

**MS06-2-4 XFEL investigation of redox crosstalk within the ribonucleotide reductase R2b-NrdI complex
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Abstract

Ribonucleotide reductase R2b contains a di-manganese carboxylate centre that generates an organic radical with the help of the oxygen-activated flavoprotein NrdI, making the R2b-NrdI complex a system with two different redox-active centres. Redox-active protein centres are a challenging target for investigation with standard single crystal synchrotron crystallography. The extended exposure to intense X-rays during data collection often leads to photoreduction of the redox-active species, impeding the determination of defined oxidation states. Serial femtosecond crystallography (SFX) utilizing an X-ray free electron laser mitigates the problem of photoreduction by shortening the X-ray exposure by several orders of magnitudes. Here we present two SFX structures of the ribonucleotide reductase R2b-NrdI complex in defined oxidation states and demonstrate structural rearrangements and crosstalk within the complex (1).

References

(1) "Redox-controlled structural reorganization and flavin strain within the ribonucleotide reductase R2b-NrdI complex monitored by serial femtosecond crystallography" Juliane John, Oskar Aurelius, Vivek Srinivas, In-Sik Kim, Asmit Bhowmick, Philipp S. Simon, Medhanjali Dasgupta, Cindy Pham, Sheraz Gul, Kyle D. Sutherlin, Pierre Aller, Agata Butryn, Allen M. Orville, Mun Hon Cheah, Shigeki Owada, Kensuke Tono, Franklin D. Fuller, Alexander Batyuk, Aaron S. Brewster, Nicholas K. Sauter, Vittal K. Yachandra, Junko Yano, Jan Kern, Hugo Lebrette, Martin Högbom bioRxiv 2022.04.14.488295; doi: <https://doi.org/10.1101/2022.04.14.488295>