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CUBIC CRYSTAL FORMS OF THE ACTIN BINDING PROTEIN PROFILIN FROM *ACANTHAMOEBA* AND *SACCHAROMYCES CEREVISIAE*

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Profilin is a regulatory component of the actin cytoskeleton in all eucaryotic cells, which binds actin, proline-rich peptides and phosphatidylinositol 4,5-biphosphate (PIP2). The crystal structures of profilin-II from *Acanthamoeba castellani* and yeast profilin from *Sacharomyces Cerevisiae* have been determined by molecular replacement and refined at 2.3 Å resolution to R=22.9%, Rfree=28.7% and R=21.1%,R_{free}=23.0%, respectively, with good geometry. Both proteins crystallized in the cubic space group $P4_332$. The structural comparisons of these two profilins with other bacterial, plant and mammalian profilins will be presented. One glycerol molecule from the cryoprotectant solvent was found to be bound in the solvent-filled pocket located near the poly-L-proline (PLP) binding site in yeast profilin. The glycerol alcohol groups form hydrogen bonds to aromatic residues involved in PLP binding in yeast profilin. These residues are conserved in all profilins and could possibly accomodate negatively charged functionalities of the PIP2 head group.

Keywords: PROFILIN ACTIN CYTOSKELETON

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MOLECULAR BASIS OF ANCHORING THE GIANT MUSCLE PROTEIN TITIN WITHIN THE SARCOMERIC Z-DISC

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Titin is a giant multi-domain protein from vertebrate striated muscles and is about 1.2 μm in length and extends through one half of the muscle sarcomere, from the Z-disk to the central M-line. It functions as a molecular ruler during sarcomere assembly and action. The very N-terminus of titin consists of two immunoglobulin-like domains, referred as Z1-Z2 domains. They tightly interact with another sarcomeric protein with a molecular weight of about 19 kDa, known as telethonine or T-cap. This protein serves, in turn, as substrate of the only protein kinase domain of titin, which is located within the M-line. We expressed, purified and crystallized the complex of telethonine with the Z1Z2 domains of titin. In an initial low-resolution structure, using small angle scattering data from EMBL/DESY, we have approximately located the binding site of telethonine on the titin N-terminus. More recently, we have obtained crystals of the separate Z1Z2-construct, the Z1Z2 domains in complex with a truncated telethonine construct, and Z1Z2 in complex with a full-length construct of telethonine, all diffracting better than 3 Å resolution. A MAD X-ray dataset from crystals of the Z1Z2-telethonine (truncated) complex has been used to produce electron density, which is of sufficient quality for structure determination. The structures of the full-length titin-telethonine complex and the separated titin Z1Z2 domains will be determined by molecular replacement. We anticipate that our structural data will provide a paradigm model for protein anchoring in filament assembly, allowing direct structural comparison of the possible changes in conformation by complex formation.

Keywords: TITIN, TELETHONINE, PROTEIN ANCHORING

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X-RAY ANALYSIS OF D(GCGAACGC): INTRA-DUPLEX AND INTER-DUPLEX HAND-IN-POCKET MOTIFS

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Many DNA structures have been described in the duplex form in general. When DNA has a function such as deoxyribozymes with catalytic activity, its three-dimensional structure is not so simple. Development of functional DNAs requires establishment of the structural basis including local motifs. The crystal structure of d(GCGAACGC) has been determined by X-ray analysis to investigate such specific motifs between the non-complementary strands. The crystal contains different two duplexes, I and II. At both ends of the duplexes, the two stems respectively consist of three contiguous Watson-Crick G:C pairs. In the central parts, the A4 residue forms a pair with A4 of the counter strand. The two A4 bases in II are in syn conformation, while one of those in I adopts syn conformation and the other one adopts anti conformation. In both duplexes, the A5 residues are bulged out, but their interacting partners are different. One is an intra-duplex hand-in-pocket motif (in I) and the other is an inter-duplex hand-in-pocket motif (between II and I). In the former motif I, the two adenine moieties of the A5 residues fold back to enter the minor groove of the same duplex and form the two hydrogen bonds (N1...H-N2 and N6-H...N3) with the G3 residues of the same strand. In the latter motif II, however, the extruded A5 residues fully extend and make a contact with the G7 residues in the minor grooves of the adjacent duplexes of I, through the two hydrogen-bonds similar to those of the motif I.

Keywords: HAND-IN-POCKET MOTIF, BULGE STRUCTURE, FUNCTIONAL DNA

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THE NEW NUCLEIC ACID DATABASE ATLAS

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The Nucleic Acid Database (NDB; **http://ndbserver.rutgers.edu/**) provides information about nucleic acid-containing three-dimensional structures. The data available consist of co-ordinates, experimental details used to determine the structures, and derived information about the geometry of the structures. The NDB Atlas, which classifies the various types of nucleic acid-containing structures into categories, is a key feature of the NDB. Within a category, each structure has an Atlas page, which highlights the special aspects of the structure using a combination of text and graphics. The NDB Atlas is being expanded by the inclusion of nucleic acid-containing structures determined by NMR. In addition, the Atlas pages are being re-designed to include links to experimental files and links to derivative data. New pictures emphasizing protein-nucleic acid interactions will be added for protein-DNA complexes. The new NDB Atlas will be a valuable resource for researchers and educators. The NDB is supported by funds from the NSF and DOE.

Keywords: DATABASES, NUCLEIC ACIDS, PROTEIN-NUCLEIC ACIDS