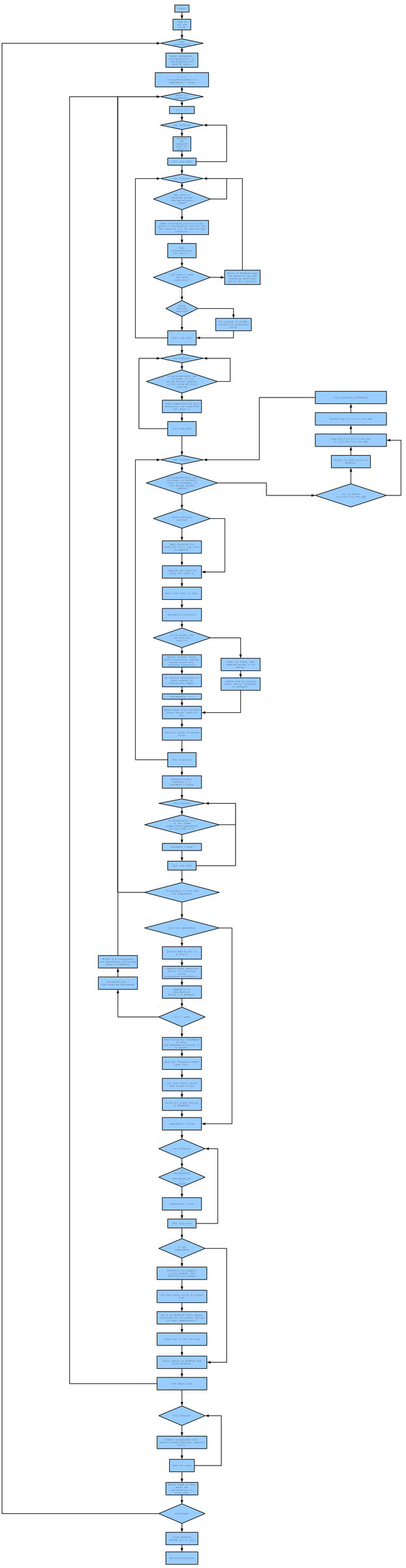
mcsad_protein.py
4-16-2012


Begin
Load in pdb file
Start
Begin Metropolis Monte Carlo
Accepted_Bonds = Bonds_Broken = Count_MC_Cycle = 0
Is a chain a 2 sampleMove = False
Start
Pick a chain
Pick a random residue
Start loop end
Start
Has chain a been checked before?
Pick a random residue
Move to another chain if the selected bond has been checked before or has no free rotations
Is residue a proline?
Move to another chain if the selected bond has no free rotations
Is a bond of length 1 selected for rotation?
Move to another chain if the selected bond has no free rotations
Pick a random rotation for chain a
Check if the bond rotation?
Move to another chain if the selected bond has no free rotations
Is a bond of length 1 selected for rotation?
Move to another chain if the selected bond has no free rotations
Check if the rotation is valid
Check if the rotation is valid
Check if the rotation is valid