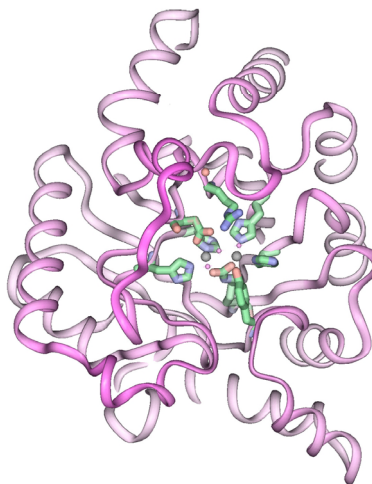


**A Comparison of Bromide Ion "Quick-Soak" and Se-Met Derivatives for Structure Determination of a Novel Hydrolase.** B. D. Santarsiero, K. Ratia, and A. D. Mesecar, The Center for Pharmaceutical Biotechnology, University of Illinois at Chicago, Chicago, IL 60607 USA.

Organophosphorus Hydrolases (OPH) are an important class of enzymes that degrade a number of organophosphorus compounds, including neurotoxins used as chemical warfare agents. A novel OPH from an extremophile has been cloned, expressed, purified, and crystallized as a target for site-directed and random mutagenesis. The native enzyme, with 333 residues, crystallizes in space group  $P3_121$  with the cell dimensions of  $a=61\text{\AA}$  and  $c=207\text{\AA}$ . The Se-Met enzyme crystallizes in the same unit cell. Three data sets were collected near the Se absorption edge on the Se-Met enzyme at APS beamline 14-BM-D to a resolution of  $2.2\text{\AA}$  for MAD analysis. In addition, a quick soak of a native crystal with KBr was used to generate a bromide ion heavy atom derivative. The crystal was flash-cooled on the coldstream, and a set of three data sets were collected near the Br absorption edge at APS beamline 14-BM-D to a resolution of  $1.9\text{\AA}$  for MAD analysis. Seven Se atoms (figure-of-merit 0.59) were found using SOLVE on the Se-Met data, and four partially-occupied bromide ions (figure-of-merit 0.30) were found with the Br data. Both SOLVE maps are excellent, and allowed for tracing of a significant part of the structure in each: RESOLVE traced 80% of the Se-Met structure, and 67% of the Br structure. Details on the structure determination and structures will be presented. The best model with 471 waters has refined to  $R(\text{cryst}) = 0.178$ ,  $R(\text{free}) = 0.212$ , and a FOM of 0.877 using one of the Br-derivative data sets.



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