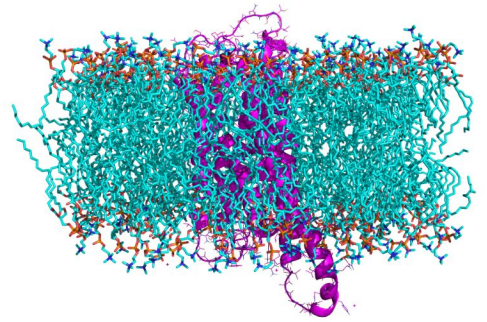
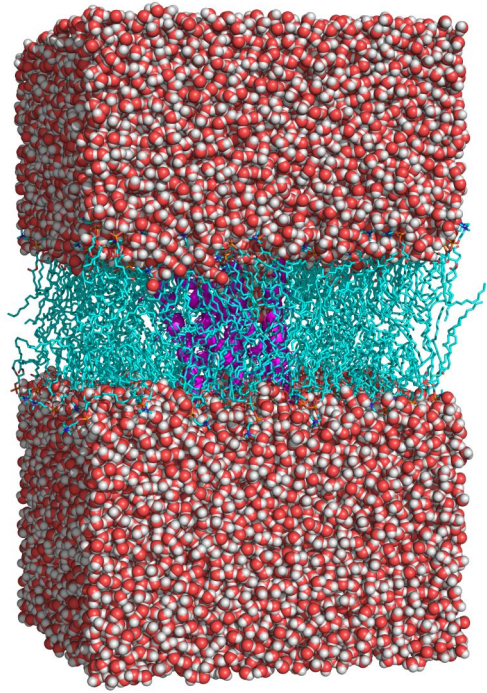


# Molecular Visualisation using PyMOL

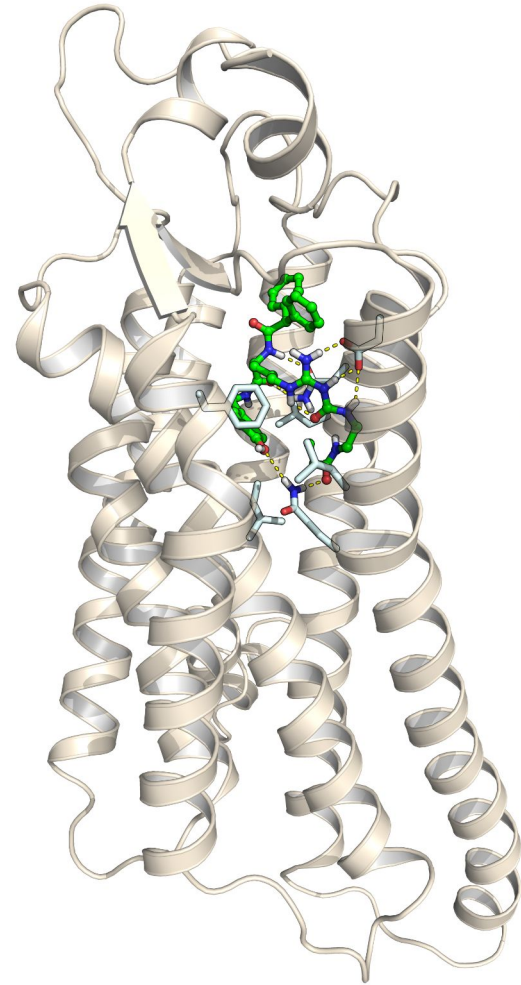
December 14 2022 | Dr. Plamen Dobrev  
Leibniz Supercomputing Centre

1. What is possible in PyMOL?
2. General Introduction to PyMOL
3. Hands-on PyMOL Demo
  1. Examples: G-Protein coupled Receptors and SARS-CoV-2 Proteins
  2. Operating PyMOL (GUI, command line)
  3. Visualizing Biomolecules
  4. Preparation of Publication-Ready Renderings
  5. Speeding up the Rendering by using Supercomputing Resources
4. Q&A

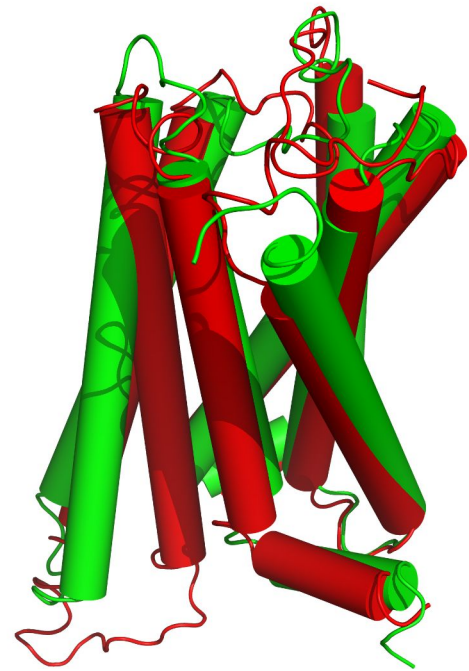
# 1. What is possible in PyMOL? Static Images



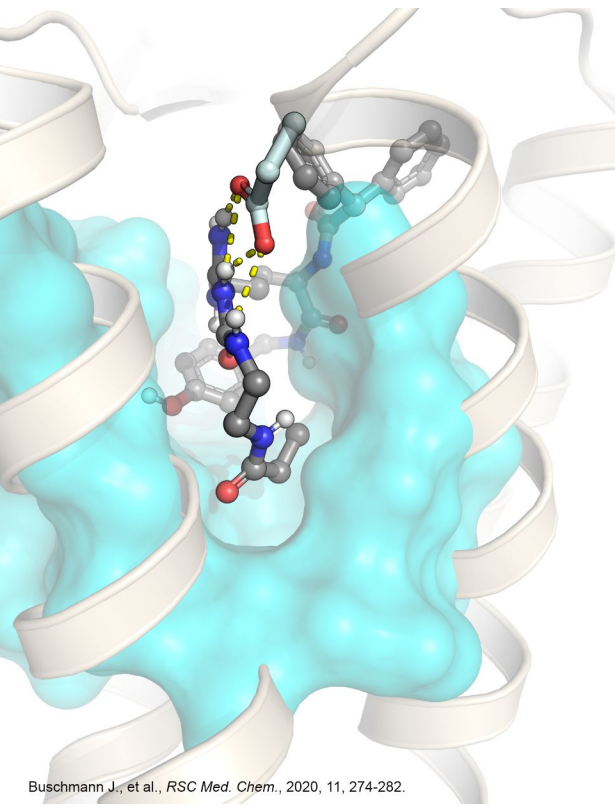
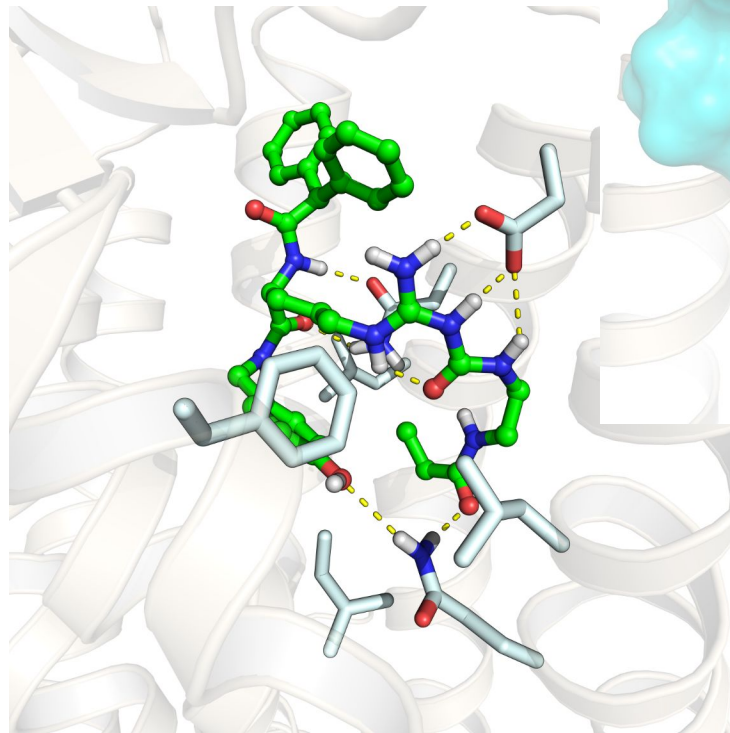
simulation boxes



cartoon  
illustration



cylindrical  
helices



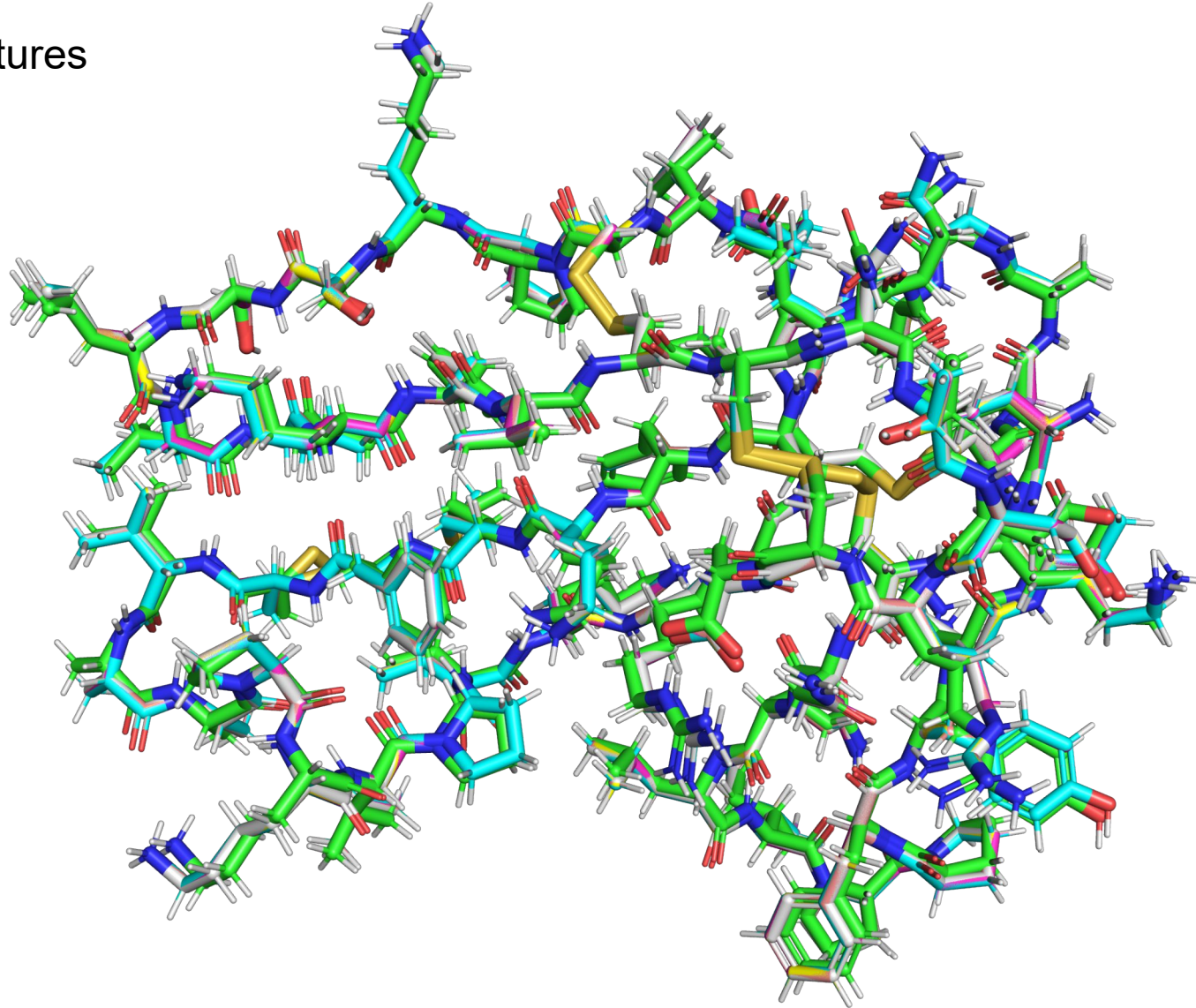
Buschmann J., et al., *RSC Med. Chem.*, 2020, 11, 274-282.

binding pocket and  
surface illustration

## 1. What is possible in PyMOL?

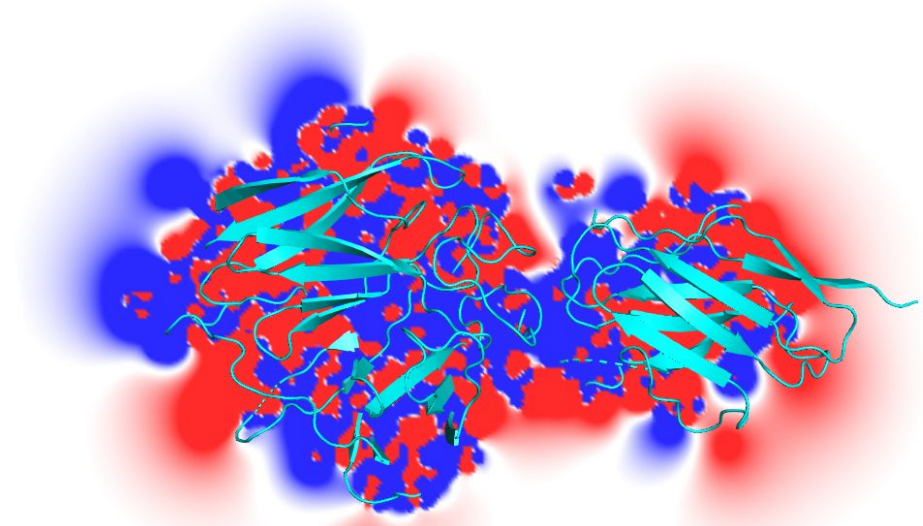
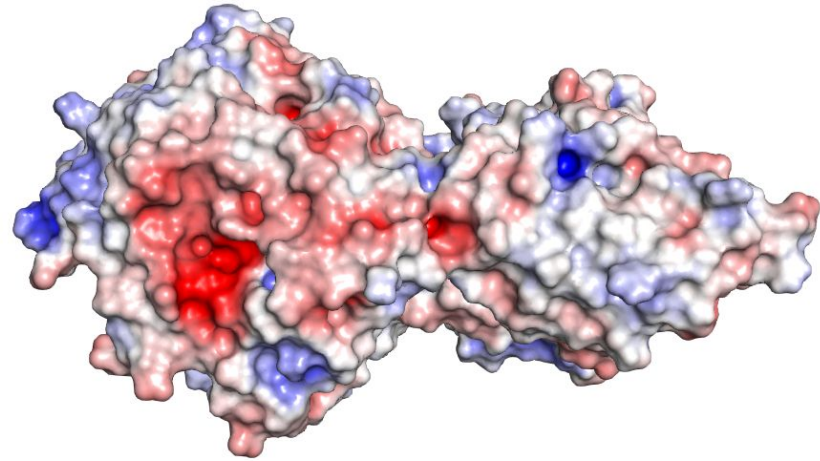
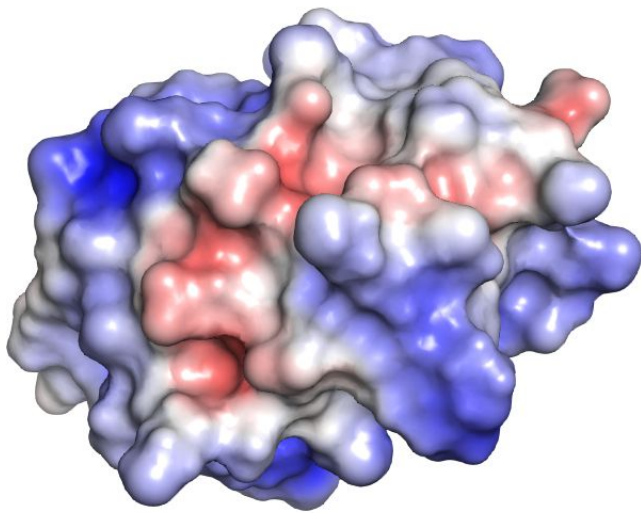
# Calculating physical properties

Optimizing protein structures



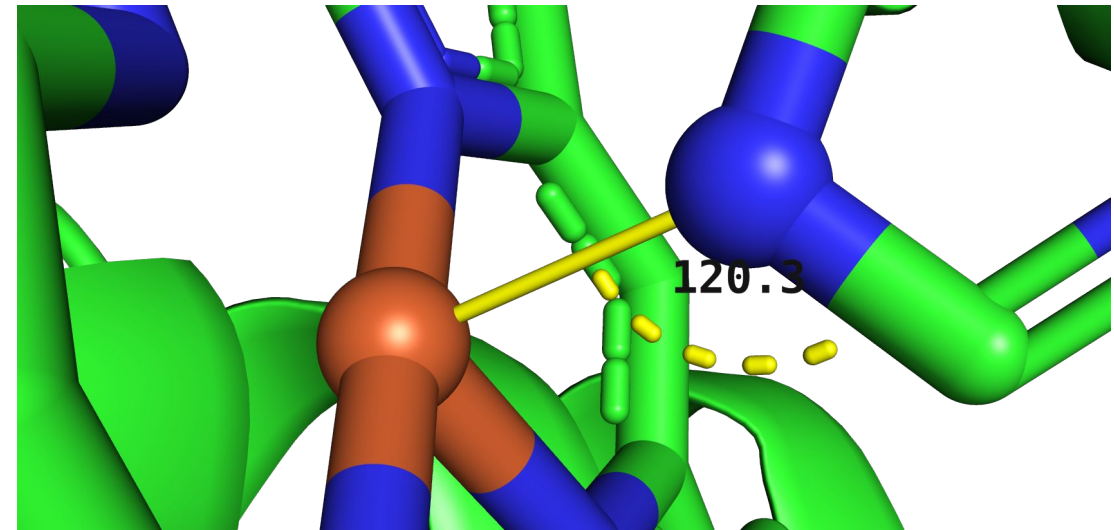
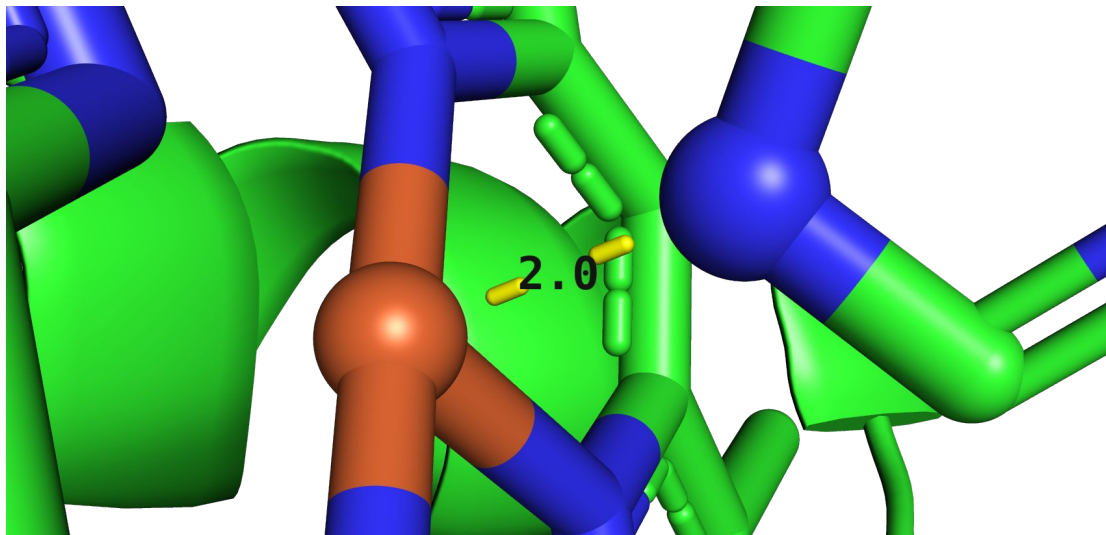
# 1. What is possible in PyMOL? Calculating physical properties

Calculating and visualizing electrostatic potential of proteins



# 1. What is possible in PyMOL?

## Measuring distances and angles



# 1. What is possible in PyMOL?

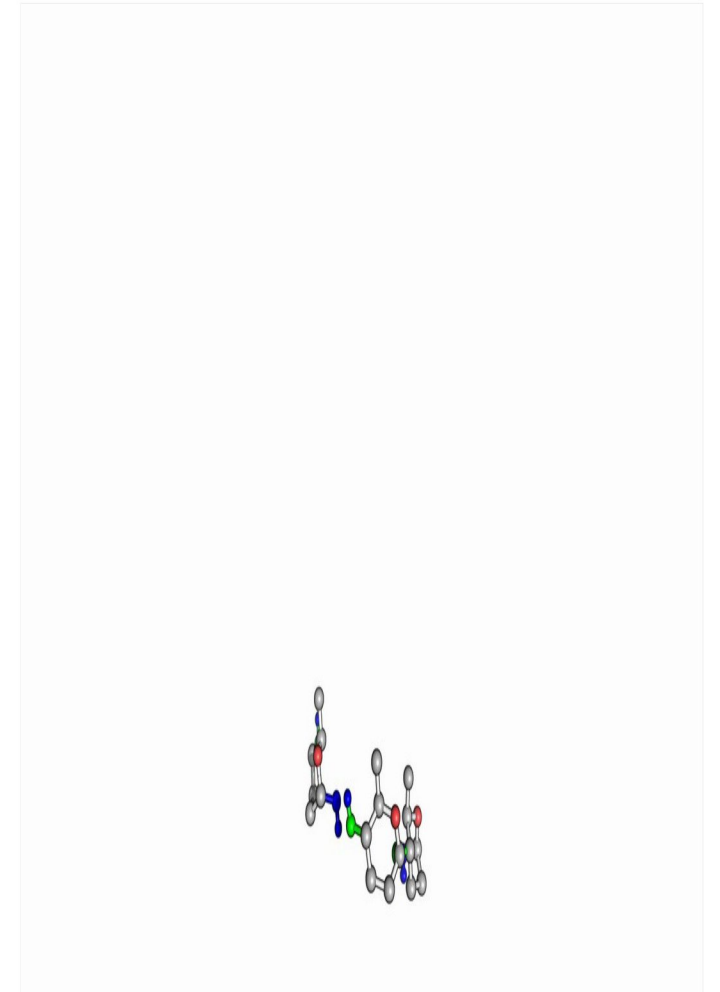
## Movies



scene loop



dynamic processes



animations

### 2.1 Resources



- PyMOL developed by Warren L. DeLano as of 1998
- written in python
- previously with a tk interface, now (from pymol 2.x) with a modern pyqt interface
  
- Incentive PyMOL
  - <https://pymol.org/2/>
  - Wiki: <https://pymol.org/dokuwiki/>
  - Command reference: <https://pymol.org/pymol-command-ref.html>
  
- Open source PyMOL
  - <https://github.com/schrodinger/pymol-open-source>
  - [https://pymolwiki.org/index.php/Main\\_Page](https://pymolwiki.org/index.php/Main_Page)



### 2.2 Installation



- Incentive PyMOL
  - <https://pymol.org/2/> (binaries for Linux, Windows and Mac)
  - <https://pymol.org/edu/> (educational-use only, no research/publications):
- Open source PyMOL
  - Anaconda packages: e.g. `conda install -c conda-forge pymol-open-source (2.5.0)`
  - Windows
    - [https://pymolwiki.org/index.php/Windows\\_Install](https://pymolwiki.org/index.php/Windows_Install)
    - Windows binaries: <https://www.lfd.uci.edu/~gohlke/pythonlibs/#pymol>
  - Linux
    - [https://pymolwiki.org/index.php/Linux\\_Install](https://pymolwiki.org/index.php/Linux_Install)
    - compile source code from <https://github.com/schrodinger/pymol-open-source>
  - Mac
    - [https://pymolwiki.org/index.php/MAC\\_Install](https://pymolwiki.org/index.php/MAC_Install)

## 2. General Introduction to PyMOL

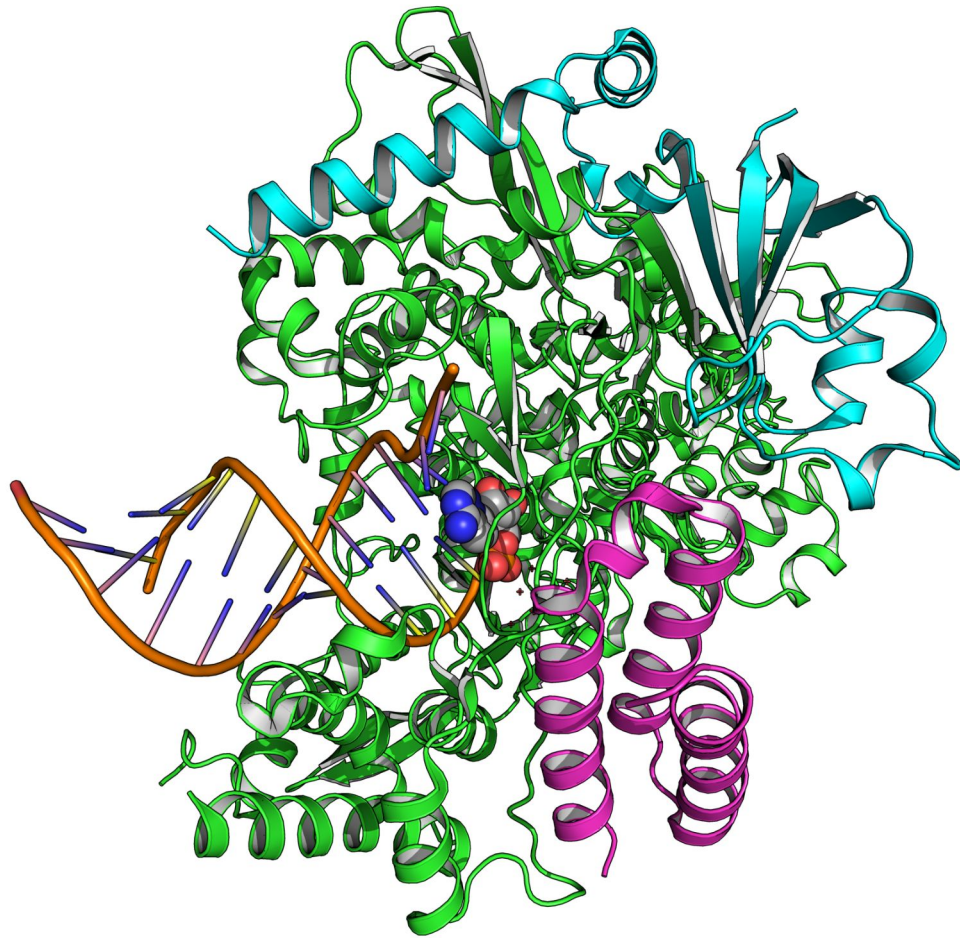
Please install Anaconda Python and PyMOL on your computer



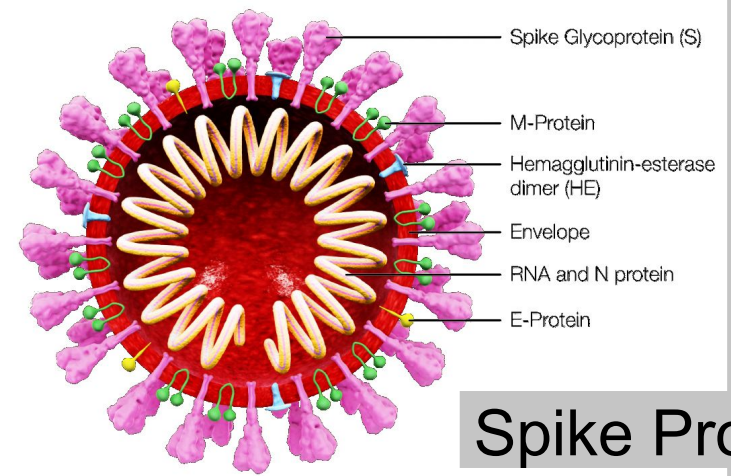
- Download Anaconda Python for your OS on <https://www.anaconda.com/products/individual> or Miniconda on <https://docs.conda.io/en/latest/miniconda.html>
- Install it on your computer
- Install pymol 2.4.0 via conda
  - Open the Anaconda Prompt and execute  
`conda install -c conda-forge pymol-open-source=2.4.0`  
`conda install -c conda-forge pmw`
- Run pymol by starting the Anaconda prompt and typing `pymol`
- Start Jupyter Notebook and open the notebook

### 3. Hands-on PyMOL Demo

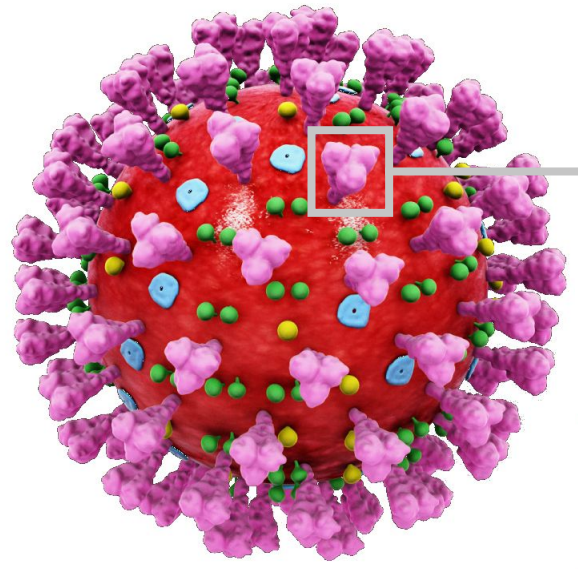
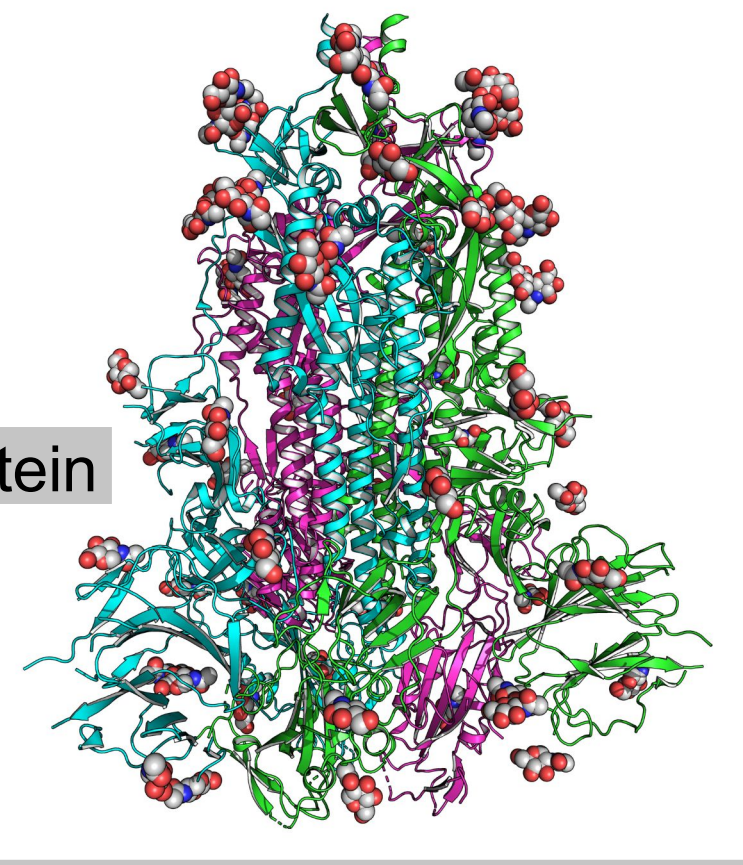
## 3.1 Examples: SARS-CoV-2 Proteins



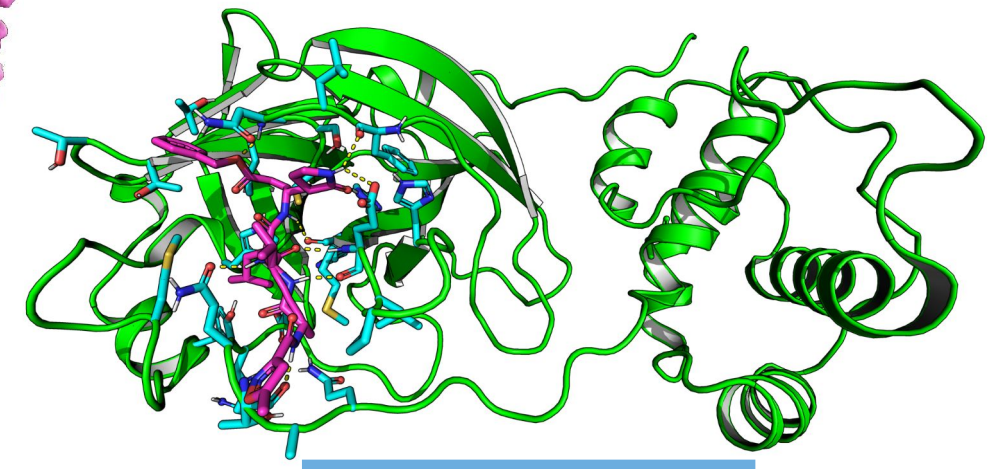
RNA-dependent RNA Polymerase



Spike Protein



Infection



Main Protease

# Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities



Bayerische  
Akademie der Wissenschaften



Since 1962  
260 Employees

**IT Service Backbone for the Advancement of Research Science  
(Munich Universities, Bavaria, Germany, Europe)**



# LRZ “SuperMUC-NG”

**Lenovo Intel (2018)**

**6,480 nodes** Lenovo ThinkSystem

**311,040 cores** Intel Xeon Skylake

**26.9 PetaFlops** Peak

**719 TeraByte** Main Memory

**70 PetaByte** Disk

New GPU accelerated cluster with Intel graphic cards is expected early in 2023

**SUPERMUC-  
NG**

## SARS-CoV-2 Variants of Concern

WHO label	PANGO lineage	First Outbreak	Earliest sample	Notable spike mutations				PDB IDs
				484	452	501	681	
Alpha	B.1.1.7	United Kingdom	Sep 2020		-	<b>N501Y</b>	<b>P681H</b>	
			Jan 2021	<b>E484K</b>	-	<b>N501Y</b>	<b>P681H</b>	7LWS, 7LWV
Beta	B.1.351	South Africa	May 2020	<b>E484K</b>	-	<b>N501Y</b>	-	7LYN, 7LYK, 7LYM
Gamma	P.1	Brazil	Nov 2020	<b>E484K</b>	-	<b>N501Y</b>	-	7M8K
Delta	B.1.617.2	India	Oct 2020	-	<b>L452R</b>	-	<b>P681R</b>	
<p><b>N501Y</b> mutation (Alpha, Beta, Gamma) may help the virus to spread more easily and infect cells</p> <p><b>E484K</b> mutation (Beta, Gamma) may help the virus sidestep some of the body's immune defences (antibody response)</p> <p><b>L452R</b> and <b>P681R</b> might help the Delta variant to spread</p>								

# Q&A

To pose a question, you can write your question  
in the “Chat” tab



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