Supporting information

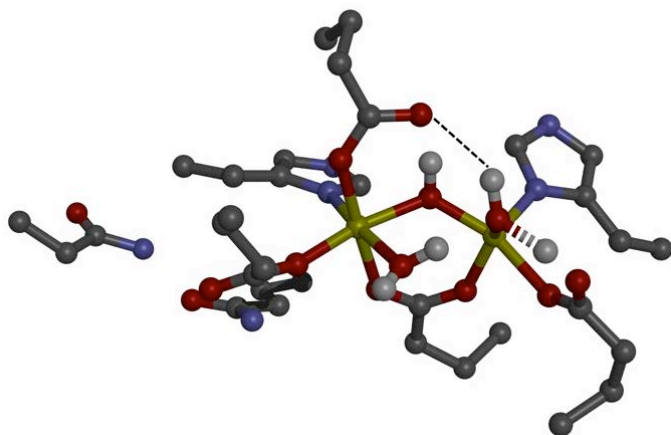**Figure S1.** Optimized geometry from the (μ-OH)(μ-OH$_2$) initial structure of MMO using truncation scheme #2. H, C, N, O, and Fe atoms are colored in white, gray, blue, red, and yellow, respectively, and the amino acid hydrogen atoms are omitted for clarity.
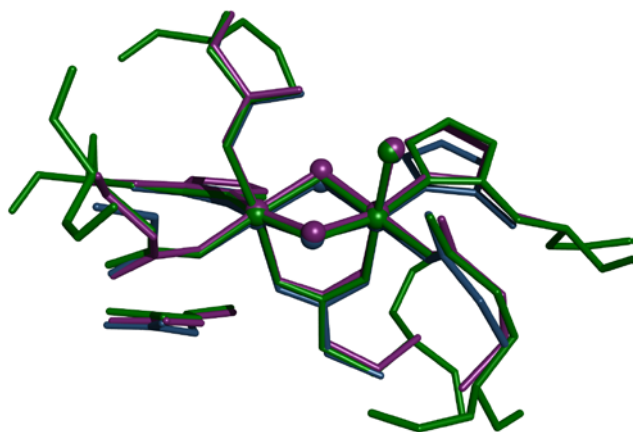

Figure S2. Overlay of models #1 (green), #2 (magenta), and #3 (blue). For clarity, all hydrogen atoms are omitted.