ADDENDUM

LATE ABSTRACTS

L.A.01

Acta Cryst. (2011) A**67,** C811

Data Quality in Area Detector Diffraction Experiments.

Mathias Meyer, *R&D CSG group, Agilent Technologies (Poland) Sp. z o.o., Rogowska 117b; PL-54-440 Wroclaw.* E-mail: Mathias.Meyer@agilent.com

Data quality of diffraction experiments depends on several factors: a) The diffractometer and the area detector hardware, b) the sample, c) the experimental procedure and d) the data reduction approach and software.

The talk will highlight key aspects of each of these factors.

The hardware revolves around the notions of absolute detectivity, overhead, minimizing systematic errors and diffractometer access.

The sample choice, mounting, protection environment is controlled within reason by the user.

The experimental procedure comprises the choice of wavelength, the geometric strategy, the mode of scan and detector operation and the decision on absolute detectivity vs. redundancy.

The data reduction software has to be optimized at extracting consistently area detector data not only under good conditions, but also under real life flaws of the practical experimental procedure.

Keywords: Detector,Quality, Experiment

L.A.02

Acta Cryst. (2011) A**67,** C811

POCKETCHECK: A comprehensive contact calculation for distinct peptide-HLA structures.

Trevor Huyton, Nektarios Ladas, Rainer Blasczyk, Christina Bade-Doeding. *Institute for Transfusion Medicine, Hannover Medical School, Hannover, Germany.* E-mail:huyton.trevor@mh-hannover.de

There have been several attempts over the years to define which positions in the HLA binding groove (pockets) influence the specificity of bound amino acids at each position in the peptide. The structural determination of the HLA molecule by X-ray crystallography has provided valuable information for understanding how peptides bind to HLA. Originally, six pockets (A-F) were defined by calculating the surface of the binding groove based upon the crystal structure of HLA-A2 [1]. Since then, x-ray crystallography has been performed for a variety of HLA alleles bound to a range of peptides, which has lead to broader pocket definitions [2].

Several studies performed peptide sequencing for allelic variants to understand the magnitude of certain mismatches on peptide specificity. We have previously described the ability of distinct HLA variants to present peptides of >10 amino acids in length [3]. In these cases it is especially important to be able to define which positions within the HLA binding cleft are in contact with a given peptide and thus influence the sequence of the peptides selected. The knowledge about individual peptide features allowed for the crystallographic analysis of selected pMHC complexes.

The Protein data bank was searched for all deposited structures of peptide:HLA-complexes http://rcsb.org/pdb and those were submitted to the contact map analysis webserver http://ligin.weizmann.ac.il/cma. The output html was piped into an InterSystems Caché "post-relational" database allowing object-oriented data storage. Tabular data with residue position, amino acid and buried surface that contact a particular peptide position were compared for >100 HLA class I structures.

These new dynamic definitions increase the precision of peptide prediction and support the characterization of individual weights for individual amino acids. This knowledge facilitates a rating of the allogenicity of mismatches and will be a further step towards intelligent HLA mismatching.

[1] M. A Saper, P.J. Bjorkman, D.C. Wiley, *J Mol Biol* 219, 277, (1991). [2] G. Chelvanayagam, *Immunogenetics* 45, 15, (1996). [3] Bade-Döding *et al*, *Haematologica*, (2011).

Keywords: Immunology, database, interaction

L.A.03

Acta Cryst. (2011) A**67,** C811

Inducing phase transitions in protein crystals by controlled crystal dehydration

Russi Silvia, Manjasetty Babu, McCarthy Andrew, Cipriani Florent & Belrhali Hassan, *EMBL Grenoble Outstation, 6 rue Jules Horowitz, 38042 Grenoble (France).*E-mail: srussi@embl.fr

Despite the success of macromolecular crystallography (MX) and the enormous advances in the field, one of the major hurdles still to be surmounted is the availability of well-diffracting crystals. As the goals of MX projects become more challenging, with a growing number of membrane proteins and huge macromolecular complexes, crystals with large solvent content and loose packing are becoming more frequent. This often results in poorly diffracting crystals that are insufficient to achieve a structural solution.

Among a variety of post-crystallisation treatments that have been described with the aim of improving crystal diffraction quality, crystal dehydration is one of the most successful one. Interestingly, dehydration may be accompanied by other remarkable changes, such as phase transitions [1], [2]. Phase transitions usually lead in a higher lattice symmetry, smaller cell volumes and reduced number of independent molecules in the asymmetric unit. The possibility to rationally induce these changes by controlled dehydration is poorly understood and an unexplored field, but the potential benefits of it (especially for those challenging and difficult structures) is indisputable.

A new humidity control device (HC1), developed at the EMBL Grenoble [3], [4] and available for on-line dehydration at the EMBL/India/ESRF beamline BM14 [5], has been used to explore its strength in a number of test cases. Allied to BM14, the HC1 allowed the systematic study of these phase transitions in a simple way and in a wide range of proteins (trypsin, insulin, lysozyme, as well as samples provided by external users). All the samples were kept under the humid air stream and characterized at different humidity levels. For those proteins in which phase transitions were observed, the best dehydration protocol was established.

The ongoing study would provide a clearer understanding of the way phase transitions take place and reveal general rules that govern this process. The results should help in the development of new tools, methodologies and crystal dehydration protocols for extended implementation at BM14 and other MX beamlines at the ESRF and to encourage crystallographers using crystal dehydration.

[1] Salunke D.M. et al. **1985,** *J Biosci* 8, 37 [2] Gupta V. et al. **2010,** *PLoS One,* 5(2), e9222 [3] Sanchez-Weatherby J. et al. **2009,** *Acta Cryst. D65*, 1237-1246 [4] Russi S. et al. **2011,** *J Struct. Biol.* doi:10.1016/j.jsb.2011.03.002 [5] http://www.bm14.eu/

Keywords: humidity control device, on-line dehydration, phase transitions