A

Check protein structure for cis peptide bonds
Molecule: 0: protein.psf
Selection: same fragment as protein

Identified cis peptide bonds
1st residue | 2nd residue | chain segment | atom | moved
GLH 8 | ALA 9 | P | P1 | none | no

Show selected cis peptide bond

Select and move atoms in cis peptide bonds
Tag atom to be moved for selected cis peptide bonds:
hydrogen | oxygen | none

Move tagged atoms for selected cis peptide bonds

Minimize/equilibration selected cis peptide bonds

Reset cispeptide plugin

I'm feeling lucky

B

C

D

AutoIMD Controls

1. Type in the atom selections for ind (top molecule):
   indmolten: same residue as within 10 of (none) or (segname P1 and
   indfixed: within 8 of indmolten

2. Choose where and how to run the simulation:
   Local using 1 processors

3. Submit your job:
   Submit | Connect | Pause | Finish | Discard

status: Waiting for user input