

## Homework Assignment #8

**Due in class Tuesday, November 28**

A rule of thumb in protein chemistry is that surface residue side chains are more flexible than buried residue side chains. But close inspection of the ASA and simulation-calculated B-factors for the inhibitor chain of 2PTC shows that not all surface residue side chains are equally flexible. For example, the following residues have large relative ASA and small B-factors: 6, 19, and 29; and the following residues have both large relative ASA and large B-factors: 46 and 49.

- a. Inspect the structure of chain I in the model 2PTC using a molecular graphics program. This structure can be obtained with one of the following commands depending on the name of your downloaded PDB file,

```
grep '^ATOM' pdb2ptc.ent | grep ' I ' > inh.pdb
```

or

```
grep '^ATOM' 2PTC.pdb | grep ' I ' > inh.pdb
```

Provide a short answer to the following question: What are common physical-chemical attributes for each the above two classes of side chains (6, 19, 29 and 20, 46, 49, 53) and how might these attributes explain the observed differences in the two classes? (Hint: Size is not a factor because the above description applies to the gamma carbons of each type of side chain).

- b. In the structure A.pdb used in your last homework assignment, residues Thr-44 and Thr-53 both have large ASA values but relatively small B factors. Inspect this structure and answer the following question: What is the likely cause of the apparent limitation in flexibility for these two exposed residue sidechains? (Hint: The answer has to do with the side chains not the backbone atoms).