Supplementary Information

Coordination design of cadmium ions at the 4-fold axis channel of the apo-ferritin cage

Satoshi Abe,^a Nozomi Ito,^a Basudev Maity,^a Chemlin Lu,^{ab} Diannan Lu^b and Takafumi Ueno*^a

^aDepartment of Life Science and Technology, Tokyo Institute of Technology, Nagatsuta-cho, Midoriku, Yokohama 226-8501, Japan

^bMinistry of Education Key Laboratory of Industrial Biocatalysis, Department of Chemical Engineering,

Tsinghua University, Beijing 100084, China



Figure S1. MALDI-TOF mass spectra of (a) apo-L161C/L165C-rHLFr and (b) apo-R168C/L169C-rHLFr.



Figure S2. Native PAGE of marker (lane 1), apo-rHLFr (lane 2), apo-L161C/L165C-rHLFr (lane 3) and apo-R168C/L169C-rHLFr (lane 4).



Figure S3. (a) Superimposed structure of apo-rHLFr (white) and apo-R168C/L169C-rHLFr (magenta). (b and c) DE loop structure with electron density map of (b) apo-R168C/L169C-rHLFr and (c) apo-L161C/L165C-rHLFr. The Cd atoms are sphere models colored with beige. $2F_0$ - F_c electron density maps at 1σ are shown in grey.



Figure S4. Close up views of 3-fold axis channels of (a) **apo-L161C/L165C-rHLFr** and (b) **apo-R168C/L169C-rHLFr**. The Cd atoms are sphere models colored with beige. The O atoms of water molecules are shown as red sphere.