Report CH/6140 ID15B

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Beamline and data collection parameters

Detector Eiger 9M
λ = 0,41 Å
Distance = 250,1652 mm
Beam size ~10 μm * 10 μm
Cell alignment: U20 with a 11 mm gap
Data collection: U20 with a 12.6 mm gap

Data collection

We were not able to obtain suitable xylanase crystals for the run.

Instead, we have collected data on a very interesting protein, a human NAD kinase (NADK), which undergoes allosteric modifications upon activation (1).
We collected data on different NADK crystals, at ambient or under high pressure: 140 MPa, 150 MPa, 190 MPa, 230 MPa.
The crystals were very fragile and melt under pressure above 2000 bar.
We tried to stabilize them with addition of glycerol, without any success.

We also collected data on a collagen-like peptide: $(Pro\text{-}Pro\text{-}Gly)_{10}$ (PPG)
The PPG crystals were very resistant to pressure, and diffracted at high resolution. We collected data at ambient pressure, 240 MPa and 860 MPa. However, we were unable to index the data with the good crystallographic cell, due to the repetitive nature of the triple helix, preventing the refinement process.

We also collected data on another model of collagen-like peptide: $(Pro\text{-}Hyp\text{-}Gly)_{10}$ (POG), where Hyp stand for hydroxyproline (denoted O). We collected data on POG crystals at ambient pressure, 250 MPa, and 540 MPa. However, the crystals were very fragile, with a lamellar packing and melt under pressure.

Scientific results

Studying NADK behavior under pressure is still very interesting, but we need to optimize the crystallization condition to obtain more resistant crystals.
To avoid the repetitive nature of the triple helix which lead to failure in the indexation and refinement processes, and to have a better chance of success, we schedule to study the behavior of another collagen-like peptide: $Pro\text{-}Hyp\text{-}Ala\text{-}(Pro\text{-}Hyp\text{-}Gly)_9$.

We also schedule to study the $(Gly\text{-}Pro\text{-}Hyp)_9$ crystals under pressure whose crystals are not lamellar, and should be more resistant to pressure.

(1) : Mary C et al., 2022 Mol Cell., 82, 32969-3311