

**A**

**cispeptide** Help

-Check protein structure for cis peptide bonds-

Molecule: 0: protein.psf

Selection: same fragment as protein

Check structure

Identified cis peptide bonds

1st residue	2nd residue	chain	segname	atom	moved
GLN 8	ALA 9	P	P1	none	no

Show selected cis peptide bond

Select and move atoms in cis peptide bonds

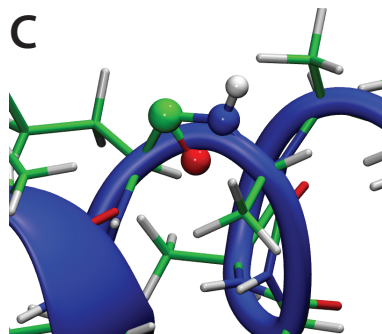
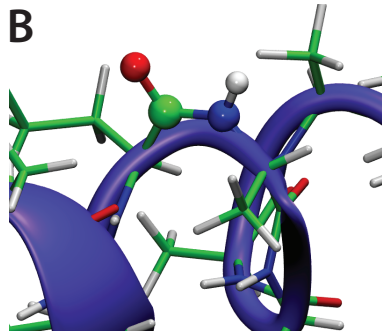
Tag atom to be moved for selected cis peptide bonds:

hydrogen oxygen none

Move tagged atoms for selected cis peptide bonds

Minimize/equilibrate selected cis peptide bonds

Reset cispeptide plugin I'm feeling lucky



**D**

**AutoIMD Controls** Help

File Settings Help

1. Type in the atom selections for imd (top molecule):

imdmolten: same residue as within 10 of (none or (segname P1 and

imdfixed: within 8 of imdmolten

2. Choose where and how to run the simulation:

Local using 1 / 1 processors

3. Submit your job:

Submit Connect Pause Finish Discard

status: Waiting for user input