

# Apicomplexa: Reproduction of 3D model figures

## Jmol Installation

1. Make sure you have Java installed on your computer. If not, you can go to this [java installation document](#) and select appropriate installation options for your operating system.
2. Once this is complete, download Jmol at this direct [download link](#) (.zip file).
3. Open the zip file, and extract Jmol.jar to any folder you like.
4. To run Jmol, simply double click on the icon of Jmol.jar, and the application will open.
  - a. Note: If you have issues with this, that means the .jar file extension might be associated with other programs by default. In this case, open the command prompt on your computer, and go to the directory which contains Jmol.jar (this can be understood simply by googling how to move through folders on the command line). Once you are in the correct directory, type into the command line: `java -jar Jmol.jar`

## Opening PDB file

1. At the top left of the application, click on the green folder, or simply File ->Open
2. Go to the directory which has the PDB files for:
  - a. *P. falciparum* sporozoites
  - b. *P. falciparum* trophozoites
  - c. *P. falciparum* gametocytes
  - d. *P. vivax* sporozoites
  - e. *P. yoelii* mixed blood stage
  - f. *P. berghei* gametocytes
  - g. *B. microti* mixed blood stage
  - h. *B. microti* tetrads
  - i. *T. gondii* bradyzoites
  - j. *T. gondii* tachyzoites
3. Click one PDB file, and click "Open"

## Modifying Visualization

You should be looking at the skeleton of the genome. To modify the figure:

1. At the top left, click on File->Console
2. Once in the console, simply **copy and paste** the below script (or drag the text into the editor) depending on which figure you are modeling.

### **Bm\_MixedBloodStage**

color background white;  
select all; wireframe 0.01;  
select :a; color translucent [175, 237, 253];  
select :b; color translucent [134, 164, 198];  
select :c; color translucent [94, 92, 143];  
select :d; color translucent [54, 20, 88];  
select PRO; define cen selected; color red; spacefill 0.02;  
select ALA; define tel selected; color blue; spacefill 0.02;  
select helium; define pir selected; color orange; spacefill 0.02;

### **Bm\_Tetrads**

color background white;  
select all; wireframe 0.004;  
select :a; color translucent [175, 237, 253];  
select :b; color translucent [134, 164, 198];  
select :c; color translucent [94, 92, 143];  
select :d; color translucent [54, 20, 88];  
select PRO; define cen selected; color red; spacefill 0.008;  
select ALA; define tel selected; color blue; spacefill 0.008;  
select helium; define pir selected; color orange; spacefill 0.008;

### **Pb\_Gametocytes & Pf\_Gametocytes**

color background white;  
select all; wireframe 0.007;  
select :a; color translucent [175, 237, 253];  
select :b; color translucent [164, 218, 239];  
select :c; color translucent [154, 200, 225];  
select :d; color translucent [144, 182, 211];  
select :e; color translucent [134, 164, 198];  
select :f; color translucent [124, 146, 184];  
select :g; color translucent [114, 128, 170];  
select :h; color translucent [104, 110, 157];  
select :i; color translucent [94, 92, 143];  
select :j; color translucent [84, 74, 129];  
select :k; color translucent [74, 56, 116];  
select :l; color translucent [64, 38, 102];  
select :m; color translucent [54, 20, 88];  
select :n; color translucent [44, 2, 75];  
select PRO; define cen selected; color red; spacefill 0.015;  
select ALA; define tel selected; color blue; spacefill 0.015;  
select helium; define pir selected; color orange; spacefill 0.015;

### **Pf\_Sporozoites**

color background white;  
select all; wireframe 0.025;

```
select :a; color translucent [175, 237, 253];
select :b; color translucent [164, 218, 239];
select :c; color translucent [154, 200, 225];
select :d; color translucent [144, 182, 211];
select :e; color translucent [134, 164, 198];
select :f; color translucent [124, 146, 184];
select :g; color translucent [114, 128, 170];
select :h; color translucent [104, 110, 157];
select :i; color translucent [94, 92, 143];
select :j; color translucent [84, 74, 129];
select :k; color translucent [74, 56, 116];
select :l; color translucent [64, 38, 102];
select :m; color translucent [54, 20, 88];
select :n; color translucent [44, 2, 75];
select PRO; define cen selected; color red; spacefill 0.06;
select ALA; define tel selected; color blue; spacefill 0.06;
select helium; define pir selected; color orange; spacefill 0.06;
```

### **Pf\_Trophozoites & Pk\_Trophozoites & Py\_MixedBloodStage**

```
color background white;
select all; wireframe 0.017;
select :a; color translucent [175, 237, 253];
select :b; color translucent [164, 218, 239];
select :c; color translucent [154, 200, 225];
select :d; color translucent [144, 182, 211];
select :e; color translucent [134, 164, 198];
select :f; color translucent [124, 146, 184];
select :g; color translucent [114, 128, 170];
select :h; color translucent [104, 110, 157];
select :i; color translucent [94, 92, 143];
select :j; color translucent [84, 74, 129];
select :k; color translucent [74, 56, 116];
select :l; color translucent [64, 38, 102];
select :m; color translucent [54, 20, 88];
select :n; color translucent [44, 2, 75];
select PRO; define cen selected; color red; spacefill 0.035;
select ALA; define tel selected; color blue; spacefill 0.035;
select helium; define pir selected; color orange; spacefill 0.035;
```

### **Pv\_Sporozoites**

```
color background white;
select all; wireframe 0.012;
select :a; color translucent [175, 237, 253];
select :b; color translucent [164, 218, 239];
select :c; color translucent [154, 200, 225];
select :d; color translucent [144, 182, 211];
select :e; color translucent [134, 164, 198];
select :f; color translucent [124, 146, 184];
```

```
select :g; color translucent [114, 128, 170];
select :h; color translucent [104, 110, 157];
select :i; color translucent [94, 92, 143];
select :j; color translucent [84, 74, 129];
select :k; color translucent [74, 56, 116];
select :l; color translucent [64, 38, 102];
select :m; color translucent [54, 20, 88];
select :n; color translucent [44, 2, 75];
select PRO; define cen selected; color red; spacefill 0.025;
select ALA; define tel selected; color blue; spacefill 0.025;
select helium; define pir selected; color orange; spacefill 0.025;
```

### **Tg\_Tachyzoites**

```
color background white;
select all; wireframe 0.017;
select :a; color translucent [175, 237, 253];
select :b; color translucent [164, 218, 239];
select :c; color translucent [154, 200, 225];
select :d; color translucent [144, 182, 211];
select :e; color translucent [134, 164, 198];
select :f; color translucent [124, 146, 184];
select :g; color translucent [114, 128, 170];
select :h; color translucent [104, 110, 157];
select :i; color translucent [94, 92, 143];
select :j; color translucent [84, 74, 129];
select :k; color translucent [74, 56, 116];
select :l; color translucent [64, 38, 102];
select :m; color translucent [54, 20, 88];
select PRO; define cen selected; color red; spacefill 0.06;
select ALA; define tel selected; color blue; spacefill 0.06;
select helium; define pir selected; color orange; spacefill 0.06;
```

### **Tg\_Bradyzoites**

```
color background white;
select all; wireframe 0.012;
select :a; color translucent [175, 237, 253];
select :b; color translucent [164, 218, 239];
select :c; color translucent [154, 200, 225];
select :d; color translucent [144, 182, 211];
select :e; color translucent [134, 164, 198];
select :f; color translucent [124, 146, 184];
select :g; color translucent [114, 128, 170];
select :h; color translucent [104, 110, 157];
select :i; color translucent [94, 92, 143];
select :j; color translucent [84, 74, 129];
select :k; color translucent [74, 56, 116];
select :l; color translucent [64, 38, 102];
select :m; color translucent [54, 20, 88];
select PRO; define cen selected; color red; spacefill 0.04;
```

```
select ALA; define tel selected; color blue; spacefill 0.04;  
select helium; define pir selected; color orange; spacefill 0.04;
```

3. Because Jmol is designed for visualizing molecules and proteins in particular, many of the predefined terms used by the program are in terms of elements (such as hydrogen, helium). This doesn't change anything when visualizing the genome, it just provides an easy way to label and color accordingly.

```
color background white;
```

This colors the background white.

```
select all; wireframe 0.007;
```

Selecting every locus (and their connections) and setting the wireframe to 0.007 increases the thickness.

```
select :a; color[175, 237, 253];
```

Colors chain 'A', or chromosome 1, light blue. This pattern follows suit for all chromosomes, in a gradient from light blue to dark purple. The images in Figure 2 of the manuscript were generated using `color[255, 255, 255]` for all chromosomes.

```
select PRO; define cen selected; color red; spacefill 0.015;  
select ALA; define tel selected; color blue; spacefill 0.015;  
select helium; define pir selected; color orange; spacefill 0.015;
```

If you open the PDB file (which you can do with any text editor), you'll see in the fourth column a list of amino acids. The amino acids listed here encode the locations of the telomeres ("ALA") and centromeres ("PRO"). At the end of certain lines, there is an "He" appended. "He" is defined as a bin containing virulence genes. When we command "select helium", we select all the bins containing virulence genes and color them orange. Similarly, we can select "ALA" and "PRO" to color the telomeres and centromeres in the same way. Centromeres are red, and telomeres are blue.

#### 4. Saving images

To save the model as showing on the screen, use command "write png" followed by a unique file name.

```
write png <3Dmodel.png>;
```

To recreate the images as shown in Figure 2 of the manuscript, first execute all commands listed above to be able to select the optimal orientation of the model. Then save the model in two separate images: one of the wireframe and one of the spheres, as follows:

```
select PRO; define cen selected; color white; spacefill 0;  
select ALA; define tel selected; color white; spacefill 0;  
select helium; define pir selected; color white; spacefill 0;  
write png <3Dmodel_wireframe.png>;
```

```
select all; wireframe 0;  
select PRO; define cen selected; color red; spacefill 0.02;  
select ALA; define tel selected; color blue; spacefill 0.02;  
select helium; define pir selected; color orange; spacefill 0.02;  
write pngT <3Dmodel_spheres.png>;
```

Import both images into powerpoint. Set the transparency for the wireframe image to 70%.  
Finally, overlay the two images, with the spheres image on top.