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Crystal Structure of a Chimeric ATP sulfurylase. Eric B. Lansdon¹, Irwin H. Segel², Andrew J. Fisher¹, ¹Dept. of Chemistry, ²Molecular & Cellular Biology, Univ. of California-Davis, Davis, CA 95616 USA.

The first step in sulfate assimilation is catalyzed by the enzyme ATP sulfurylase to form adenylyl 5'-phosphosulfate (APS) from sulfate and ATP. Crystal structures of various ATP sulfurylases have been determined. Two closely related sulfurylases from *Penicillium chrysogenum* and *Saccharomyces cerevisiae* show very similar features including a sulfurylase domain and an extra C-terminal domain. Both of these enzymes are hexamers. This C-terminal domain in *P.c.* acts as an allosteric domain which binds an allosteric effector (PAPS) to shift the enzyme into a T-state conformation. However, the C-terminal domain from *S.c.* does not have allosteric activity and yet the C-terminal domain is conserved, probably to promote hexamerization. Two large regions in the *S.c.* primary sequence are missing which are used in *P.c.* to bind the allosteric effector. Only the necessary parts of the domain that are used for quaternary contacts are conserved between these two proteins. In this study, we switched the allosteric domain of *P.c.* ATP sulfurylase with the C-terminal domain of *S.c.* ATP sulfurylase. The chimeric protein is catalytically active and *S.c.* C-Terminal domain also promotes hexamerization of the protein. Interestingly, the chimera is more heat stable than wild type *P.c.* and *S.c.* ATP sulfurylase. The crystal structures of this chimeric enzyme yield clues about the role of the allosteric domain in catalysis and the allosteric transition of *P.c.* ATP sulfurylase.