

As in PDB , knowledge of basic components like nucleotides and proteins are present in the form of text so finding their presence can be done using the text file version of pdf. Now we should analyse the spatial information and the differences which are created using the basic biological components . As the relative structural conformation is important to us .

Say we focus on spike protein of Covid 19 :

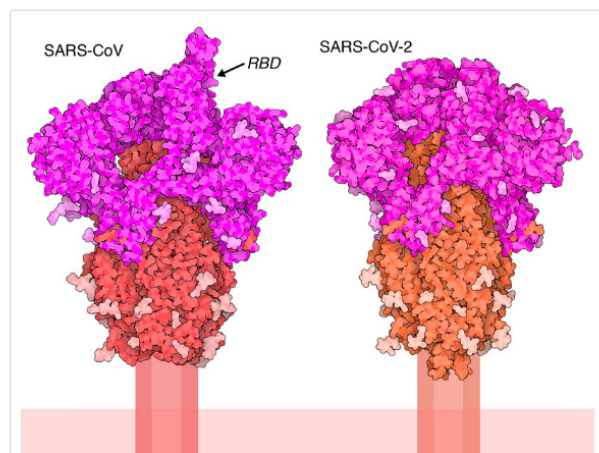
SARS-CoV-2 Spike

Coronavirus spike protein binds to receptors on cell surfaces, and is a target for vaccine development.

The research community has quickly mobilized to fight the current SARS-CoV-2 pandemic, building on years of work on the previous SARS-CoV virus. The spike protein of this virus will be a central figure in this fight, since it is the primary target of antibodies that provide immunity against the virus. The surfaces of coronaviruses are covered with these spikes, giving them their distinctive crown-like appearance in electron micrographs. The spikes initiate the process of infection, binding to receptors and then fusing with the cell membrane to release the viral genome inside. Many other enveloped viruses use similar spike-like proteins to infect cells, including influenza hemagglutinin, and the envelope glycoproteins of HIV-1 and ebola.

Cut to Size

The spike protein is composed of three identical chains, that together form a complex with a small domain inside the virus, a membrane-spanning segment, and a large ectodomain that extends outward from the virus. In addition, the spike is a glycoprotein: the ectodomain is covered with sugar chains that help to mask the virus from the immune system. The structures of SARS-CoV and SARS-COV-2 spikes shown here (PDB entries 6crz and 6vxx) include only the ectodomain, and as you can see, they are very similar. Each chain is synthesized in one piece, but then is clipped by cellular proteases into two functional pieces. The outer S1 fragment, colored magenta, binds to cellular receptors, and the S2 fragment, colored red, directs fusion of the virus with the cell. Both of these structures include only portions of the many sugar chains that coat the spike, since the sugars are highly flexible and difficult to observe.



<https://pdb101.rcsb.org/motm/246>

The structures of SARS-CoV and SARS-COV-2 spikes shown here :

