

Poster Presentation

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Native SAD Structure Solution from Merohedrally Twinned Data

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Up until now, comparatively few structures were solved by native SAD. Recent advances in multi crystal averaging [1] have shown that native SAD can be applied to an increasing number of cases. Though theoretically possible [2], successful structure solutions from twinned data have not been reported yet. Here, we report the structure solution of the human Centromere protein M from a merohedrally twinned crystal with a twinning fraction of 0.45 in the space group P3. The data were collected at the bending magnet beamline X06DA at the Swiss Light Source, which is equipped with the in-house developed multi-axis goniometer PRIGo and the PILATUS 2M detector. A highly redundant 2.2 Å dataset was collected in a number of different crystal orientations. A substructure solution could only be obtained after 50000 SHELXD [3] tries. Automatic model building after phasing and density modification resulted in a model with the majority of residues built correctly. We will present this particularly difficult case together with other more routine cases, all solved with the same experimental setup and at the beamline X06DA.

[1] Q. Liu, T. Dahmane, Z. Zhang, *et al.*, *Science*, 2012, 336, 1033, [2] Z. Dauter, *Acta Crystallographica Section D*, 2003, 2004-2016, [3] G. Sheldrick, *Acta Crystallographica Section A*, 2008, 112-122

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