

Supplemental Figure S3. Superposition of monofunctional mitochondrial *Rn*ECH and *At*MFP2-ECH active sites.

A, Ribbon diagram of the AtMFP2-ECH domain with hexanoyl-CoA from mono-functional RnECH domain (Bell, A.F., et~al. (2002) Chem~Biol~9, 1247-1255) imposed. The black dotted line is the disordered loop of the AtMFP2-ECH domain. B, The AtMFP2-ECH active site with the sigmaA weighted 2Fo-Fc electron density contoured at a 1.2 σ level. The hexanoyl-CoA substrate from the RnECH structure is imposed. The side chains labels are only displayed in subfigure C for clarity. Black dotted lines are hydrogen bonds. C, The superposition with RnECH domain in orange carbon atoms (magenta water, green substrate) and AtMFP2 in the same orientation as in subfigure B.