

SARS-CoV-2 genome sequences were available in January 2020
 Rosetta@home volunteers modeled structures of important gene sequences soon after
 and continue to model structures for researchers around the world

<https://rosetta.bakerlab.org>

Robetta Project - Structure Prediction - admin - Log out

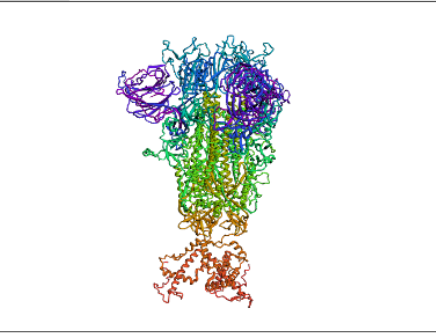
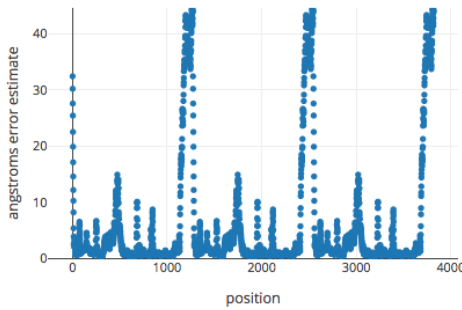
SSGCID - BewuA.18655.a Spike glycoprotein S Download Models

Job ID	Status	Method	Username	Target	Length	Date (PST)	Expiration Date (PST)
15652	Complete	Structure prediction	ssgcid	SSGCID - BewuA.18655.a Sp...	1273	8 Feb 2020	-

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sequence: MFVFLVLLPLVSSQCWNLTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPFFSNVTWFHAIHVSNGTKRFDNPVLPFNDGVYFASTEKSNIIIRGWIFGTTL
deepconcf: -EEEEEEEE-EEEE-EE-EE-EEEEEE-EE-EE-EEEEEEEE-EEEEEE-
psipred:  -EEEEEE-EEEE-EE-EE-EEEEHH-HHHEEEEE-EE-EE-EEEEEE-EEEE-
spider3:  EEEEEEE-EEEE-EE-EEEEEE-EEEEEE-EEEEEE-EEEEEE-EEEEEE-
disopred:
tmhmm:
  
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Model 1 Model 2 Model 3 Model 4 Model 5

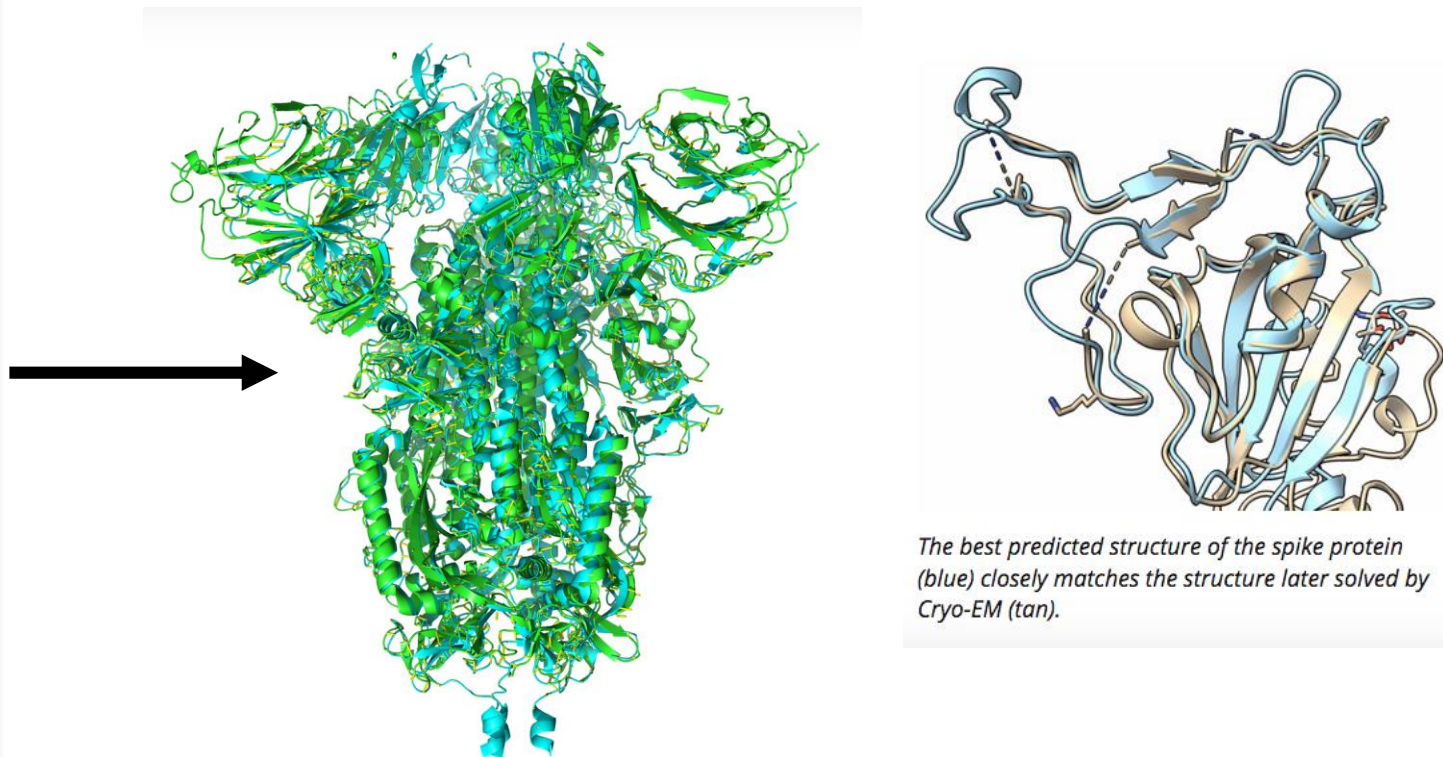



Color by - | Download - | View Powered by 3Dmol.js

Domain ID	Domain	Parse	Confidence	Modeling Method	Model Span	Length	Date (PST)
15556	1	1	0.50	comparative modeling	1-1273	1273	9 Feb 2020

POWERED BY BOINC


Superposition of R@h model of Spike protein
 Within 1.6 angstroms rmsd to 6vxx covering 2236 CA atoms



PDB RCSB Molecule of the Month

Spike protein 6vxx released March 2020 from David Veessler's lab at the UW Biochemistry Department
RBD with ACE2 receptor also released from Qiang Zhou's lab at Westlake University, Zhejiang Province, China

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Educational portal of  **Celebrating 20 YEARS OF Molecule of the Month**

Molecule of the Month By Category By Date By Title

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

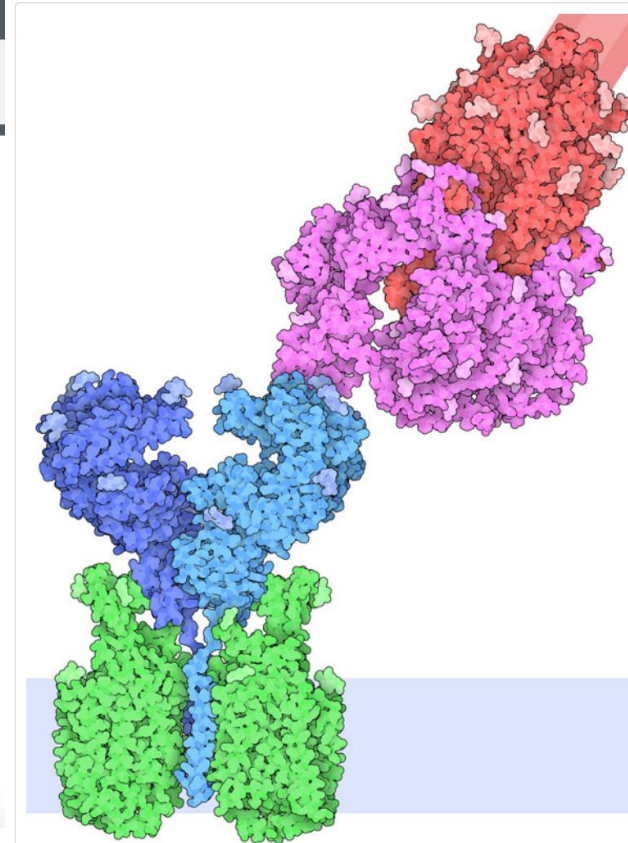
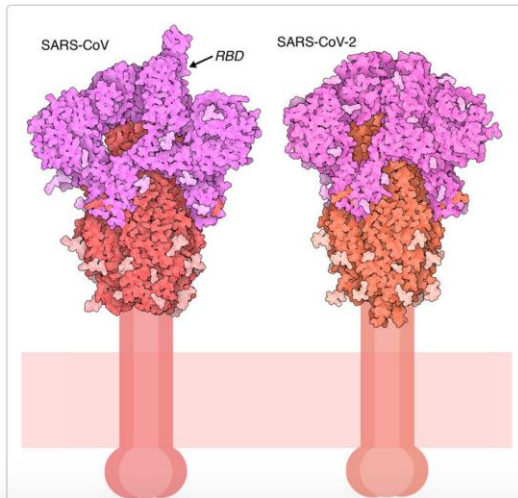


Illustration of a complex of the spike protein (red and magenta) bound to its receptor ACE2 (blue). ACE2 is part of a complex with the amino acid transporter B0AT1 (green). The cell membrane is shown schematically in light blue at the bottom.

Receptor Binding

Spike protein binds to ACE2 (angiotensin-converting enzyme 2) on the surface of cells. ACE2 is an enzyme that activates angiotensin, a peptide hormone involved in control of blood pressure. ACE2 is found on lung, heart, kidney, and intestinal cells, making these cells the target for infection by the virus. PDB entry 6m17 reveals the complex of ACE2 with the receptor-binding domain of the SARS-CoV-2 spike. In the complex, ACE2 is also bound to the amino acid transporter B0AT1. The illustration was created by superimposing this complex with the structure of the spike protein in PDB entry 6vxx.

Rosetta@home updates since last call

1. Added Linux-ARM platform with help from the ARM development community including Rex St. John, Dmitry Moskalchuk, David Tischler, Lloyd Watts, and Sahaj Sarup

~6000 Linux-ARM hosts with credit (over 135 million credits)
2. Updated Rosetta application to latest source (for COVID related jobs)
3. Fixed various server issues with the database, crediting (use raw PFC), and client job cache (base on run time preference) in response to feedback from the forum