

Microsymposium

MS82.O04

Crambin - record in crystallographic resolution for a biological macromolecule

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A couple of years ago a study was presented that set the record for the highest X-ray crystallographic resolution for a biological macromolecule [1]. The structure of the small protein crambin was determined to 0.48 Å resolution - this almost doubled the amount of available experimental data. Crambin is a small protein consisting of 46 amino acids belonging to the thionin family. Although the protein and its structure has long been known, it lacks any obvious enzymatic activity and has a hard-to-guess biological function. The protein crystallizes readily and serves as an excellent specimen for exploring the limits of resolution of the diffraction. The results demonstrated the possibilities that can be offered by a high-energy synchrotron source. The structure refined with Refmac, Shelxl and Mopro revealed a wealth of details. Bonding electron density became visible along the main chain. However, no fundamental additional structural features could be detected in comparison to the previously collected data set to 0.54 Å resolution. The availability of extremely high-resolution data is certainly of great help to drive further software development and methods for data interpretation. The question will always remain as to what the true limits are in terms of what can be seen in a biological macromolecule. Here we will present the results of our recent efforts in interpretation of such ultra-high resolution data.

[1] Schmidt A, Teeter M, Weckert E, Lamzin VS. (2011) *Acta Crystallogr. F Struct. Biol. Cryst. Commun.* 67, 424-428.

Keywords: refinement, high-resolution, crambin