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Keywords: V-ATPase, asymmetric, rotation mechanism

MS08.P06

Acta Cryst. (2011) A67, C264 Structural analysis of MamA, a magnetosome associated protein from two different magnetospirillium species

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Tetra- tricopeptide repeat (TPR) is a structural motif found as such or forming part of a bigger fold in a wide range of proteins. It serves as a template for protein-protein interactions and mediates multiprotein complexes [1]. MamA is a unique, highly abundant, Magnetosome associated protein and predicted to contain 5 TPR motifs as well as predicted putative one. Magnetosome is a subcellular organelle that consists of a linear-chain assembly of inner membrane invaginations each able to biomineralize and enclose a ~50-nm crystal of magnetite or greigite. Magnetosome allows magnetotactic bacteria, a diverse group of aquatic microorganisms, to orientate themselves along geomagnetic fields in search of suitable environments [2]. MamA is one of the most characterized magnetosome-associated proteins in vivo and yet, its function is not clear [3-5]. Here, we report on the crystallization and structure analysis of recombinant M. magneticum (AMB-1) and M. gryphiswaldense (MSR-1) MamA deletion mutants. The structures were determined to a resolution of 2.0 Å and confirmed MamA fold as a five TPR motifs containing protein.

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Keywords: TPR containing proteins, Magnetosome, Magnetotactic bacteria

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The mechanisms of self-assembly of the vault, the largest cytoplasmic ribonucleo-protein complex

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Vaults are the largest cytoplasmic ribonucleo-protein particles found in numerous eukaryotic species. They were first observed in 1986 as contaminants in preparations of clathrin-coated vesicles from rat liver. Rat liver vault comprises three kinds of proteins: the major vault protein (MVP), the vault poly(ADP-ribose) polymerase (VPARP), the telomerase- associated protein 1 (TEP1) and a small untransrated RNA consisting of 141 bases (vRNA). The mass of rat liver vault is about 10 MDa, and the particle shell measures about 700 Å in length and about 400 Å in maximum diameter. Most vault particles are present in the cytoplasm, but few of them (about 5% of the total vault fraction) localize to the nucleus. Several studies suggested that vaults might play an important role in the multi-drug resistance (MDR) of cancer cells. Human vRNAs have the ability to bind mitoxantrone, a chemotherapeutic compound, and they may play an important role in the export of toxic compounds (Gopinath et al., Nucleic Acids Res., **33**, 4874-4881 (2005)). The recent study shows that vaults may be involved in innate immunity (M. P. Kowalski et al., Science **317**, 130-132 (2007)). However, their cellular function remains unclear.

We have determined the x-ray structure of rat liver vault at 3.5Å resolution in 2008 [1, 2]. X-ray structure reveals that vault particle has 39-fold dihedral symmetry and shell is made up of 78 identical MVP chains. Each MVP monomer folds into 12 domains: nine structural repeat domains, a shoulder domain, a cap-helix domain, and a cap-ring domain. Side-by-side hydrophobic interactions of the cap-helix domain play a key role for self-assembly of the half-vault. N-terminal residues of MVP domain 1 form intermolecular interactions around two-fold axis including anti-parallel sheet and ionic bond. In this session, we will discuss the mechanisms of self-assembly of the vault.

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Keywords: vault, ribonucleo-protein complex, self-assembly

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Modeling the organization of molecules in collagen using the paracrystal concept

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A characteristic feature of the dense phases formed by fibershaped molecules is their organization into parallel rods packed in a hexagonal or pseudo-hexagonal lateral network. This is typically the case for the collagen triple helices inside fibrils, as confirmed by recent X-ray diffraction experiments carried out on highly crystallized fibers obtained by immersing the freshly extracted fibers in a salt-controlled medium.

However such diffraction patterns also generally exhibit additional features in the form of diffuse scattering, which is a clear signature of a low degree of lateral ordering. Only few studies have analyzed and modeled the lateral packing of collagen triple helices when the structure is disordered. Some authors have used the concept of shortrange order but this approach does not contain any echo of a hexagonal order. In this study [1], we use an analytical expression derived from the paracrystal model which retains the hexagonal symmetry information and leads to a good agreement with the experimental data in the medium-angle region. This method is quite sensitive to the degree of disorder and to the inter-object distance. One clear result is that the shift in peak positions, generally attributed to variations in intermolecular distances, can also arise from a change in the degree of ordering without any significant modification of the distances. This underlines the importance of evaluating the degree of ordering before attributing a shift in peak position to a change in the unit-cell. This