MS3-03 **ISW1a crystal resolution improvements through packing engineering.** Kazuhiro Yamada,[a] David F. Sargent,[a] & Timothy J. Richmond [a], [a] *Institute of Molecular Biology and Biophysics, ETH-Honggerberg, 8093 Zurich, Switzerland*
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Yeast ISW1a is classified as a member of the Imitation SWItch (ISWI) subgroup of the SWI2/SNF2 superfamily of ATP-dependent chromatin remodelers. The main function of ISW1a is the repression of gene expression through modulation of nucleosome positioning. ISW1a is a hetero-dimeric complex comprised of the 135 KDa Isw1 subunit and the 94 KDa Ioc3 subunits. Isw1 contains an N-terminal ATPase domain connected by a linker to a C-terminal domain which is composed of three consecutive subdomains HAND, SANT and SLIDE (HSS). The Ioc3 protein does not share any significant sequence homology to any structually characterized domain. We have solved the crystal structure of ISW1a (ΔATPase) complex both with and without bound duplex DNA at resolutions of 3.60 ($P6_522$) and 3.25 (H32) Å, respectively [1]. In both structures, there is one ISW1a complex in the asymmetric unit. In terms of biological significance, these structures revealed not only an entirely new protein fold architecture of Ioc3 carrying a novel recognition motif for a specific DNA sequence, but also SANT and SLIDE were proven to take topologically unique DNA binding forms. Of interest to crystallographers, the ISW1a crystal in the absence of DNA displayed resolution improvements after introducing point mutations which increased salt bridging in the crystal packing interface, and ISW1a-DNA crystal also exhibited the improvements only after applying dehydration and slow cooling techniques during the post crystal treatment. Taking both these results into account, the introduction of a point mutation at the crystal packing interface and the dehydration and slow cooling methodologies could represent more general tools to improve resolution for poorly diffracting crystals.

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Keywords: chromatin; crystal diffraction; crystal structures

MS3-04 **Getting the best data using photon counting pixel detectors.** Marcus Mueller,[a] Meitian Wang,[b] Clemens Schulze-Briese,[a] [a]*DECTRIS Ltd., Switzerland,* [b]*Swiss Light Source at Paul Scherrer Institut, Switzerland*
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The data collection parameters used in a diffraction experiment have a strong impact on the quality of the acquired data. The selection of parameters has to account for the application of the data in various phasing methods or high-resolution refinement [1]. Furthermore, experimental factors like crystal characteristics, available experiment time, and the properties of X-ray source and detector have to be considered. CCD detectors have been for many years the prevalent type of detectors used in macromolecular crystallography. Most recommendations for data collection strategies as well as the experience of the experimenters are based on the characteristics of this detector type. Recently, hybrid pixel X-ray detectors that operate in single-photon-counting mode became available for macromolecular crystallography [2,3]. The commercially available PILATUS hybrid pixel detector is now in standard user operation at an increasing number of macromolecular crystallography synchrotron beamlines. Hybrid pixel detectors have fundamentally different characteristics and offer various advantages over CCD detectors [3,4]: (i) No readout noise and no dark current. (ii) A sharp point spread function of one pixel. (iii) Millisecond readout times and high frame rates. (iv) A high dynamic range of 20 bits. To fully exploit the advantages of hybrid pixel detectors, different data collection strategies than those established for CCD detectors have to be applied because of the different characteristics of the two types of detectors. Fine φ-slicing is a strategy particularly well suited for hybrid pixel detectors because of the fast readout time and the absence of readout noise. This strategy was systematically investigated collecting a large number of data sets from crystals of four different proteins to investigate the benefit of fine φ-slicing on data quality with a noise-free detector in practice. The results show that fine φ-slicing can substantially improve scaling statistics and anomalous signal [5]. Furthermore, unpublished results on the influence of the detector readout time on data quality will be presented.

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