

## The Coronavirus Structural Task Force

Andrea Thorn

*Institut für Nanostruktur und Festkörperphysik, Universität Hamburg, Luruper Chaussee 149 (Bldg. 610 - HARBOR), Germany  
andrea.thorn@uni-hamburg.de*

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 1000 structures covering 18 of the SARS-CoV-2 viral proteins have been released in a span of a few months. These structural models serve as the basis for research to understand how the virus hijacks human cells, for structure-based drug design, and to aid in the development of vaccines. However, errors often occur in even the most careful structure determination -and may be even more common among these structures, which were solved quickly and under immense pressure. The Coronavirus Structural Task Force [1] has responded to this challenge by rapidly categorizing, evaluating and reviewing all of these experimental protein structures in order to help downstream users and original authors. In addition, the Task Force provided improved models for key structures online, which have been used by Folding@Home, OpenPandemics, the EU JEDI COVID-19 challenge and others. We set up a website ([www.insidecorona.net](http://www.insidecorona.net)) and a database containing our evaluation and revised models; we met online every day, working on an automatic structure evaluation and revising individual structures. We also engaged in outreach activities, writing blog posts about the structural biology of SARS-CoV-2 aimed at both the scientific community and the general public, refining structures live on Twitch and offering a 3D printable virus model for schools. In the beginning, there were no tenured academics in the Coronavirus Structural Task Force; we were an ad hoc collaboration of 24 researchers across nine time zones, brought together by the desire to fight the pandemic. Still, we were able to rapidly establish a large network of COVID-19 related research, forge friendships and collaborations across national boundaries, spread knowledge about the structural biology of the virus and provide improved models for in-silico drug discovery projects.

- [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., Stüb, 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>

**Keywords: coronavirus, structural biology, biocrystallography, cryo-em, validation**