Crystal structure of dicamba monooxygenase: A Rieske nonheme oxygenase that catalyzes oxidative demethylation

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Supplemental Material

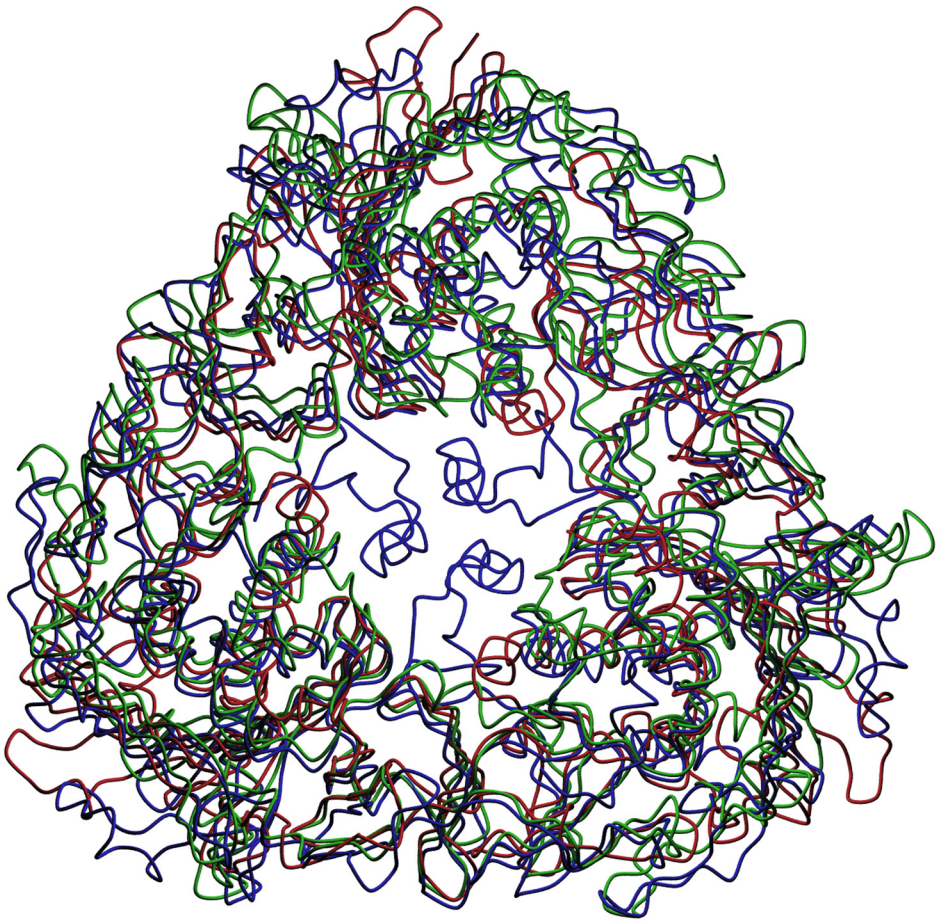

Figure S1: Superposition of OMO, CARDO and DMO. The backbone traces of OMO is shown is blue, CARDO in green and DMO in red. There is clear similarity in the core regions of the proteins, but notable differences in the central pore and loop regions. The average Cα RMSD between DMO and the other two proteins is 2.5 Å.

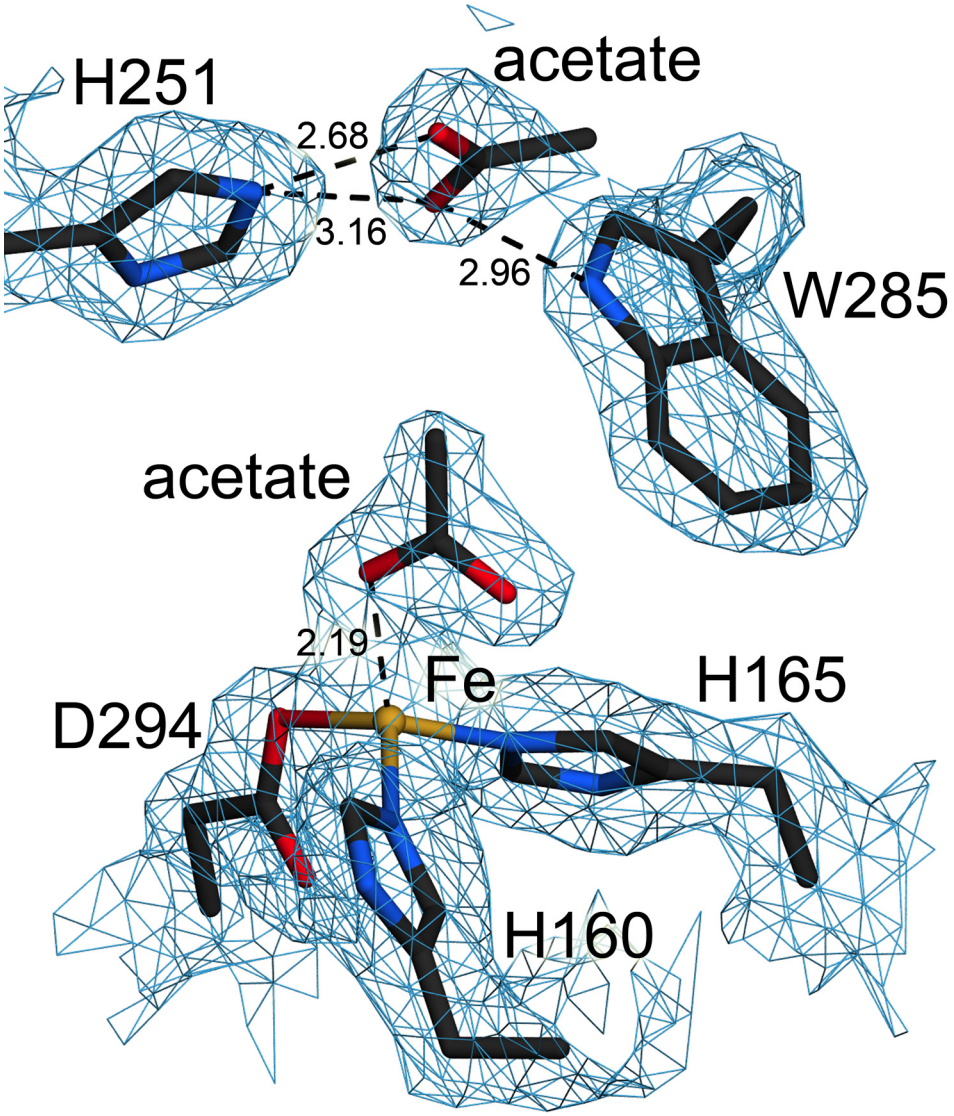

Figure S2: Bound acetate ions in the active site of free DMO. $2mF_O$-DF_C electron density contoured at 1.0σ (blue) is shown for the 1.75 Å resolution structure of free DMO. Both H251 and the mononuclear iron site in the DMO active site are associated with acetate from the crystallization buffer in this structure. The sidechains of H251 and W285 makes nearly identically hydrogen bonds with the carboxylic acid moiety of dicamba and DCSA, indicating a high intrinsic affinity for a carboxylate at this location. The mononuclear iron site is associated with acetate in this monomer (A), but dioxygen in monomer B (Figure 7).