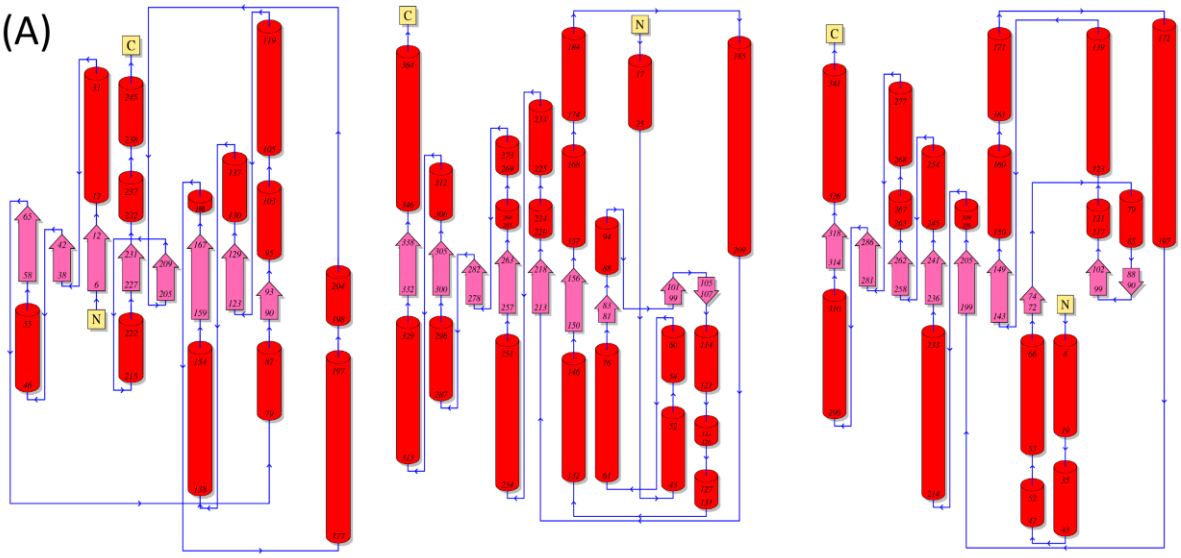
Supplementary Material

Structure determination

The input diffraction data were prepared and converted for use in *Auto-Rickshaw* using programs of the *CCP*4 program suite (Winn et al., 2011) without any applied resolution cutoff. Δ*F*-values were calculated using the program *SHELXC* (Sheldrick, 2008). All of the 12 heavy atoms requested per monomer were found using the program *SHELXD* (Schneider & Sheldrick, 2002). The correct hand for the substructure was determined by *ABS* (Hao, 2004) and *SHELXE* (Sheldrick, 2008). Initial phases were calculated after density modification with *SHELXE*. The twofold noncrystallographic symmetry (NCS) operator was found by *RESOLVE* (Terwilliger, 2000). Density modification, phase extension and NCS-averaging were performed using the program *DM* (Cowtan, 1994). 97% of the model (663 amino acids in two chains) was built automatically by *ARP*/*wARP* (Morris *et al.*, 2004; Perrakis *et al.*, 1999). The resulting model was used as an input for the MR-SAD-protocol of *Auto-Rickshaw* including initial model refinement in *CNS* (Brünger *et al.*, 1998; Brünger, 2007) and *REFMAC5* (Murshudov *et al.*, 1997). The model was afterwards completed iterative by manual inspection and model advancement in *Coot* (Emsley & Cowtan, 2004; Emsley *et al.*, 2010) followed by refinement in *REFMAC*5.

(A)

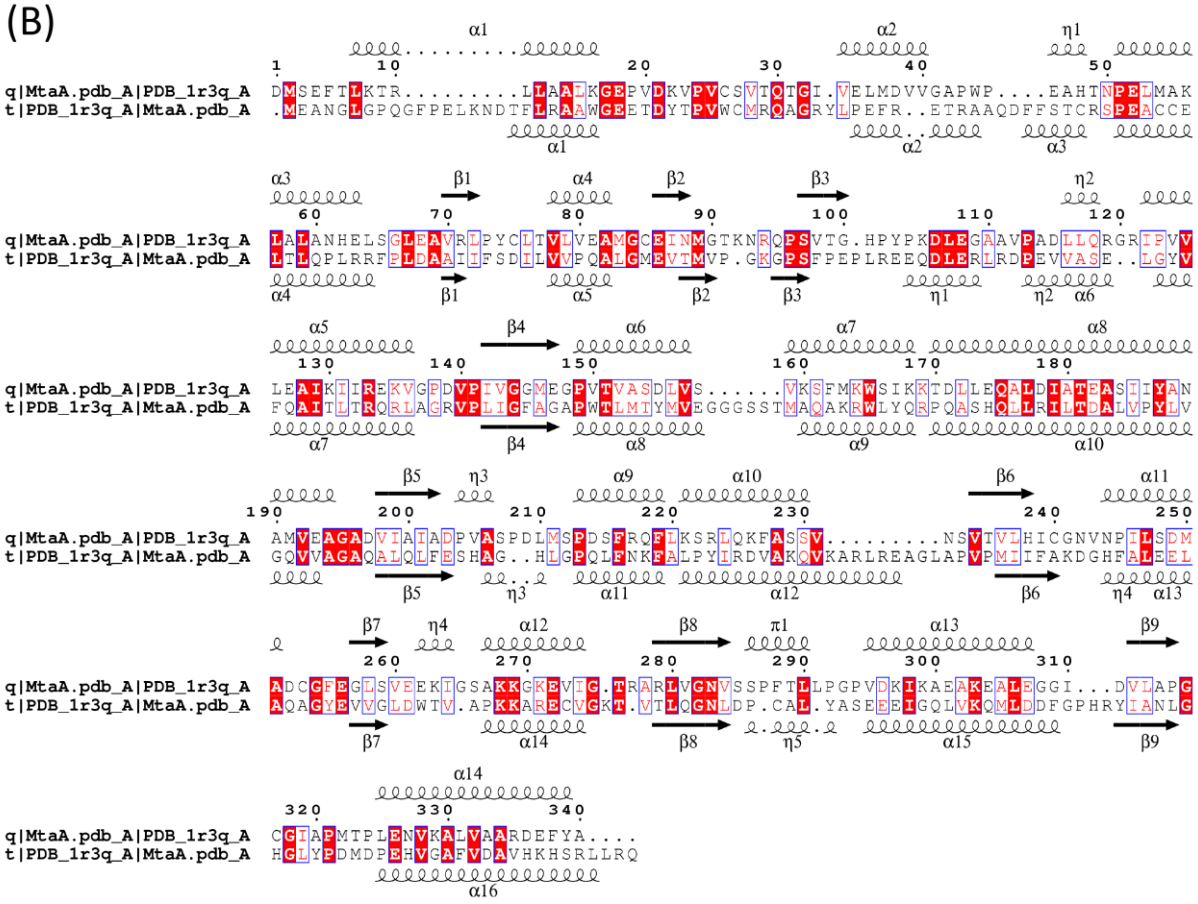


human uroporphyrinogen(III)-decarboxylase (pdb-entry: 1r3q)

chicken triosephosphate-isomerase (pdb-entry: 1tim)

corrinoid: coenzmye M methyl-transferase from *M.mazei* (pdb-entry: 4ay8)

(B)



Supplementary Fig. S1. (A) Topology diagrams of human uroporphyrinogen(III)decarboxylase (PDB-entry 1r3q), the closest structural homologue to MtaA and chicken triosephosphate-isomerase (PDB-entry 1tim) and MtaA. Plots were generated using pdbsum (Laskowski (2001, 2007, 2009), Laskowski et al. (1997, 2005). (B) Structure-based sequence alignment of MtaA from *M. mazei* with its closest structural homologue, the human uroporphyrinogen(III)decarboxylase (PDB-entry 1r3q). The structural-sequence alignment was performed with pdbefold (Krissinel & Henrick, 2004). The final figure was prepared with the program ESPript (Gouet et al., 1999) using a similarity score of "0.7 0.5 B". Residues that are identical between MtaA and uroporphyrinogen(III)decarboxylase are shown in *white* on a *red* background. Residues that are similar (score <0.7) are shown in *red* within *blue* frames. *Red boxes* in the sequence highlight identical residues and *white boxes* highlight similar residues.