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#!/usr/bin/python
__author__ = "morganlnance"
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HW2 Question 3 (Workshop #2 Exercise 2)
This program makes an alpha helix of a specified length
out of alanines. Phi and psi values are idealized.
This program dumps the resulting pose as 'helix.pdb'
         ./make_helix.py <number of helix residues>
Usage:
Example: ./make_helix.py 20
##########
# IMPORTS #
##########
import sys
from pyrosetta import init, \
    pose_from_sequence, PyMOLMover
#############
# ARGUMENTS #
############
try:
    n_helix_residues = int(sys.argv[1])
except:
    print "\nGive me an integer for the number of helix residues.\n"
    sys.exit()
#######
# MAIN #
#######
# initialize pyrosetta and load the pose
init()
pose = pose from sequence("A"*n helix residues, "fa standard")
# PyMOLMover for visualization
pmm = PyMOLMover()
pmm.keep_history(True)
# ideal phi and psi values
phi = -60
psi = -45
# set phi and psi
pmm.apply(pose)
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for ii in range(1, pose.size()+1):
    pose.set_phi(ii, phi)
    pose.set_psi(ii, psi)
    pmm.apply(pose)
pose.dump_pdb("helix.pdb")
```