

RStudio interface showing a script editor, environment pane, and package list.

Script Editor:

```
1 # ---
2 title: "Running PyMOL from R Notebook"
3 output: html_notebook
4 # ---
5
6 {r}
7 use_condaenv("r-reticulate")
8
9
10
11 {python}
12 from pymol import cmd
13 cmd.do("reinitialize")
14 cmd.do("fetch 6VXX")
15 cmd.do("zoom (resi 614 and chain A)")
16 cmd.label(selection="chain A and resi 614 and name C8", expression="'%s-%s' % (resn,resi)")
17 cmd.do("set label_color, black; set label_size, 48")
18 cmd.do("set stick_radius, 0.12")
19 cmd.do("hide cartoon; show sticks")
20 cmd.do("set ray_shadows, 0")
21 cmd.do("draw")
22 cmd.do("png /Users/blaine/D614Greticulate.png, 800, 500, dpi=300")
23
24
25 {r}
26 # will install with conda
27 py_install("jupyter", channel="conda-forge")
28
29
30
31 ![Coronavirus SARS2 Spike Protein site 61.](/Users/blaine/D614Greticulate.png){#id .class
width=50% height=50%}
```

Environment Pane:

Package	Version
agrep1	<Promise>
all.equal.character	<Promise>
all.equal.default	<Promise>
all.equal.environment	<Promise>
all.equal.envRefClass	<Promise>
all.equal.factor	<Promise>
all.equal.formula	<Promise>
all.equal.language	<Promise>
all.equal.list	<Promise>
all.equal.numeric	<Promise>
all.equal.POSIXt	<Promise>
all.equal.raw	<Promise>
all.names	<Promise>
all.vars	<Promise>
allowInterrupts	<Promise>
anyDuplicated.array	<Promise>
anyDuplicated.data.frame	<Promise>
anyDuplicated.matrix	<Promise>
anyNA.data.frame	<Promise>
anyNA.numeric_version	<Promise>
anyNA.POSIXlt	<Promise>
aperm.table	<Promise>
arrayInd	<Promise>
as.array.default	<Promise>
as.character.condition	<Promise>
as.character.Date	<Promise>
as.character.error	<Promise>
as.character.factor	<Promise>

Package List:

Package	Version
ColorBrewer	1.1-2
Rcpp	1.0.4.6
RcppEigen	0.3.3.7.0
RcppParallel	5.0.2
reshape2	1.4.4
reticulate	1.16
rlang	0.4.6
rmarkdown	2.3
rpart	4.1-15
rprojroot	1.3-2
rconnect	0.8.16
rstan	2.19.3
rstanarm	2.19.3
rstantools	2.1.0
rstudioapi	0.11
scales	1.1.1
shiny	1.5.0
shinyjs	1.1

Console:

```
done
> use_condaenv("r-reticulate")
PyMOL>reinitialize
PyMOL>fetch 6VXX
TITLE Structure of the SARS-CoV-2 spike glycoprotein (closed state)
Executveload-Detail: Detected mmCIF
Cmdload: loaded as "6VXX".
PyMOL>zoom (resi 614 and chain A)
PyMOL>set label_color, black; set label_size, 48
Setting: label_color set to black.
PyMOL>set stick_radius, 0.12
Setting: stick_radius set to 0.120000.
```

Figure:

The figure displays a 3D molecular model of the SARS-CoV-2 spike glycoprotein in its closed state. The protein is shown as a green ribbon structure. A specific residue, ASP-614, is highlighted in red and labeled. The structure is set against a black background with stick representations for the atoms.