

# Structural Analysis of Severe Acute Respiratory Syndrome Coronavirus-2 Proteins: Exploring Mutations in Nsp13

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Severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), discovered in December 2019, caused the COVID-19 global pandemic. SARS-CoV-2 belongs to the family, Coronaviridae, which is composed of positive-stranded RNA viruses. These viruses are known to have one of the largest RNA viral genomes, which consists of approximately thirty-thousand base pairs. The SARS-CoV-2 genome encodes both non-structural proteins, which assist in replication of the virus upon infection, and various structural and assembly proteins. As part of a virtual summer research experience with the RCSB PDB, we studied how SARS-CoV-2 proteins evolved during the first six months of the COVID-19 pandemic by exploring amino acid sequence and 3D atomic-level structure using various structural bioinformatics tools, including Clustal Omega ([www.ebi.ac.uk/Tools/msa/clustalo/](http://www.ebi.ac.uk/Tools/msa/clustalo/)) for sequence alignments and phylogenetic trees; Mol\* ([molstar.org](http://molstar.org)) for 3D molecular visualization; and Foldit ([fold.it](http://fold.it)) for structural/energetic effects of sequence mutations. The focus of this poster is SARS-CoV-2 non-structural protein 13 (Nsp13), a 596-residue protein consisting of five domains. Nsp13 functions as a helicase, unwinding double-stranded RNA. Helicase activity depends on NTP hydrolysis, catalyzed by six conserved active site residues. Nsp13 synergizes with the viral RNA-dependent RNA polymerase, a heterotetramer consisting of once copy of Nsp7, two copies of Nsp8, and one copy of Nsp12. Nsp13 represents a potential target for discovery and development for small molecules that combat SARS-CoV-2. Studying the structure of this protein will enhance our understanding of its mechanism of action and ways to inhibit the enzyme.

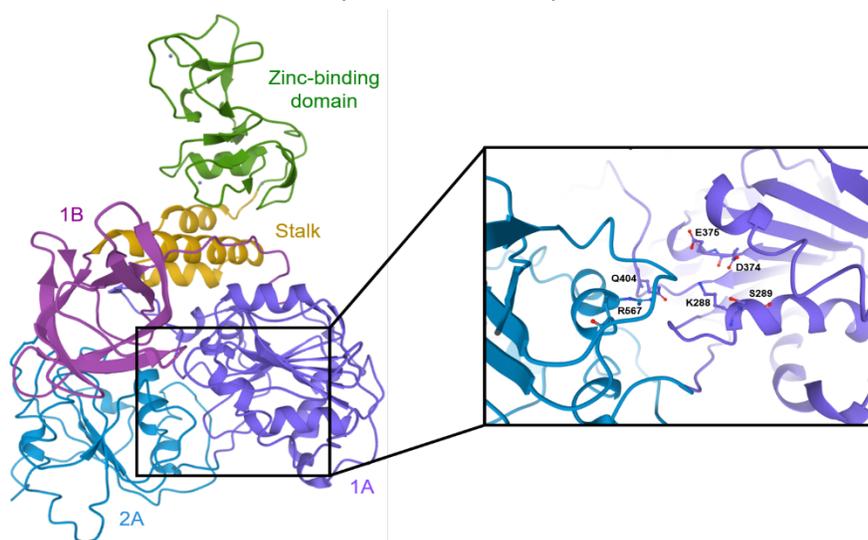


Figure 1.