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Near-Physiological-Temperature Serial Femtosecond X-ray Crystallography Reveals Novel Conformations of SARS-CoV-2 Main Protease Active Site

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Radiation damage is one of the major limitations of x-ray crystallography. XFELs provide ultrafast and ultrabright X-ray pulses allowing data collection without secondary radiation damage at ambient temperature. Here, we determined the crystal structure of Severe Acute Respiratory Syndrome CoronaVirus-2 main protease by serial femtosecond x-ray crystallography. To compare the structural changes caused by radiation damage, we calculated the radiation damage on our structure and compared it to other main protease structures that are obtained from different x-ray sources. Our work not only shows the effect of radiation damage but will also provide structural dynamics of the main protease for drug repurposing and structure-based drug design studies against SARS-CoV-2.

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