

s8a.m5.p3 **Towards an atomic structure of intermediate filaments.** S.V. Strelkov¹, H. Herrmann², N. Geisler³, R. Zimbelmann², A. Lustig¹, U. Aebi¹ and P. Burkhard¹, *1 M.E. Müller Institut, Biozentrum der Universität Basel, 4056 Basel, Switzerland, 2 German Cancer Research Center, Heidelberg, 3 Max Planck Institute for Biophysical Chemistry, Göttingen, Germany.*

Keywords: coiled coils, intermediate filaments, macromolecular assemblies.

10nm-wide intermediate filaments (IFs) represent an essential component of the cytoskeleton in most eukaryotic cells. The elementary unit of the IF structure is an elongated dimer with its major central part being a parallel α -helical coiled coil. The filament formation proceeds via a specific multistage association of the dimers. We set a goal of determining the atomic structure of human IF protein vimentin using X-ray crystallography. The wild-type protein is not suitable for crystallisation because of its elongated shape and intrinsic tendency to assemble into filaments. To overcome this problem, we have produced and characterised more than 20 partially overlapping vimentin fragments with lengths ranging between 39 and 330 residues. Diffraction quality crystals were obtained for five fragments. The structures of the Z2B and Cys2 fragments could be solved to 1.9 and 2.3Å resolution, respectively. Both fragments belong to the segment 2B of the coiled coil while the second one also reveals a coiled-coil stutter. The 1.4Å structure of the C1A fragment corresponding to the highly conserved N-terminal region of the vimentin 'rod' features a monomeric α -helix. We expect that determining crystal structures of further fragments will gradually allow us to compile a molecular model for the full-length vimentin dimer. This approach will be eventually extended to establishing the architecture of complete filaments at atomic resolution.

s8a.m5.p4 **The crystal structure of the *Clostridium thermocellum* CelS, the major enzymatic component of the cellulosome.** B.G. Guimarães[§], H. Souchon[§], J.H.D. Wu[#], P.M. Alzari[§], *§Unité de Biochimie Structurale – Département d'Immunologie, Institut Pasteur, 25 rue du Dr. Roux 75724 Paris Cedex 15. #Department of Chemical Engineering, University of Rochester, Rochester, New York 14627-0166.*

Keywords: cellulosome, cellobiohydrolase, 3D structure.

The anaerobic thermophilic bacterium *Clostridium thermocellum*, produces an extracellular system, the cellulosome, which is very efficient to degrade cellulose. The cellulosome is a multi-protein complex consisting of more than 14 subunits, most of which possess glycosidase activity. Among these, the cellobiohydrolase CelS is the most abundant. We report the crystallization and the structure determination at 2.2 Å resolution of the *C. thermocellum* CelS complexed with cellobiose.

CelS crystals belong to space group P2₁2₁2₁ with cell dimensions $a = 147.8$ Å, $b = 207.4$ Å, $c = 213.5$ Å and six molecules in the asymmetric unit. The crystal structure was solved by molecular replacement techniques using the 3D structure of endocellulase CelF of *C. cellulolyticum* as a model. Structure refinement is in progress and the final CelS model will be presented and analyzed.

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