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Supporting information for article:

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

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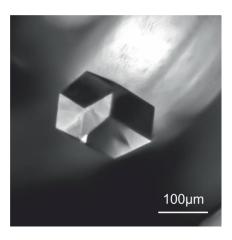


Figure S1 Hexagonal-prism crystal of *Mex*MCL as obtained in this work.

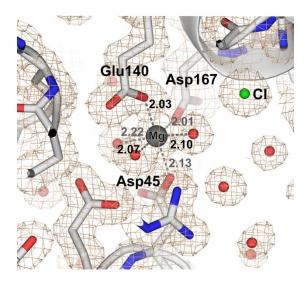


Figure S2 $2mF_{\rm O}-DF_{\rm C}$ electron density around the Mg²⁺-binding site map contoured at 1σ .

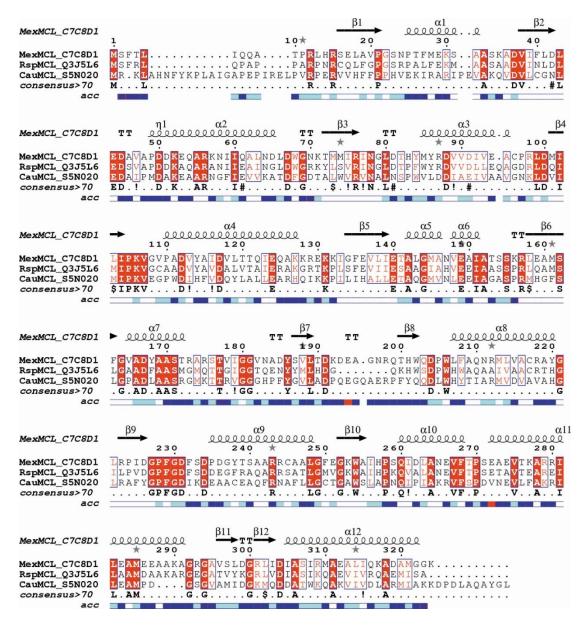


Figure S3 Sequence alignment of characterized MCL enzymes: *Mex*MCL, *Rsp*MCL and *Cau*MCL; UniProt ID's C7C8D1, Q3J5L6, and S5N020, respectively. *Mex*MCL has close sequence identity with both *Rsp*MCL (57%) and *Cau*MCL (30%). The alignment was prepared with Espript 3.0 (Robert & Gouet, 2014).

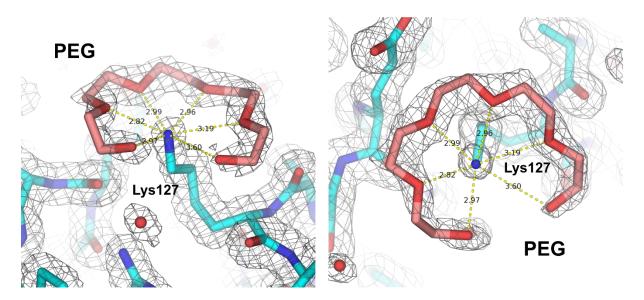


Figure S4 Ring-shaped electron density (contoured at 1 σ) around the amino sidechain of Lys127 (*blue*), modeled as a crown-ether-like complex between PEG and the positively charged amino group.