The trick in biology is to select, from the thousands of facts that you know, the three that are relevant to your problem, and to not be disturbed that they contradict each other.

Eric Wieschaus
(paraphrased)

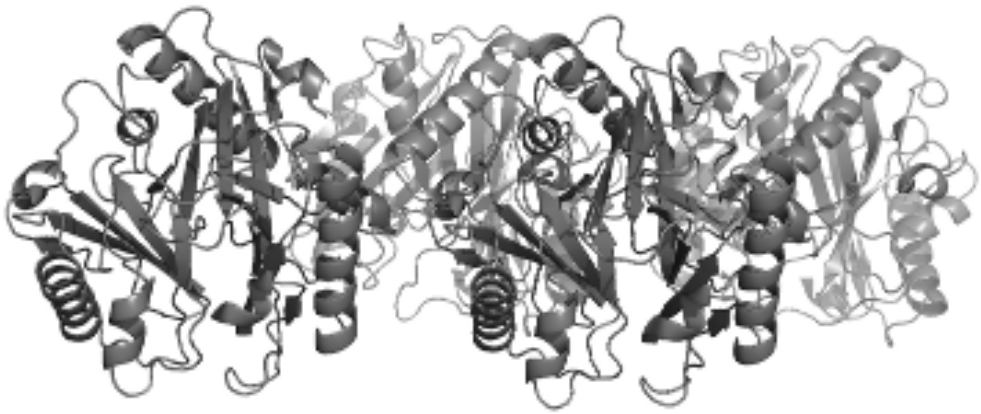
3D Structures

Mark Voorhies

4/6/2012

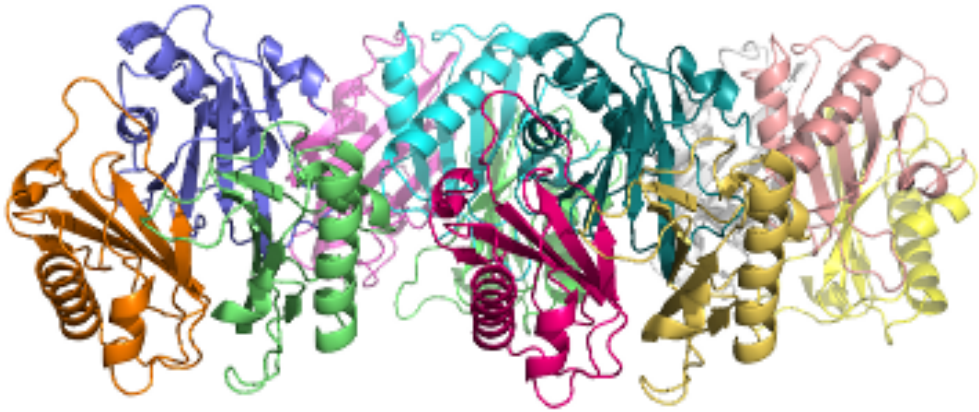
Orienting ourselves

```
select all
color grey
hide everything
show cartoon
```



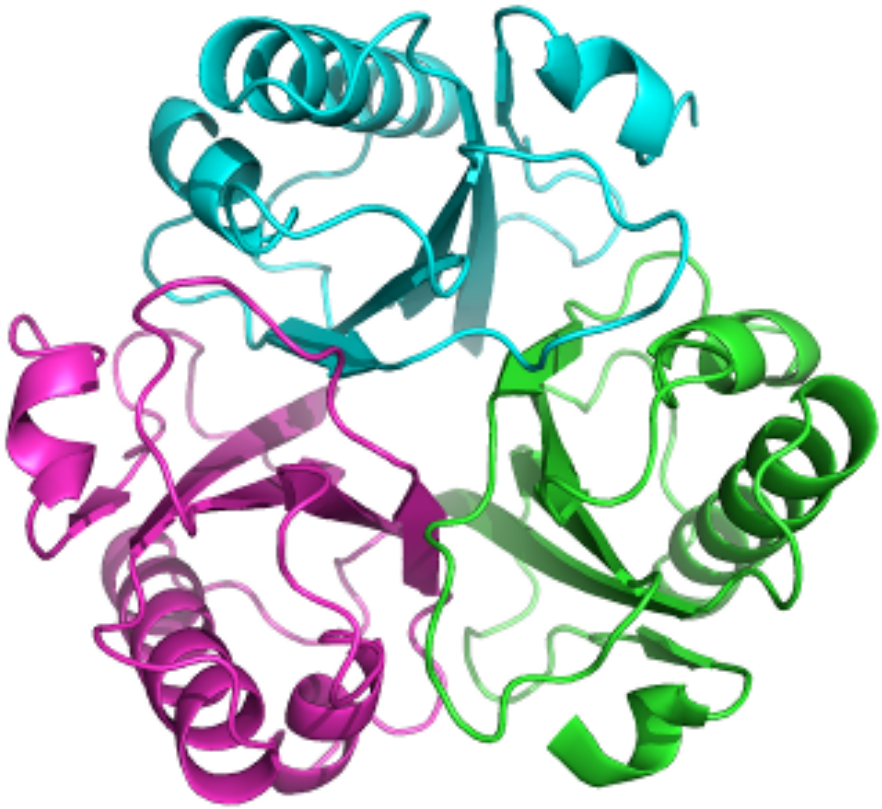
Orienting ourselves

2CHT $\rightarrow$ C $\rightarrow$ by chain $\rightarrow$ by chain



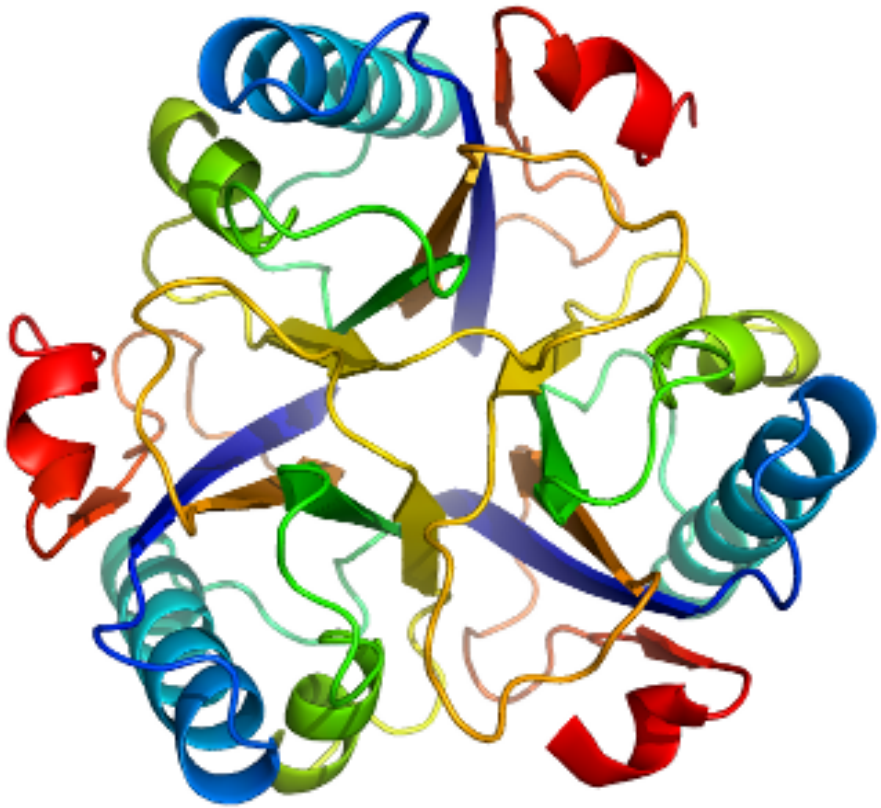
Pick one trimer in the unit cell

```
select all
hide everything
select trimer1, chain a+b+c
show cartoon, trimer1
orient trimer1
```



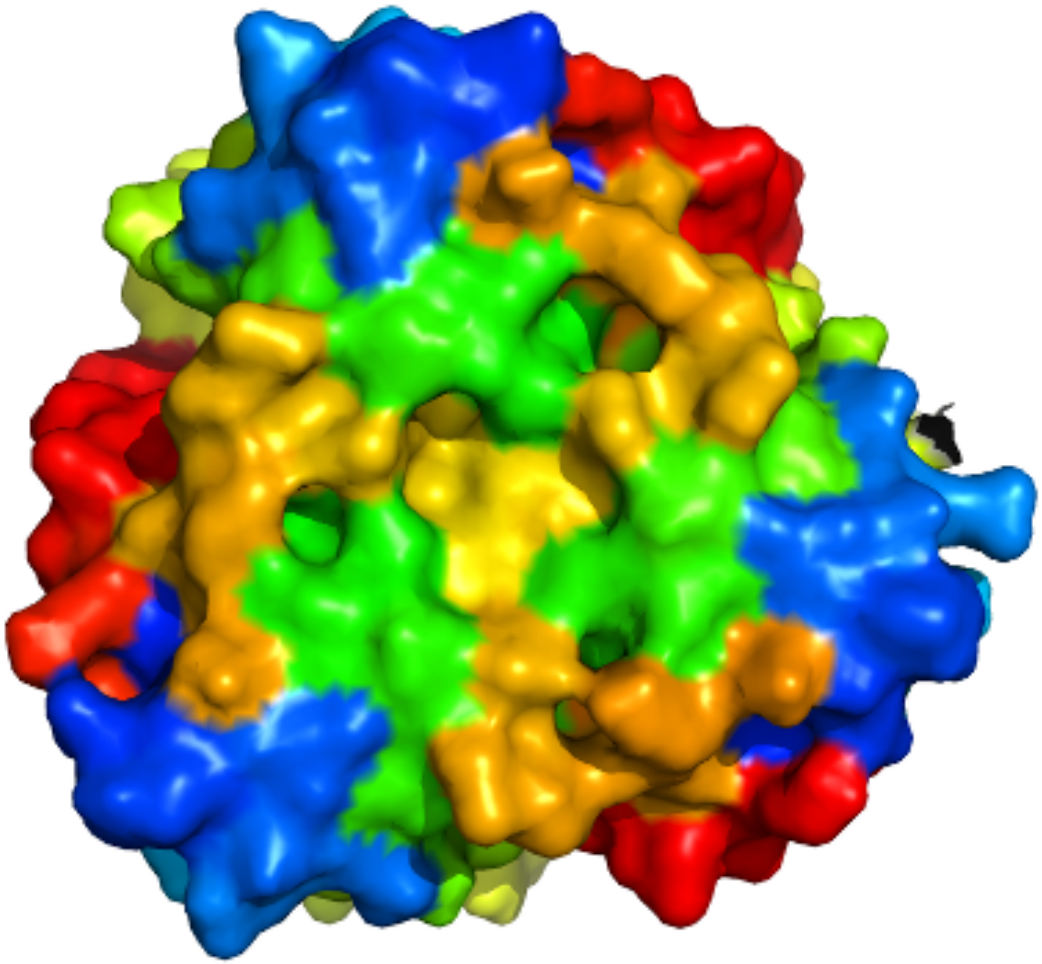
Orient ourselves on the primary structure

trimer1 $\rightarrow$ C $\rightarrow$ by chain $\rightarrow$ chainbows



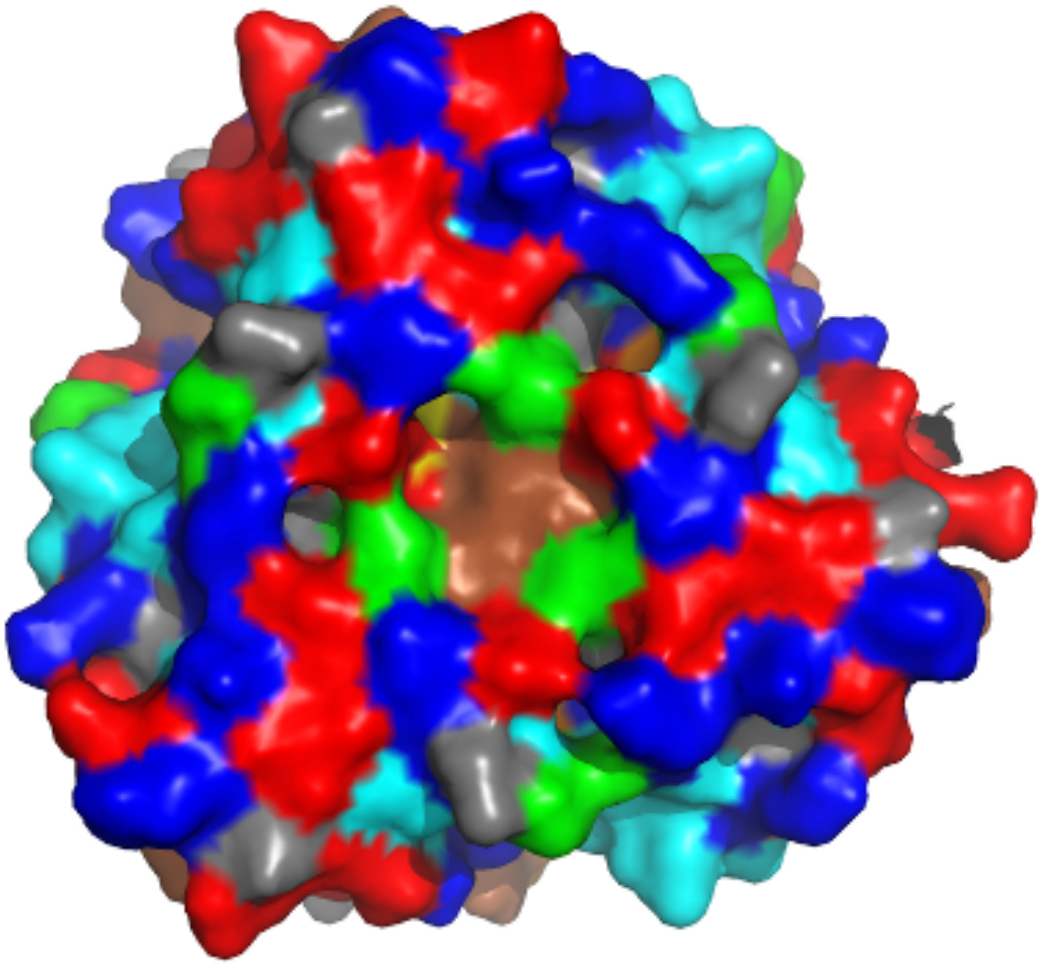
Show Conolly solvent accessible surface

```
show surface, trimer1
```



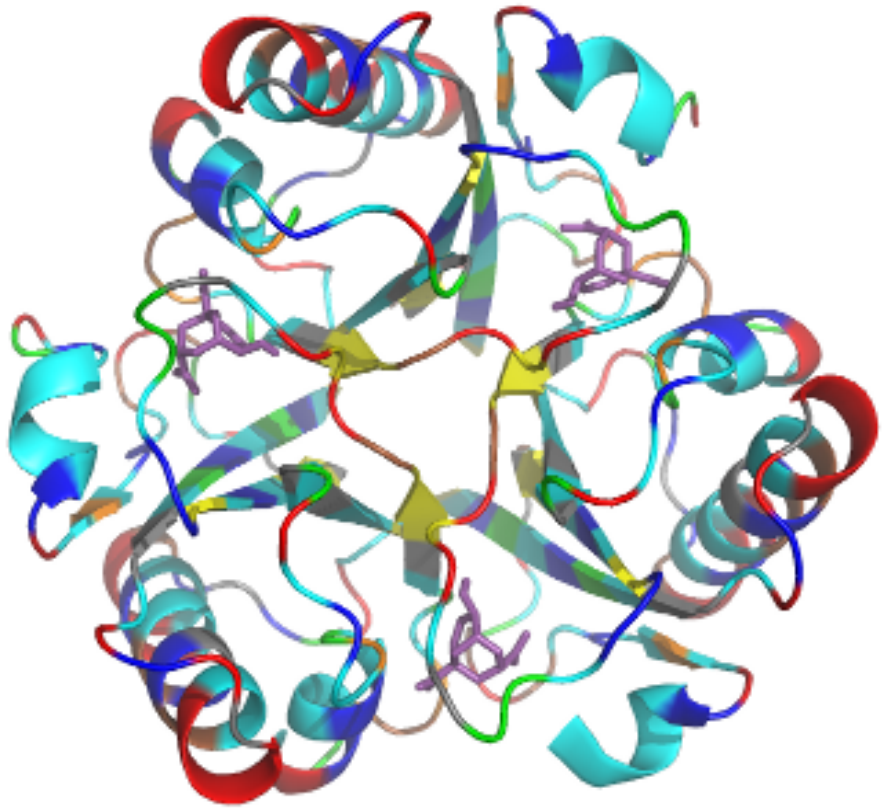
Run a custom coloring script

`@properties.pml`



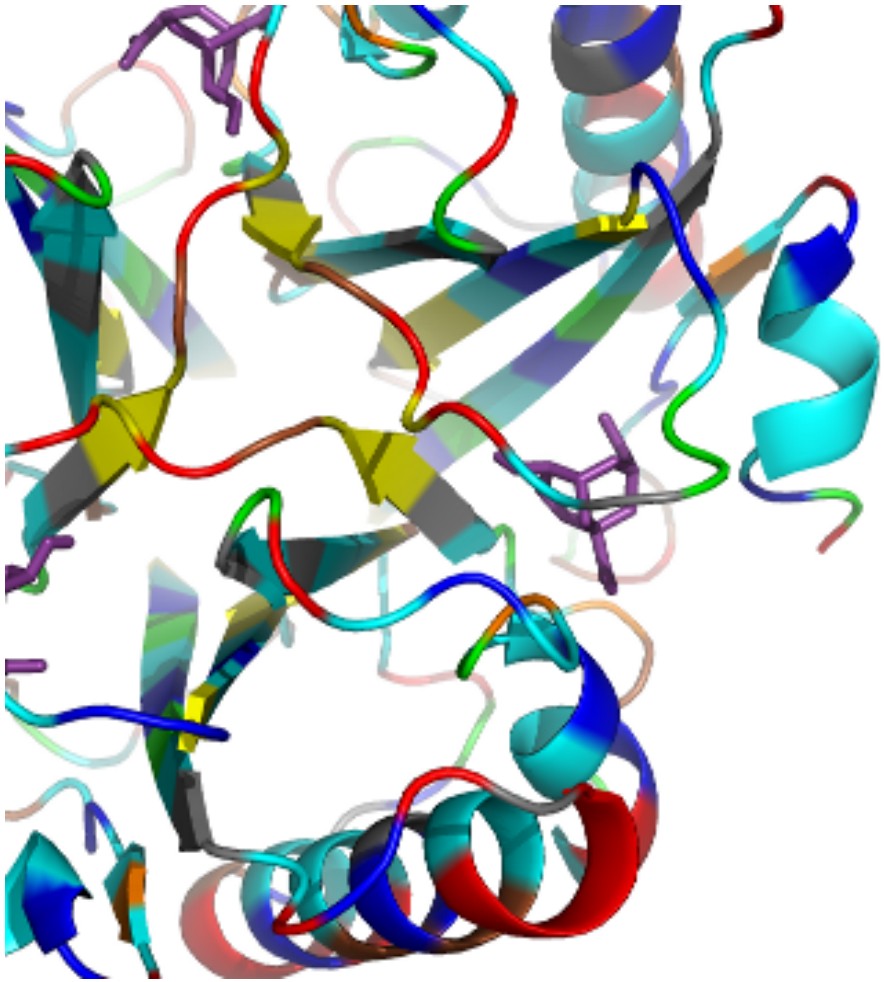
Find the ligands

```
select all
hide everything
show cartoon, trimer1
select protein, not het
select ligand, het and not resn hoh
show stick, ligand
```



Orient on one active site

```
select ligA, resi 201
orient ligA
```



Find the active site residues

```
select g1, protein within 5.0 of ligA
select g2, byres g1
show stick, g2
```