PYMOL

"Is this region of the protein surface likely to be positive, negative, or neutral relative to the rest of the protein?"

PyMOL provides such answers for proteins by performing an automated calculation

that amounts to smoothing out the local charge density from nearby atoms (within 10 β ngstroms), without taking

into account solvent screening effects. To perform this calculation, select

**Actions/generate/vacuum electrostatics/protein contact potential**.

After a minute or two, PyMOL will create a new object with the protein shown

as an electrostatic surface colored blue in the positive regions and red the negative regions.

You can then CTRL−click−and−drag along the slider to change the color levels.

**Alignments**

**Sequence Based**

PyMOL can perform sequence-driven structure alignment through 

the **A**→**Action**→**Align** menu, shown in Figure 25. You can align

all proteins to a currently selected one (**A**→**Action**→**Align**→**All**

**to this)**, or align proteins one by one (**A**→**Action**→**Align**→**To**

**Molecule)**. Finer control over the alignment process can be exercised

by creating selections that represent the two regions to be

aligned. In this case, one selection (e.g. sel01) should be created in

the target molecule and a second independent selection (e.g. sel02)

should be created in the molecule to be aligned. Then for selection

sel02, you click on the **A**→**Action**→**Align**→**To Selection**→**sel01**

to perform a superposition based on only those two regions.

Alignments performed using the **A**→**Action** menu are based on a

protein sequence alignment followed by an interactive structure

superposition, and only the CA atom positions are considered.

Greatest control over alignment can be exercised by typing an

align command in the command line. For example, the kinase

structure 1uwh actually contains two copies of the enzyme, chains

A and B, whereas 1t46 only contains one copy. The default alignment

of 1t46 and 1uwh matches only the 1uwh B chain. To force

alignment of 1t46 against the "A" chain of 1uwh, type the following

command: **align 1t46////CA, 1uwh//A//CA**. This

command uses selection macros, which are discussed in the

Advanced Features at the end of this tutorial. PyMOL comes

with a more robust alignment command called super. Use

super if align doesn’t do so well.

**Try It—Quickly Align Multiple Structures to One Target**

Let’s align all of the kinase proteins in our session to 1Z5M. For 1Z5M, choose **A**→**Action**→**Align**→**All to this**. All

enabled proteins should now be aligned to 1Z5M. To see the alignment more clearly, please select

**S**→**Show**→**As**→**Ribbon**.