

## **Supporting Information**

### **Application of a Spherical Harmonics Expansion Approach for Calculating Ligand Density Distributions around Proteins**

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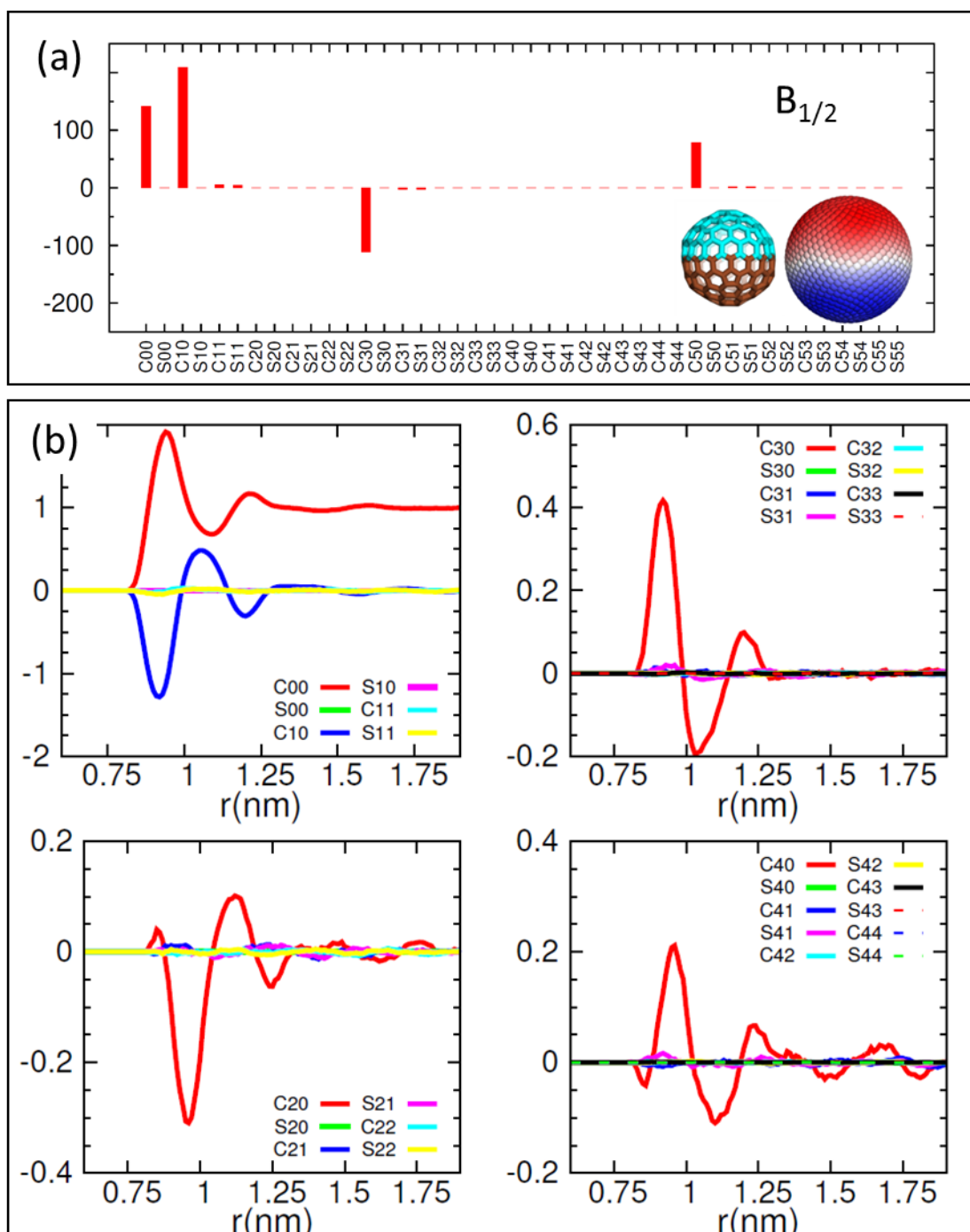


Figure S1. (a) Spherical harmonic coefficients for the hydrophilic atom distribution in  $B_{1/2}$ . (b) Spherical harmonic coefficients for the water distribution around  $B_{1/2}$ .

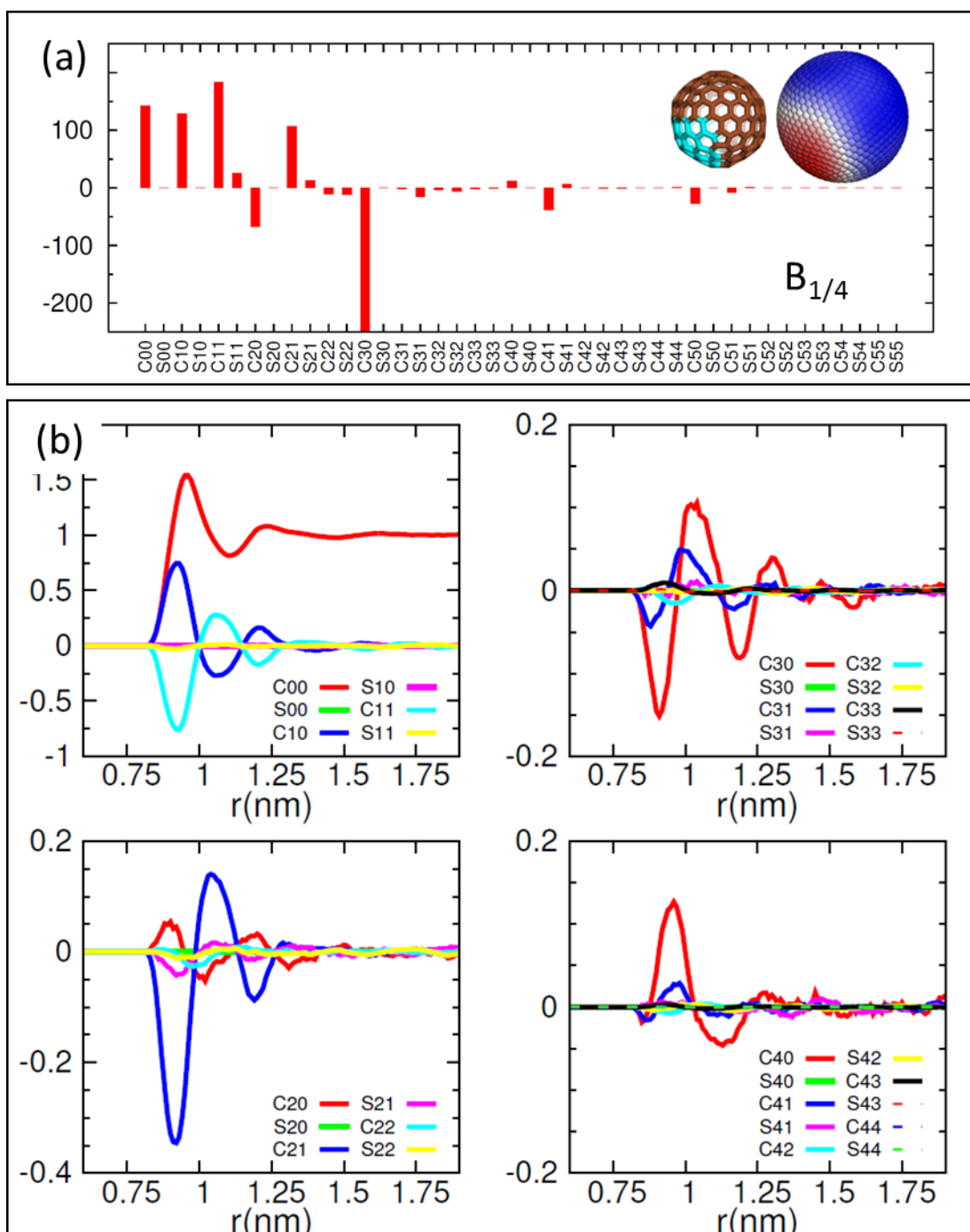


Figure S2. (a) Spherical harmonic coefficients for the hydrophilic atom distribution in  $B_{1/4}$ . (b) Spherical harmonic coefficients for the water distribution around  $B_{1/4}$ .

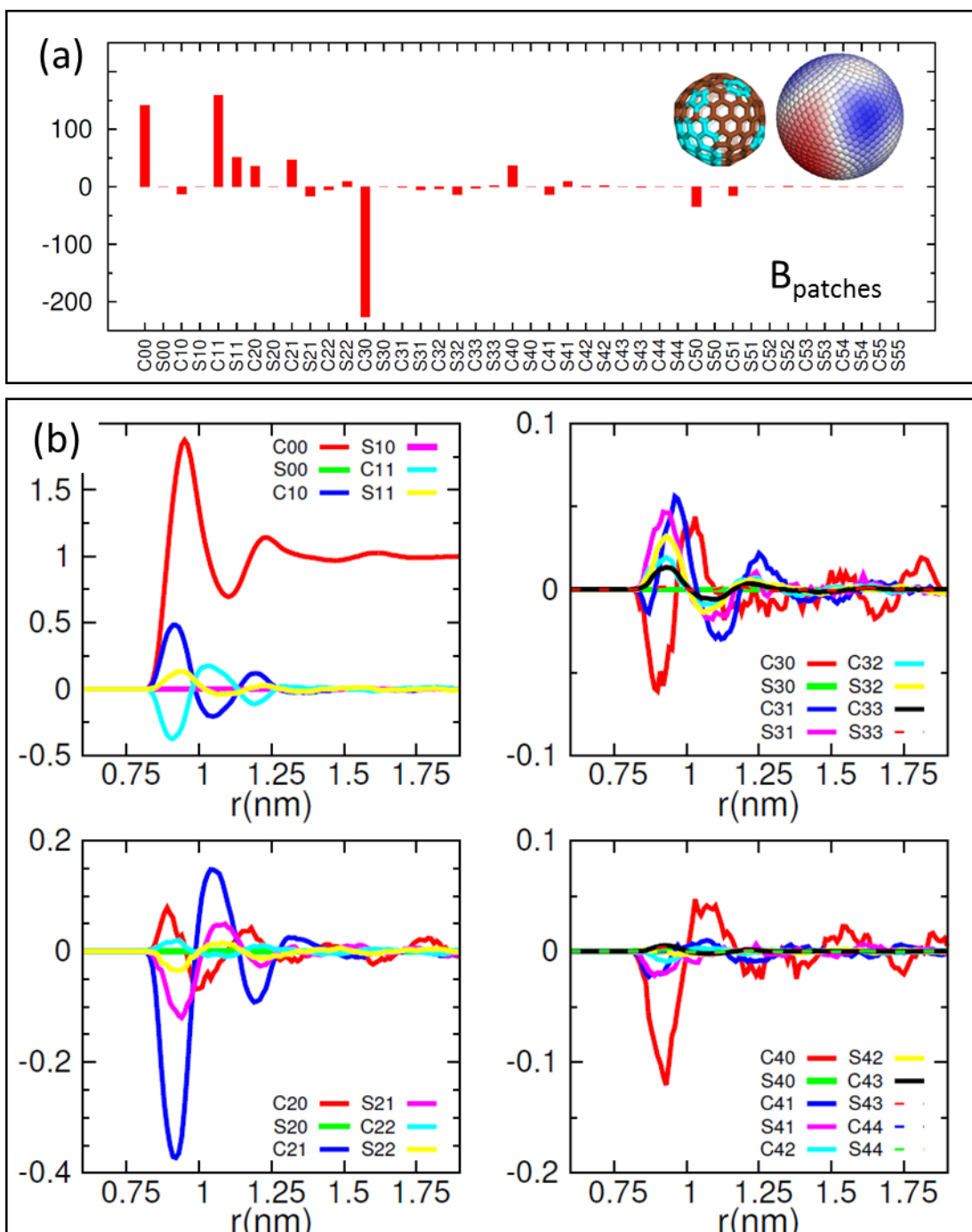


Figure S3. (a) Spherical harmonic coefficients for the hydrophilic atom distribution in  $B_{\text{patches}}$ . (b) Spherical harmonic coefficients for the water distribution around  $B_{\text{patches}}$ .

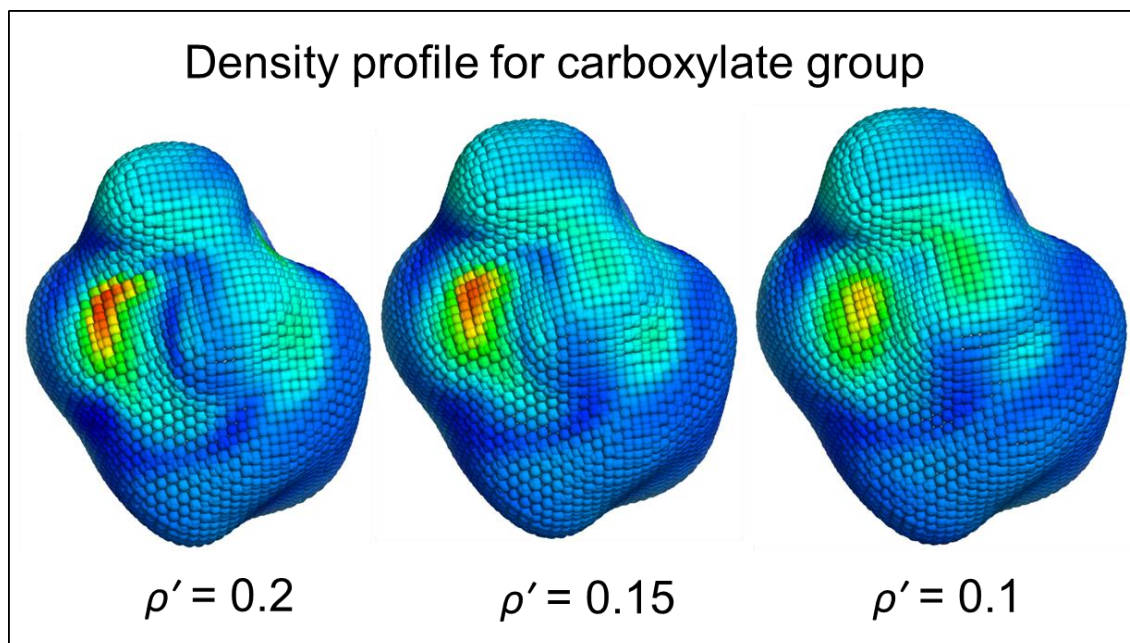


Figure S4.  $\rho/\rho_0$  values plotted for the carboxylate group of Capto MMC ligand at different interfaces around ubiquitin. Red indicates regions of high ligand density ( $\rho/\rho_0 \sim 200$ ) while blue indicates regions of low ligand density ( $\rho/\rho_0 \sim 1$ ).