

## E0033

**Protein Model Validation in Structural Genomics- the SECSG Perspective.** W. Tempel<sup>1</sup>, Z.J. Liu<sup>1</sup>, W.B. Arendall III<sup>2</sup>, S.R. Wang<sup>2</sup>, D.C. Richardson<sup>2</sup>, J.S. Richardson<sup>2</sup>, J. Rose<sup>1</sup>, B.C. Wang<sup>1</sup>, Southeast Collaboratory for Structural Genomics, <sup>1</sup>Dept. of Biochemistry and Molecular Biology, Univ. of Georgia, Athens, GA, <sup>2</sup>Dept. of Biochemistry, Duke Univ. Medical Center, Durham, NC, USA.

The determination of reference structures for the complete range of protein families has emerged as a preeminent goal of structural genomics. Therefore, quality assurance of the models gains added importance. At the Southeast Collaboratory for Structural Genomics (SECSG), additional validation steps precede the tests performed during model deposition at the Protein Databank. In addition to crystallographic criteria such as Rfree and difference maps, we use updated Ramachandran and side chain rotamer criteria, and also all-atom contact analysis as implemented in the MolProbity web tools [Lovell et al. (2003) *Proteins* **50**: 437]. Furthermore, model validation is no longer confined to the final refinement cycles but has become an integral part of model refinement. This can avoid model bias, speed convergence, and ultimately produce superior results by all criteria. Herein we compare the quality of SECSG models with typical crystal structures at comparable data resolution that have been deposited at the PDB by other laboratories.

Supported by NIGMS, IBM, Georgia Research Alliance and University of Georgia.