"Enhanced peer review" - rebuilding early SARS-CoV-2 structures in ISOLDE

Tristan Ian Croll

University of Cambridge, Cambridge, United Kingdom tic20@cam.ac.uk

The first few months of the SARS-CoV-2 pandemic illustrated, in many ways, the level of maturity and essential nature of modern structural biology. The outbreak was given official pandemic status on 11 Feb 2020 - six days *after* the release of the first crystal structure of the main protease; the first cryo-EM structure of the spike protein was released just two weeks later. These were the first of a flood of new structures - most, in a strong break with tradition, released well before the associated manuscripts. This, combined with the recent decision by the worldwide Protein Data Bank to allow re-versioning of submitted structures by the authors, allowed for an almost unprecedented scenario: while the experimentalists worked to get these critically important structures solved as quickly as possible, specialists in model building and refinement could check and (where necessary) improve their models, returning the results to the original authors often before their papers were ever published.

In this talk I will discuss some of my observations arising from inspecting and rebuilding some three dozen early SARS-CoV-2 and SARS-CoV-1 structures. In a great many respects, the remarkable improvement in the rate of modelling errors between SARS-CoV-1 and -2 structures shows just how far the field has come. However, the devil is in the details, and various classes of repeated errors in the modern structures point to the need for further improvement in model-building and validation methods.

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