acephala (kale) [2] and solved the crystal structure by molecular replacement method. The model structure, Lepidium WSCP (PDB code: 1WYA), shares 41% identity of primary sequence. Kale WSCP possesses a homo-tetrameric structure consisting of 19 kDa subunits, and each monomer contains one Chl but no carotenoid, as in the case of Lepidium WSCP.

The remarkable structural feature is that all four Chls are packed in a hydrophobic core at the inter-subunit interface. Because the Chls are secluded from solvent, it is unlikely that the excitation energy of Chl transfers to oxygen and generates radical species.

[1] Schmidt K. *et al*., *Biochemistry*, 2003, **42**, 7427. [2] Horigome D., Satoh H., Uchida A., *Acta Cryst*., 2003, **D59**, 2283.

Keywords: WSCP, chlorophyll, oxygen radical

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Group-subgroup Relations, Twinning, and Rigid-body Vibration (TLS) in a Bio-crystal: Analogy to Inorganic Structures

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The crystal structure of native methylenetetrahydromethanopterin dehydrogenase, **Mtd-nat**, from *Methanopyrus kandleri* (a= 120 Å, b= 151 Å, c= 220 Å, β=90.0º, *mmm* Laue symmetry due to twinning) was shown to own monoclinic symmetry (C2) by group theory arguments. The structure is closely related to that of the Se-methionine labelled protein, **Mtd-Se**, (a= 120 Å, b=151 Å, c= 110 Å, $C222_1$, structure solution by MAD) differing only by small reorientations of about 1° of the hexameric structural units. Standard tests for twinning were negative; the twinning was recognized using l=odd reflections only.

The structural units in the Mtd-Se crystals feature a striking anisotropic rigid body libration of the hexameric units as shown by TLS refinement (at 1.55 Å resolution) which is consistent with the static reorientation in the Mtd-nat crystals [1].

The relation between the two crystal structures, the rigid body libration in one, as well as the characteristic twinning of the other suggest an analogy to the structural changes at certain kinds of phase transitions described by group-subgroup relations which imply twinning, 'soft' lattice vibration modes, and which are well studied in inorganic structural chemistry and solid state physics.

[1] Warkentin E., Hagemeier C. H., Shima S., Thauer R. K., Ermler U., *Acta Cryst*., 2005, D**61**, 198-202.

Keywords: group-subgroup relations, twins, TLS refinement

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Phasing with Iodine and an X-ray Home Source

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The goal of the present work is focused on the phasing strategy employed to elucidate the crystal structure of the protein N-acetylglucosamine-6 phosphate (GlcNAc6P) deacetylase from *E. coli* [1]. GlcNAc6P deacetylase is an enzyme of the amino sugar catabolism pathway, catalyzing the conversion of the GlcNAc6P in to GlcN6P. The crystal structure was phased by SIRAS using low resolution (2,9Å) iodine anomalous scattering. Native crystals[1] were soaked in a cryo-solution consisting of 1.2 M NaH_2PO_4 and 0.7 M NaI for 10 min. A high redundancy dataset (694° angular sector) was collected on a rotating anode at 100K, resulting in 1,676,880 observed and 21,619 independent reflections. Seventeen iodine sites of partial occupation (1.0-0.3) were found with SHELXD and the output correlation coefficients between the observed and calculated SFs differences were 34.73% (all) and 18.93% (weak data). Phase calculation was carried out with the program SOLVE. Phase extension to 2Å resolution, based on a native data set collected at a synchrotron source [1], and succeeding density modification steps were performed with program RESOLVE. An initial hybrid model was built by merging residues traced in different runs and sub cycles of ARP/WARP model building. Some insights on the refined structure will be presented.

[1] Ferreira F. M., *et al.*, *Acta Cryst.*, **D56**, 670.

Keywords: phasing, SIRAS, GlcNAc6P deacetylase

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Structural Comparison and Analysis of the Substrate Specificities of Purine Nucleoside Phosphorylases

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The reversible phosphorolysis of purine and pyrimidine nucleosides is an important reaction in the salvage pathway, where cleavage of glycosidic bond yields a free base and ribose-1-phosphate. Structural studies reveal that only two folds exist, which provides the basis to classify the nucleoside phosphorylases into two families: nucleoside phosphorylase-I and nucleoside phosphorylase-II. Nucleoside phosphorylase-I enzymes share a common single-domain subunit, have either a homotrimeric or a homohexameric quaternary structure, and accept both purine and pyrimidine substrates. Nucleoside phosphorylase-II enzymes share a common two-domain subunit fold with a dimeric quaternary structure, and are specific for pyrimidine nucleosides [1]. Purine nucleoside phosphorylases (PNPs) belong to the nucleoside phosphorylase-I family. Typically, homohexameric PNPs cleave inosine, guanosine and adenosine, while homotrimeric PNPs cleave guanosine and inosine but not adenosine; however, exceptions have been observed.

Fifteen known structures of homohexameric and homotrimeric PNPs from bacterial and mammalian species are analyzed based on sequence alignment, phylogenetic analysis and substrate specificity. While conservation of key active site residues is observed in both bacterial and mammalian PNPs, there is significant sequence divergence between the two classes of PNP. Comparison of the active sites from known structures of the trimeric and hexameric PNP family members provides insight to the structural basis of substrate specificity.

[1] Pugmire M., Ealick S.E., *Biochem. J*, 2002, **361**, 1.

Keywords: purine nucleoside phosphorylase, active site, substrate specificity

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Examination of the Mechanism of Carbamate Kinase by Structural Analyses

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Carbamate kinase (EC 2.7.2.3) catalyzes the reversible reaction $NH_2COO^- + ATP \leftrightarrow NH_2COOPO_3^{2-} + ADP$ serving to synthesize ATP from carbamoyl phosphate in microorganisms [1].

Since CK catalysis involve phosphoryl group transfer, the enzyme CK may have the residues which stabilize intermediate during phosphate transfer. To clarify this point we have determined the three-dimensional structure of carbamate kinase of *Pseudomonas aeruginosa* bound to carbamoyl phosphate and ADP by X-ray crystallography. The structural analysis provides the information on substrate binding and catalysis in CK.

Comparing Apo form of CK with ADP&CP bound form, there's a large conformational changes that cover CP binding pocket. Detailed examinations of the part where the conformational changes happened showed some H-bond and ion pair with Phosphate group of Carbamyl phosphate drove these changes.

Through these structural data, we could suggest a procedure of Pa Carbamate kinase reaction and provide some insights of mechanism of reaction.