I (1) (4T)
930	A
1124	V (2) (3G)

C

	STATES			
aa POSITIO N	Kolkata	Gujarat	Kerala 29	Kerala 166
271	Q	R	Q	Q
408	R	R	I	R
614	G	G	D	D
930	A	A	A	V
1124	V	G	G	G

Figure 2: Mutation analysis of isolates from Kolkata, Gujarat and Kerala

- A. Multiple sequence alignment of Spike protein sequence of Kolkata isolate with sequences obtained from other parts of India. Sites of mutation are showed in Red
- B. Tabulation of amino acid mutations among isolates from Kolkata. Mutations are shown in red. Number/s in parenthesis show number of isolates that showed the amino acid type.

$\Delta\Delta G$: 0.905 kcal/mol (Stabilizing)

$\Delta\Delta G$ ENCoM: 4.756 kcal/mol
(Stabilizing)

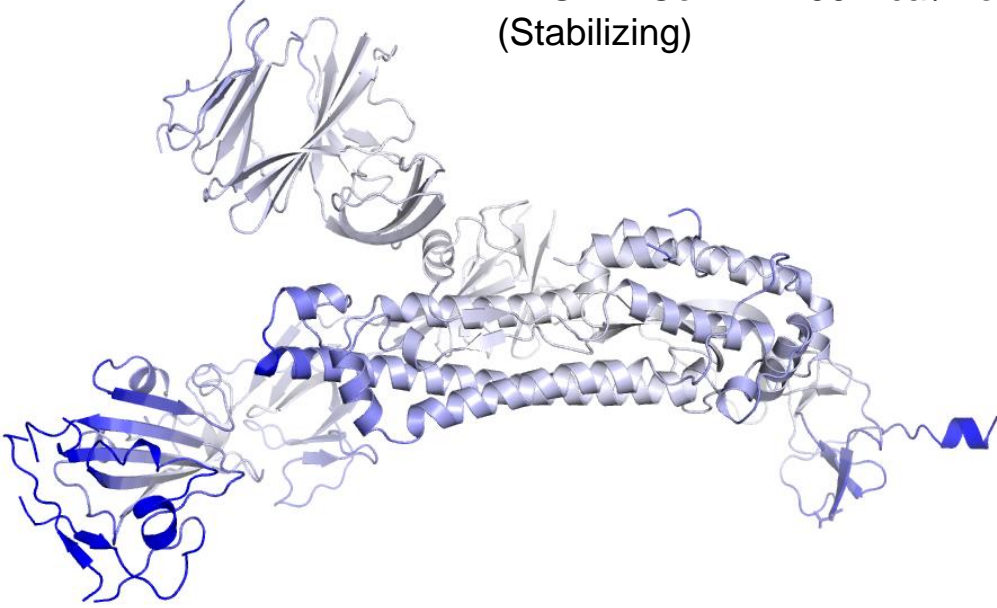


Figure 4: Δ Vibrational Entropy Energy Between Wild-Type and Mutant.

Δ Vibrational Entropy Energy Between Wild-Type and Mutant

$\Delta\Delta S_{\text{Vib}}$ ENCoM: -4.445 kcal.mol⁻¹.K⁻¹ . Amino acids were coloured as per the vibrational entropy change due to mutation. Blue represents rigidification of structure

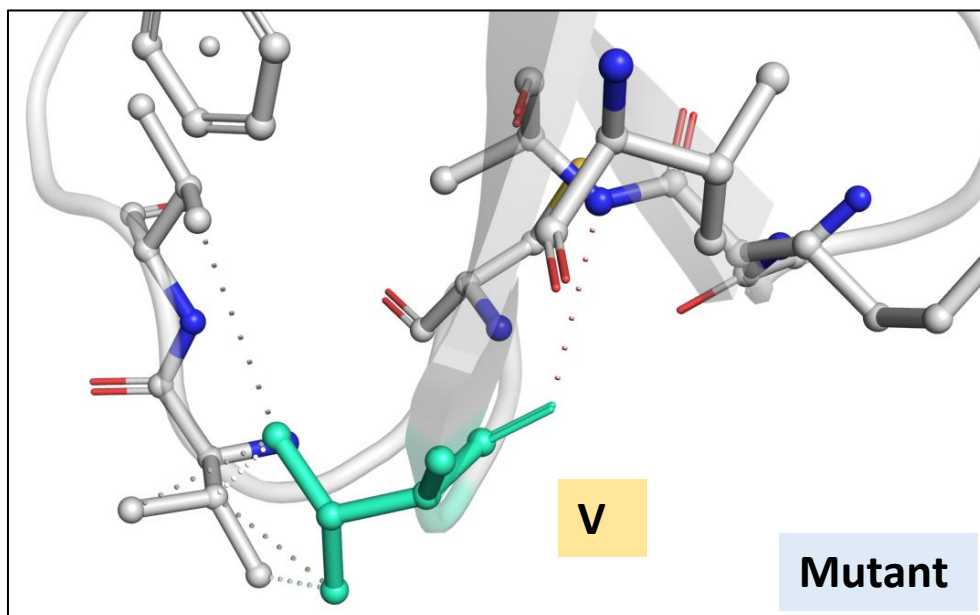
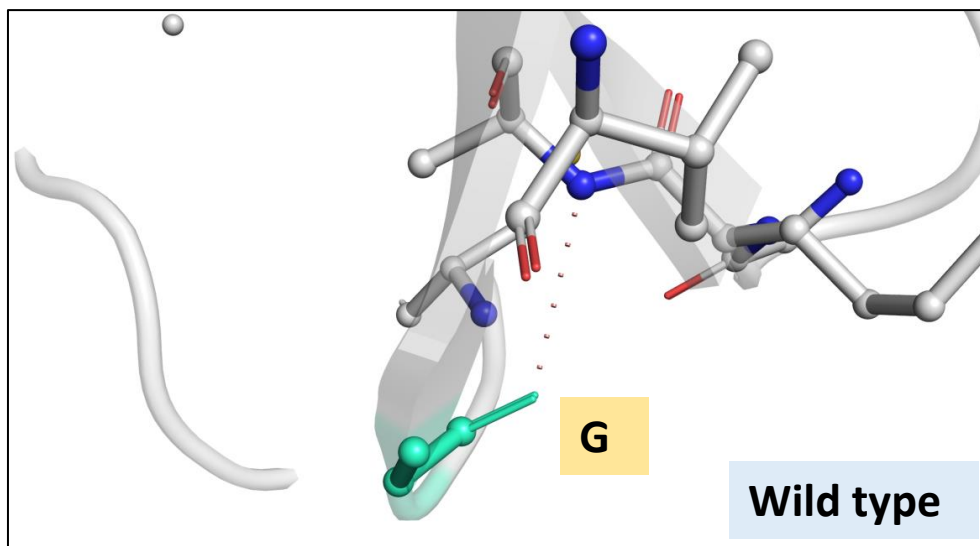


Fig. 5 : Interatomic Interaction

Wild-type and mutant residues are colored in light-green and are also represented as sticks alongside with the surrounding residues which are involved on any type of interactions

