Supporting

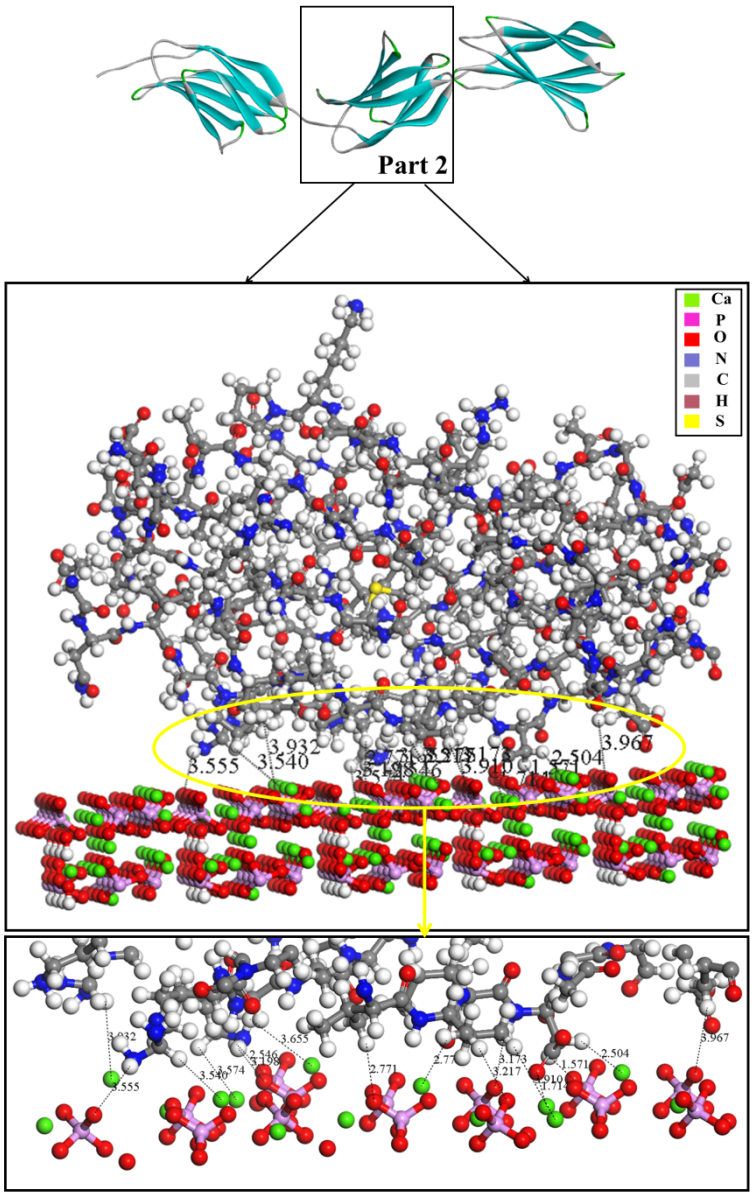

Fig. S1. Adsorption configurations of rhCol I (Part 2) on (001) surface and its local enlargementation. In order to clearly observe the interaction between protein and HAP, no water molecules are shown.

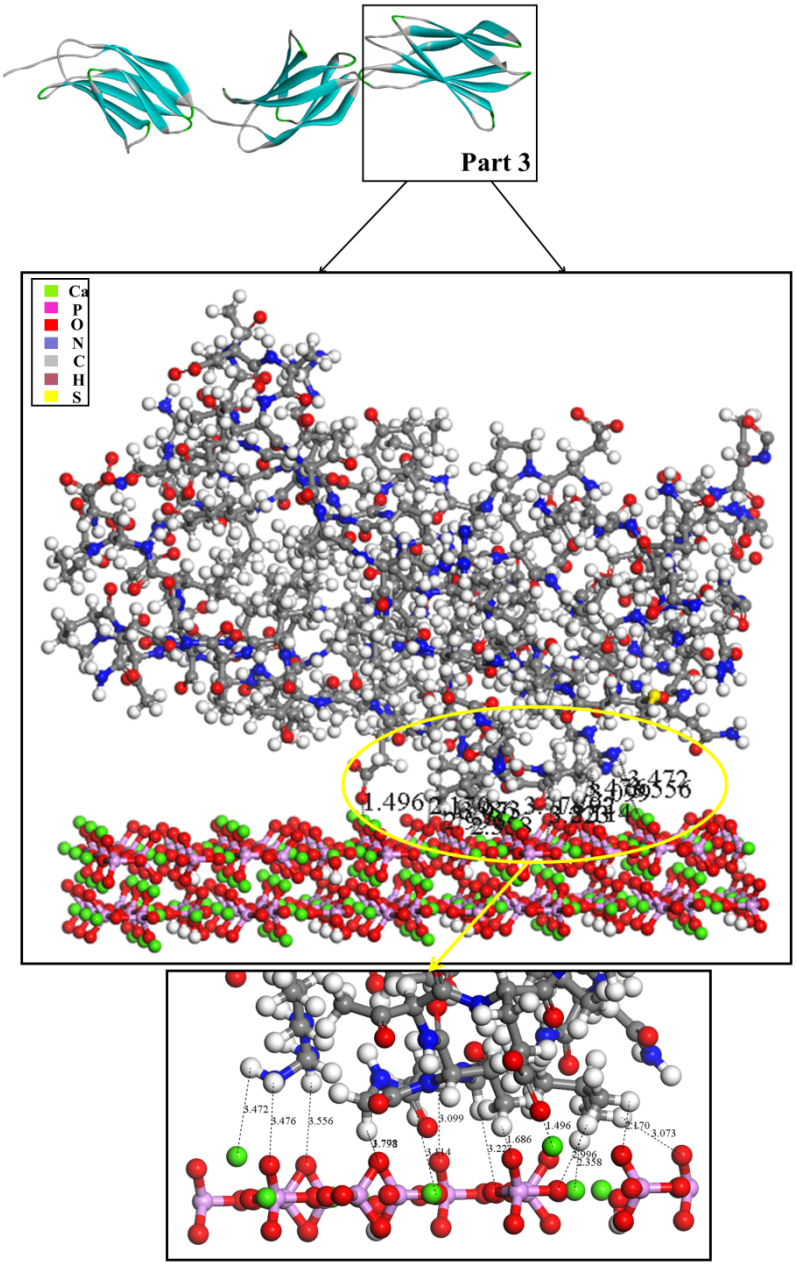

Fig. S2. Adsorption configurations of rhCol I (Part 3) on (001) surface and its local enlargementation. In order to clearly observe the interaction between protein and HAP, no water molecules are shown.

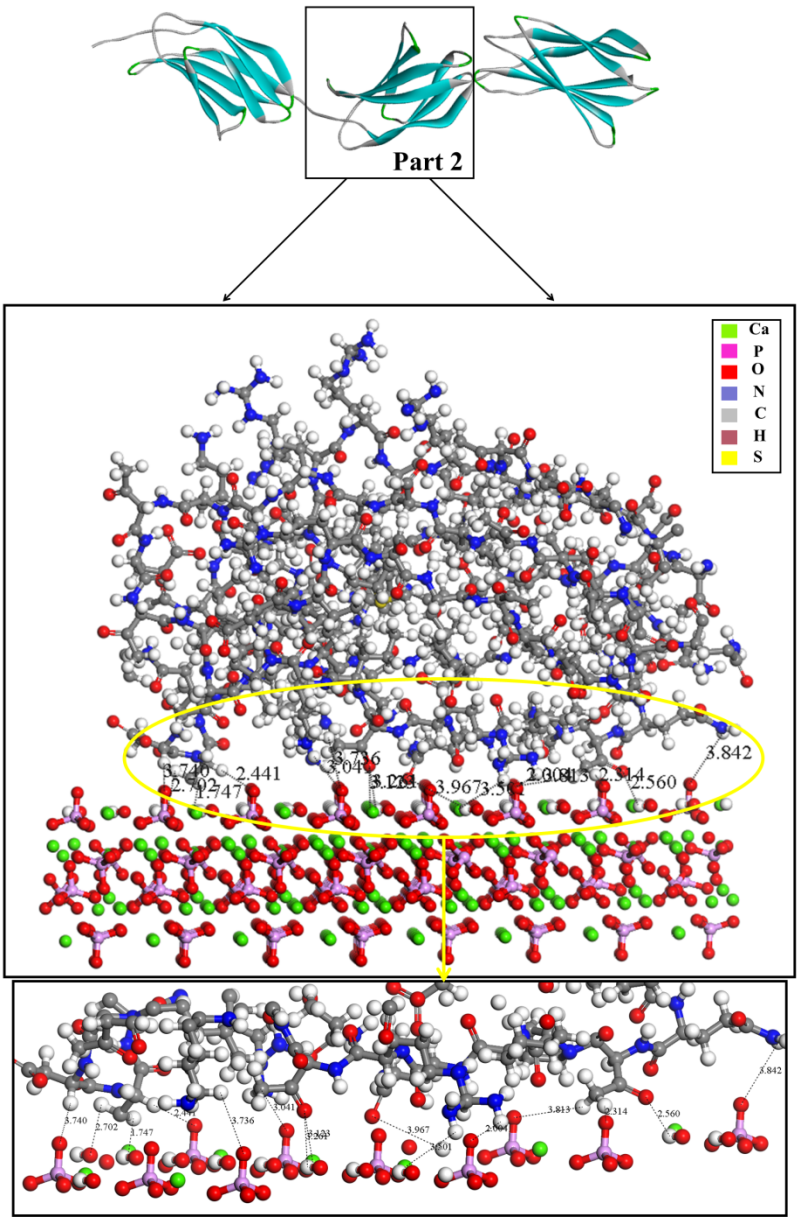

Fig. S3. Adsorption configurations of rhCol I (Part 2) on (100) surface and its local enlargementation. In order to clearly observe the interaction between protein and HAP, no water molecules are shown.

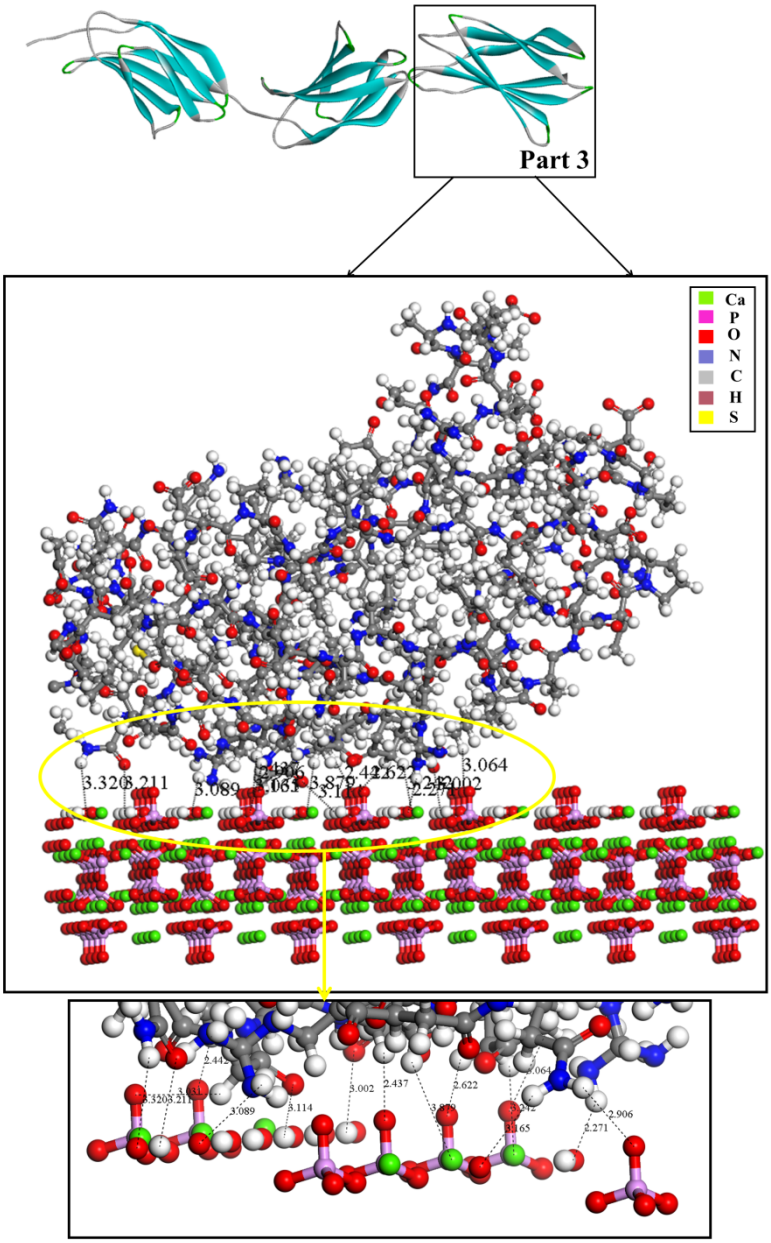

Fig. S4. Adsorption configurations of rhCol I (Part 3) on (100) surface and its local enlargementation. In order to clearly observe the interaction between protein and HAP, no water molecules are shown.

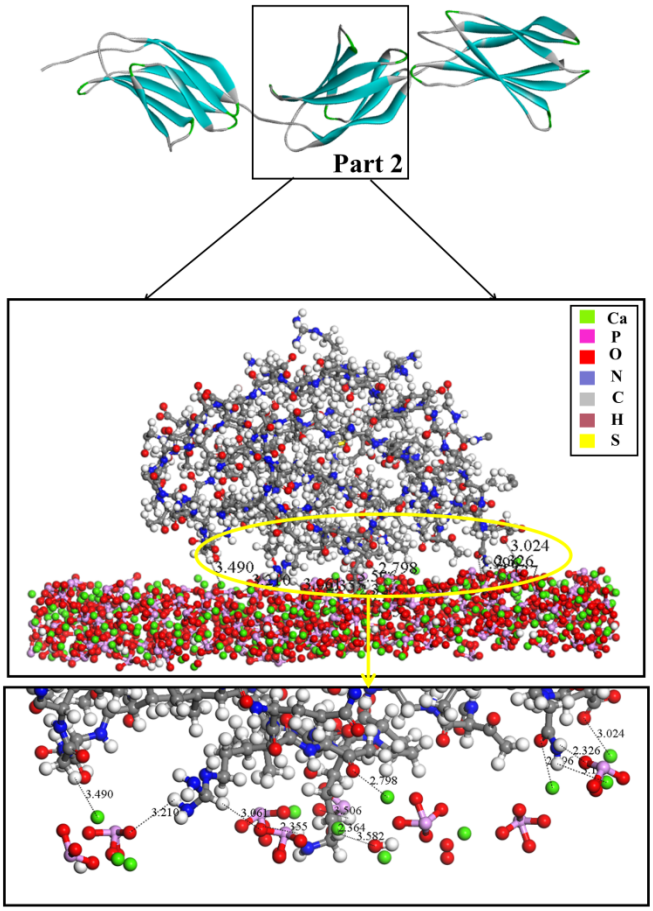

Fig. S5. Adsorption configurations of rhCol I (Part 2) on (211) surface and its local enlargementation. In order to clearly observe the interaction between protein and HAP, no water molecules are shown.

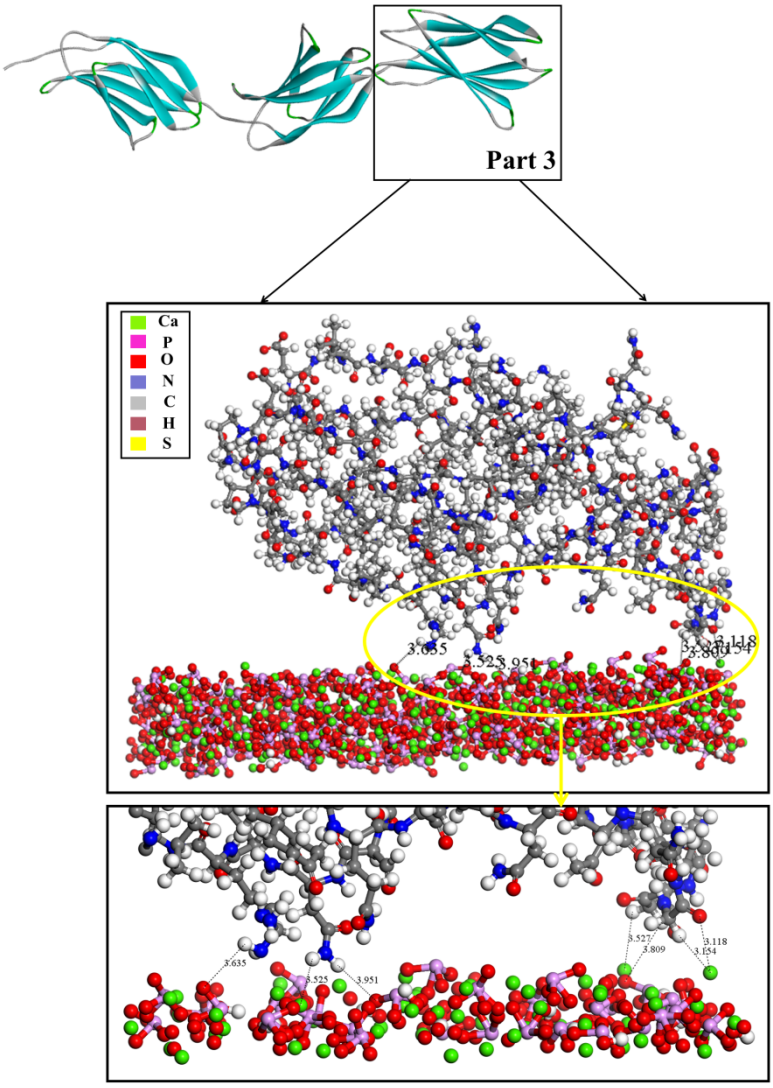

Fig. S6. Adsorption configurations of rhCol I (Part 3) on (211) surface and its local enlargementation. In order to clearly observe the interaction between protein and HAP, no water molecules are shown.

Information regarding the force field

In Dreiding force field, the potential of various atoms was described as a non-bonded and bonded force. The Non-bond force between particles in dreiding force field is described by the Lennard–Jones (LJ) formalism. This formalism is a mathematically simple relation about the interatomic force between a pair of

particles[1]. This simple relation was stated by Lennard Jones[2] for the first time. This simple atomic interaction stated as Eq. (1):

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6} \right] \quad r \ll r_c \qquad (1)$$

In Eq. (1), σ is the distance at which the function is zero; ε is the depth of the potential well, and rij is the distance between the two atoms. In MD simulations, both σ and ε constants related to the kind of particles in the MD simulation package.

The bonded forces consist of bond angle bend, bond strength, and dihedral angle torsion terms. The bond and angle strength stretch in dreiding force field are calculated by harmonic oscillator equations as (2) and (3) formulas:

$$E_r = \frac{1}{2} k_r (r-r_0) \qquad (2)$$

$$E_\theta = \frac{1}{2} k_\theta (\theta-\theta_0) \qquad (3)$$

In these formulas, k_θ and k_r are harmonic oscillator constants. θ_0 is the equilibrium value of angles, and r_0 is the atomic bond length. Dihedral term in atomic interaction described with Eq. (4) and its coefficients are chosen from Dreiding force field[3]:

$$E = k \left[1+d \cos(n\varphi) \right] \qquad (4)$$

In Eq. (4), k is an oscillator constant with +1 or −1 rates and the integer number is n[3].

References

[1] Karimipour A, Amini A, Nouri M, *Comput. Part. Mech.*, 2021, 8, 737-749.

[2] Lennard-Jones J E, *Proc. Roy. Soc. A*, 1924, 106, 463-477.

[3] Mayo S L, Olafson B D and Goddard W A, *J. Phys. Chem.*, 1990, 94, 8897-8909.