

## Supplementary Table

**Table S1:** Comparison of volume of 4 major clefts for wild type and mutant protein

| Clefts          | Wild type<br>protein<br>( $\text{\AA}^3$ ) | Mutant<br>protein<br>( $\text{\AA}^3$ ) |
|-----------------|--|---|
| 1(in red)       | 4580.30                                    | 4257.56                                 |
| 2(in pink)      | 3238.75                                    | 3304.97                                 |
| 3(in<br>yellow) | 1701.84                                    | 1716.61                                 |
| 4(in blue)      | 1149.19                                    | 855.14                                  |