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Combined neutron- / X-ray crystal diffraction reveals switches for Fe(II) / Fe(III) binding in the cyanobacterial iron binding protein FutA that are resolved by XFEL X-ray induced photoreduction

Thursday 5 December 2024 13:05 (35 minutes)

Marine cyanobacteria are main contributors to carbon and nitrogen fixation, yet they are limited by iron availability. The most abundant and smallest photosynthetic organism on Earth is the cyanobacterium *Prochlorococcus* that can thrive in low nutrient waters. Interestingly, in contrast to most cyanobacteria that possess two FutA proteins to bind Fe(II) and Fe(III), *Prochlorococcus* has a single FutA iron binding protein, but the mechanism that would allow this single FutA protein to bind two different iron charge states remained unknown. Here we used neutron and X-ray diffraction to characterise FutA iron binding in different oxidation states at room temperature. The neutron diffraction study characterised the oxidised Fe(III) iron binding state, while a home source X-ray diffraction dataset revealed a reduced Fe(II) iron binding state. We characterised X-ray induced photo-reduction of the iron centre by spectroscopy. To study the transition between states we optimised crystallisation for serial experiments and designed a novel X-ray pump probe experiment that used an attenuated XFEL pulse for photoreduction, followed by a productive pulse to record data. The experiments reveal an alternative positioning of the Arg203 side chain in the second coordination shell of iron to maintain an overall charge neutral binding site for Fe(II) and Fe(III) states. This molecular switch provides a plausible mechanism for iron binding promiscuity. PNAS 121 (2024): e2308478121.

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