Acta Cryst. (2002). A**58** (Supplement), C217

THE ROLE OF Sec1 AND COMPLEXIN IN NEUROTRANSMISSION

W. Weissenhorn[1] J. Kadlec[1] A. Bracher[1] H. Betz[2]
[1]EMBL, Grenoble, France [2]Max-Planck-Institute for Brain Research, Frankfurt, Germany

Nerve terminals release neurotransmitters from vesicles into the synaptic cleft upon transient increases in intracellular Ca^{2+}. This process requires the formation of trans SNARE complexes and is regulated by accessory proteins including nsec1 and COMPLEXIN (CPX). Here we present the crystal structure of neuronal squid Sec1 from squid, which was solved by MAD at 2.4 Å. S-Sec1 folds into a modular arch-shaped three-domain assembly. Comparison of structures of squid s-Sec1 from different crystal forms, and rat nsec1 bound to syntaxin-1a (Misura et al. (2000), Nature 404, 355-362) indicates potential conformational rearrangements in domain 1 and 3. A hinge region between domains 1 and 2 may be involved in binding/release of SYNTAXIN (SX), which may also affect the conformational flexibility of the helical hairpin of domain 3. The release of SX from nsec1 is thought to follow SNARE complex formation. Neuronal SNARE complexes then bind to CPX, which couples neurotransmission to an increase in intracellular calcium. The crystal structure of a squid core CPX/SNARE complex solved by molecular replacement at 2.95 Å resolution shows a helical segment of CPX that binds in anti-parallel fashion to the four-helix bundle of the core SNARE complex. CPX interacts at its C-terminus with SX and SYNAPTOBREVIN around the ionic zero layer of the SNARE complex. We propose that CPX is part of a multi-protein complex that regulates membrane fusion of docked vesicles at a late pre-fusion stage.

Keywords: NSEC1, SNARES, COMPLEXIN

Acta Cryst. (2002). A**58** (Supplement), C217

CRYSTAL STRUCTURE OF PEA Toc34 - A NOVEL GTPase OF THE CHLOROPLAST PROTEIN TRANSLOCON

C. Hsiao[1] Y. Sun[2] F. Forouhar[1] H. Li[1] S. Tu[1] C. Chen[3]
[1]Institute of Molecular Biology, Academia Sinica, Nankang, Taipei, Taiwan 115, R.O.C. [2]Department of Life Science, National Tsing Hua university, Hsinchu, Taiwan 300, R.O.C. [3]Institute of Biomedical Sciences, Academia Sinica, Nankang, Taipei, Taiwan 115, R.O.C.

Toc34, a 34 kDa integral membrane protein, is a member of the Toc (translocon at the outer-envelope membrane of chloroplasts) complex that associates with precursor proteins during protein transport across the chloroplast outer membrane. Here we report the crystal structure of the cytosolic part of pea Toc34 complexed with GDP and Mg at 2.0 Å resolution. In the crystal, the Toc34 molecules exist as dimers with features resembling the ones found in a small GTPase complexed with a GTPase activating protein (GAP).

Gel-filtration, however, revealed that dimeric and monomeric forms of Toc34 coexisted in phosphate saline buffer (pH 7.2) solution. Mutation of Arg 128, an essential residue for dimerization, to alanine led to the formation of only a monomeric form whose GTPase activity is significantly reduced compared to that of the wild-type Toc34. These results together with a number of structural features unique to Toc34, suggest that each monomer acts as a GAP on the other interacting monomer.

Keywords: PROTEIN IMPORT CHLOROPLAST TRANSLOCON

Acta Cryst. (2002). A**58** (Supplement), C217

EXTENSION OF RASMOL TO DISPLAY SURFACES, TO HANDLE CML/XML AND OTHER NEW FEATURES

H. J. Bernstein[1,2] F. C. Bernstein[2]
[1]Dowling College, Oakdale, NY 11769, USA [2]Bernstein + Sons, Bellport, NY 11713, USA

RasMol by R. Sayle, is a heavily used, well-established, open-source, molecular graphics program. Visualization of macromolecular surfaces is helpful in understanding intermolecular contacts and interactions. Existing versions of RasMol show both solid and translucent dotted van der Waals surfaces, and P. Valadon's RasTop variant of RasMol shows Richards-Connolly solvent accessible surfaces as translucent dotted surfaces. We extend the existing surface presentation logic in RasMol to show either van der Waals or Richards-Connolly surfaces as solid, transparent, or translucent surfaces and to allow a single surface to optimally envelop multiple conformers.

Another important new feature is the extension of the input and output capabilities of RasMol to support the Chemical Markup Language (CML), the Extensible Markup Language (XML), and Yet Another Extended Data Framework (YAXDF) thus extending the existing macromolecular Crystallographic Information File (mmCIF) and core CIF support. Other changes to RasMol, such as multilingual Unicode support, multiple molecule support, and bond editing will be discussed.

Keywords: SURFACES, GRAPHICS, RASMOL

Acta Cryst. (2002). A**58** (Supplement), C217

QUANTITATIVE VISUALIZATION OF MOLECULES AND THEIR PROPERTIES

C. Bajaj
Center for Computational Visualization Computer Sciences & TICAM University of Texas at Austin TEXAS TX USA

I shall describe multiresolution geometry data structures used for the visualization of molecular shape and associated properties (electrostatics, interaction potentials, ...). These geometry data structures while volumetric, allow for smooth piecewise polynomial spline approximations of molecular surfaces, corresponding to level sets of electron density. I shall also describe algorithms for topological, and metric quantification of molecular shape and associated properties via differential and integral calculations of the spline representation. The collection of data structures and algorithms should provide useful support for a range of rapid molecular manipulations, including quantifying shape and properties complementarity, structural analysis, molecular docking, and molecular animation visualization.