



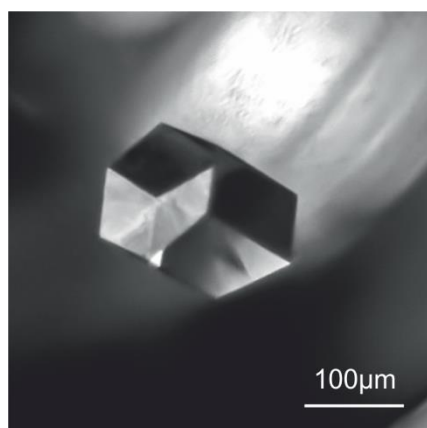
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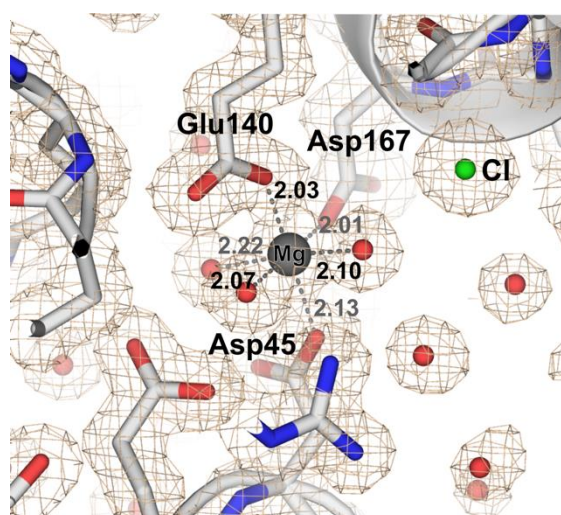
**Supporting information for article:**

**Structure of *Methylobacterium extorquens* malyl-CoA lyase: CoA-substrate binding correlates with domain shift**

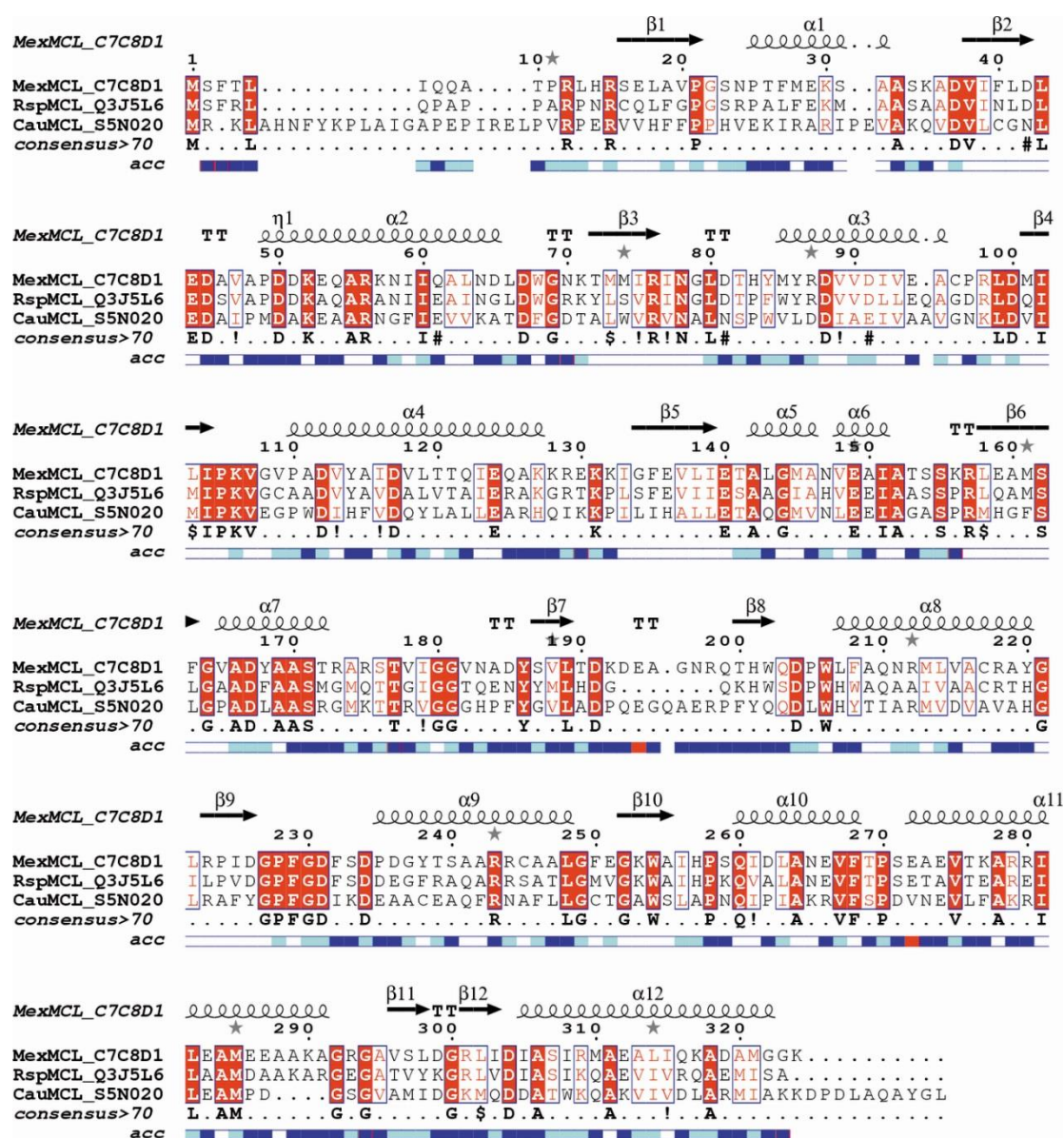
**Javier M. González, Ricardo Marti-Arbona, Julian C.-H. Chen and Clifford J. Unkefer**

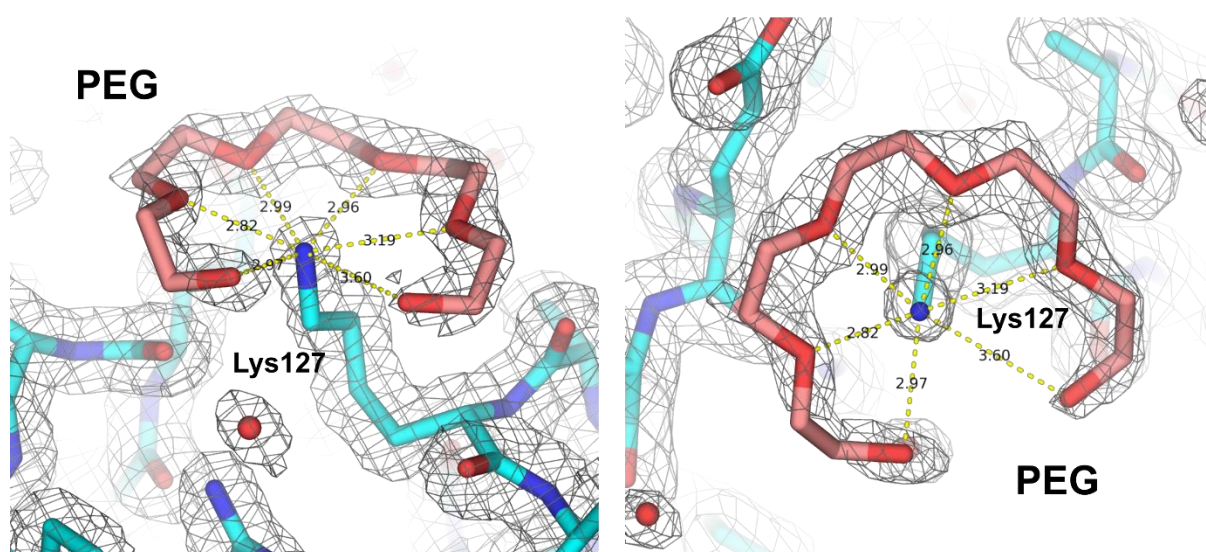


**Figure S1** Hexagonal-prism crystal of *MexMCL* as obtained in this work.



**Figure S2**  $2mF_o - DF_c$  electron density around the  $Mg^{2+}$ -binding site map contoured at  $1\sigma$ .





**Figure S4** Ring-shaped electron density (contoured at  $1\sigma$ ) around the amino sidechain of Lys127 (*blue*), modeled as a crown-ether-like complex between PEG and the positively charged amino group.