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DATABASES LINKED TO ELECTRONIC PUBLICATIONS

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An important new development of the WWW version of the Inorganic Crystal Structure Database ICSD has been made with the help of Brian McMahon for the IUCr and maintainers of electronic journals for several large commercial publishers. ICSD can now retrieve the complete electronic text and abstract for articles in these journals. To understand the importance of this, connect to our demonstration ICSD server **http://barns.ill.fr/dif/icsd/**, select the "normal screen" and enter a trivial search request. (Remember that the demonstration server only contains 4% of the 62,000 entries in the ICSD database). For example if you search for 'Elements' O and 'Jrnl Coden' ACCRA then click on 'References' you will obtain direct links to the Acta Cryst. abstracts of the individual articles, with further links to the full papers. Something similar can be done for many other crystallography journals, such as the American Mineralogist, J. Solid State Chem. etc.

Not all issues are available electronically, and many require a subscription, but it is often sufficient for the lab. library to subscribe, and the electronic version will become automatically available to all local computers. American Mineralogist is making electronic versions of older issues available at no cost, and IUCr journals (Acta Cryst A, B, C, JAC etc) have complete electronic articles back to 1948 !

We believe that the coupling to electronic issues of journal articles will be a decisive advantage for ICSD-for-WWW, which can already compare structures, calculate bond lengths and bond-charge, and display powder diffraction patterns and 3D structures.

Keywords: ICSD 'ELECTRONIC PUBLISHING' INTERNET

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FUELING PEPTIDE TRANSPORT: STRUCTURE OF AN ABC ATPase DOMAIN OF TAP, THE TRANSPORTER ASSOCIATED WITH ANTIGEN PROCESSING

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The transporter associated with antigen processing (TAP) is an endoplasmic reticulum (ER) resident protein that transports cytosolic peptides generated by the proteasome to the ER lumen for loading onto MHC class I molecules. TAP is an ABC transporter formed of two subunits, TAP1 and TAP2, which each has a membrane-spanning domain and an ATPase domain. In the ER membrane, TAP forms a peptide-loading complex with MHC class I molecules and their specific chaperone, tapasin, as well as the more general ER chaperones calnexin, calreticulin, and the thiol oxidoreductase ERp57. We report the structure of the C-terminal ABC ATPase domain of TAP1 (cTAP1) bound to ADP. cTAP1 forms an L-shaped molecule with two domains, a RecA-like domain and a small α-helical domain. The diphosphate group of ADP interacts with the P-loop. Residues thought to be involved in γ-phosphate binding and hydrolysis show flexibility in the ADP-bound state as evidenced by their high B factors.

Comparisons of cTAP1 with other ABC ATPases from the ABC transporter family as well as ABC ATPases involved in DNA maintenance and repair reveal key regions and residues specific to each family. Three ATPase subfamilies are identified which have distinct adenosine recognition motifs, as well as distinct subdomains that may be specific to the different functions of each subfamily. Differences between TAP1 and TAP2 in the nucleotide-binding site may be related to the observed asymmetry during peptide transport.

Keywords: ANTIGEN PRESENTATION, ABC TRANSPORTER, ATPASE

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THREE-DIMENSIONAL STRUCTURE OF THE BACTERIAL PROTEIN TRANSLOCASE AT 8 Å RESOLUTION

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The Sec machinery is responsible for the export and membrane integration of most secreted and membrane proteins in bacteria. In the inner membrane, a channel is formed by the association of SecY, SecE and SecG. The complex active in protein translocation is thought to consist of up to 4 SecYEG units each predicted to contain up to 15 membrane-spanning α-helices. These three membrane proteins have been over-expressed in E. coli, purified as a complex and crystallized in two dimensions (1). Electron cryo-microscopy and image processing of tilted crystals show that the crystals are formed of two membranes interacting through the cytoplasmic domains of the protein and related to each other by a two-fold screw axis. This atypical crystal architecture was confirmed by thin section and freeze-fracture analysis. The unit cell (a = 104 Å, b = 57 Å, α = 90°) contains two asymmetric units, each embedded in a membrane. The asymmetric unit is composed of a SecYEG dimer, within which a two-fold non-crystallographic symmetry relates the two monomers. The monomeric complex contains 15 transmembrane helices. In the centre of the dimer is a 16 x 25 Å cavity that is closed on the periplasmic side. This apparent channel is lined by a pair of highly tilted helices that may act as a gate for protein translocation.

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Keywords: ELECTRON CRYO-MICROSCOPY, SECYEG, 2-D CRYSTALS

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STRUCTURAL BASIS FOR THE INTERACTION BETWEEN FG-NUCLEOPORINS AND NTF_2

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Despite many recent advances in the field of nuclear trafficking, the precise molecular mechanism by which nuclear transport factors and their cargoes pass through nuclear pores remains controversial.

There is, however, an emerging consensus that the translocation step is mediated by interactions between transport factors and nuclear pore proteins (nucleoporins) that contain characteristic tandem sequence repeats based on phenylalanine-glycine (FG) rich cores. FG-repeat nucleoporins frequently contain domains with twenty or more repeats and appear to contain little regular secondary structure. Interactions with nucleoporins containing F_xFG repeat cores are crucial for the nuclear import of RanGDP mediated by nuclear transport factor 2 (NTF_2). To address the precise nature of the NTF_2-FxFG interaction, we have determined the crystal structure of a complex of yeast NTF_2 ($yNTF_2$) and a FxFG peptide. Although we have previously described trigonal crystals of wild-type $yNTF_2$ complexed with a fragment of a FxFG-repeat containing nucleoporin, merohedral twinning frustrated attempts to solve their structure using molecular replacement. However, we found that the $yNTF_2$-N77Y mutant fortuitously crystallized in space group $P2_1$ and so was not subject to merohedral twinning.

This enabled us to determine the crystal structures of both $yNTF_2$-N77Y alone and also when complexed with a peptide containing a single FxFG repeat core. These structures have enabled us to evaluate the precise manner in which FxFG nucleoporin cores interact with this nuclear transport factor at 1.9 Å resolution and show that residues from both chains of the dimeric molecule form the FxFG binding site on NTF_2.

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Keywords: NUCLEAR TRAFFICKING, COMPLEX, NUCLEOPORINS