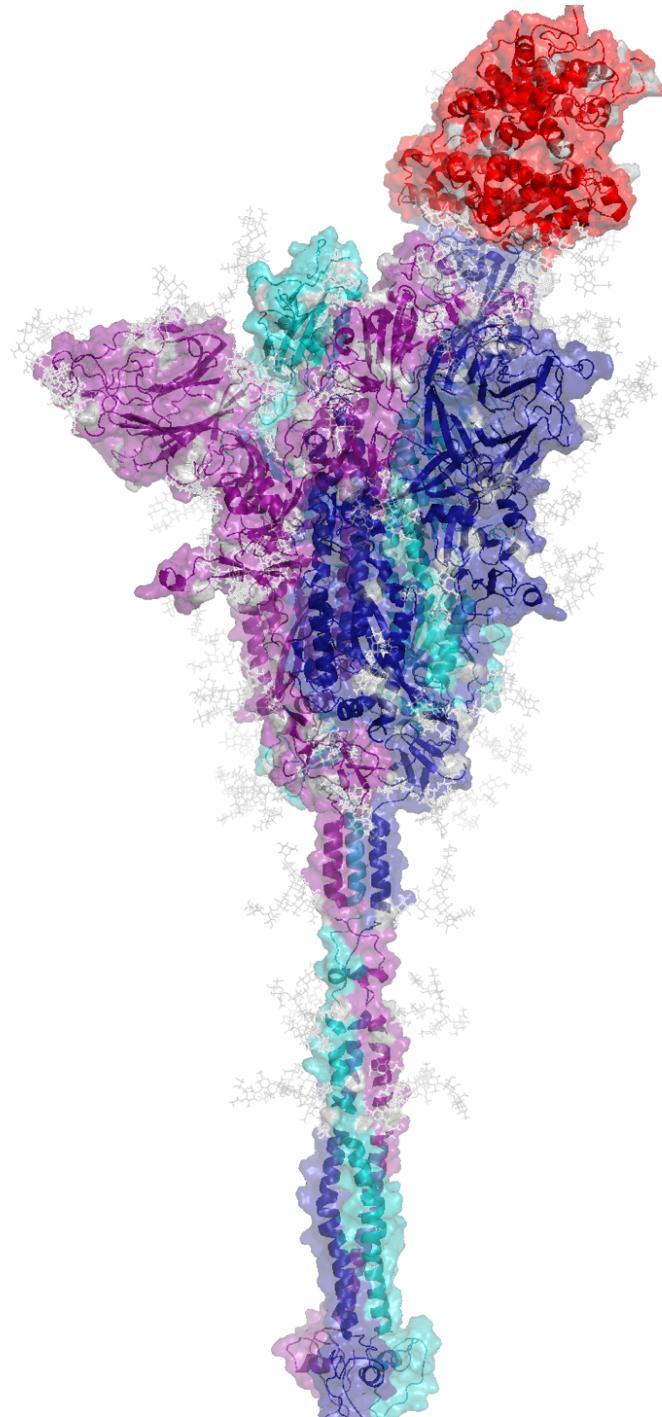


Modeling Spike-Antibody Complexes



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[Tutorial Files are available on GitHub](#)

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Introduction

Proteins are essential biomolecules that perform a wide range of important functions in living organisms, such as catalyzing chemical reactions, transporting molecules, and providing structural support. The structure of a protein refers to a sequence of amino acids that make up the protein and the three-dimensional arrangement of atoms in space.

The importance of protein structure lies in the fact that it directly influences protein function. The specific shape of a protein allows it to interact with other molecules, such as ligands or receptors, in a highly specific manner. A slight change in protein structure can have a significant impact on its function and may lead to a loss of activity or altered activity that can result in disease or other biological processes.

Protein structure is essential for protein function, and understanding protein structure is crucial for the development of new drugs, understanding genetic diseases, and advancing our understanding of biological processes at the molecular level. Molecular modeling is a biophysical method that uses computers to model protein structures and simulate their dynamic behavior. By modeling and simulating protein structure and dynamics, we can gain new insights in protein structure and function that is otherwise inaccessible through current experimental techniques.

The SARS-CoV-2 Spike protein is the primary target for SARS vaccine development. The Spike protein is composed of three identical subunits and is embedded in the membrane of the SARS-CoV-2 virus. The Spike protein binds to the ACE2 host cell receptor to initiate infection and is targeted by antibodies to neutralize the virus. Developing an understanding of the Spike protein structure is essential to developing effective therapeutics and vaccines. A common approach to vaccine development is to study and compare structures of the Spike protein, the Spike-ACE2 complex, and Spike-antibody complexes to determine the structural components necessary for viral infection and effective neutralization by antibodies.

[This video of the SARS-CoV-2 life cycle](#) was made using computer models and simulations of the Spike protein and other SARS-CoV-2 viral components. This tutorial will provide a step-by-step guide to comparing Spike, Spike-ACE2, and Spike-antibody models using the PyMol software. Not all topics can be covered in a short workshop so relevant links will be provided throughout the text for interested users to conduct further learning. The [PyMol Wiki](#) provides many tutorials that cover the many different functions of PyMol.

Software

Installation

Installing PyMol

1. Navigate to [PyMol software download page](#) and select the image that corresponds to your operating system.
2. Double click on the file to launch the installer.
3. Follow the instructions to install PyMol.
4. If you are familiar with conda and prefer a conda install you can also follow the on-screen instructions for conda installation.

Other software

There is other visualization software freely available:

- [ChimeraX](#)
- [VMD](#)
- [Blender](#)
 - Requires the Molecular Nodes plugin
 - For advanced users

Simulation Software

The software used for simulations is separate from visualization software. Due to computational demand, these simulations typically run rather slowly on a laptop computer. It is better to use a GPU workstation or server to run simulations. If you would like to check out some simulation software, [NAMD](#) is freely available, provides user documentation and tutorials, and integrates well with VMD, PyMol, and ChimeraX. There are other simulation software suites available as well.

Tutorial Files

The files for this tutorial are available on the profile [@ScientistAsh on GitHub](#).

These files are based on previously published models^{1–3} that can be found on the [CHARMM-GUI website](#).

References

- (1) Woo, H.; Park, S.-J.; Choi, Y. K.; Park, T.; Tanveer, M.; Cao, Y.; Kern, N. R.; Lee, J.; Yeom, M. S.; Croll, T. I.; Seok, C.; Im, W. Developing a Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein Model in a Viral Membrane. *J. Phys. Chem. B* **2020**, *124* (33), 7128–7137. <https://doi.org/10.1021/acs.jpcb.0c04553>.
- (2) Choi, Y. K.; Cao, Y.; Frank, M.; Woo, H.; Park, S.-J.; Yeom, M. S.; Croll, T. I.; Seok, C.; Im, W. Structure, Dynamics, Receptor Binding, and Antibody Binding of the Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein in a Viral Membrane. *J. Chem. Theory Comput.* **2021**, *17* (4), 2479–2487. <https://doi.org/10.1021/acs.jctc.0c01144>.
- (3) Cao, Y.; Choi, Y. K.; Frank, M.; Woo, H.; Park, S.-J.; Yeom, M. S.; Seok, C.; Im, W. Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. *J. Chem. Theory Comput.* **2021**, *17* (10), 6559–6569. <https://doi.org/10.1021/acs.jctc.1c00552>.

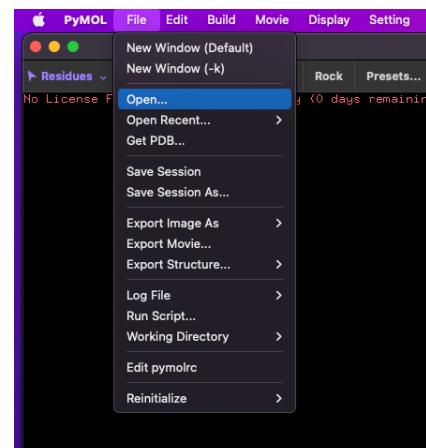
Working with PyMol Objects

In this section you will learn the basic functions of PyMol and the best visualization strategies for looking at the SARS-CoV-2 Spike-ACE2 receptor complex. We will start with loading the Spike-ACE2 complex and displaying the Spike protein bound to the ACE2 receptor. The Spike protein is a homotrimer, composed of 3 identical subunits. The Spike protein also has glycans, or sugar molecules, that are added on to asparagine residues after the protein is translated.

Loading The Spike-ACE2 Complex PDB File

The first step is to load the Spike-ACE2 complex. The pdb file, spike_ace2.pdb¹ contains the atomic coordinates for the SARS-CoV-2 Spike protein, glycans, and ACE2 receptor.

1. Start a PyMol session by double clicking on the PyMol logo. If you installed using conda, you may have to launch your conda environment and call pymol from the command line.
2. Click the Skip Activation button.
3. In the PyMol Menu at the top of the screen, choose File → Open...
4. A File Browser window will appear. Navigate to and select the spike_membrane.pdb file.



You can also drag a file from a file browser window and drop the file into the PyMol viewing window.

PyMol can download a pdb file from the PDB website when the computer is connected to the internet.

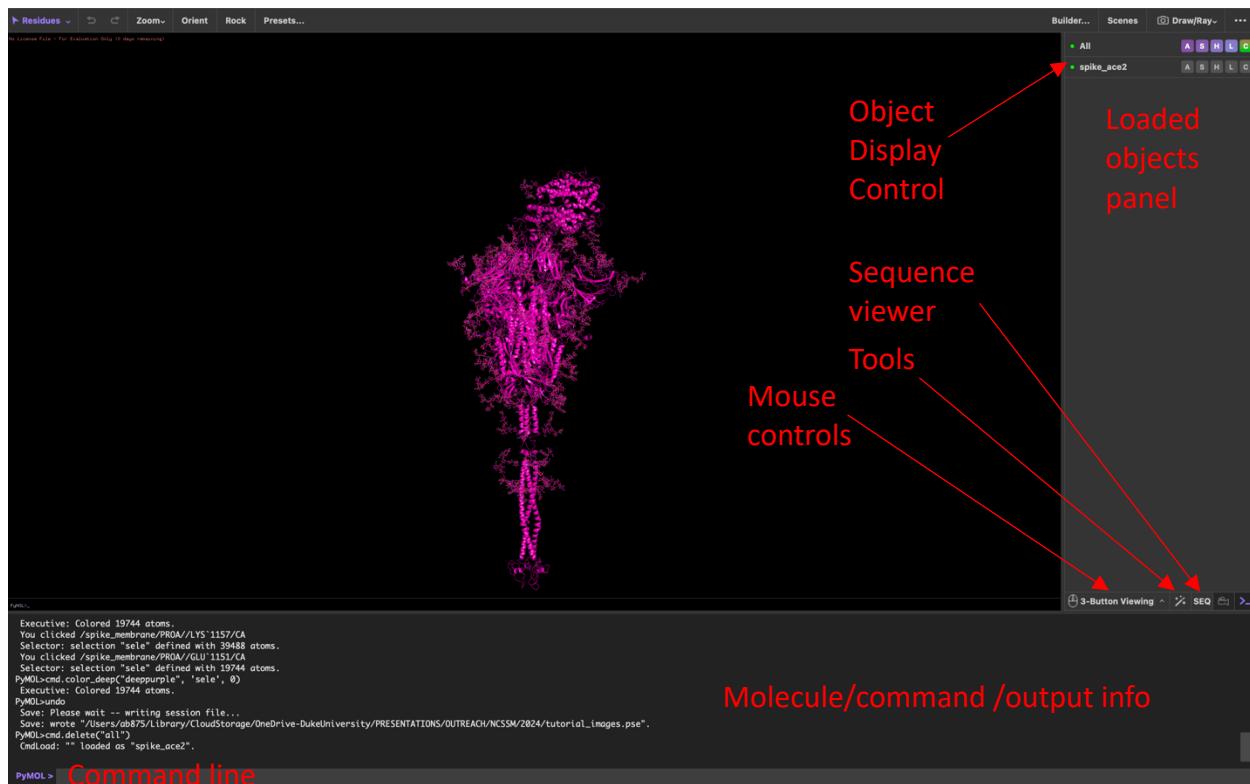
1. Click File > Get PDB...
2. Type the four letter PDB code of the protein in PDB ID entry box
3. Press the Download button.

PyMol will download the pdb file automatically. You can also select to download the X-ray crystallography maps if you select those options.

Now, the SARS-CoV-2 Spike protein, it's associated glycans, and an ACE2 receptor will appear in the PyMol display window. The figure below shows the PyMol viewing window after loading the

spike-membrane PDB file and controls where the various controls are for changing the view and renderings.

The first thing we want to do to build a good rendering is orient the molecule. How you orient the molecule, depends on what you want to show or view. For this tutorial we will view the stalk of the Spike protein sticking out from the bottom of a the receptor binding domain. Use the left mouse button to reorient the Spike protein so that the stalk is pointing towards to bottom of the screen as in the figure below.

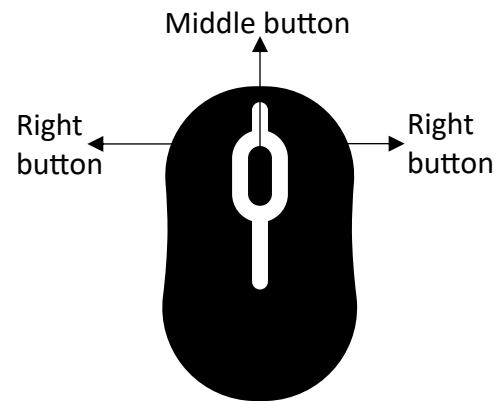


Protein Data Bank: The Protein Data Bank (PDB) is a database that contains the atomic coordinates for experimentally and computationally determined protein structures. Often the first step in modeling proteins is to find a structure of the protein, or a closely related protein, in the PDB. [You can browse the PDB here.](#)

Mouse Controls

PyMol is easiest to use with a three-button mouse as shown in the figure to the right. The mouse buttons control the display window:

1. The right button will zoom the view in/out.
2. The left button will rotate the view.
3. The middle button will move the view.



To center the view around a specific atom:

1. Hover the mouse cursor over the atom of interest.
2. Quickly click and release the middle mouse button.

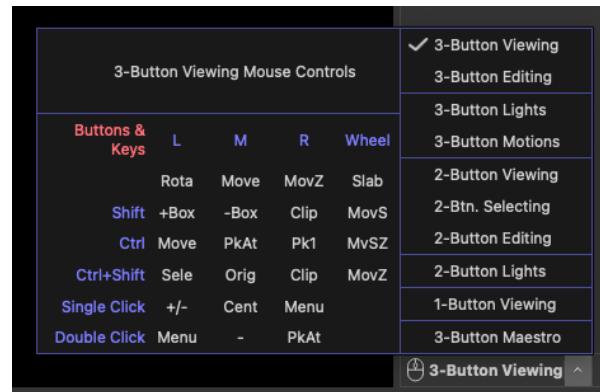
It may also be useful to change the clipping plane or camera as well. The clipping plan and camera controls are described in the table below.

Keyboard	Scroll Wheel Action
No Modifier Key Pressed	Expands or Shrink Slab
Shift Key Pressed	Moves Slab Relative to Camera
Ctrl Key Pressed	Moves Camera and Slab Together
Ctrl and Shift Keys Pressed	Zooms the Camera

<https://pymol.org/dokuwiki/doku.php?id=mouse:clipping>

Typically, you will use PyMol in 3-button viewing mode. However, you may want to change to editing mode or to a two- or one-button mouse mode. To change the mouse mode:

1. Navigate to the bottom right corner of the PyMol viewing window.
2. Click on the carrot icon (^) next to the mouse button.
3. Select the mouse mode you like.

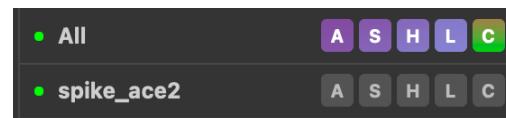


Mouse Control Cheat Sheet: Note that you can view the mouse controls by clicking on the carrot icon (^) and viewing the table to the left of the mode selection panel. You can learn more about PyMol clipping and camera controls at [PyMol clipping controls](#) and [PyMol camera controls](#).

Building a Visualization of the Spike-ACE2 Complex

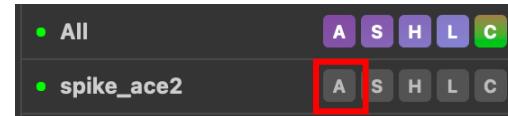
PyMol can display the Spike-ACE2 complex in various ways using both the graphical interface and the command line. The command line offers more flexibility, but the graphical interface is easier to use and provides all the basic functionality needed for publication-quality images.

Each molecule loaded in PyMol is designated as a unique object shown in the object panel. Each object loaded in PyMol has a five-button control panel next to the object name. Using these five buttons, you can create a molecule rendering in the colors and styles of your choice. Additionally, PyMol has a graphical interface for controlling the representation in all loaded objects simultaneously at once. In this section, you will build a representation of the Spike-ACE2 complex.



The Action Button

The action button is denoted by the letter 'A'. The A button next to the object labeled 'All' will apply the action to all loaded objects. To apply an action to only a single object, use the action button next to the listed object. In this case, we will use the action button next for the spike_ace2 object. The action button has controls for:



1. Centering/orienting objects
2. Copy/rename/delete objects
3. Tools for various calculations

Save a Session: To save a PyMol session, use the file menu bar at the top. Click File > Save As... save as a new file or File > Save to save updates to a pre-existing file. A file browser window will pop up and you can save the file in the folder of your choice with a descriptive title. The PyMol session file can be opened by double clicking in a file browser window.

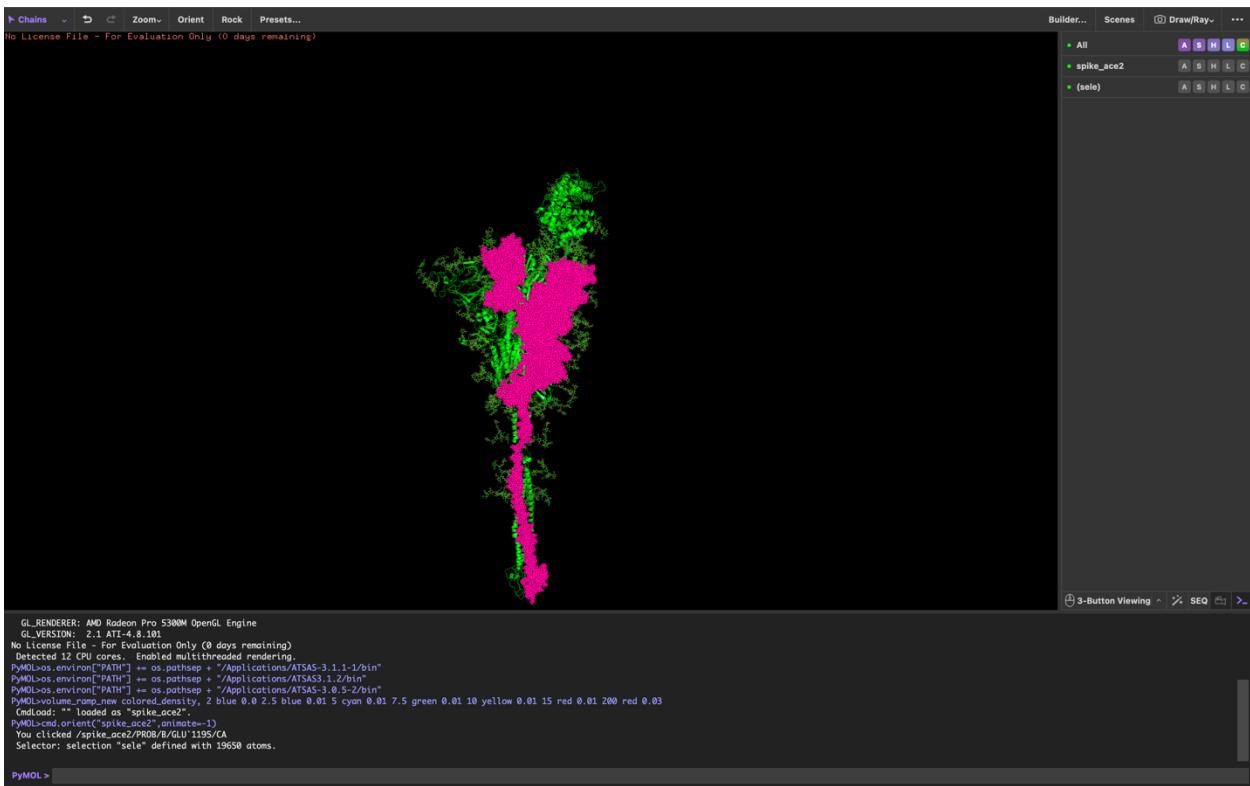
Selections

Selections allow you to apply actions to a specific part of a protein, like a chain or residue type. The default selection mode in PyMol is Residues, so that clicking will select a residue. For this tutorial, we want to render the different chains in different colors so we will change to the Chain selection mode.

1. Click the Residues button in the top left corner of the PyMol visualization window.
2. Select Chains.

Now the mouse selection mode is Chains and you can select specific chains to apply renderings to. Above the membrane there are three helices. Click on the helix in the front to select it. You should now see your chain selection as in the figure below.

This is the basic way of making selections. More complex selections can be made by using the command line. For this tutorial we will rely on the mouse selection mode to build a rendering of the spike-membrane protein.



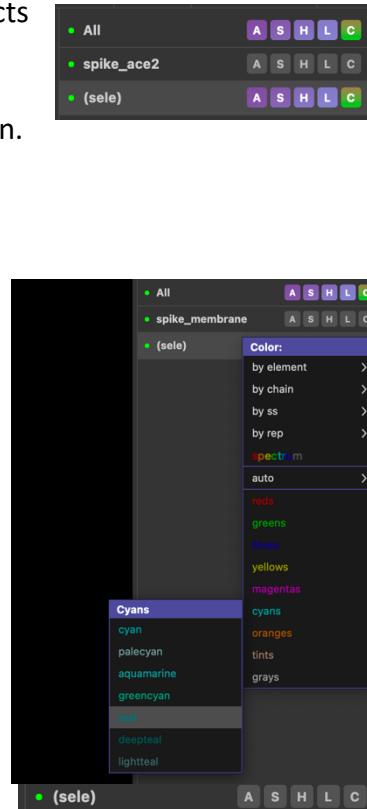
Note that a new object name '(sele)' will appear in the loaded objects panel.

Re-click selection or click away from molecule to unselect a selection.

The Color Button

Now we will use the color button, together with the mouse selection mode, to render the three different chains of the spike protein and the ACE2 in a different colors.

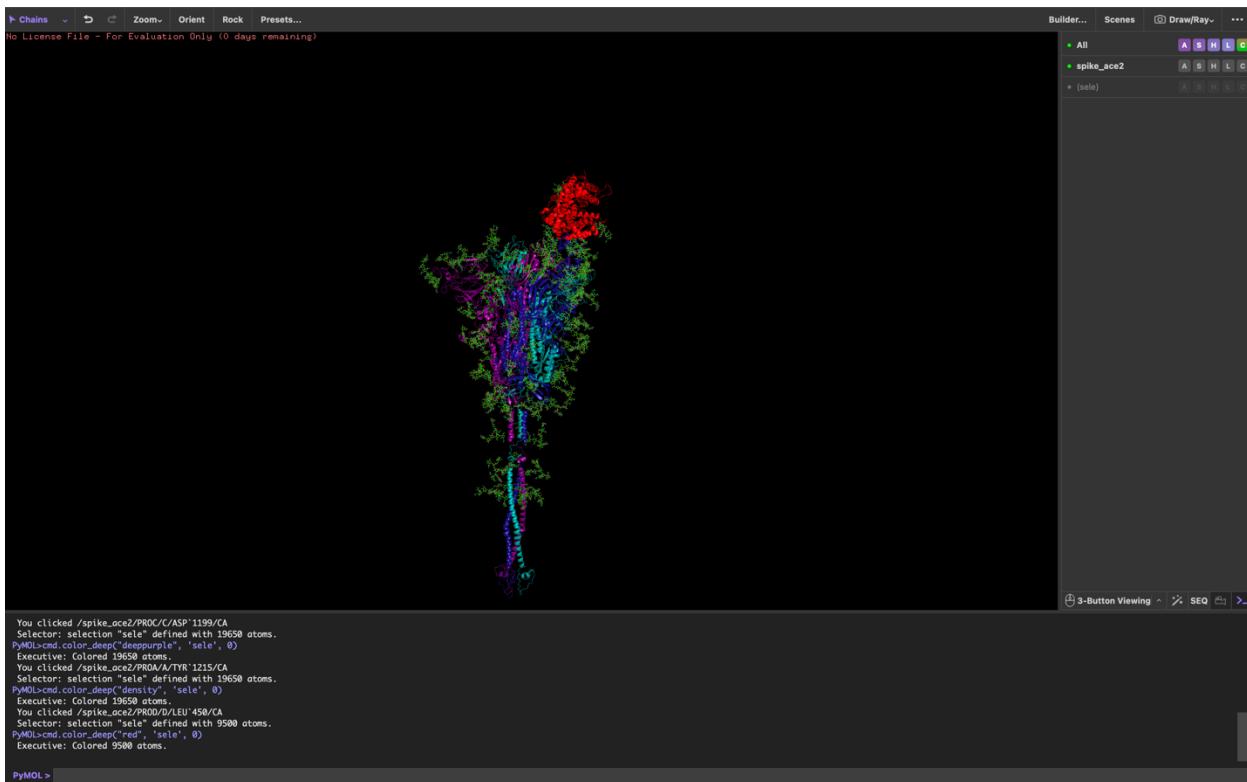
1. Click on C for the `sel` object.
 2. Select a color of your choice. I used the `teal` option from the `cyan` menu.
 3. Click the background of the PyMol viewing window to deselect the chain.



4. Repeat these steps for the other two helices.

You should now see the Spike protein with each chain in a different color.

There is one remaining chain sticking off the top of the Spike protein. This is the ACE2 receptor. Use the above steps to color the ACE2 receptor red. You should now have a representation that looks similar to the figure below.



Using the Command Line

To visualize the glycans and their connecting asparagine (ASN) residues we need to use the command line for selections. In the command line type:

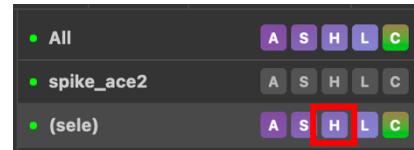
`sele resn BGL or resn AMA or resn BGA or resn ANE or resn BMA or resn AGA or resn AFU or resn ASN`

The above command will select all the glycan and ASN residues, which connect the glycans to the protein.

The Hide Button

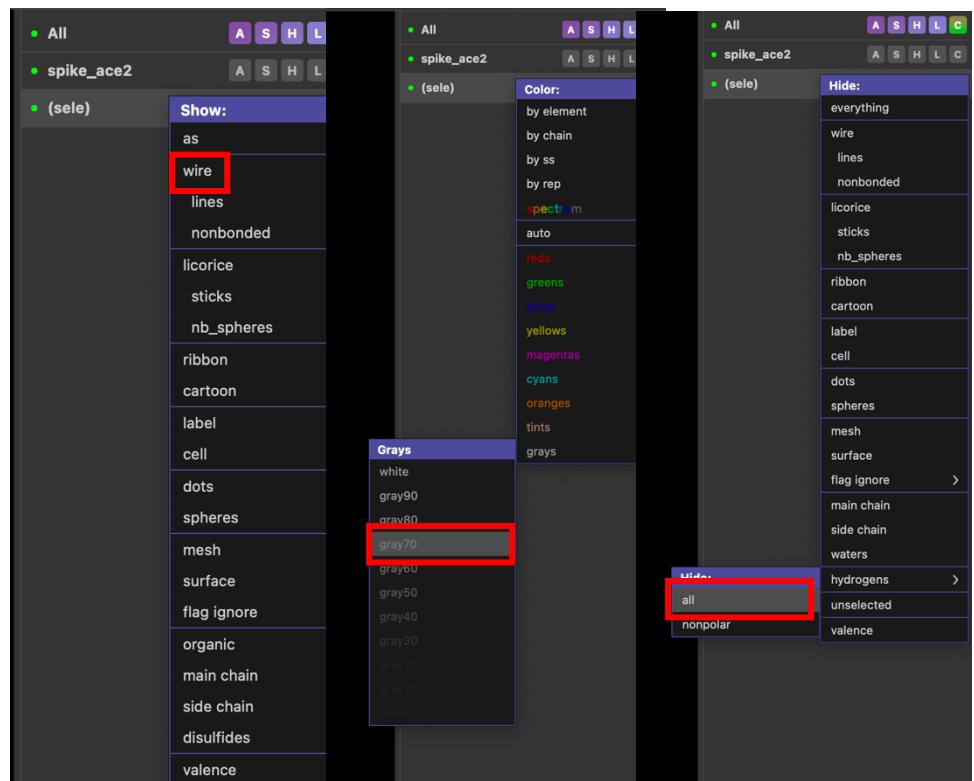
The hide button has tools for hiding selections, objects, and representations. For now, we will use the hide button to hide the default renderings of the glycan residues.

1. Ensure that the selection from the above command is still active.
2. Click the H button next to the (sele) object.
3. Click Everything to hide everything.

*The Show Button*

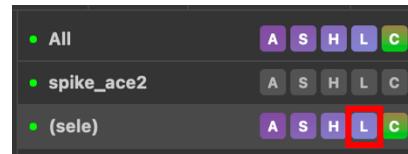
The show button has tools for changing the representations of objections and selections. For this tutorial we will show the glycan and ASN residues in grey wires.

1. Click the S button next to the (sele) object.
2. Click the wire button.
3. Click the C button next to the (sele) object.
4. Select grey70.
5. Click the H button next to the (sele) object.
6. Go to the bottom and hover over hydrogens and then click all to hide the hydrogens and simplify the rendering.



The Label Button

The label button has tools for adding labels to various elements. However, it is normally easier to save image and add labels afterwards, so we will not use the label functions in this tutorial.



Typically, renderings for publication will use white as the background color. To change the background color:

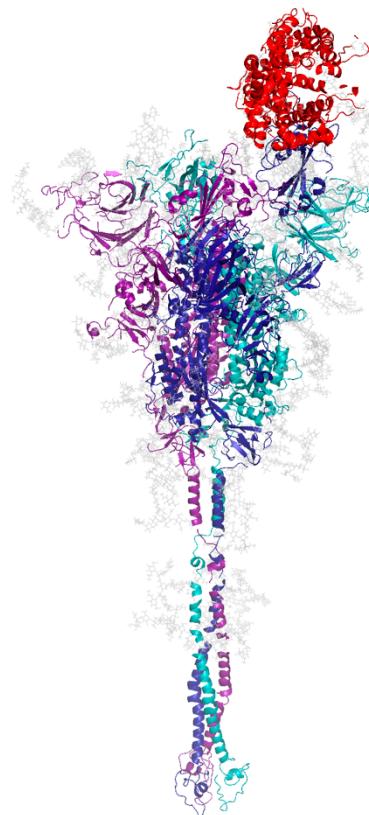
7. Click Display drop down in the PyMol menu bar.
8. Hover over the Background menu and select White.

You should now have a Spike-ACE2 complex model that looks something like that shown below. It is okay if you used different coloring and drawing methods.

Advanced Display Settings: More display setting options, such as setting the display background to white, exist under the Display drop down in the PyMol menu bar.

Rendering Settings: Each of the rendering options has default selections. But various properties of each rendering style and color can be altered. You can access the rendering settings via the Settings drop down in the menu bar at the top of the PyMol window.

Save a Rendering: You can save a rendering in several different image file formats. In the PyMol menu, click on the File drop down menu and then hover over Export Image As... and select the desired format. PNG is recommended.



Examining the Spike-ACE2 Receptor Binding Site

SARS-CoV-2 viral infection is initiated when the Spike protein binds to the ACE2 receptor on the host cell. By examining the interface of the Spike-ACE2 complex, we can learn a tremendous amount of information about the structural mechanisms that allow this binding, and thus infection, to occur. In this section you will learn how to examine the Spike-ACE2 receptor complex.

One extremely useful aspect of modeling is the ability to interrogate protein structures at atomic resolution. This way we can identify specific residues and interactions that are likely important for function. Residues that are identified as important for a specific function can then be mutated and tested for altered function in experiments. When looking at receptor and antibody binding, it is helpful to know which specific residues make up the binding sites. In this section we will examine the ACE2 receptor binding sites on the Spike protein.

Identifying Binding site Contacts

One extremely useful aspect of modeling is the ability to interrogate protein structures at atomic resolution. This way we can identify specific residues and interactions that are likely important for function. Residues that are identified as important for a specific function can then be mutated and tested for altered function in experiments. When looking at receptor and antibody binding, it is helpful to know which specific residues make up the binding sites. In this section we will examine the ACE2 receptor and C105 antibody binding sites on the Spike protein.

To visualize the important contacts in the Spike-ACE2 binding site, we first need to select the relevant chains that are in contact with the ACE2. In this case, it is the dark blue Spike chain from the image above.

1. Change the mouse selection mode to Chains.

- Click on the dark blue Spike chain and the red ACE2 chains in the PyMol visualization window.

We should now have two chains selected. Now we will identify the contacts in the binding site.

- Click the A button next to the (sele) object.
- Hover over the polar contacts menu.
- Select the between chains option.

You will not notice much difference in the rendering. To view the contacts we need to zoom in on the binding site.

In the object panel you should see a new object name sele_interchain_polar containing the polar contacts between Spike and ACE2. We will use this object to zoom in on the binding site contacts.

- Click the A button next to the sele_interchain_polar object.
- Click zoom to zoom in.

In this view you will see that the contacts are represented by dashed yellow lines with the distance between the contacts labeled. But it is still hard to tell which residues are interacting with each other. To display the interacting residues, we need to reactivate the chain selections for the ACE2 and Spike chains.

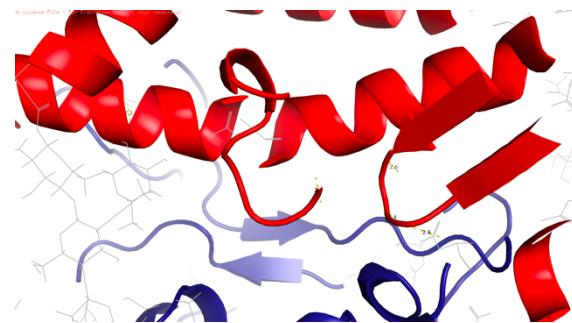
- Reactivate selection by clicking the sele object button or by selecting Chains selection mode and clicking the red ACE2 chain and the dark blue Spike protein chain.
- Click the S button next to the (sele) object.

The screenshot shows the PyMol software interface. At the top, there is a toolbar with buttons for All (purple), spike_ace2 (green), and (sele) (grey). Below the toolbar is a context menu with the following structure:

- Action:**
 - delete selection
 - rename selection
 - zoom
 - orient
 - center
 - origin
 - drag coordinates
 - clean
 - modify >
 - preset >
 - find >
 - align >
 - remove atoms
 - hydrogens
 - duplicate
 - copy to object
 - extract object
 - masking >
 - movement >
 - compute >
- Polar Contacts:**
 - within selection
 - involving side chains
 - involving solvent
 - excluding solvent
 - excluding main chain
 - excluding intra-main ch
 - just intra-side chain
 - just intra-main chain
 - to other atoms in objec
 - to others excluding solv
 - to any atoms
 - to any excluding solvent
 - between chains**
- Find:**
 - polar contacts >
 - any contacts >
 - halogen-bond interac >
 - salt-bridge interactio >
 - pi interactions >
 - clashes >

The screenshot shows the PyMol software interface with the following object panel:

- All (purple)
- spike_ace2 (green)
- (sele) (grey)
- sele_interchain_polar (grey)



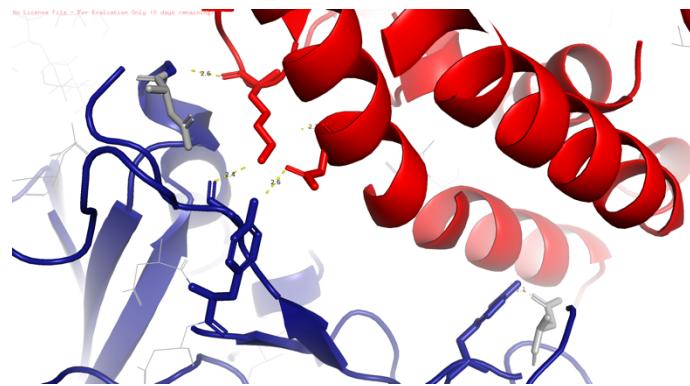
3. Click licorice to show the residues in sticks rendering.
4. Click the (sele) object to hide it.

Simplify Contacts Rendering

Use the left mouse button to rotate the view and identify the specific residues that are connected by the dotted yellow lines. These are the polar contacts identified by the find contacts tool we ran above. We would like to show only these contacts in sticks while hiding the other residues.

1. Change the mouse selection mode to Residues.
2. Use the mouse to select the residues that are connect by the yellow lines.
3. Next to the spike_ace2 object click the H button and hide the licorice representation.
4. Next to the (sele) object, click the S button and show the licorice representation of the selected residues.
5. Next to the (sele) object, click the H button, then hydrogens, and then all to hide all hydrogens and simplify the rendering.
6. Click the A button next to the sele_interchain_polar object and zoom on the interface.

Now you should have a rendering of the specific polar contacts between the ACE2 receptor and the Spike protein like that shown in the figure. These contacts are important for how the Spike protein binds to the receptor to initiate infection in the host cell.



Examining the C105 Antibody Epitope

The ACE2 receptor binds to the receptor binding domain (RBD) of the Spike protein. C105 is a SARS-CoV-2 neutralizing antibody that binds to an epitope on the RBD of the Spike protein. In this section we will compare the Spike-ACE2 receptor complex with the Spike-C105 antibody complex to gain insight into how this antibody works to neutralize the SARS-CoV-2 virus. This structure of C105 antibody contains two chains, one heavy chain and one light chain, that both make important contacts with the Spike protein. We will look at how the two chains interact with the Spike protein.

Antibody structures: Antibodies consist of four protein chains: two identical heavy chains and two identical light chain, held together by disulfide bonds. Light chains are smaller than heavy chains and contain one variable and one constant domain. The heavy chains contain one variable domain and three constant domains. The variable domains have high sequence variability and are responsible for the specificity of the antibody. The constant domains determine the antibody class and antibody belongs to. The structures shown throughout this tutorial show one heavy chain and one light chain for simplicity.

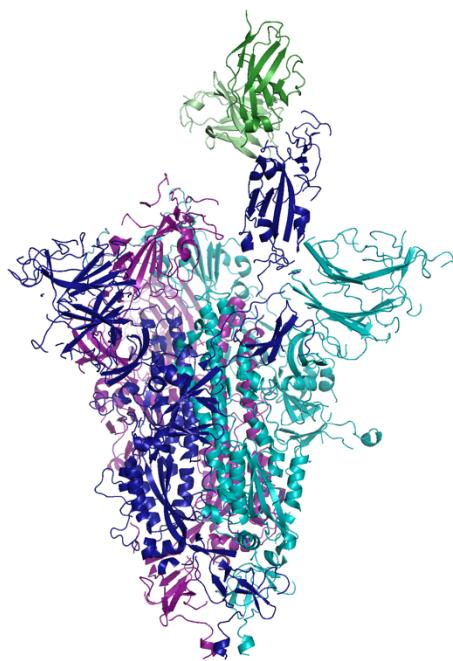
We now have the Spike-C105 antibody complex loaded PyMol. Notice how these structures are aligned perfectly with one another. Now, we want to simplify the view so we can focus on the Spike-C105 binding interface, just as we did for the Spike-ACE2 receptor binding interface.

1. Click the `spike_ace2` object button to hide the `spike_ace2` object.
2. Click the `sele_interchain_polar` object button to hide the `spike_ace2` binding interface contacts.
3. Change the mouse selection mode to **Chains**.
4. Use the mouse to select one of the Spike chains.
5. Click the `C` button next to the `(sele)` object and select a color for the chain. I used the same coloring scheme as for the Spike-ACE2, except I colored the antibody chains green instead of red.
6. Repeat steps 4-5 for the rest of the chains.

To examine and compare binding sites, we will hide the glycan residues in this structure.

1. Click the `H` button next to the `spike_c105` object.
2. Click **Licorice** to hide sticks.

You should now have two objects loaded and rendered such that you can visualize the Membrane-Spike-ACE2-C105 model as seen in the image below. You can selectively view one model or the other by clicking on the object button to hide/show your rendering.



To leverage the structural analysis above to improve vaccine and drug design, we need to determine what residues are important in the Spike-C105 antibody complex. To identify specific contacts at the binding interface, you can follow the same procedure as described in [Identifying Binding site Contacts](#). You may also want to try finding other contact types as well.

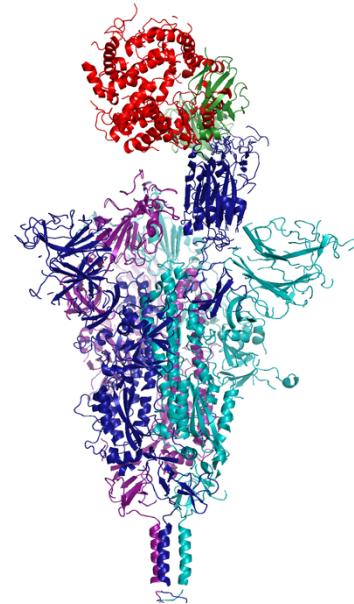
If you explore the binding site further, you will find that the complete set of interacting residues at the Spike RBD-C105 epitope is complex. There are many residues interacting with each other. One of the difficulties in modeling is being able to sift through the overwhelming amount of data that can be extracted from these structures. By continuing to explore this interface you may be able to find interactions I have not already mentioned! Can you find any?

Interaction distances: Different types of bonds have different interaction distances. While covalent and ionic bonds occur usually $<3\text{\AA}$, electrostatic interactions can occur distances of $>12\text{\AA}$. Selecting the proper distance cutoff for viewing an interacting partner is somewhat of an arbitrary choice but should be influenced by the type of interactions you would like to study, the research question you are considering, and feasibility of displaying/analyzing all residues. You can try to change the cutoff value to see the different residues you pick up.

Compare Binding Sites

To compare the binding site of ACE2 to the C105 antibody epitope, we will want to activate both models aligned to each other at the same time. These models have already been aligned to we just need to view both models together to compare them. Click on the objects to show both the spike_ace2 and spike_c105 models at the same time. You should now have a figure similar to that shown to the right.

What should be readily apparent is that the C105 antibody in green is overlapping with the ACE2 receptor in red. The binding site for the C105 antibody overlaps with the binding site for the ACE2 receptor, thus acting as a blocking molecule. When the C105 antibody is bound to the Spike protein the ACE2 receptor cannot bind, preventing the SARS-CoV-2 from initiating infection. This is one structure-based mechanism by which the C105 antibody works to fight the SARS-CoV-2 virus.



As you can see by working through the exercises above, the RBD is primary structural component of the Spike protein that moves upon C105 antibody binding. This antibody also partially overlaps with the ACE2 receptor when bound to the Spike protein, indicating that both the ACE2 and C105 antibody cannot be bound at the same time. By analyzing and comparing the structures of the ACE2-bound Spike with the C105 antibody-bound Spike we can determine that the C105 antibody works to neutralize the Spike protein in part by competing with ACE2 for binding to the Spike protein and by shifting the position of the RBD, thus altering the structure, and therefore function, of the Spike protein.

Watching Trajectories

As you can see, examining single structures can be invaluable in providing insight into specific structural features in the Spike protein that are important for receptor and antibody binding. However, many proteins are also structurally dynamic and can exist in more than one structure. We call the set of structures a protein can exist in a conformational ensemble. Different structures in the conformational ensemble can have different functional states, including inactive, so understanding how proteins move between different structures is another important component of studying protein structures. We use computer simulation techniques to simulate protein models and examine their movements. In this section we will load a molecular dynamics simulation of the Spike protein and examine the structural dynamics in the Spike protein.

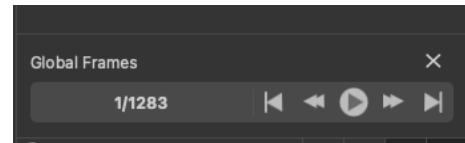
First, we need to download the trajectory file.

1. Download the trajectory file from [CHARMM-GUI COVID-19 Archive](#) and save it to your desired location.
2. Decompress the download files by double-clicking.

Now we need to load the trajectory. Trajectory files contain atomic velocities but no coordinates. Therefore, trajectory files must be loaded as data into a coordinate file.

1. Click the All object to hide all renderings.
2. Load the `spike_membrane.pdb` file into PyMol using your preferred file loading method.
3. Load the trajectory file by dragging the file from the file browser window and dropping the file in the PyMol viewing window.
4. When prompted, select `spike_membrane` as the object to load the trajectory file into. Trajectory files can be large so loading the DCD file may take a few minutes.
5. Update the rendering of the model as you wish.

In the bottom right corner of the PyMol window a Global frames trajectory viewer will appear. This tool allows you to play and navigate through the trajectory. Click the play button to watch the Spike protein dynamics. What do you see? Do you notice anything interesting?



You can see how the spike protein waves back and forth when it is embedded in the membrane. These motions are important for function of the Spike protein and the exposure of different antibody epitopes.

PyMol is not the best visualization software for viewing trajectories. [VMD](#) is a better software for viewing trajectories. A tutorial similar to this one, covering the same topics with the same files, can be found online [here](#).

Summary

In this workshop we skimmed over how to use the PyMol software to load and visualize Spike protein models and simulation files and how to examine these files to gain insight into the Spike function. The exercises covered in this workshop are only a small subset of the various computational tools and techniques that computational biophysicists use to explore and understand protein structures and function. Visit the [PyMol Wiki](#) to learn more about some of these other tools. There are also other software packages that are freely available (see [Software](#)) with many how-to articles online. You should try these out as well. You can learn more about the theory underlying these computational tools (as well as some experimental methods) at the [Physical Lens on the Cell](#) blog. And remember, you can always find interesting and important protein structures at the [Protein Data Bank](#) website.