## MS07 O1

**Is there a Sevres standard for protein structures?** Alexander Wlodawer[a], Mariusz Jaskolski[b], Zbigniew Dauter[a], [a]*Macromolecular Crystallography Laboratory, National Cancer Institute, Frederick, MD, USA.* [b]*Department of Crystallography, A. Mickiewicz University, Poznan, Poland.*
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**Keywords: refinement, restraints, validation**

Limited resolution of the diffraction data collected for most of protein crystals do not allow their models to be refined without introduction of stereochemical restraints. Traditionally, the libraries of geometrical targets have been constructed on the basis of well-refined crystal structures of amino acids or small peptides. These standards may not be completely appropriate for large protein structures, where some specific intra- and intermolecular interactions may cause certain stereochemical features to adopt conformations rarely observed in less strained small molecules. The availability in the PDB of a number of protein models refined at ultra-high resolution offers the possibility of creating a library of protein geometry built on most accurately refined protein models. However, even the best refined models display some degree of variability in the analogous structural features, therefore the geometrical targets cannot be treated as a "holy Grail", but should be accompanied by appropriate weights, allowing for a degree of flexibility. The targets of various restraints (very often too tight in the current practice) and the level of corresponding weights appropriate in various circumstances will be discussed, and illustrated with the examples taken from the recent depositions in PDB.

## MS07 O2

**Improvement of Crystallographic Data near Corners in Mosaic CCD Detectors.** A.S. Arvai[1], S. Brockhauser[2], G. Cioci[3], GA. Leonard[3], A. McCarthy[2], S. McSweeney[3], C. Müller-Diekmann[3], C. Nielsen[1], D. Nurizzo[3], R. B.G. Ravelli[2], and X. Nguyen-huu[1], [1] *Area Detector Systems Corp, Poway CA, USA,* [2] *EMBL, 6 rue Jules Horowitz, 38042 Grenoble, France* [3]*ESRF, rue Jules Horowitz, 38042 Grenoble, France.* E-mail: gordon.leonard@esrf.fr

Large area fast-readout CCDs have become the detector of choice for modern Macromolecular Crystallography synchrotron beam lines. These mosaic detectors are flat-field corrected in order to give a uniform response over the whole surface area. Nevertheless, it has been observed that crystalline diffraction intensities are often underestimated when recorded near the corners of a CCD module. We believe that this effect is primarily due to a variation of the point spread function from the center to the corner of each module. The location of these corners on 3x3 and 4x4 CCD detectors often has significant negative impact on structure solution when important medium resolution reflections are measured in these areas. A method to construct and apply a correction for this effect is presented along with some examples showing improvement in R-factors, anomalous signal, and the ability to solve a structure.

## MS07 O3

**Tandem use of crystallography and mass spectrometry to sequence *ab initio* HPBP** Eric Chabriere[a], Mikael Elias[a] Hélène Diemer[b], Frédérique Renault[c], Carlos Contreras-Martel[d], Alain Van Dorsselaer[b] ,[a]*LCM3B, Nancy Universtit.* [b]*LSMBO, Strasbourg.* [c]*CRSSA, France.* [d]*LCCP, IBS, Grenoble.*
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**Keywords: *ab initio* sequencing, gene missing, atherosclerosis**

The Human Phosphate Binding Protein (HPBP) is a serendipitously discovered apolipoprotein from human plasma that binds phosphate [1]. Amino acid sequence relates HPBP to an intriguing protein family that seems ubiquitous in eukaryotes. These proteins, named DING according to the sequence of their four conserved N-terminal residues, are systematically absent from eukaryotic genomes database [2]. As a consequence, HPBP amino acids sequence had to be first assigned from the electronic density map at 1.9 Å. Then, an original approach combining X-ray crystallography and mass spectrometry provides the complete and *a priori* exact sequence of the 38kDa HPBP. This first complete sequence of a eukaryotic DING protein will be helpful to study HPBP and the entire DING protein family which could be involved in various diseases (atherosclerosis, kidney stone, HIV, rheumatoid arthritis)

[1] Morales R., Berna A., Carpentier P., Contreras-Martel C., Renault F., Nicodeme M., Chesne-Seck M.L., Bernier F., Dupuy J., Schaeffer C., Diemer H., Van-Dorsselaer A., Fontecilla-Camps J.C., Masson P., Rochu D.**,** Eric Chabriere**,** *Structure,* 2006, 14, 601-609 (2006)
[2] Berna A., Bernier F., Chabriere E., Perera T., Scott, K., *Intl. J. Biochem. Cell Biol.*, 2007 In press.

## MS07 O4

**The wwPDB remediation project** Ganesh J. Swaminathan[a], Bohdan Schneider[b], [a]*European Bioinformatics Institute, Cambridge, U.K.* [b]*Research Collaboratory for Structural Bioinformatics, Piscataway, USA.* E-mail: jawahar@ebi.ac.uk

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The worldwide Protein Data Bank (wwPDB) [1], [2] is a group of organizations that act as data centres for deposition, processing and distribution of data in the Protein Data Bank (PDB) [3]. Its mission is to maintain a single PDB archive of macromolecular structural data that is freely and publicly available to the global community. The members are RCSB PDB (USA), BMRB (USA), MSD-EBI (Europe) and PDBj (Japan).
The evolution of experimental methods, functional knowledge of proteins, and methods used to process PDB data have introduced inconsistencies into the archive since its inception in 1971. The wwPDB (http://www.wwpdb.org/) has collaborated on a project to remediate the PDB archive and create a new set of corrected files. All existing entries have been reviewed and errors have been corrected where possible in order to ensure the uniformity of archived entries and allow scope for future developments in structural biology. Some of