



Figure 1. The structure of tau peptide ²¹⁵LPTPPTREP²³⁰ with $2mF_o - DF_c$ electron density contoured at the level of 0.5σ . The sidechain of R230 has not been modeled due to the lack of sufficient electron density

Keywords: intrinsically disordered proteins, protein tau, Fab fragment, peptide conformation

MS12. Crystallization and crystal treatment

Chairs: Terese Bergfors, Matthew Bowler

MS12-O1 Successful crystal formation - the journey from idea to fruition

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The availability of well-ordered crystals is essential to structure determination by X-ray crystallography. Nucleation is the first step that determines the crystallization process hence a search for the ultimate nucleating agent (nucleant) is ongoing. An ideal nucleant should induce efficient heterogeneous nucleation of crystals in a controlled manner and be effective in finding new crystallization condition and in improving crystal quality. It should be stable, easy to handle, and readily dispensed by robotics into numerous crystallization nano-droplets. This talk will discuss the strategies and the research of several years [1-4] resulting in our latest results [5] of the design, fabrication and validation of the first non-protein nucleating agents that can be used for the automated screening and optimization of any bio-macromolecule. These nucleants are dispensed using commercially available robots and their utilization bypasses the concerns associated with seeding, solid and viscous heterogeneous nucleants. The application of these materials is simple, quick, and 20 nanolitres is sufficient for each trial, thereby providing a potent tool for scientists in academia and industry endeavouring to increase their success. References [1] Chayen *et al.* (2001) *J. Molecular Biology* **312**, 591-595 [2] Chayen, N.E. *et al.* (2006) *Proc. Natl. Acad. Sci. U. S. A.* **103**, 597-601 [3] Saridakis *et al.* (2011) *Proc. Natl. Acad. Sci. U. S. A.* **108**, 11081-11086 [4] Khurshid *et al.* (2014) *Nature Protocols* **9**, Pages: 1621-1633 [5] Khurshid *et al.* (2015) *Acta Crystallographica D* **71**, 534-540. <http://www.iucr.org/news/research-news/smart-crystallization> <http://www.imperialinnovations.co.uk/CRMIP>

Keywords: crystallization, nucleation, proteins, macromolecules, automation, robotics