

MS08 Serial crystallography, obtaining structures from many crystals

MS08-1-6 Iron binding and photoreduction in the ABC transporter subunit FutA
#MS08-1-6

R. Bolton ¹, M. Machelett ¹, D. Axford ², A. Royant ³, T. Schrader ⁴, T. Tosha ⁵, H. Suigimoto ⁵, J. Worrall ⁶, G. Evans ², M. Hough ², R. Owen ², I. Tews ¹

¹University of Southampton - Southampton (United Kingdom), ²Diamond Light Source - Didcot (United Kingdom), ³Institut de Biologie Structurale - Grenoble (France), ⁴Jülich Centre for Neutron Science - Garching (Germany), ⁵RIKEN SPring-8 Center - Hyogo (Japan), ⁶University of Essex - Colchester (United Kingdom)

Abstract

Oceanic primary production by marine cyanobacteria is a main contributor to carbon and nitrogen fixation on earth. *Prochlorococcus* is the most abundant photosynthetic organism on Earth, responsible for a comparable carbon fixation to the net global primary production from agriculture. The ecological success is rooted in genome reduction and ability to thrive in nutrient depleted waters. The single FutA protein in *Prochlorococcus* has a function in iron uptake through as a periplasmic binding protein to the specialised ABC where it would bind iron in the ferric state (Fe³⁺). However, in the cytosol FutA proteins are known to bind ferrous iron (Fe²⁺).

Studies of metal binding proteins are hampered by X-ray induced photoreduction, in this case leading to conversion from the ferric to the ferrous oxidation state. We used serial femtosecond crystallography (SFX) and neutron diffraction to obtain crystallographic structures of the oxidised state, revealing penta-fold coordination of the metal. X-ray induced photoreduction using rotation methods and serial synchrotron dose series (SSX) then gave access to the reduced ferrous state. Structural changes were mapped at room temperature several dose points up to 110 kGy before global radiation damage becomes too severe, defining the sweet spot of such analyses in this case.

References

Beale JH, Bolton R, Marshall SA, Beale EV, Carr SB, Ebrahim A, Moreno-Chicano T, Hough MA, Worrall JAR, Tews I, Owen RL. Successful sample preparation for serial crystallography experiments. *J Appl Crystallogr.* 52 (2019), 1385-1396.

Horrell S, Axford D, Devenish NE, Ebrahim A, Hough MA, Sherrell DA, Storm SLS, Tews I, Worrall JAR, Owen RL. Fixed Target Serial Data Collection at Diamond Light Source. *J Vis Exp.* 2021 Feb 26, 168.