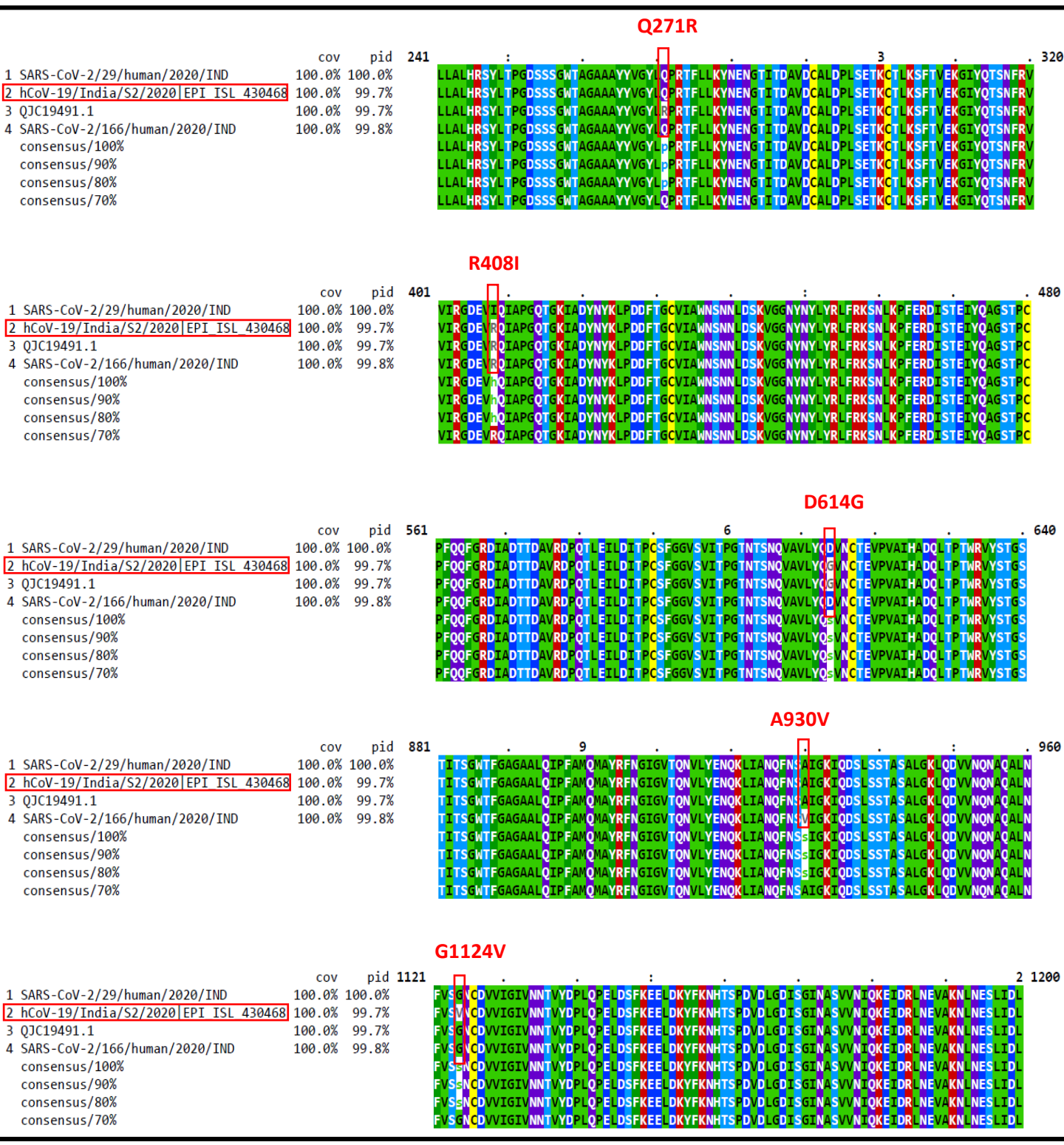
Virus Name	Accession Number	Region of Collection Within West Bengal
hCoV-19/India/S2/2020	EPI_ISL_430468	Kolkata
hCoV-19/India/S11/2020	EPI_ISL_430467	East Medinipur
hCoV-19/India/S5/2020	EPI_ISL_430465	Darjeeling
hCoV-19/India/S3/2020	EPI_ISL_430464	Kolkata
hCoV-19/India/S6/2020	EPI_ISL_430466	Tehatta

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

A



B

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

C

	STATES			
aa POSITION	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.

A

```
 *          *          *          *
YEPQIITTDNTFVSGNCDVVIGIVNNTVYDPLQPE
HHHHHH        HHHHHH        HHHH
EEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEE
  T       T     T           T       T
HHEEEEEEEEEEEETEEEEEEEEEEEEEEEEEEHHTH
```

Wuhan, China

B

```
 *          *          *          *
YEPQIITTDNTFVSVNCDVVIGIVNNTVYDPLQPE
HHHHHH        HHHHHHHHHH        HHHH
EEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEE
  T       T                 T       T
HHEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEHHTH
```

Kolkata, India

Mutation: G1124V

Four helices (H) added at positions 1123,1124,1125,1126

1 turn (T) lost at position 1124

Figure 3: Effect of mutation at position 1124 on secondary structure of Spike protein

A. Secondary structure of Spike protein of Wuhan isolate (the area around the residue 1124 has been shown)

B. Secondary structure of Spike protein of Kolkata isolate showing effect of mutation on the secondary structure.

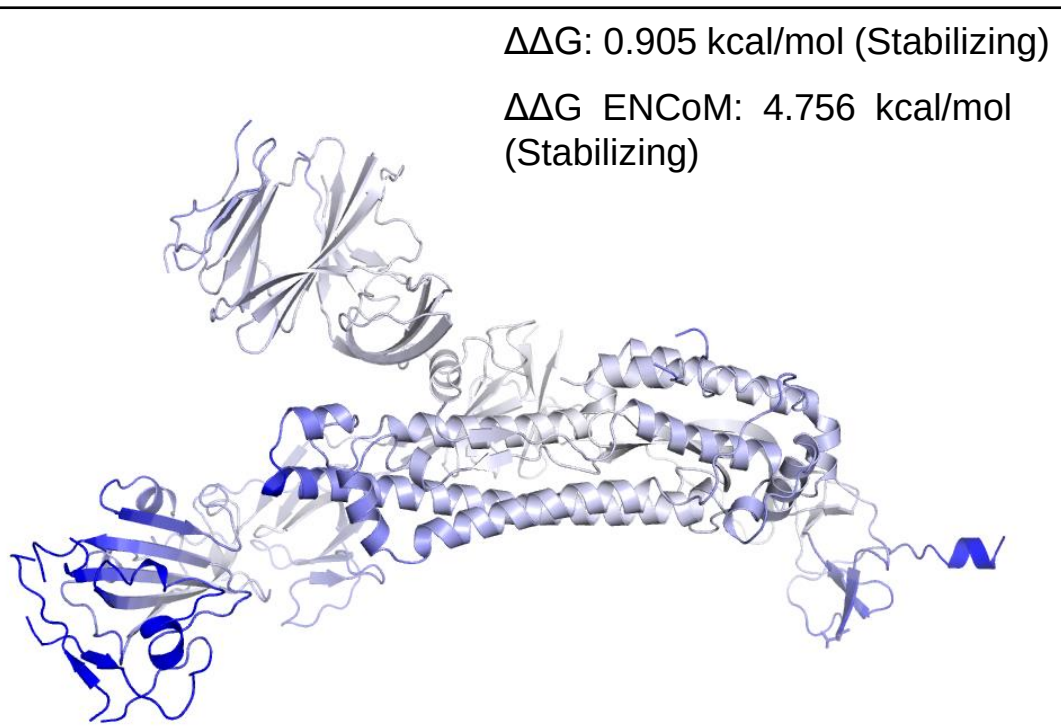


Figure 4: Δ Vibrational Entropy Energy Between Wild-Type and Mutant. Δ Vibrational Entropy Energy Between Wild-Type and Mutant $\Delta\Delta S_{Vib}$ ENCoM: -4.445 $kcal.mol^{-1}.K^{-1}$. Amino acids were coloured as per the vibrational entropy change due to mutation. Blue represents rigidification of structure

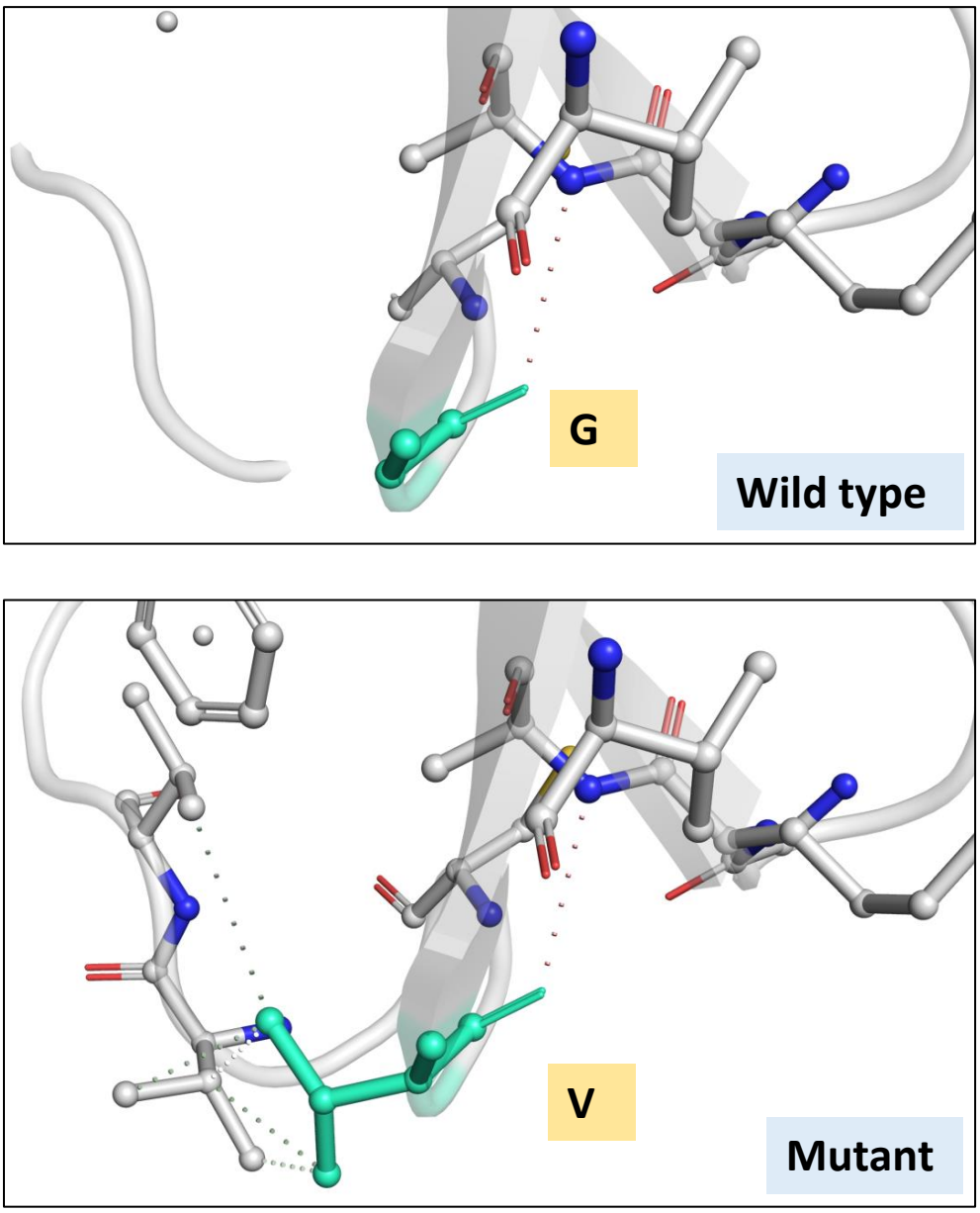


Fig. **5 : Interatomic Interaction**
Wild-type and mutant residues are colored in light-green and are also represented as sticks alongside with the surrounding residues which are involved on any type of interactions

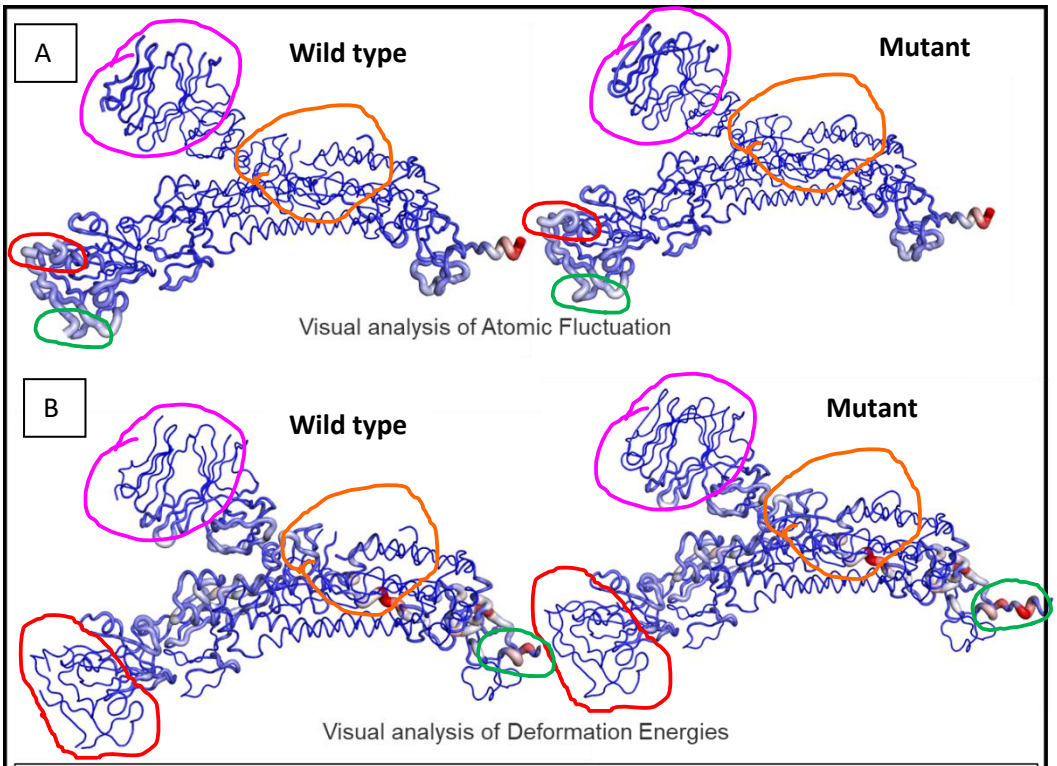


Fig. 6 : A. Analysis of atomic fluctuations
B. Visual analysis of deformation energies.
Magnitude of fluctuation and deformation has been shown using thin to thick tube coloured blue (low), white (moderate) and red (high)