Poster Presentation

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Monoclinic HEWL derivative structure at 0.75 Å resolution

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Tris-dipicolinate lanthanide complex, Na_3 .[Ln(DPA)³], where DPA stands for pyridine-2,6 dicarboxylate, has been proven to be especially interesting to produce derivative crystals with high phasing power [1]. The lanthanide complex can act as a cross-linking agent, which binds at the interface between protein molecules, leading to a supramolecular interaction at the crystal scale [2]. In the case of hen egg-white lysozyme (HEWL), derivative crystals obtained by co-crystallization with Yb(DPA)₃³- belong to the space group C2, in similar crystallization conditions that normally lead to the tetragonal form $P4_32_12$. Data were collected on a derivative crystal up to a resolution of 0.75 Å at the EMBL beamline P13 at PETRA III at DESY (Hamburg, Germany). Taking advantage of the high the resolution and the strong anomalous signal of the Yb³+ (f" = 5.2 e⁻ at 17 keV), the structure was solved by both SAD and ab initio methods. Data collection, experimentally phased electron density maps and the structure, especially with respect to the vicinity of the lanthanide binding sites, will be discussed.

[1] G. Pompidor, O. Maury, J. Vicat, et al., Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 762-769., [2] G. Pompidor, A. D'Aléo, J. Vicat, et al., Angewandte Chemie International Edition, 2008, 47, 3388-3391.

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