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The Coronavirus Structural Taskforce

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The Coronavirus Structural Task Force [1] was an ad hoc collaboration of mostly junior researchers across nine time zones, brought together by the desire to fight the pandemic.

Most of us are crystallographic methods developers and as early as February 2020, we started evaluating the structures of macromolecules in SARS-CoV and later SARS-CoV-2 as they became available from the Protein Data Bank. We found that many could be improved. A website (www.insidecorona.net) and a database containing the evaluations and revised models were set up to aid in-silico drug discovery and other downstream research. Newly deposited structures are analysed as they come out by a bespoke structure evaluation/comparison pipeline. In addition, many individual structures were revised manually, atom-by-atom. In order to spread knowledge about the structural biology of the virus, we also reviewed the literature, putting the molecular models into a larger context for the rapidly growing community of researchers - drug developers, bioinformaticians, crystallographers - tackling the COVID-19 pandemic. We established a large network of COVID-19 related research, and forged friendships and collaborations across national boundaries.

As public outreach is so important right now, we also refine structures live on Twitch, write articles and offer a 3D printable virus model for schools.

[1] Croll, T., Diederichs, K., Fischer, F., Fyfe, C., Gao, Y., Horrell, S., Joseph, A. P., 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. (2020). *BioRxiv*. doi:10.1101/2020.10.07.307546.

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