The crystallographic R-factor of current model is 19.2% for 69,264 unique reflections with Fo > 2sFo in the range of 8.0 - 2.3 Å. The root mean square deviations from ideal stereochemistry are 0.008Å for bond lengths and 1.05° for bond angles. The structural basis for the extreme thermostability of this enzyme will be discussed.

**PS04.01.114 CRYSTALLOGRAPHIC STUDIES ON THE BIFUNCTIONAL PTERIN-4A-CARBINOLAMINE DEHYDRAZTASES FROM HUMAN LIVER AND PSEUDOMONAS AERUGINOSA.** Dietrich Suck, Ralf Ficner, Uwe H. Sauer, Gunter Stier, EMBL, Meyerhofstrasse 1, 69117 Heidelberg, Germany

The bifunctional protein pterin-4a-carbinolamine dehydratase (PCD) is a cytoplasmic enzyme involved in the regeneration of tetrahydrobiopterin, an essential cofactor of several monoxygenases. PCD is also found in cell nuclei forming a tight complex with the transcription factor HNF1. PCD binds to the dimerization domain of HNF1 and accordingly it is called dimerization cofactor of HNF1 (DCoH) as well. The functional enzyme PCD is a homotetramer while it interacts as a dimer with the dimeric HNF1.

The crystal structure of tetrameric PCD/DCoH from rat/human liver was solved by MIR and refined to a R-factor of 22% at 2.7 Å resolution (1). The single domain monomer (12 kDa) comprises three α-helices packed against one side of a fourstranded, antiparallel β-sheet. The homotrimer displays 222 symmetry and can be viewed as a dimer of dimers. In this dimer two monomers form an eight-stranded, antiparallel β-sheet with all helices packing against it on one side. In the tetramer the interface between both dimers is a central four helix bundle where each of the monomers contributes one helix to it. The concave, hydrophobic surface of the eightstranded β-sheet of the dimers is reminiscent of the face of the eightstranded β-sheet of the dimer. The concave, hydrophobic surface of the eightstranded β-sheet of the dimers is reminiscent of the face of the eightstranded β-sheet of the dimer.

The crystal structure was solved using a bacterial homologue of PCD/DCoH, called PhhB, which is a bifunctional ectozyme, also catalyzing the hydrolysis and the formation of tetrahydrobiopterin. There are 5 disulfides. The structure, and alignment of ADPR cyclase and CD38 sequences, suggests that the active site resides in the cleft between domains. Key residues for activity appear to be Trp77, His85, Thr96, Gln98, Asp99, Gly103, Tyr104, Asn107, Ser108 and Trp140. The structure was solved using a NCS averaged MIR map based on 6 derivatives. The current R-factor for all data in the range 8.0-2.4Å is 0.22 (Rfree 0.31).


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**PS04.01.116 STRUCTURAL STUDIES OF A BACTERIAL HELICASE.** Helga Hoyer, Dietmar Rötelke, Cornelia Bartsch and Wolfram Saenger, Institut für Kristallographie, Freie Universität Berlin Takustr 6, 14195 Berlin, Germany

Helicase RepA is a typical helicase of the bacterial replication system. The enzyme unwinds double stranded DNA after binding to a flanking single stranded region. This process is fueled by ATP hydrolysis. Single crystals of suitable size for x-ray crystallographic studies have been grown by the vapour diffusion method. They diffract to 2.8 Å resolution using synchrotron radiation. Space group was assigned to P2₁, with cell dimensions of a=105 Å, b=180 Å, c=115 Å, β=95°. In agreement with electron microscopy studies we found that the protein is comprised of 6 identical 30 kDa subunits, forming a hexameric ring. The search for heavy atom derivatives is in progress.

**PS04.01.117 THREE-DIMENSIONAL STRUCTURE OF O-ACETYLSERINE SULFHYDROLASE FROM SALMONELLA TYPHIMURIUM.** P. Burkhardt*, E. Hohenester*, G.S.J. Raou#., P.F. Cook# and J.N. Jansonius*, *Department of Structural Biology, Biozentrum, University of Basel, Switzerland. #Department of Biochemistry, The University of Texas Southwestern Medical Center, Forth Worth, Texas, U.S.A

The A-isozyme of O-acetylserylhydrolase (OASS), an α-dimeric pyridoxal 5'-phosphate-dependent enzyme isolated from Salmonella typhimurium catalyses the synthesis of L-cysteine from O-acetyl-L-serine and sulfide. The pyridoxal form of the enzyme has been crystallized in the ortho-riboflavin space group P2₁2₁2₁ with cell constants a=54.3 Å, b=96.9 Å and c=144.4 Å. The crystals diffract to 2.3 Å and contain one dimer per asymmetric unit. The subunit molecular weight is 34000.

The structure has been solved by MIRAS-phasing of six heavy atom derivatives and refinement is underway (current R-factor is 22% at 2.7 Å). OASS has a sequence similarity of about 30% to trypanothione synthase-ß (TRPSß) but less than 20% of the residues are identical. Both enzymes have the same fold, but there are some major differences: The interface to the α-subunit in TRPSß...