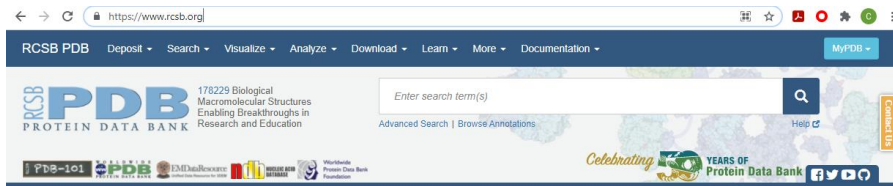
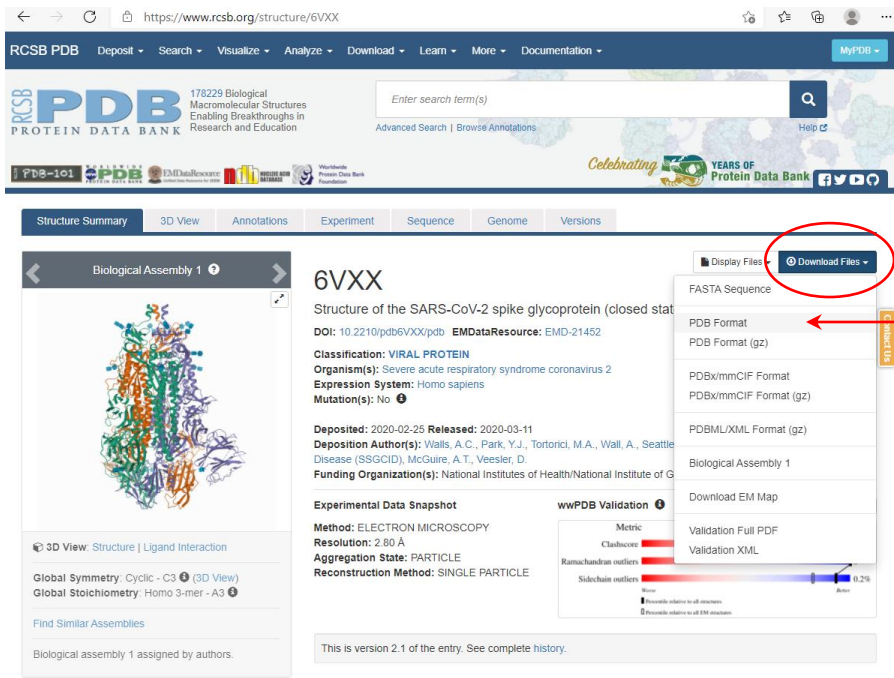


Resource for downloading structural data: www.rcsb.org

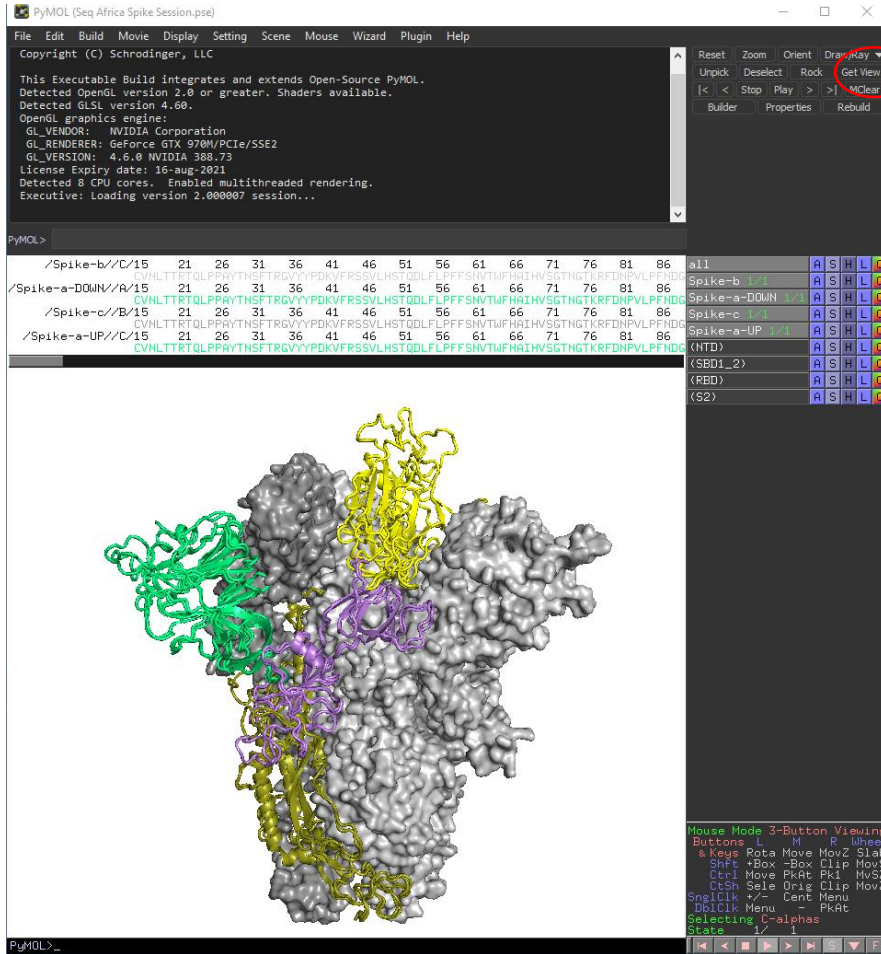


Search for proteins using keywords eg: “SARS-CoV-2 Spike”
Search for proteins using PDB ID eg: “6VXX”



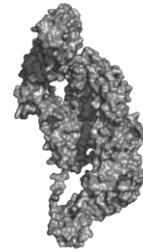
Download Files (dropdown menu)
PDB format

Premade Pymol session file: Seq Africa Spike Session.pse



Run Get View

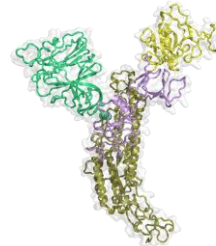
```
set_view (\nPyMOL> -0.239942104, -0.088808551, -0.966634452,\nPyMOL> 0.970393002, 0.003266835, -0.241166592,\nPyMOL> 0.024566753, -0.995957255, 0.085405558,\nPyMOL> -0.030103562, -0.035919264, -536.363952637,\nPyMOL> 207.847229004, 192.204620361, 184.289764404,\nPyMOL> -1891.301635742, 2968.634765625, -20.000000000 )
```



Spike C - surface view



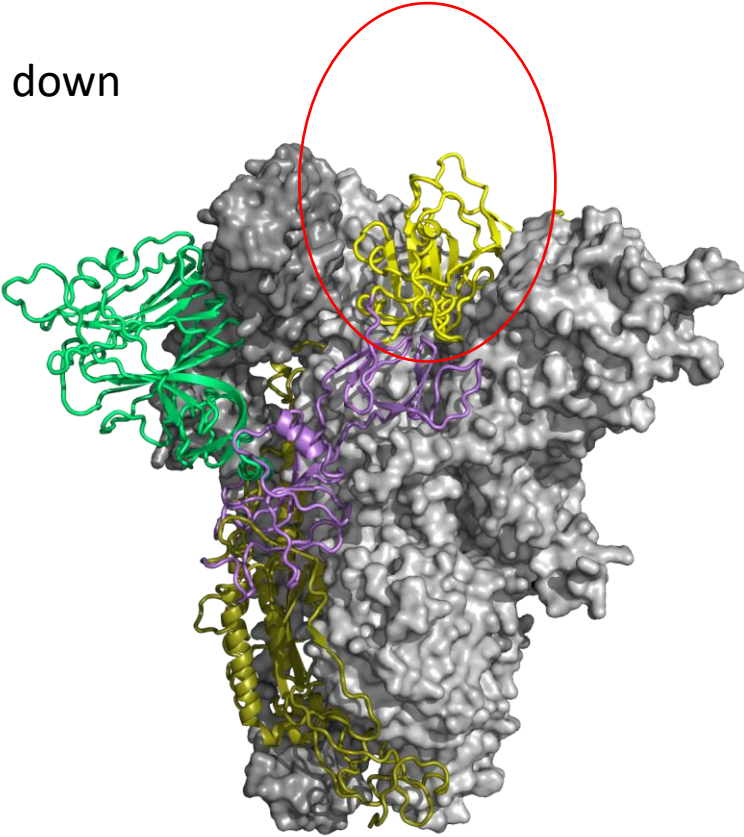
Spike B - surface view



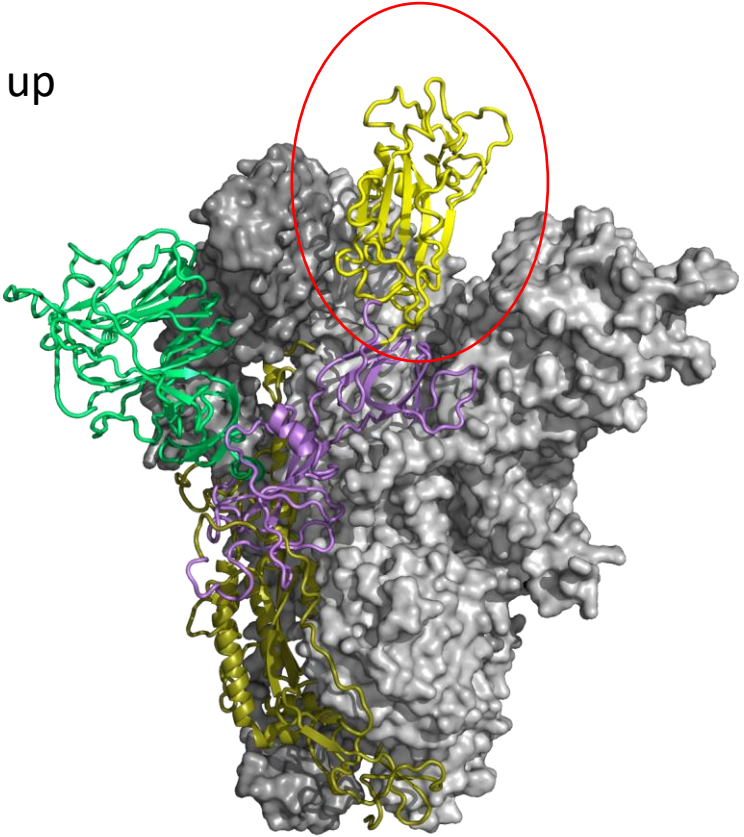
Spike A - cartoon view

Prepared two views:

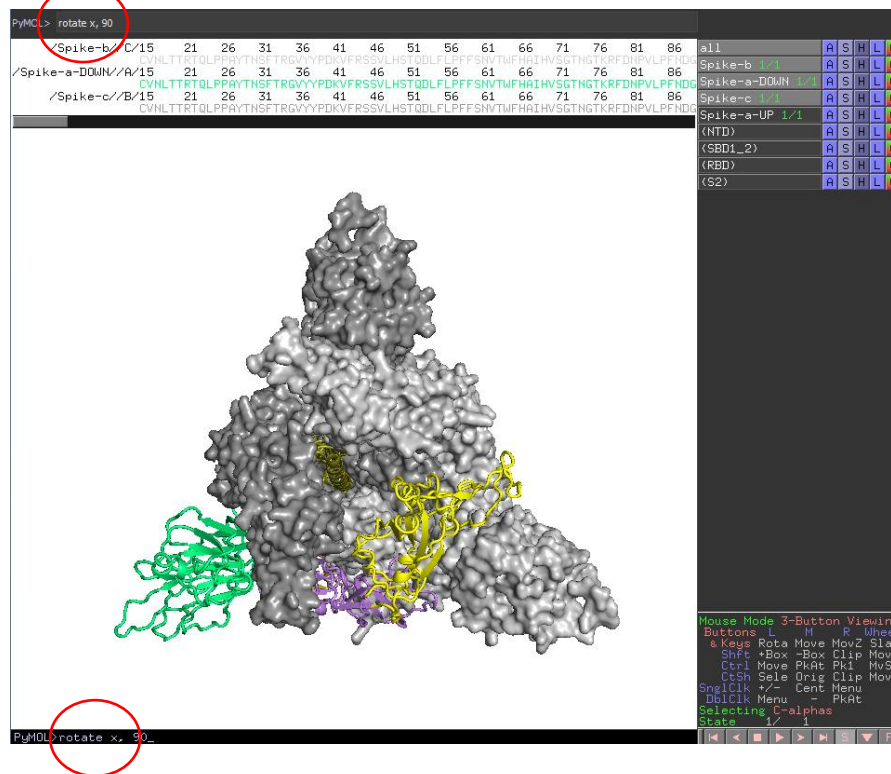
RBD down



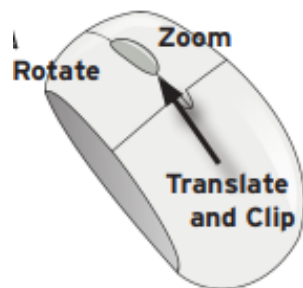
RBD up



Command: rotate x, 90 will change the view to “top view” (as approached by cell / ACE2)



Rotate x, -90 will return the view to “side view”



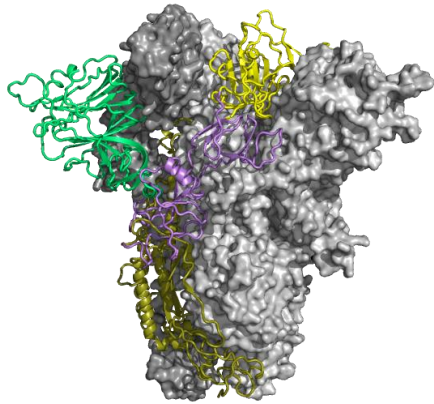
Mouse controls

Left button: Click within molecule to rotate

Right button: Zoom

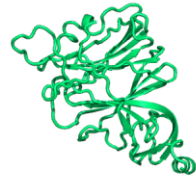
Middle button: Slice

Spike Trimer

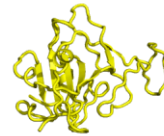


Premade domain selections

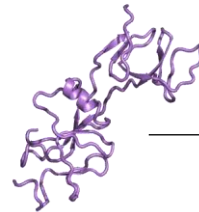
all	A	S	H	L	C
Spike-b 1/1	A	S	H	L	C
Spike-a-DOWN 1/1	A	S	H	L	C
Spike-c 1/1	A	S	H	L	C
Spike-a-UP 1/1	A	S	H	L	C
<NTD>	A	S	H	L	C
<SBD1_2>	A	S	H	L	C
<RBD>	A	S	H	L	C
<S2>	A	S	H	L	C



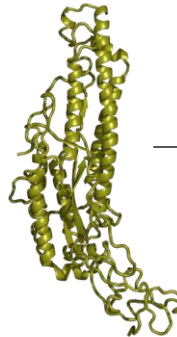
N-Terminal Domain
(NTD)



Receptor Binding Domain
(RBD)



Sub-Domain 1
Sub-Domain 2
(SBD1 and SBD2)



S2
(Fusion machinery)

Command: select 501, resi 501

Selection will be named 501

Selection will include all residue 501

Point and click to select residue 501 in chain A (Up or Down)

OR

PyMOL>select 501, resi 501
Selector: selection "501" defined with 32 atoms.

PyMOL>

/Spike-b	481	486	491	496	501	506	511	516	521	526	531	536	541	546	551	all	A	S	H	L	C	
RDISTEIQRGSTPCNGVEGFNCYFPLQSYGLPTNNG																	Spike-b 1/4	A	S	H	L	C
/Spike-a-DOWN	481	486	491	496	501	506	511	516	521	526	531	536	541	546	551		Spike-a-DOWN 1/21	A	S	H	L	C
RDISTEIQRGSTPCNGVEGFNCYFPLQSYGLPTNNG																	Spike-c 1/4	A	S	H	L	C
/Spike-c	481	486	491	496	501	506	511	516	521	526	531	536	541	546	551		Spike-a-UP 1/4	A	S	H	L	C
RDISTEIQRGSTPCNGVEGFNCYFPLQSYGLPTNNG																	(NTD)	A	S	H	L	C
/Spike-a-UP	481	486	491	496	501	506	511	516	521	526	531	536	541	546	551		(SBD1_2)	A	S	H	L	C
RDISTEIQRGSTPCNGVEGFNCYFPLQSYGLPTNNG																	(RBD)	A	S	H	L	C
/Spike-a-UP	481	486	491	496	501	506	511	516	521	526	531	536	541	546	551		(S2)	A	S	H	L	C
RDISTEIQRGSTPCNGVEGFNCYFPLQSYGLPTNNG																	(501)	A	S	H	L	C

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

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip Mov5
Ctrl Move PKAT Pk1 Mov5
Ctrl Move Drag Ctrl Mov5
Space 1/2 Cent Menu
DBClick Menu - PKAT
Selecting C-alphas
State 1/ 1

Select "A" for action menu
Choose rename selection

Backspace sele, and enter the new name here
Renaming sele to: 501

I have selected default to C-alpha
You may choose any, residue is common

Show the selected residue in a way that stands out

The screenshot shows a protein structure on the left and a command list on the right. The command list includes: all, Spike-b, Spike-a-DOWN, Spike-c, Spike-a-UP, (NTD), (SBD1_2), (RBD), (S2), and (S01). The 'S' column for each command is highlighted in red. A red arrow points from the 'S' in the (S01) row to the text 'Select "S" for show menu'.

Select "S" for show menu

The 'Show' menu is open, showing various display options. The 'spheres' option is highlighted with a red oval. A red arrow points from this oval to the text 'Choose spheres'.

Choose spheres

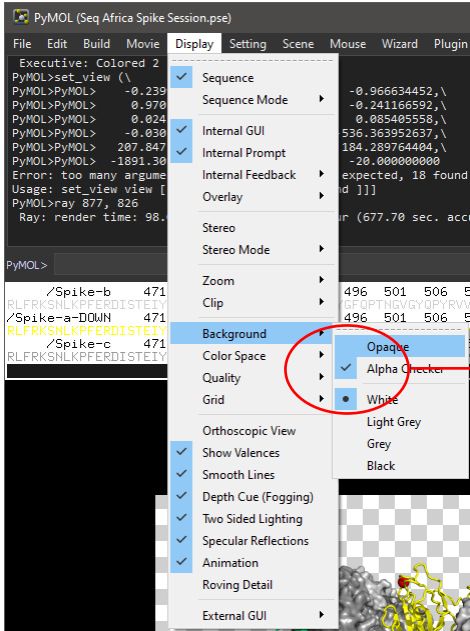
The screenshot shows the protein structure with the selected residue highlighted in red. The command list on the right is the same as in the first screenshot, but the 'C' column is highlighted in red. A red arrow points from the 'C' in the (S01) row to the text 'Choose "C" for colour (color) menu'.

Choose "C" for colour (color) menu

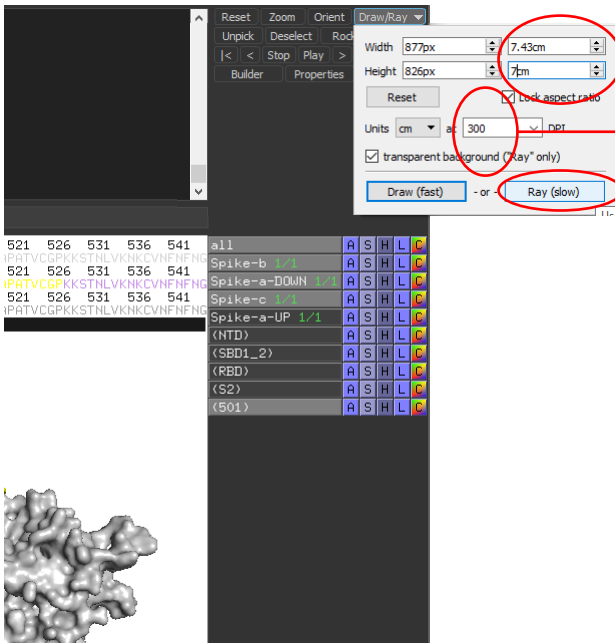
The 'Color' menu is open, showing various color options. The 'red' option is highlighted with a red oval. A red arrow points from this oval to the text 'Choose red'.

Choose red

Generate an image



Navigate to Display → Background → uncheck opaque or select white



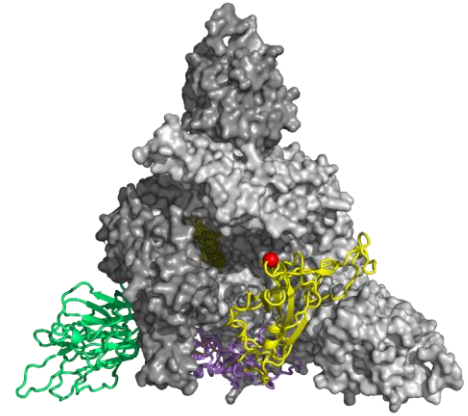
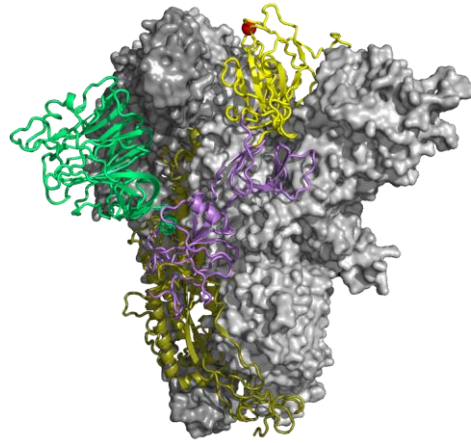
Choose image dimensions
Choose image resolution
“Ray”

Then choose “save image to file”
Or navigate to File → Export image as → PNG

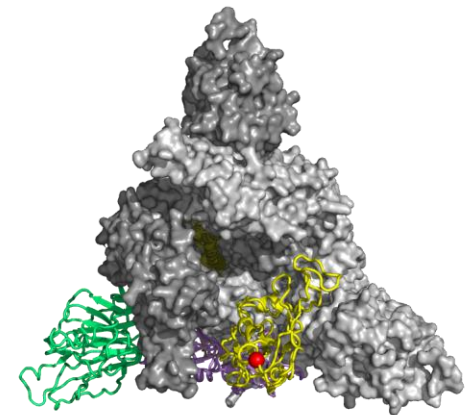
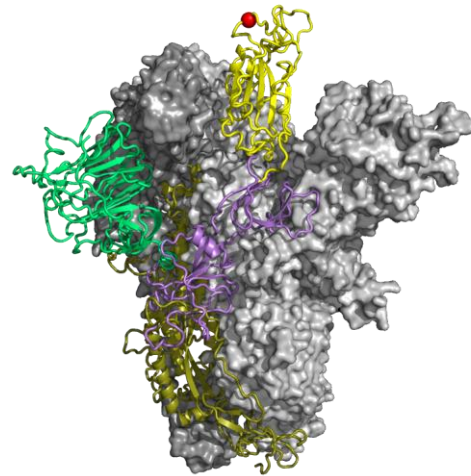
Side View

Top View

RBD down



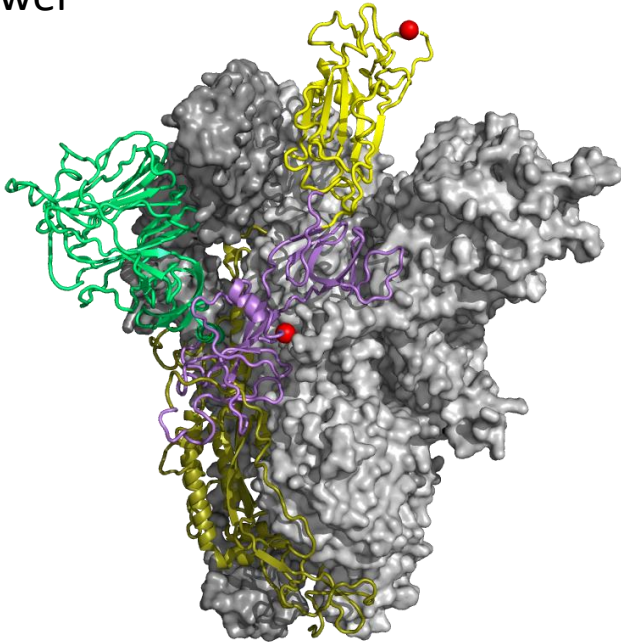
RBD up



Exercise

Generate an image of SARS-CoV-2 spike trimer, with one RBD in the UP position, showing residue positions 484, and 614 as red spheres.

Answer



Contact:

Constantinos Kurt Wibmer

kurtw@nicd.ac.za