

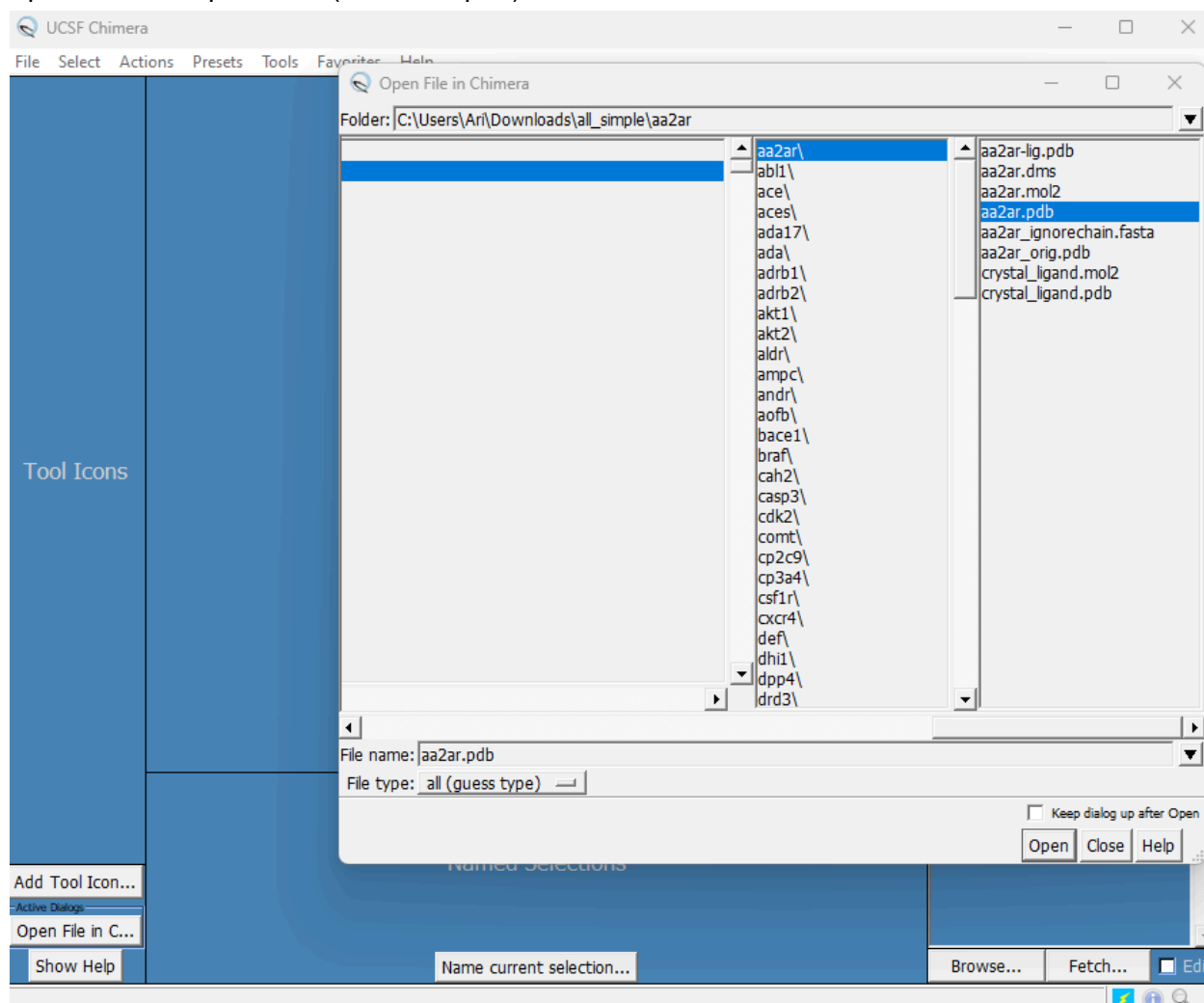
Download Chimera link - <https://www.cgl.ucsf.edu/chimera/download.html>

Chimera MS and DMS file tutorial:

<https://www.cgl.ucsf.edu/chimera/docs/UsersGuide/dms.html#writedms>

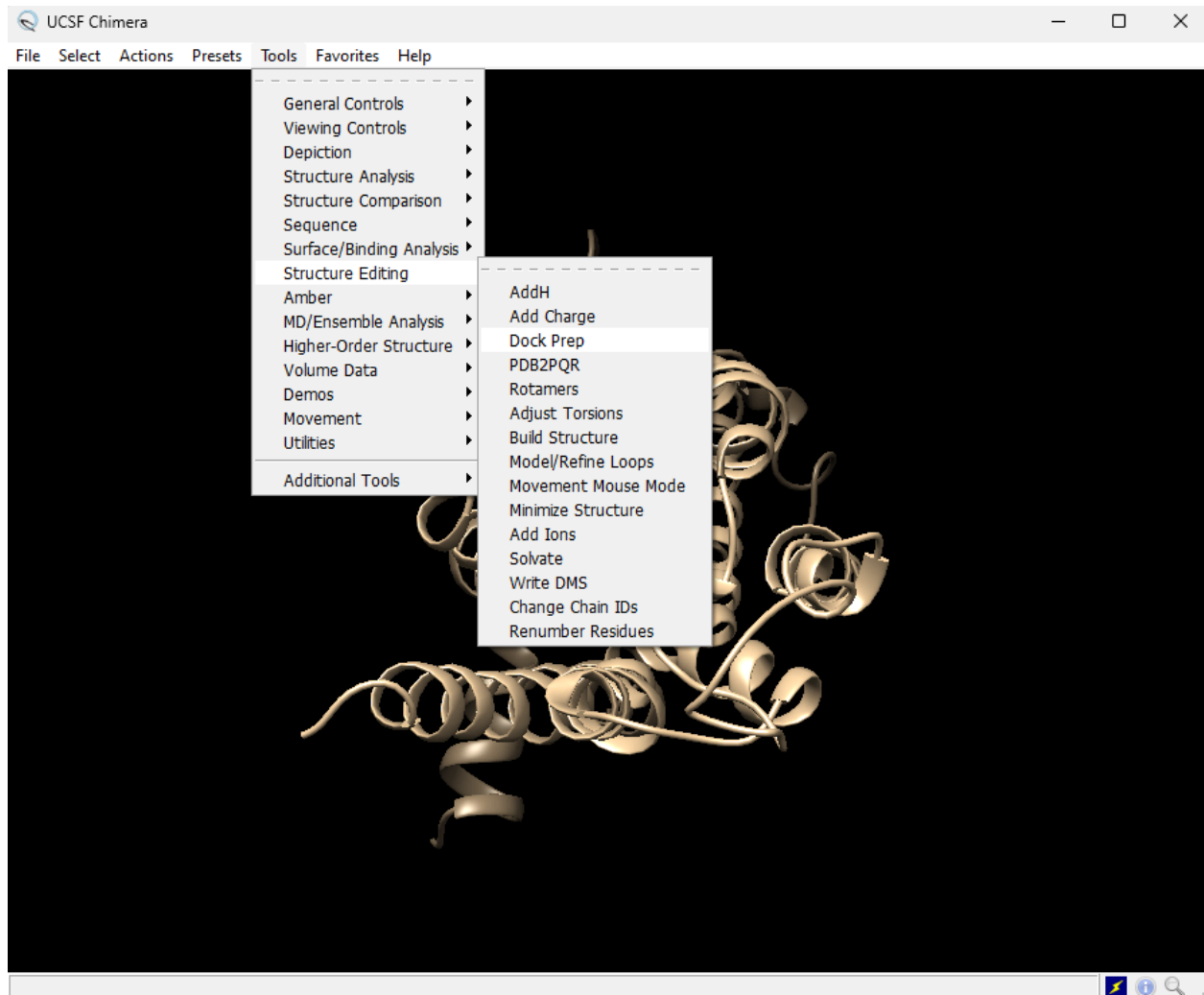
Using aa2ar as an example (you do not need to repeat aa2ar)

Open the a receptor PDB (i.e. aa2ar.pdb)

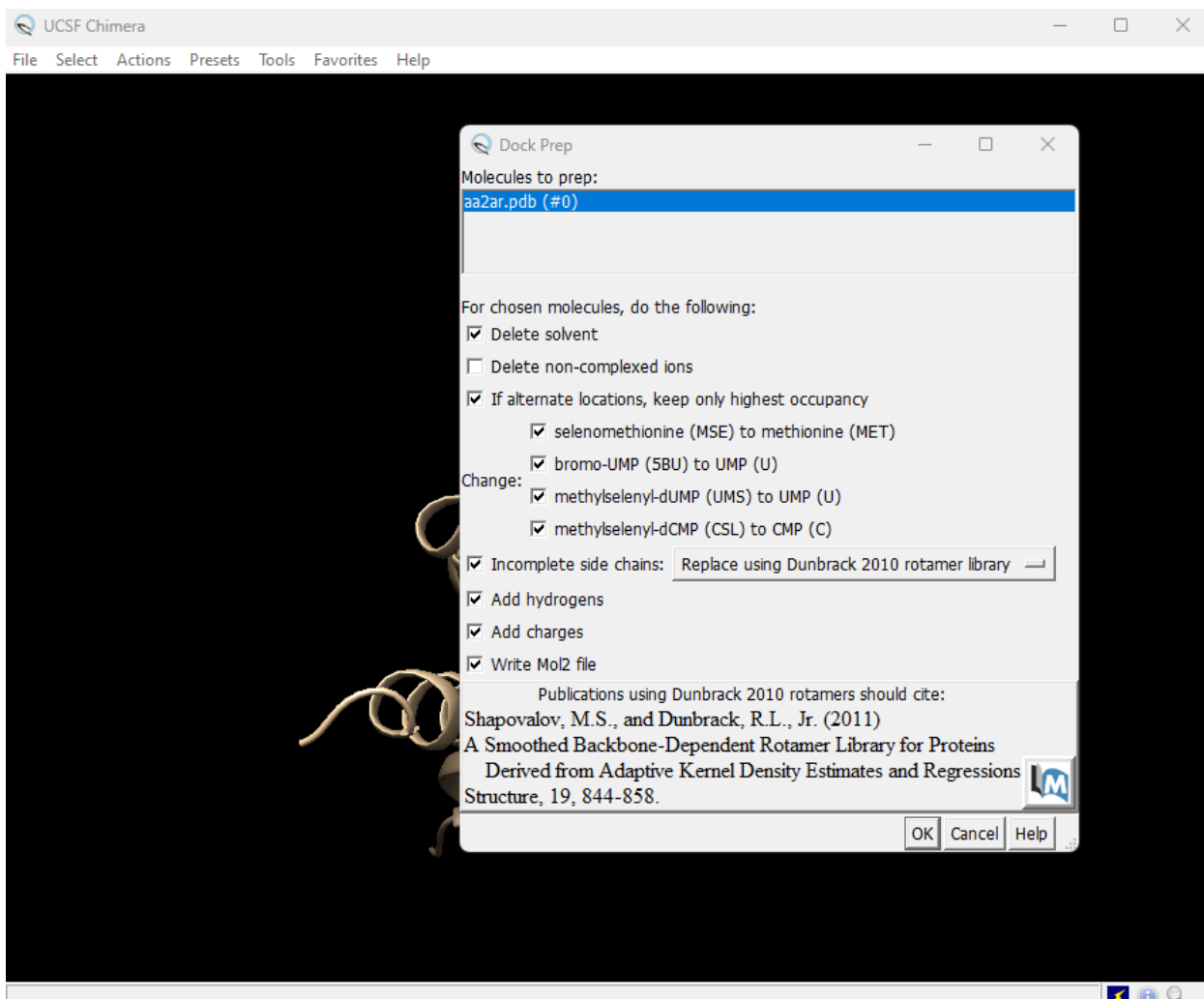


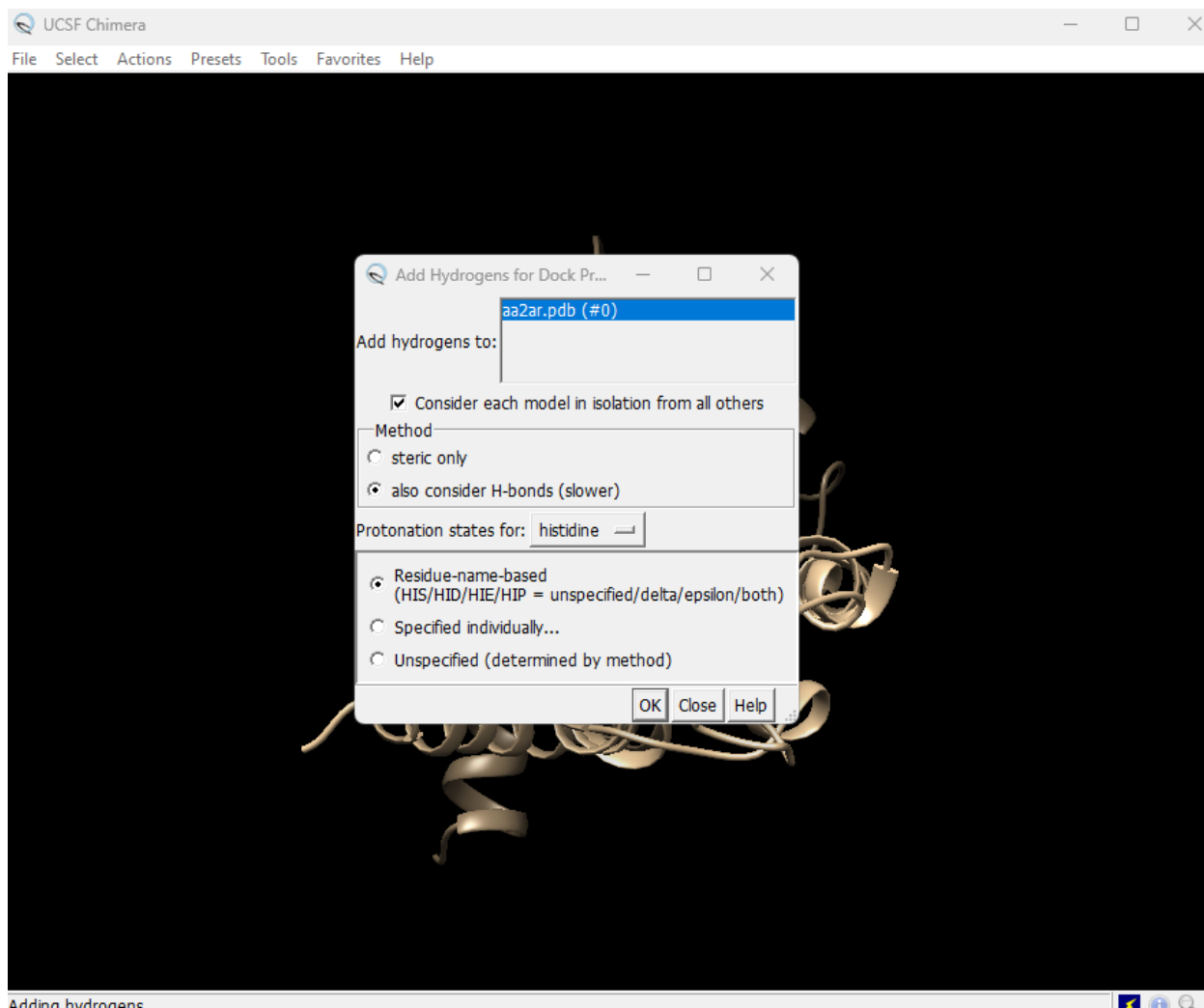
Creating dock6 mol2 file:

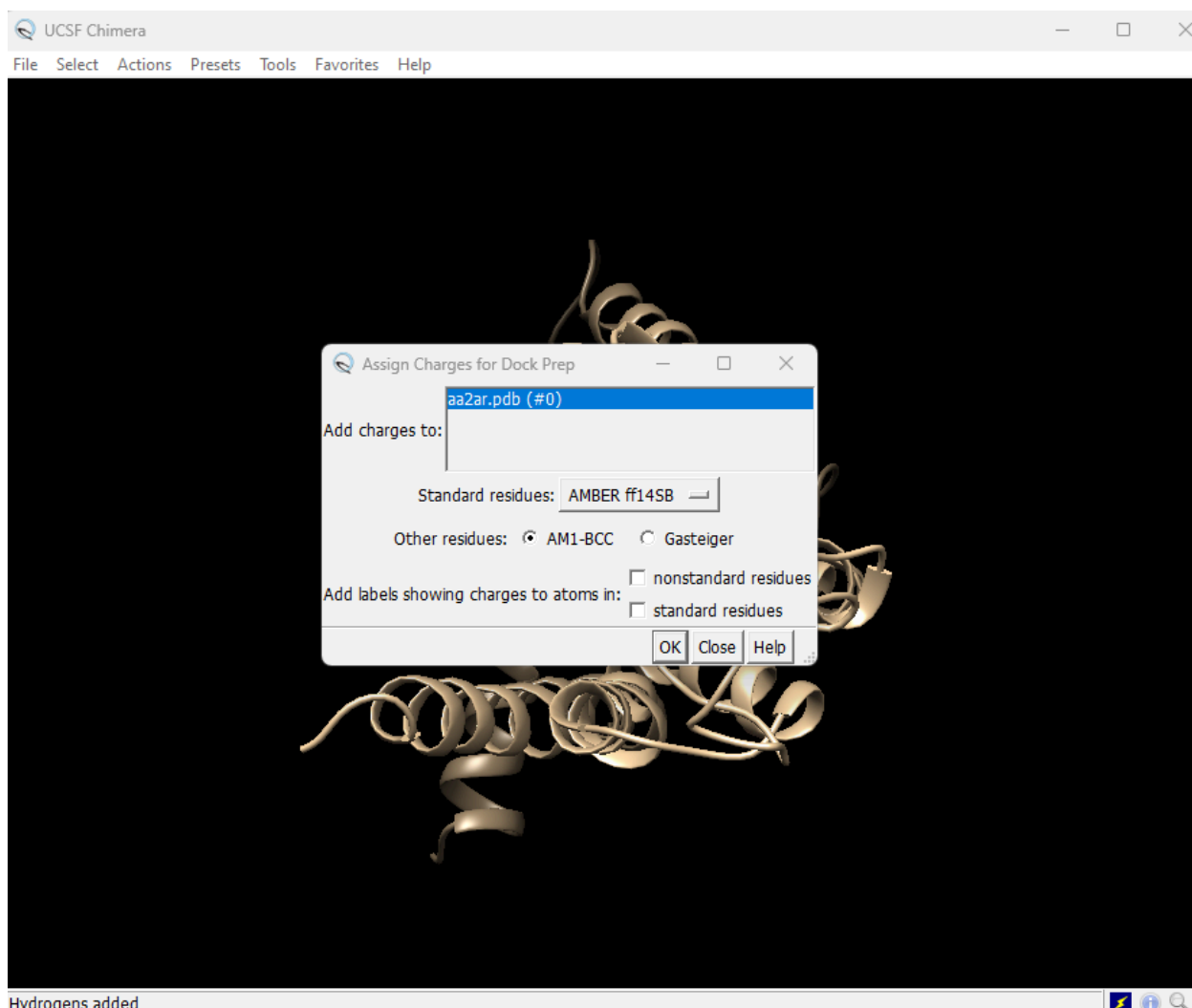
1. Go to Tools->Structure Editing->Dock Prep



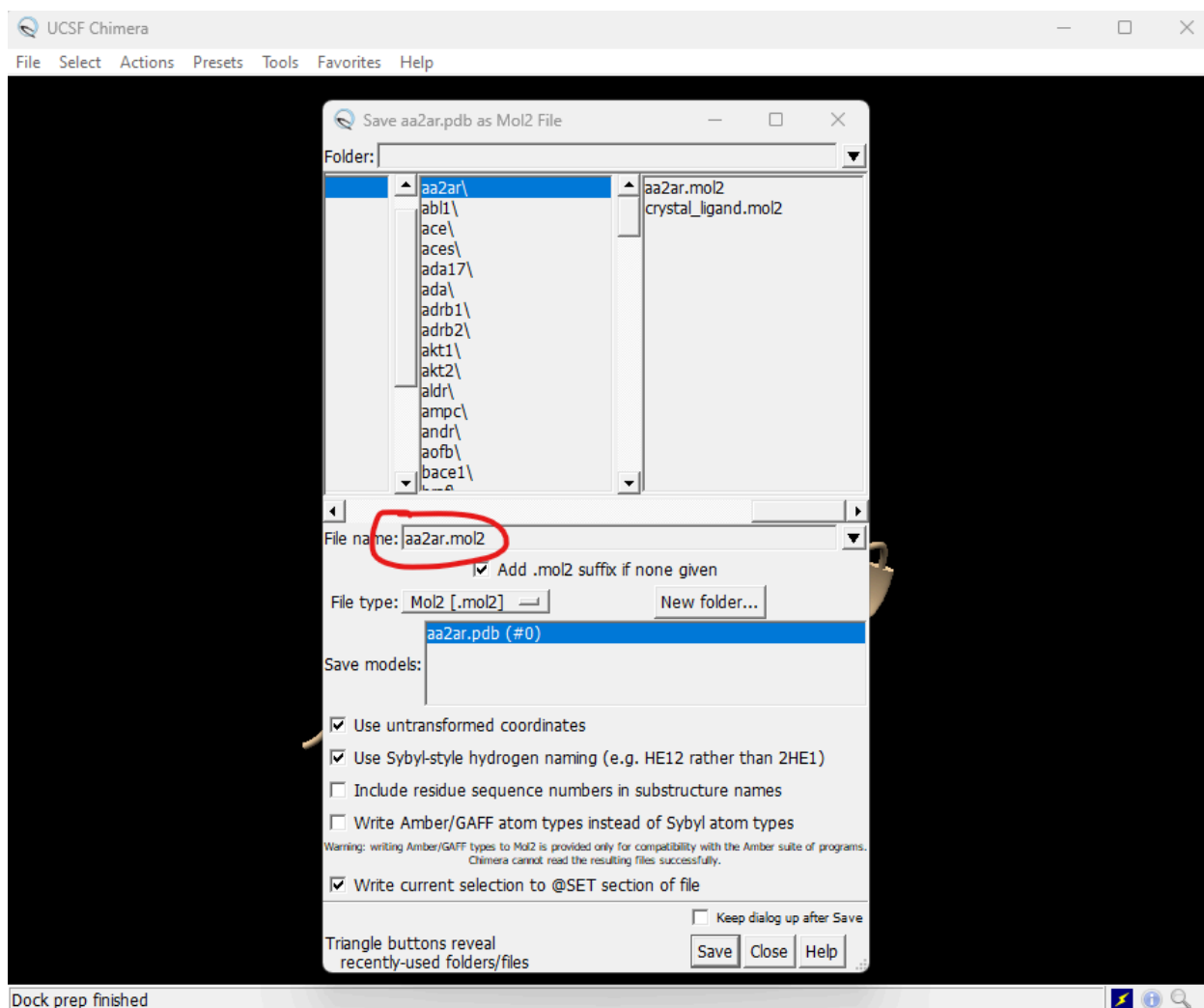
2. Use default settings:







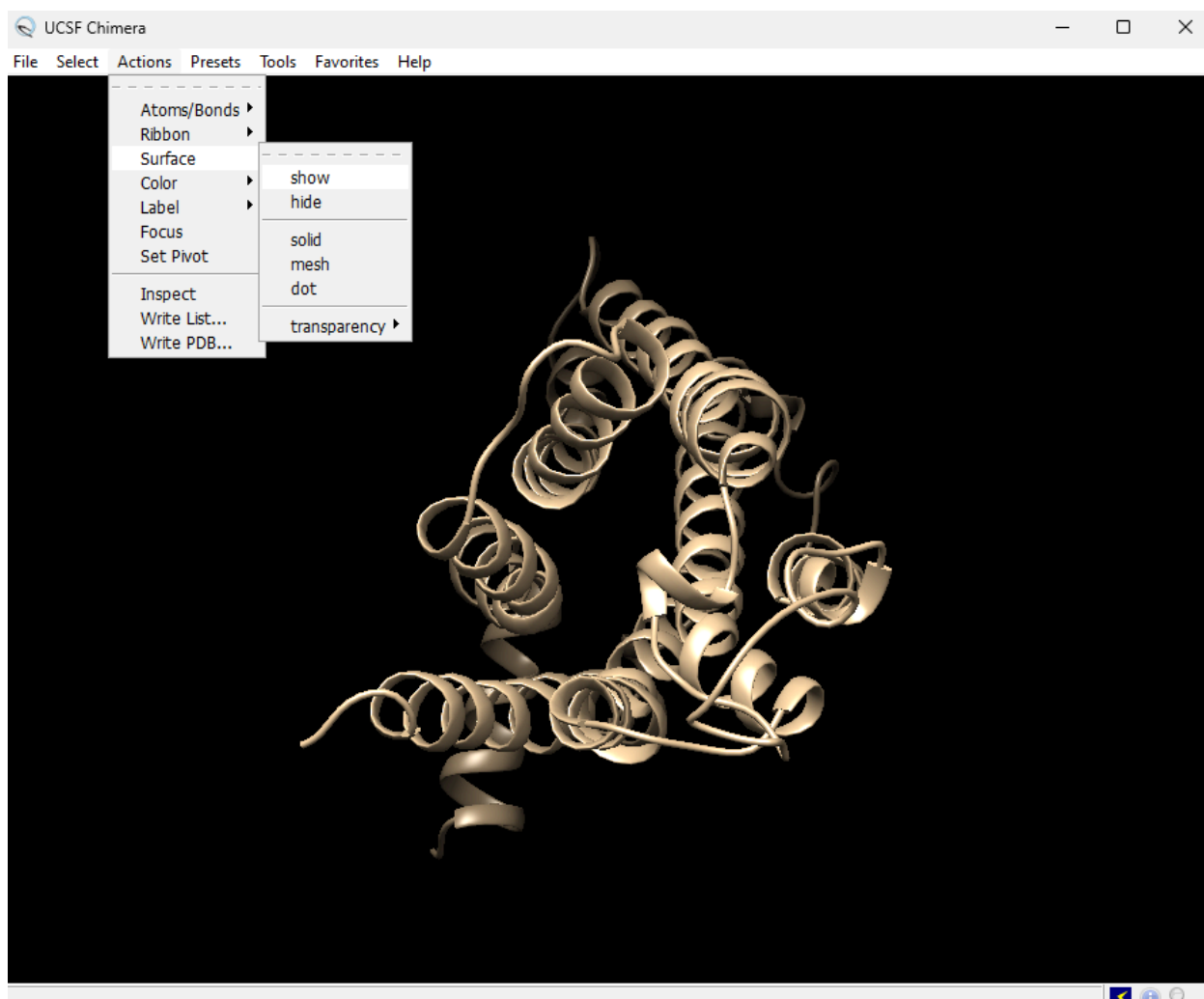
3. Save as system.mol2 (i.e. aa2ar.mol2); Ideally save this in all_simple or in a new folder in the github repository for dock inputs. I can set something up

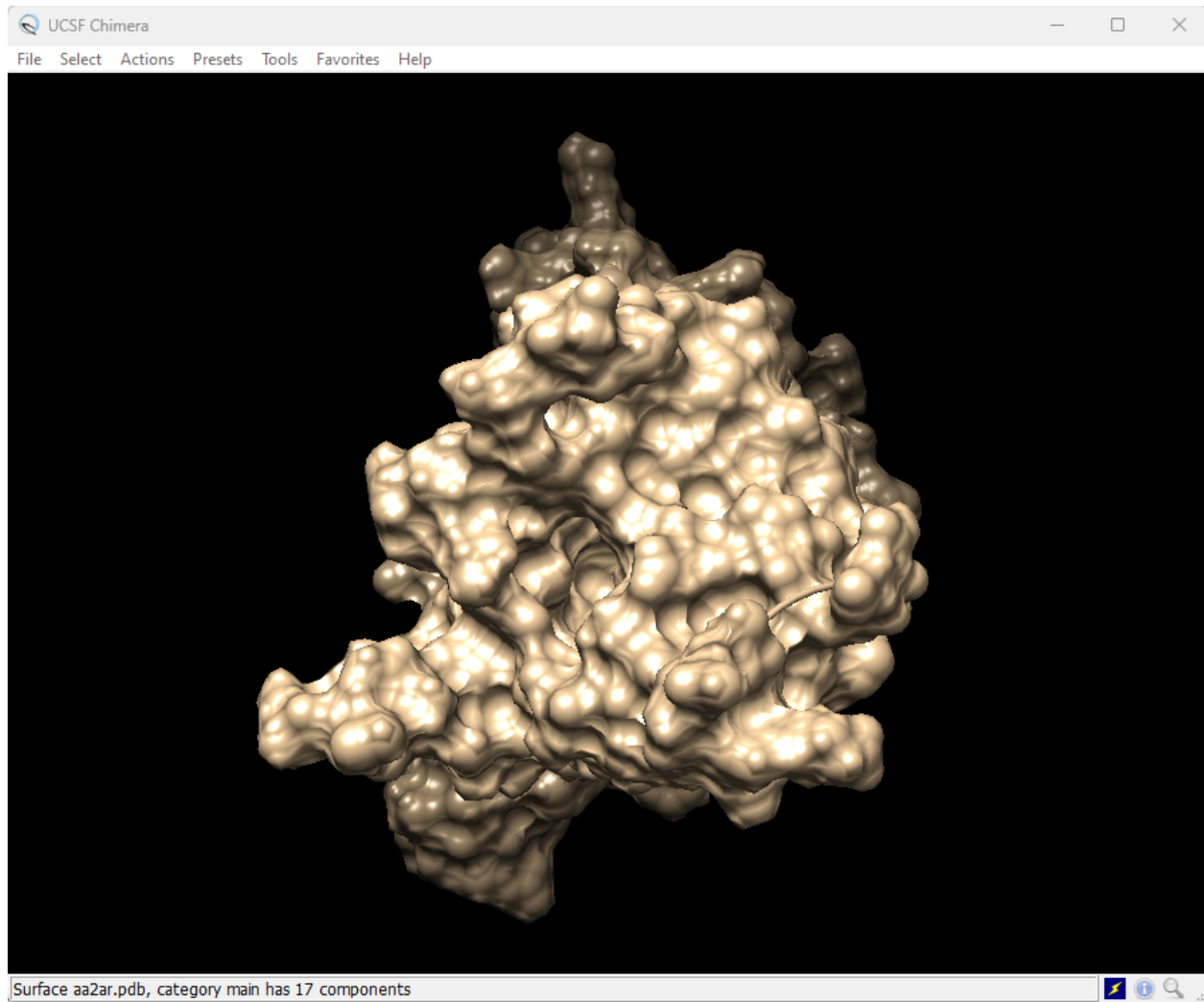


Keep receptor pdb open for creating DMS surface!

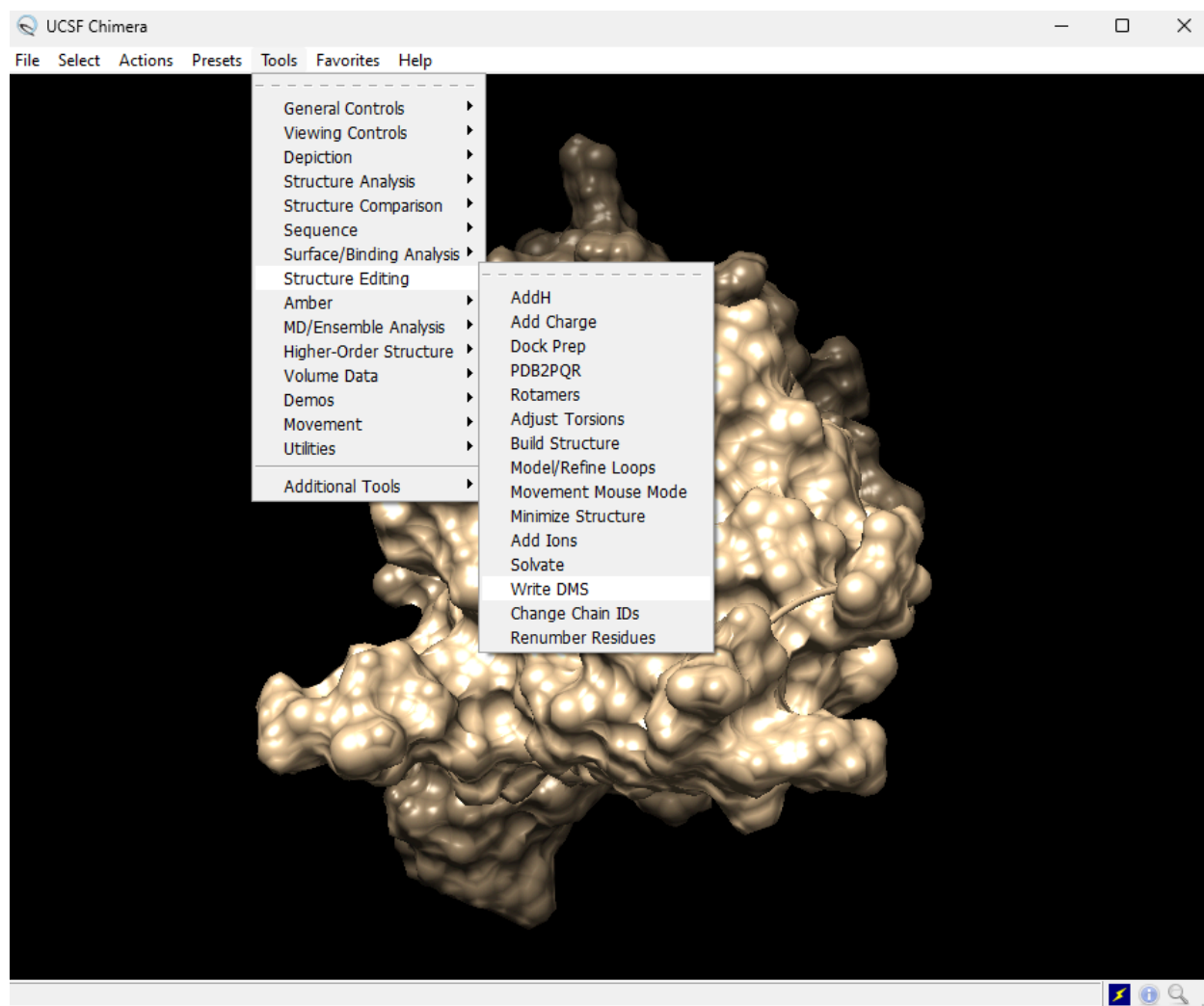
Make DMS of receptor:

1. Create surface of receptor: Actions->Surface->show

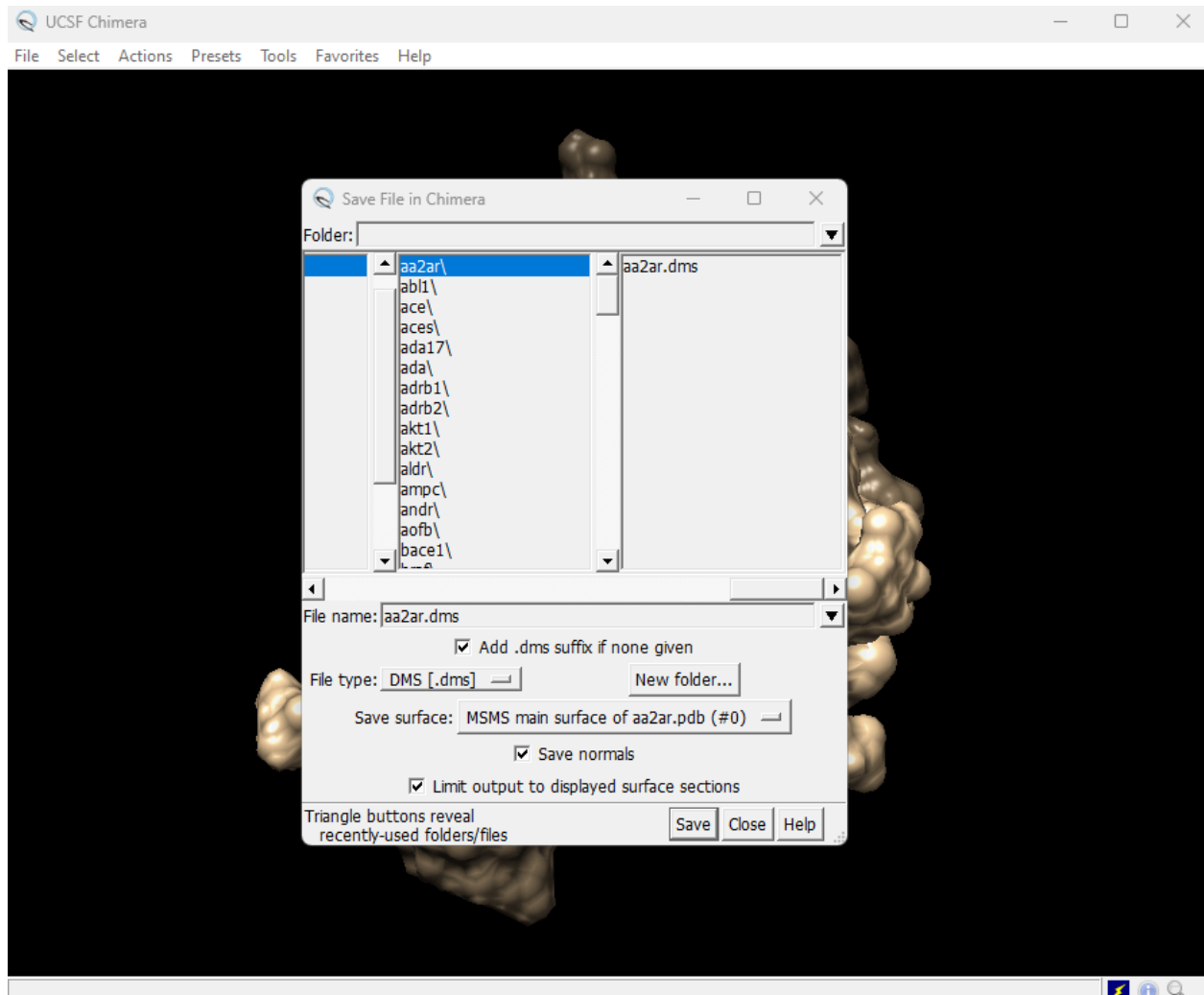




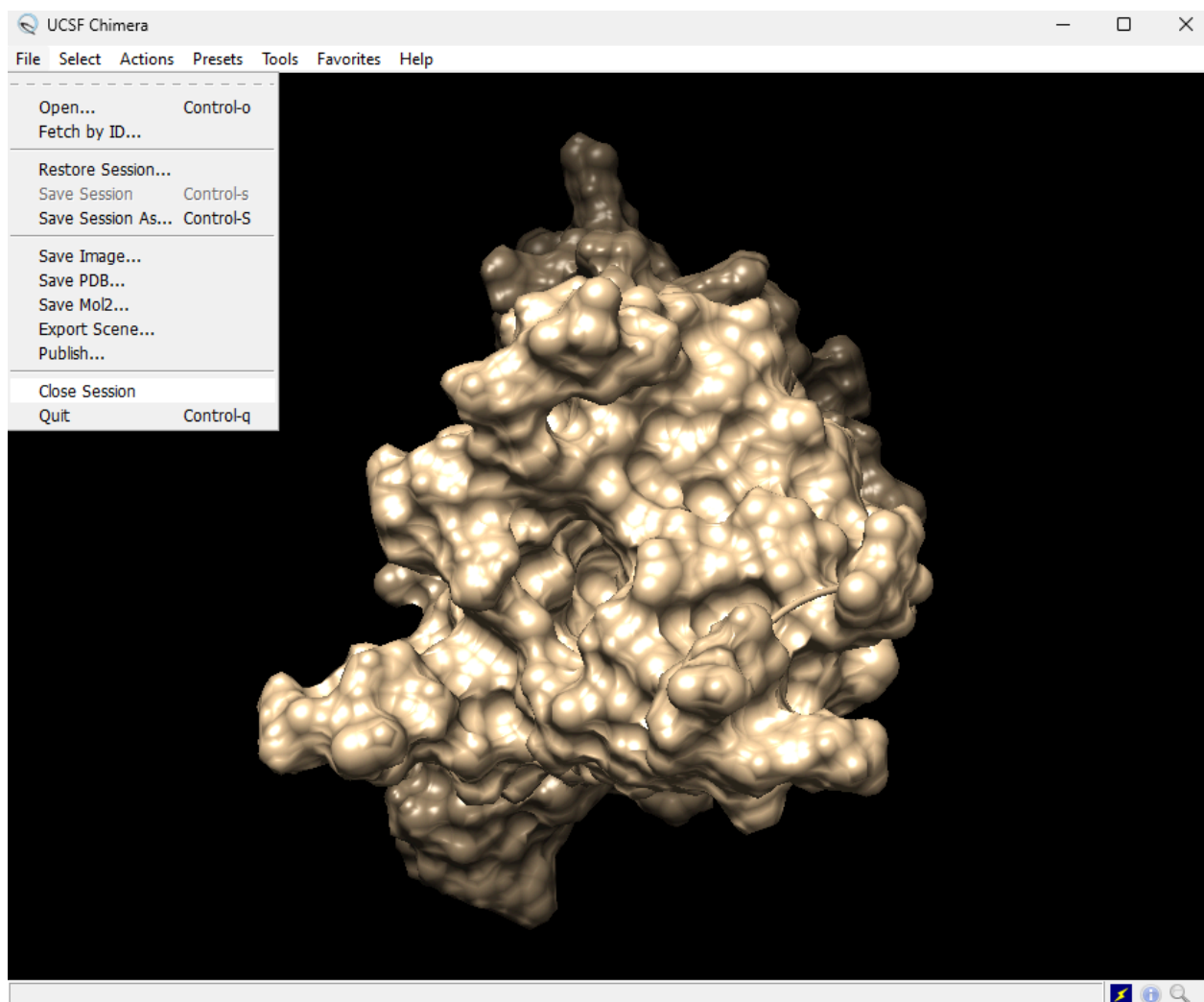
2. Write the surface to DMS: Tools->Structure Editing->Write DMS



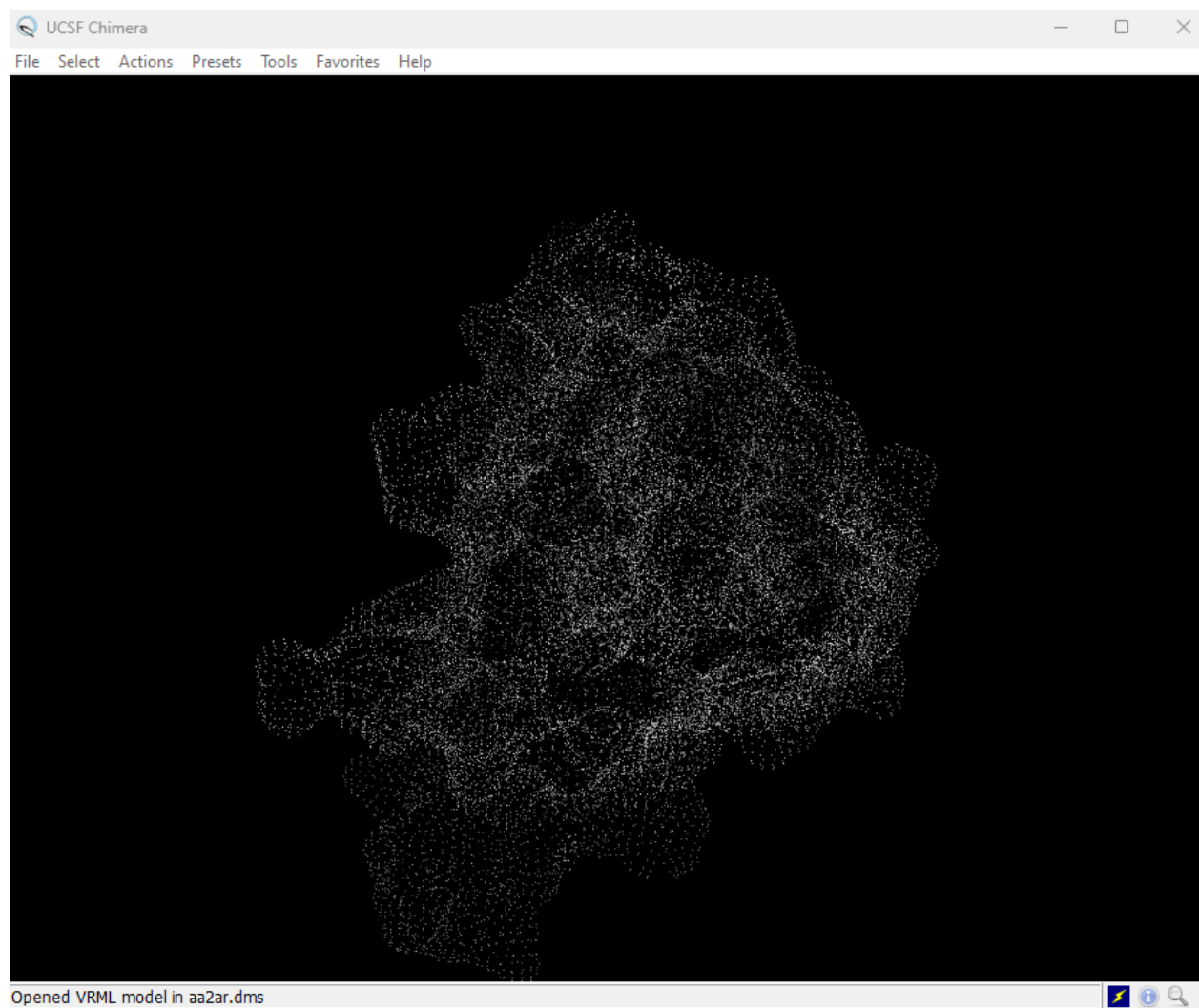
3. Save DMS file; i.e. aa2ar.dms



Close session with pdb file (not close entire chimera program to avoid startup): File->Close Session



(OPTIONAL) View dms file:



Receptor surface and mol2 locations:
Creating folders in the internship github repository