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The Coronavirus Structural Taskforce

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During the COVID-19 pandemic, structural biologists rushed to solve the structures of the 28 proteins encoded by the SARS-CoV-2 genome in order to understand the viral life cycle and to enable structure-based drug design. In addition to the 204 previously solved structures from SARS-CoV-1, over 2000 structures covering SARS-CoV-2 viral proteins have been released in a span of a 2 years. As structural models are available, researchers from different backgrounds use them as a basis for further analysis. Molecular dynamics simulations, docking studies and bioinformatics modelling are just an example of the possible use of those data. However, all modelling is prone tov error and structural biology is not immune to that. I will present here the efforts of the Coronavirus Structural Task Force [1], a spontaneous gathering of scientists who tried to target the issue by fixing errors when possible, sharing our findings with the broader community and communicating about the culture of errors in structural biology. A few key findings, as well as a wider discussion about the role of open science in the current days will be the core of my presentation.

[1] Croll, T., Diederichs, K., Fischer, F., Fyfe, C., Gao, Y., Horrell, S., Joseph, A., Kandler, L., Kippes, O., Kirsten, F., Müller, K., Nolte, K., Payne, A., Reeves, M.G., Richardson, J., Santoni, G., Stäb, S., Tronrud, D., Williams, C, Thorn, A*. (2021) Making the invisible enemy visible (2021) Nature Structural & Molecular Biology 28, 404–408 https://doi.org/10.1038/s41594-021-00593-7

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