

Advanced Scripting Workshop

Part 1: Interactive Command Line

To get familiar with the PyMOL command line, enter the following commands one by one.

Make use of **auto-completion** (**Tab** key) for command-, color- and representation names!

```
# download PDB file (most important command! :-))  
fetch 1a00
```

```
# show only cartoon representation  
as cartoon
```

We have loaded hemoglobin, which is a hetero-tetramer of two alpha and two beta chains. Let's color alpha different from beta.

```
# hemoglobin alpha  
color orange, chain A+C
```

```
# hemoglobin beta  
color marine, chain B+D
```

Right now we only see polymer chains, because other molecules don't have a cartoon representation (we did "as cartoon"). Let's show "sticks" (bonds) for non-polymer atoms.

```
show sticks, not polymer
```

```
# automatically set the camera on the heme cofactor of the first chain  
orient resn HEM and chain A
```

Small molecules are better visualized with color-by-element and bond orders.

```
# color non-carbon atoms by element  
color atomic, not elem C
```

```
# show bond orders  
set valence
```

