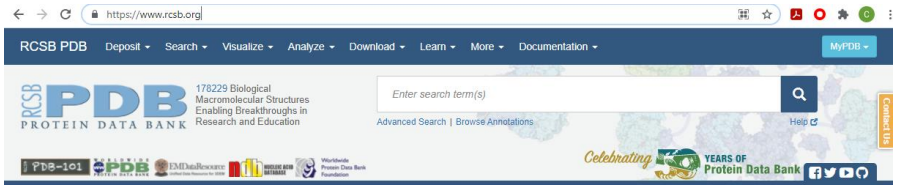
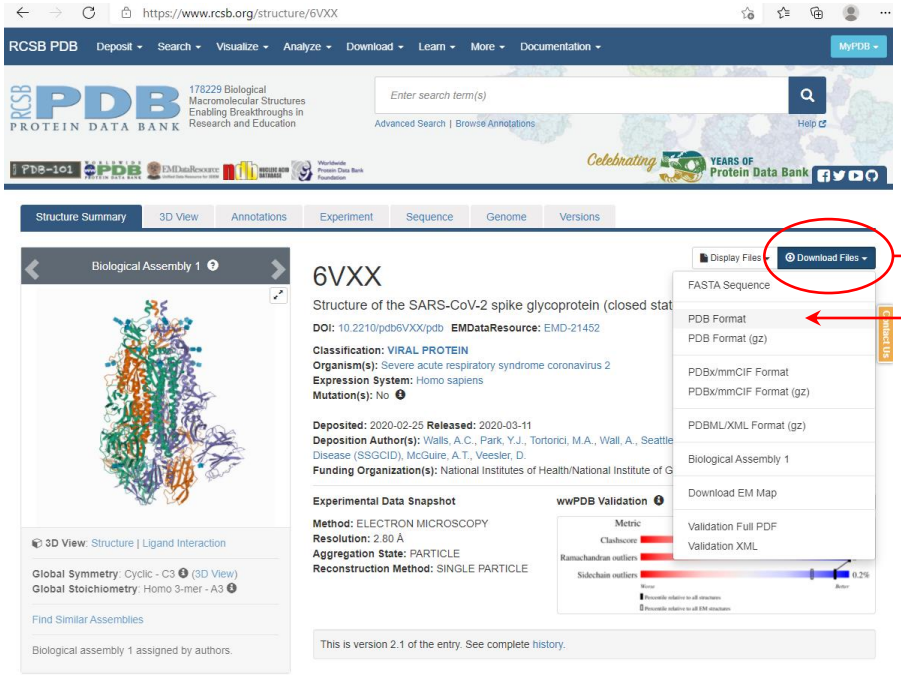
Resource for downloading structural data:
www.rcsb.org

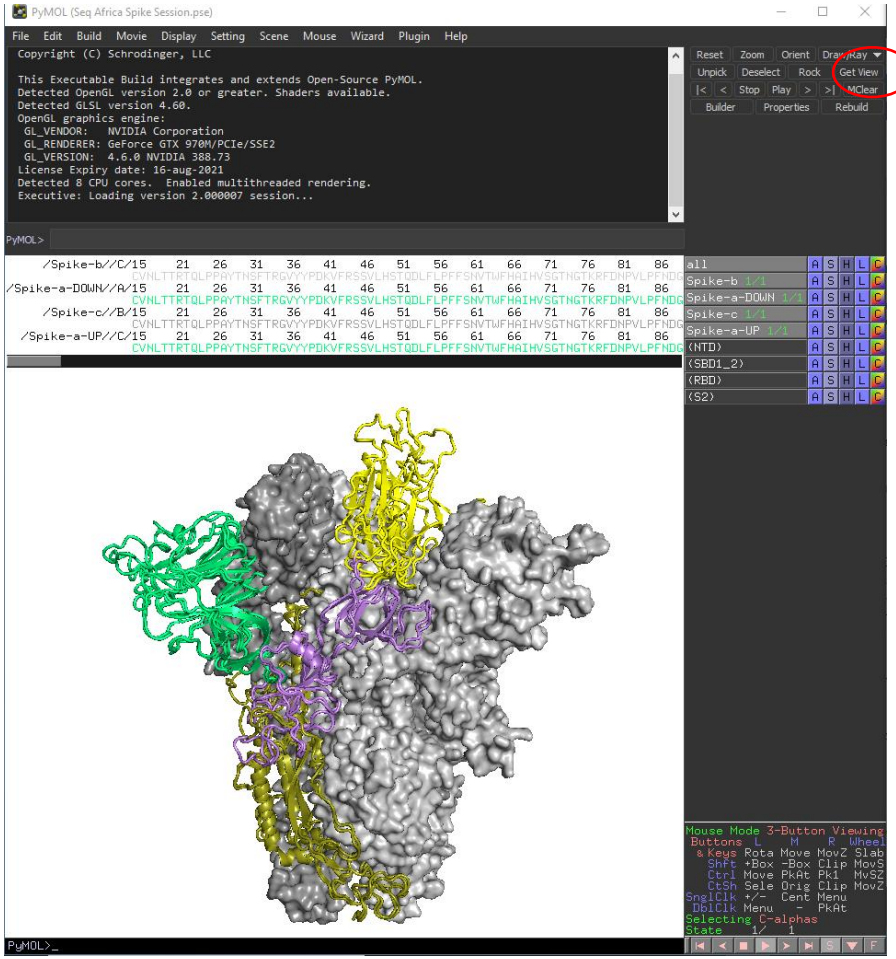


Search for proteins using keywords eg: “SARS-CoV-2 Spike”
Search for proteins using PBD ID eg: “6VXX”



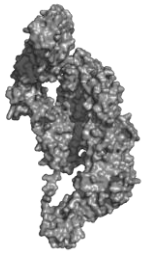
Download Files (dropdown menu)
PDB format

Premade Pymol session file: Seq Africa Spike Session.pse

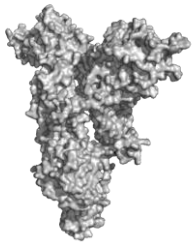


Run Get View

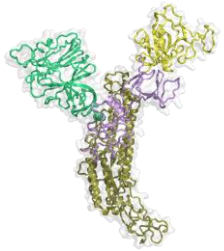
```
set_view (\
PyMOL>    -0.239942104,   -0.088808551,   -0.966634452,\
PyMOL>     0.970393002,    0.003266835,   -0.241166592,\
PyMOL>     0.024566753,   -0.995957255,    0.085405558,\
PyMOL>    -0.030103562,   -0.035919264, -536.363952637,\
PyMOL>   207.847229004,  192.204620361,  184.289764404,\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



Spike C - surface view



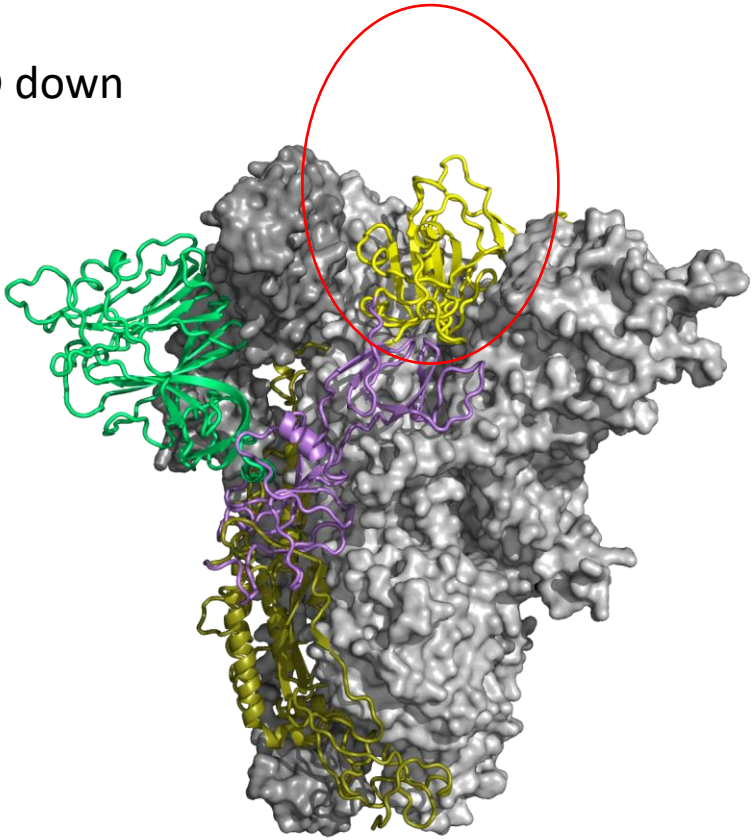
Spike B - surface view



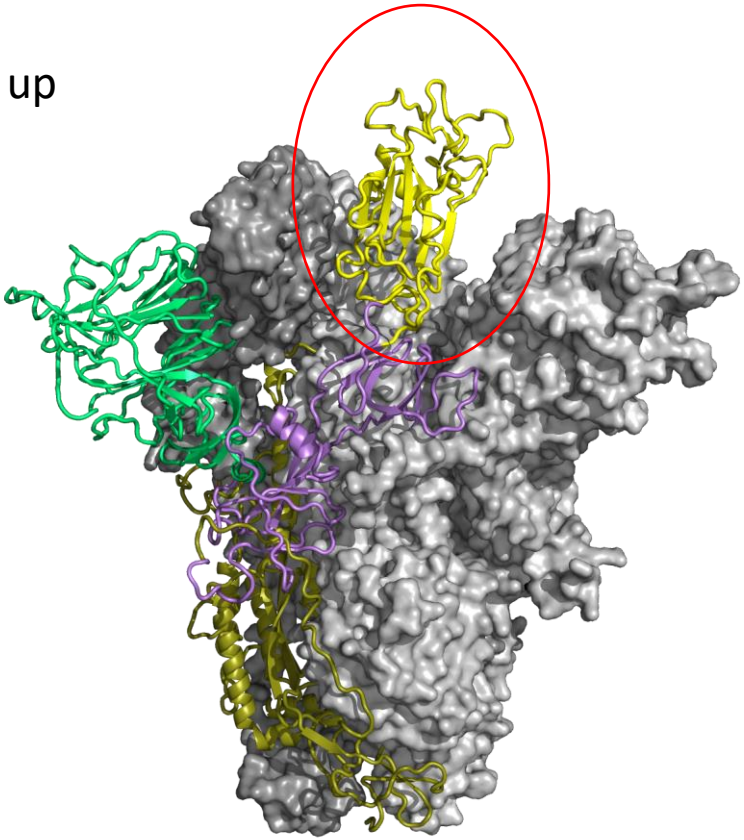
Spike A - cartoon view

Prepared two views:

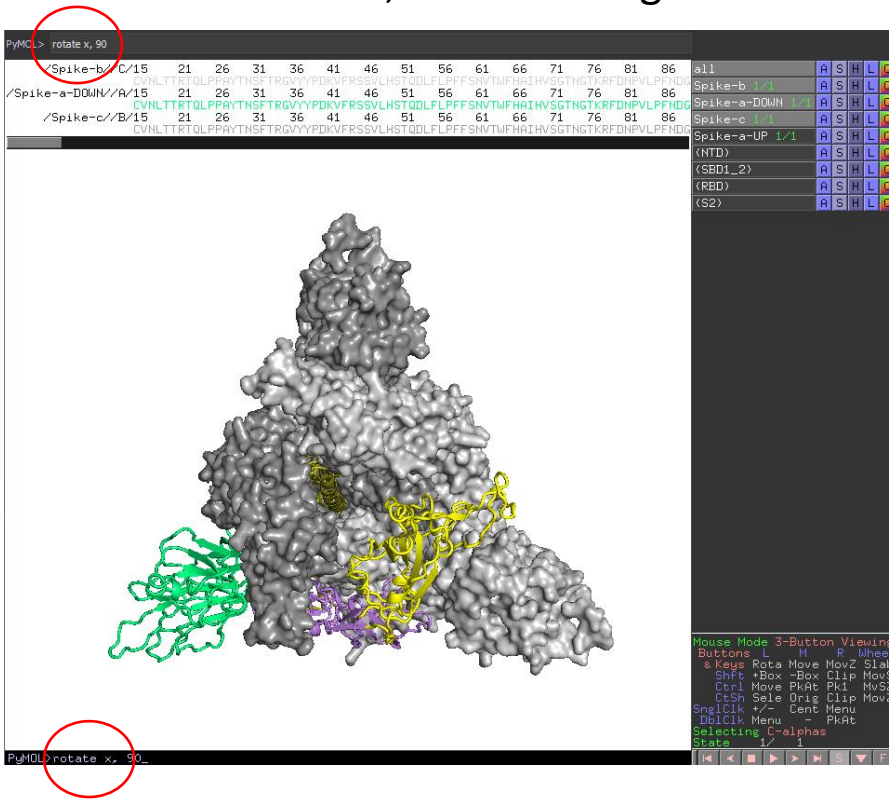
RBD down



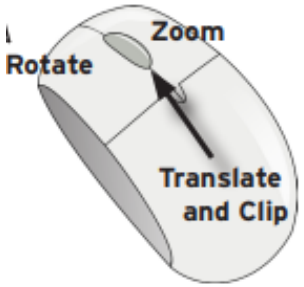
RBD up



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



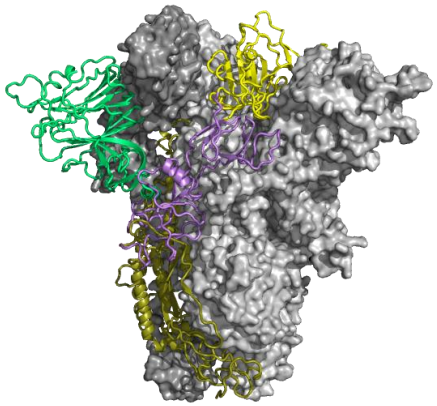
Rotate x, -90 will return the view to “side view”



Mouse controls

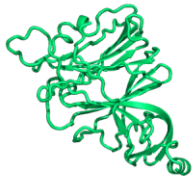
Left button:	Click within molecule to rotate
Right button:	Zoom
Middle button:	Slice

Spike Trimer

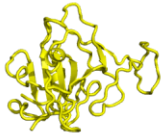


Premade domain selections

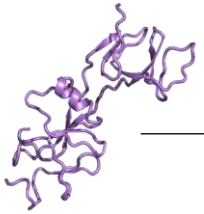
all	A	S	H	L	C
Spike-b 1/1	A	S	H	L	C
Spike-a-DOWN 1/1	A	S	H	L	C
Spike-c 1/1	A	S	H	L	C
Spike-a-UP 1/1	A	S	H	L	C
(NTD)	A	S	H	L	C
(SBD1_2)	A	S	H	L	C
(RBD)	A	S	H	L	C
(S2)	A	S	H	L	C



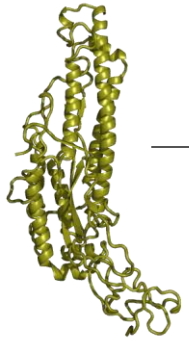
N-Terminal Domain
(NTD)



Receptor Binding Domain
(RBD)



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



S2
(Fusion machinery)

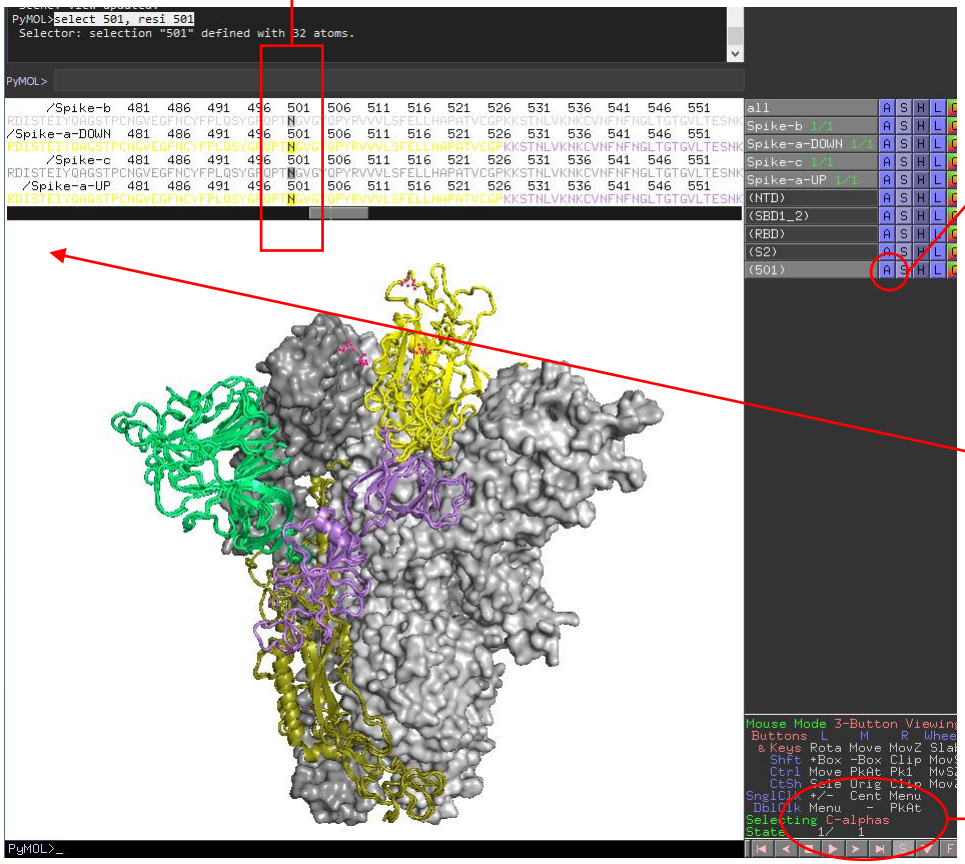
Command: select 501, resi 501

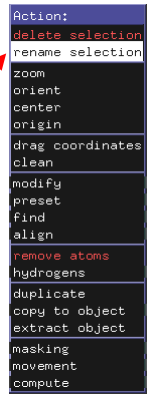
Selection will be named 501

Selection will include all residue 501

OR

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



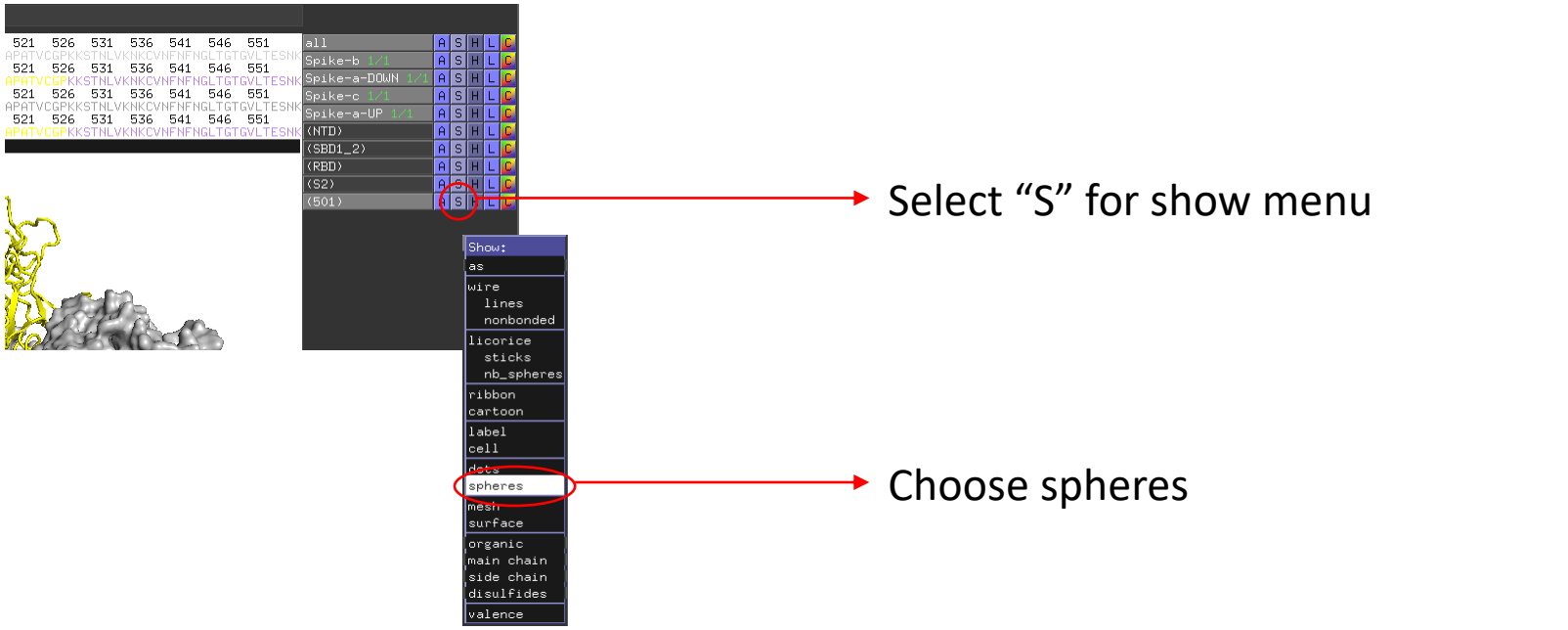


Select “A” for action menu
Choose rename selection

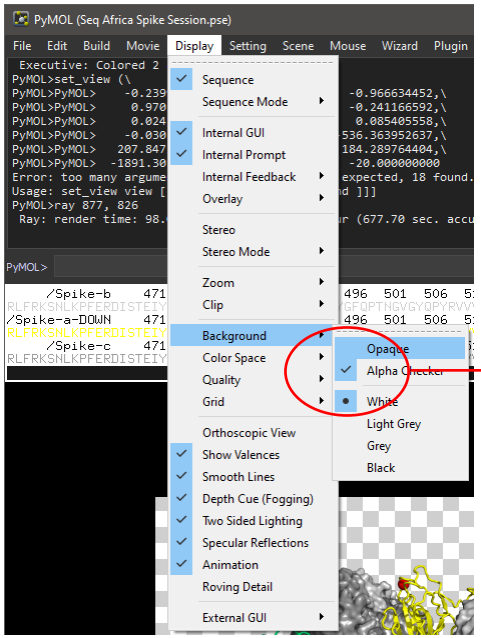
Backspace sele, and enter the new name here
Renaming sele to: 501

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

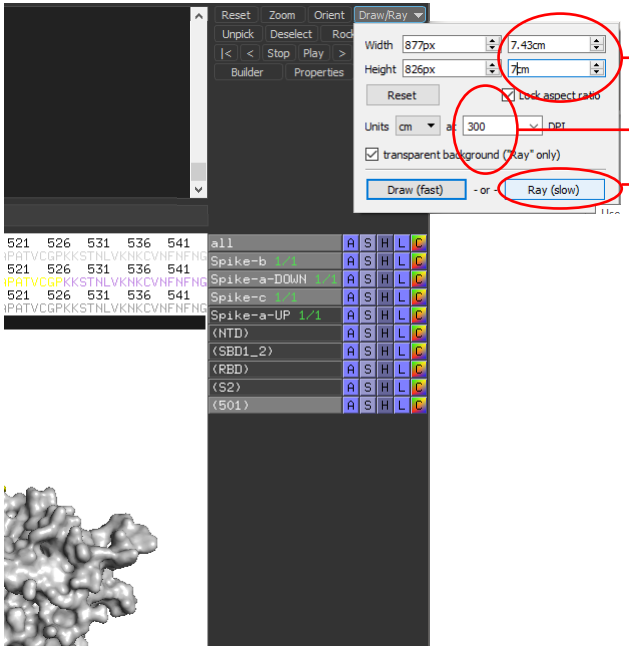
Show the selected residue in a way that stands out



Generate an image



Navigate to Display → Background → uncheck opaque
or select white



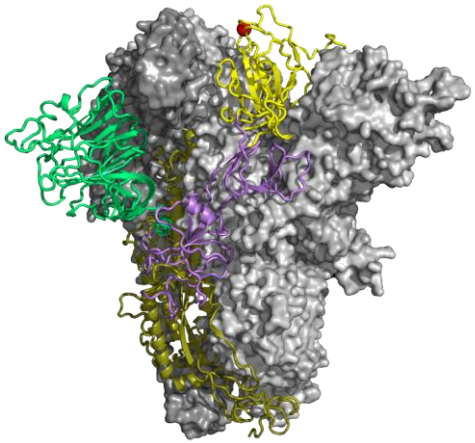
Choose image dimensions
Choose image resolution”
“Ray”

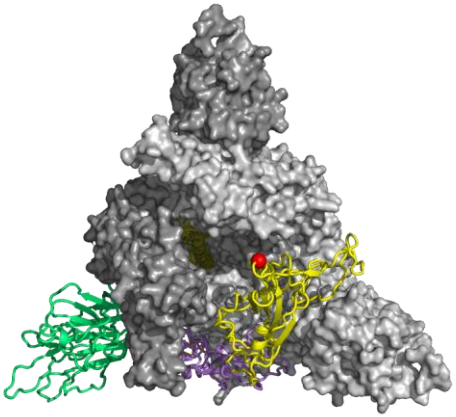
Then choose “save image to file”
Or navigate to File → Export image as → PNG

Side View

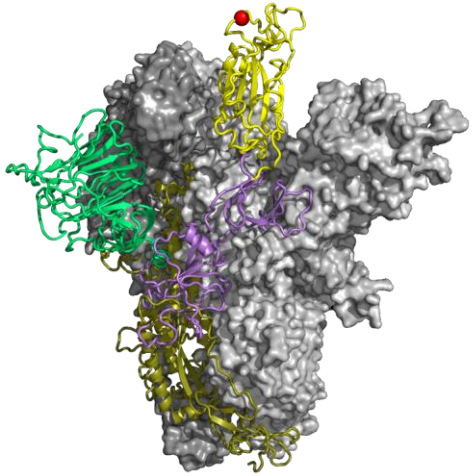
Top View

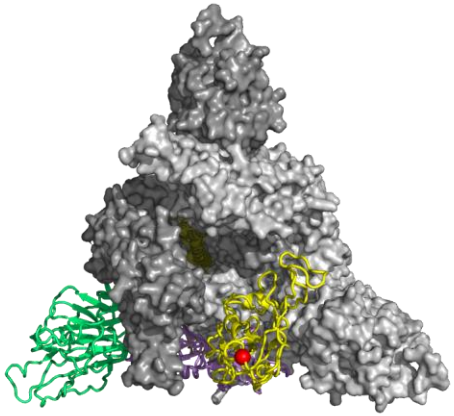
RBD down





RBD up

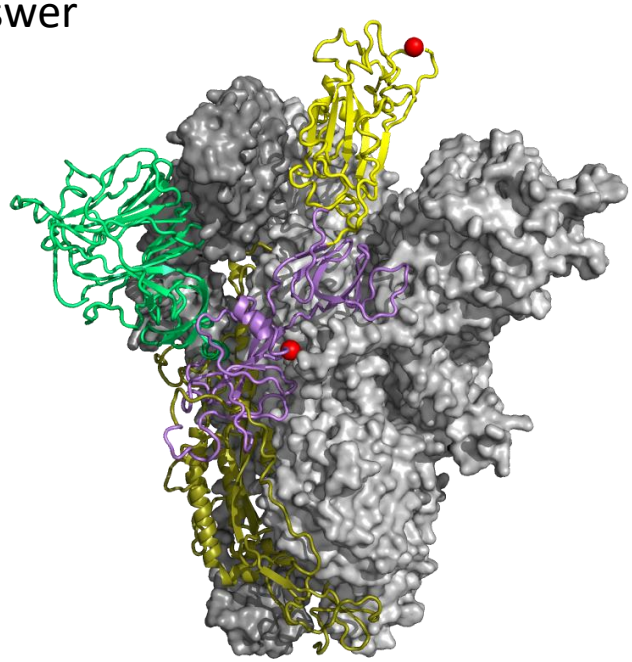




Exercise

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



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