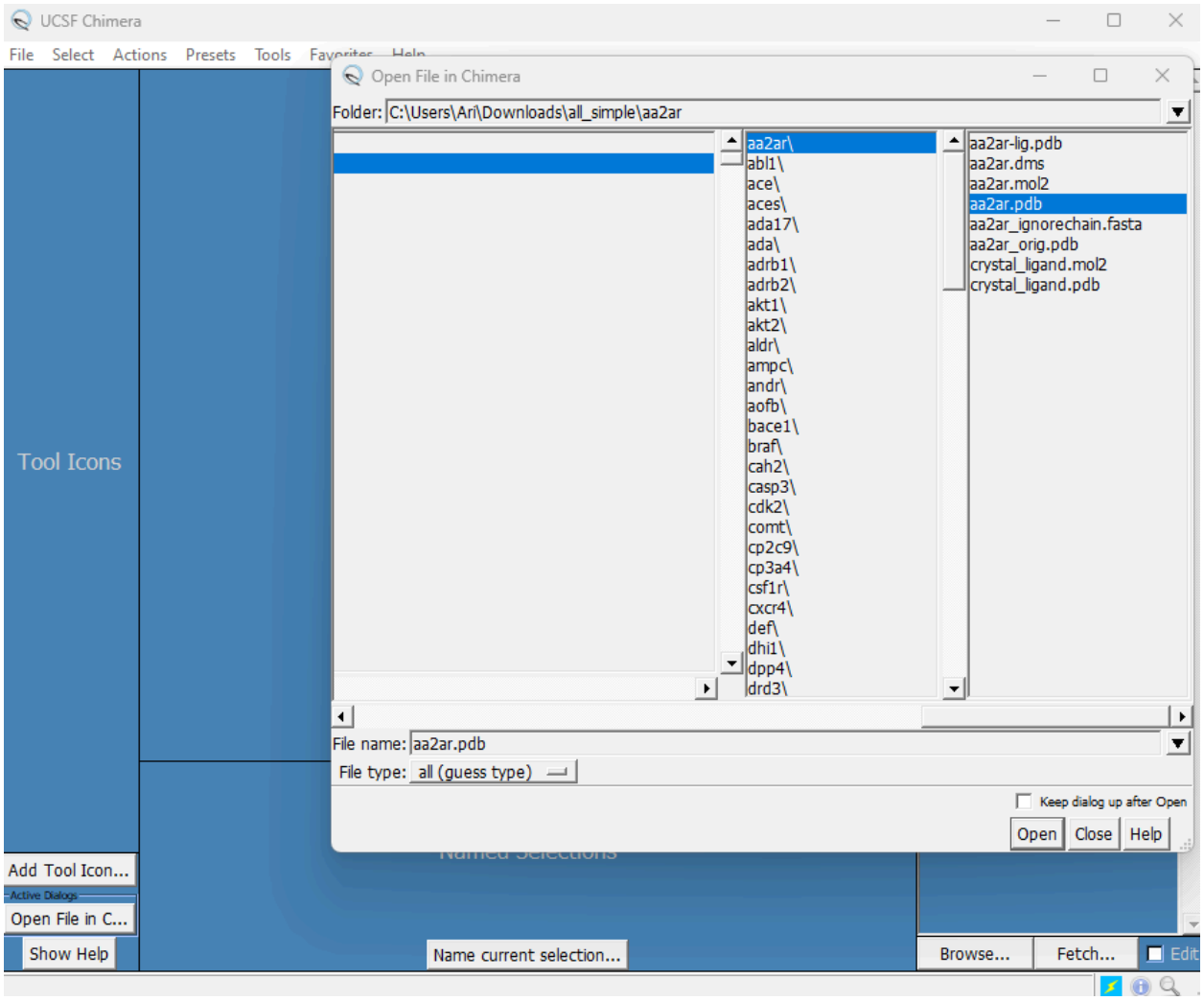
Download Chimera link - https://www.cgl.ucsf.edu/chimera/download.html

Chimera MS and DMS file tutorial:
https://www.cgl.ucsf.edu/chimera/docs/UsersGuide/dms.html#writedms

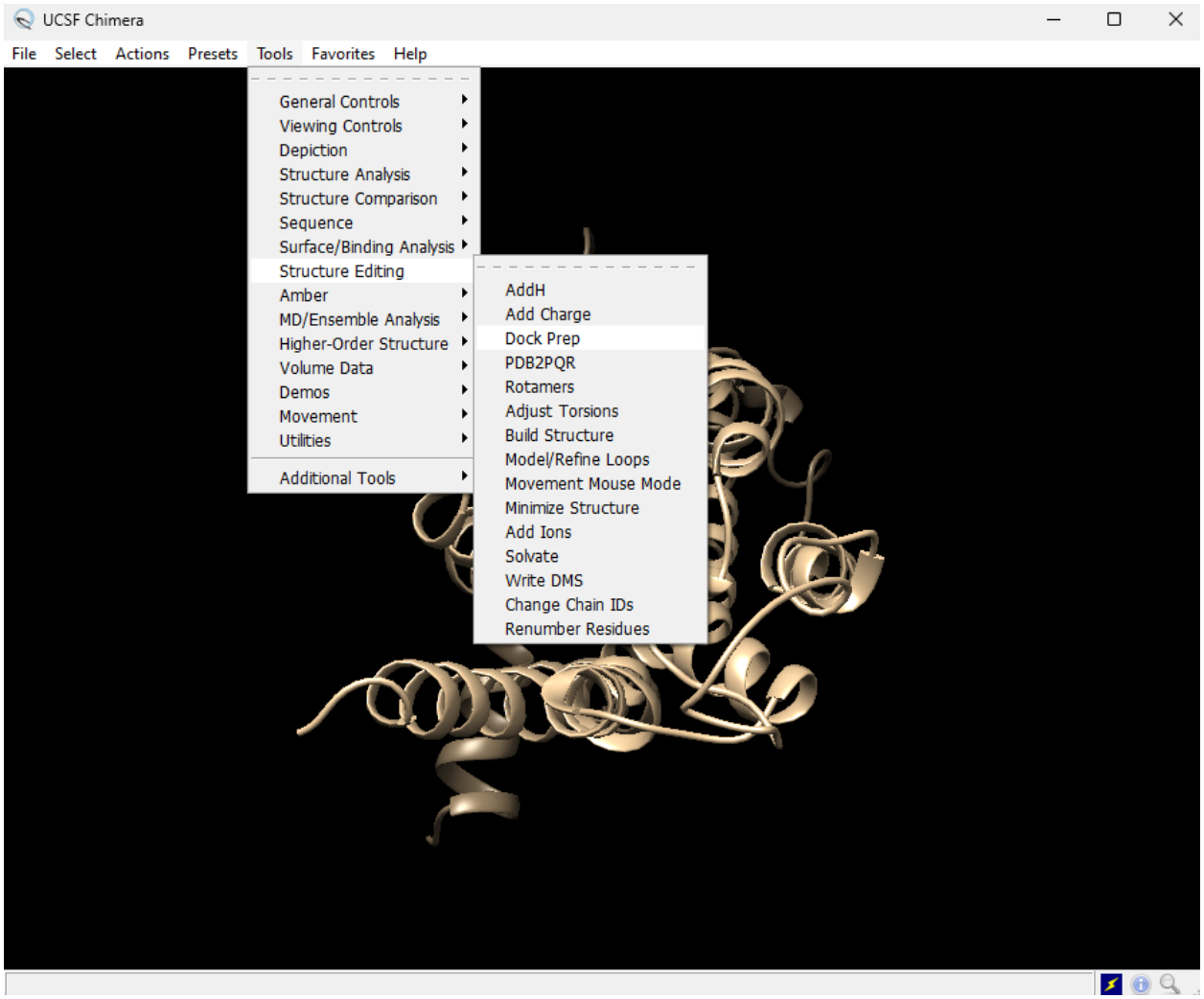
Using aa2ar as an example (you do not need to repeat aa2ar)

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

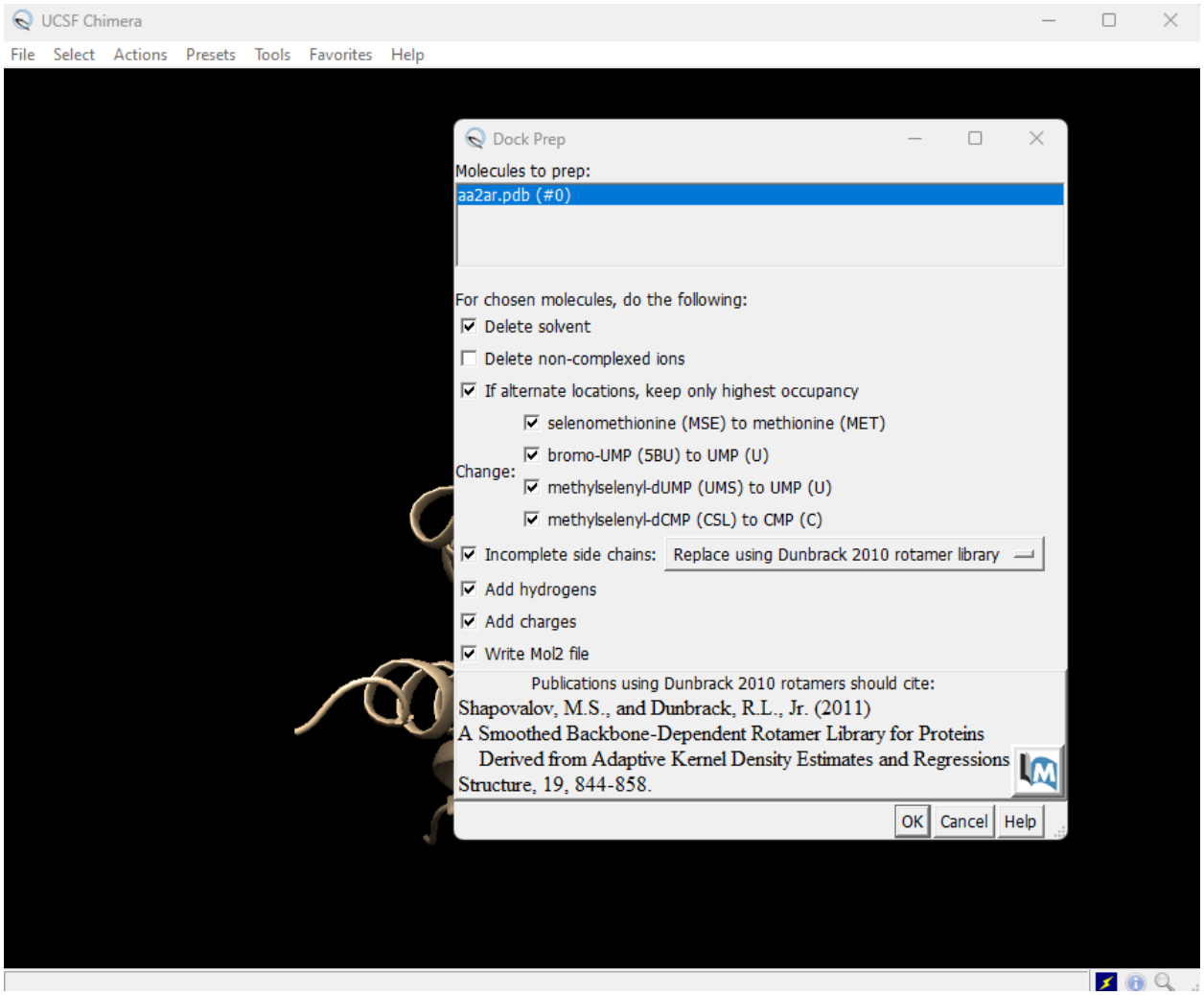


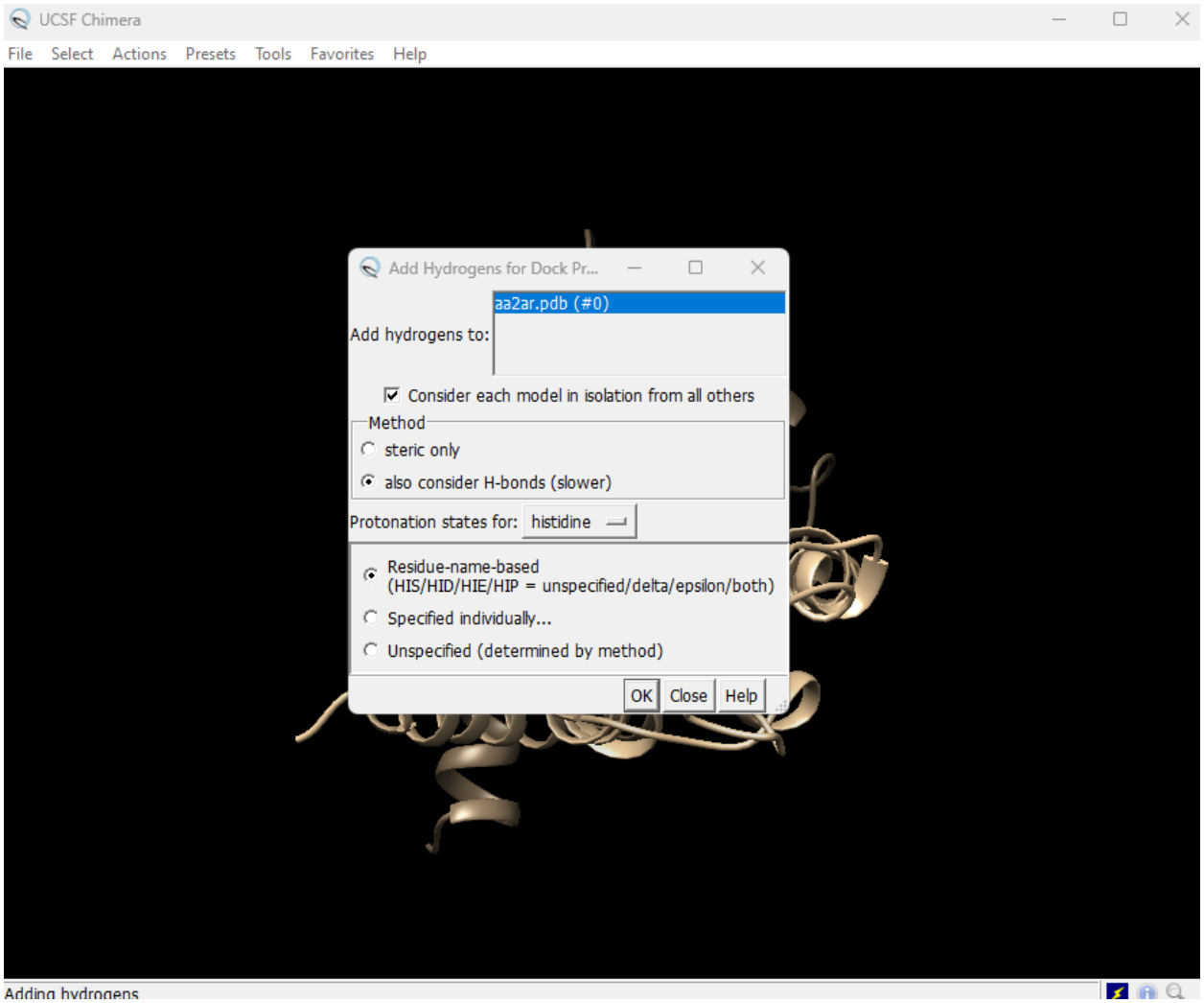
Creating dock6 mol2 file:

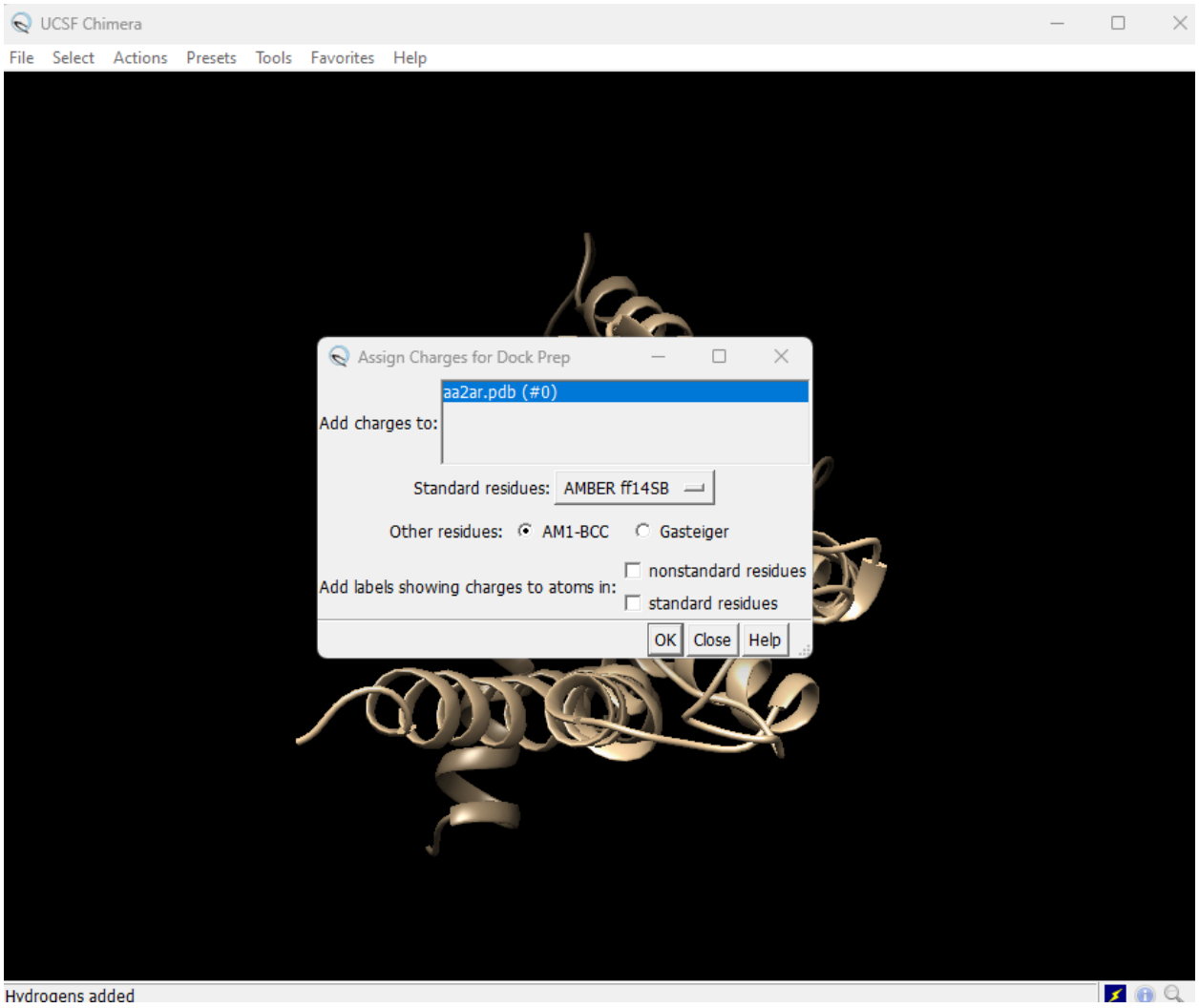
1. Go to Tools->Structure Editing->Dock Prep



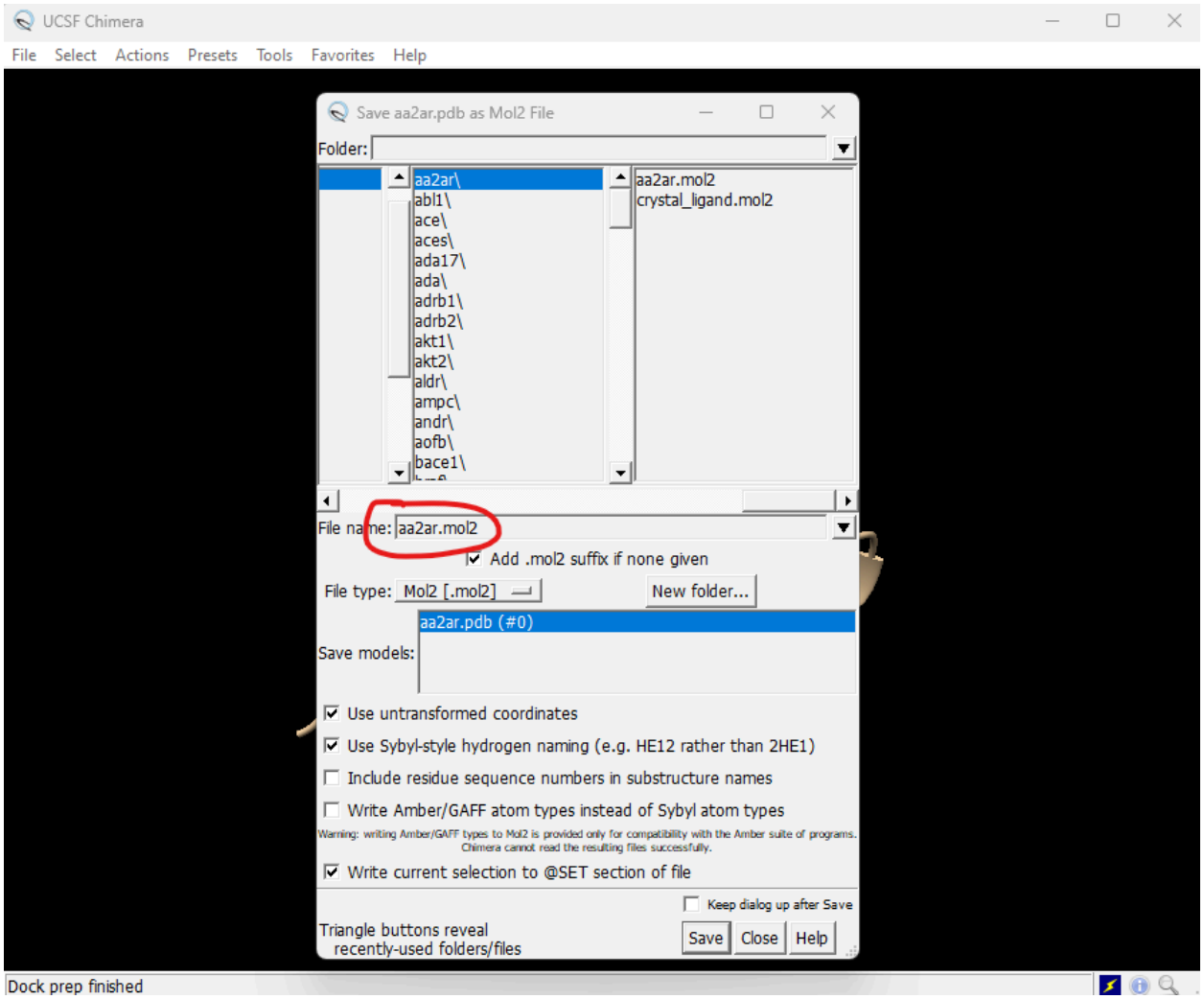
2. Use default settings:


UCSF Chimera
File Select Actions Presets Tools Favorites Help
Dock Prep
Molecules to prep:
aa2ar.pdb (#0)
For chosen molecules, do the following:
Delete solvent
Delete non-complexed ions
If alternate locations, keep only highest occupancy
Change:
selenomethionine (MSE) to methionine (MET)
bromo-UMP (5BU) to UMP (U)
methylselenyl-dUMP (UMS) to UMP (U)
methylselenyl-dCMP (CSL) to CMP (C)
Incomplete side chains:
Replace using Dunbrack 2010 rotamer library
Add hydrogens
Add charges
Write Mol2 file
Publications using Dunbrack 2010 rotamers should cite:
Shapovalov, M.S., and Dunbrack, R.L., Jr. (2011)
A Smoothed Backbone-Dependent Rotamer Library for Proteins
Derived from Adaptive Kernel Density Estimates and Regressions
Structure, 19, 844-858.
OK
Cancel
Help


UCSF Chimera
File Select Actions Presets Tools Favorites Help
Add Hydrogens for Dock Pr...
Add hydrogens to:
aa2ar.pdb (#0)
Consider each model in isolation from all others
Method
steric only
also consider H-bonds (slower)
Protonation states for: histidine
Residue-name-based
(HIS/HID/HIE/HIP = unspecified/delta/epsilon/both)
Specified individually...
Unspecified (determined by method)
OK Close Help
Adding hydrogens



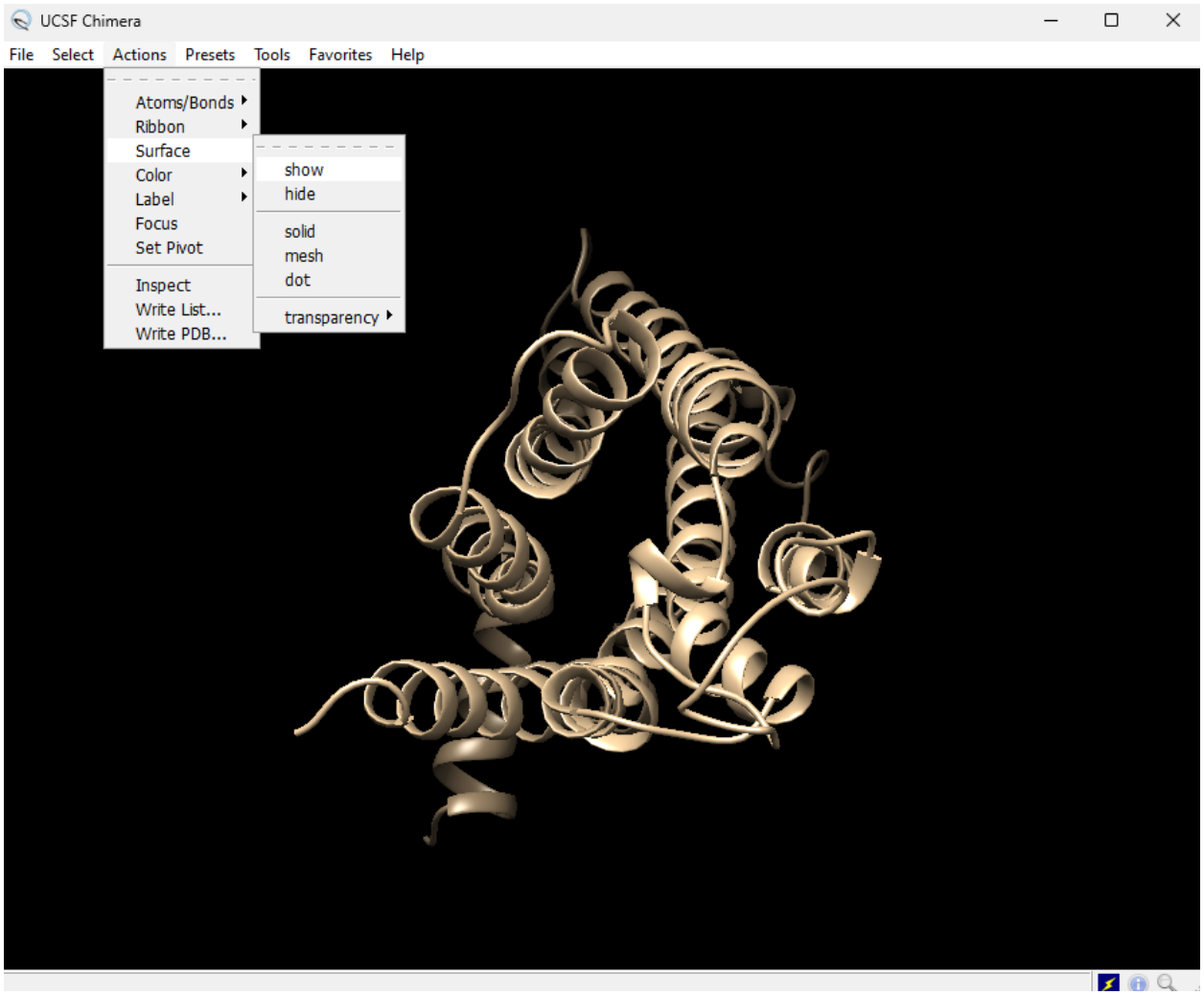
3. Save as system.mol2 (i.e. aa2ar.mol2); Ideally save this in all_simple or in a new folder in the github repository for dock inputs. I can set something up

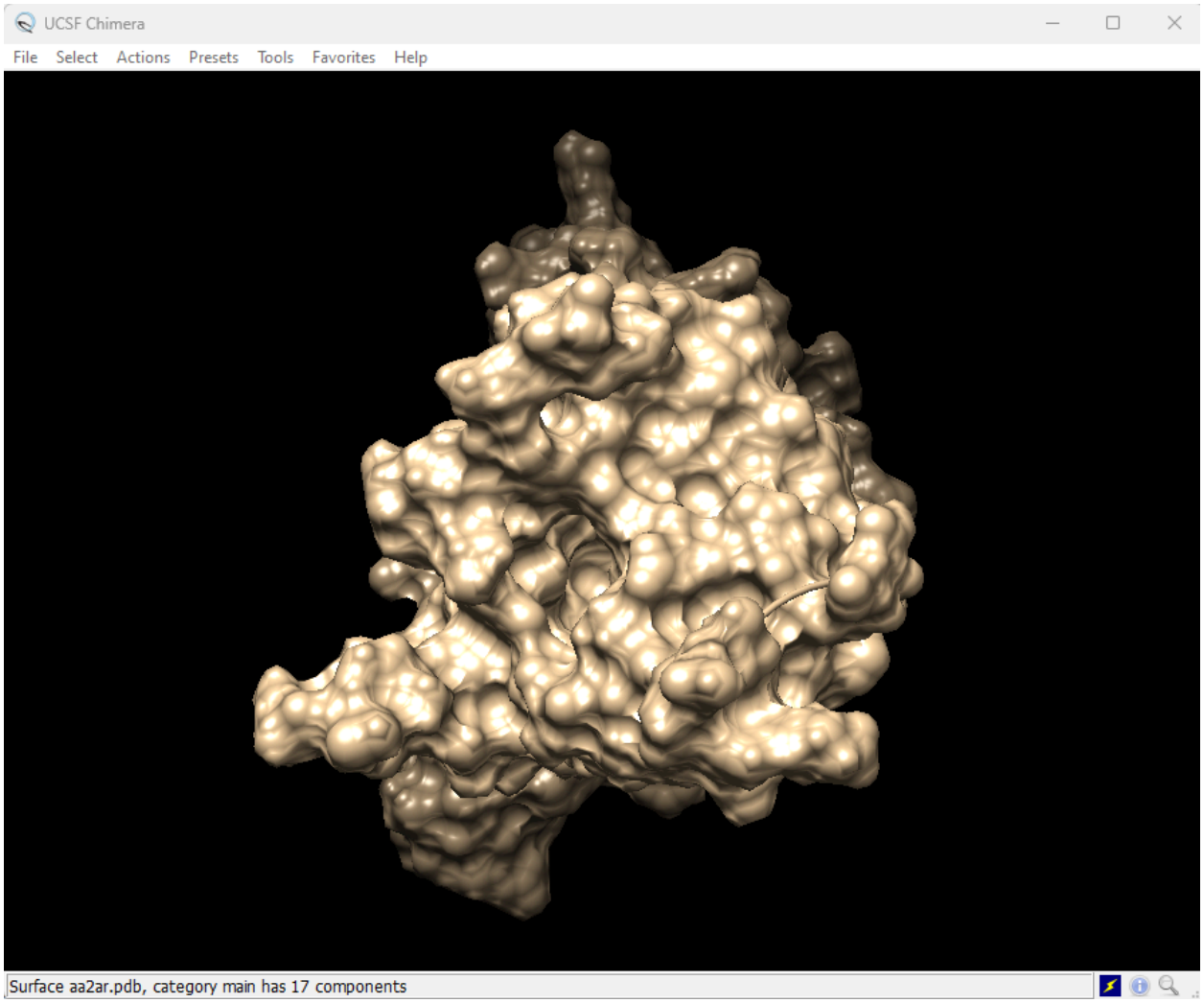


Keep receptor pdb open for creating DMS surface!

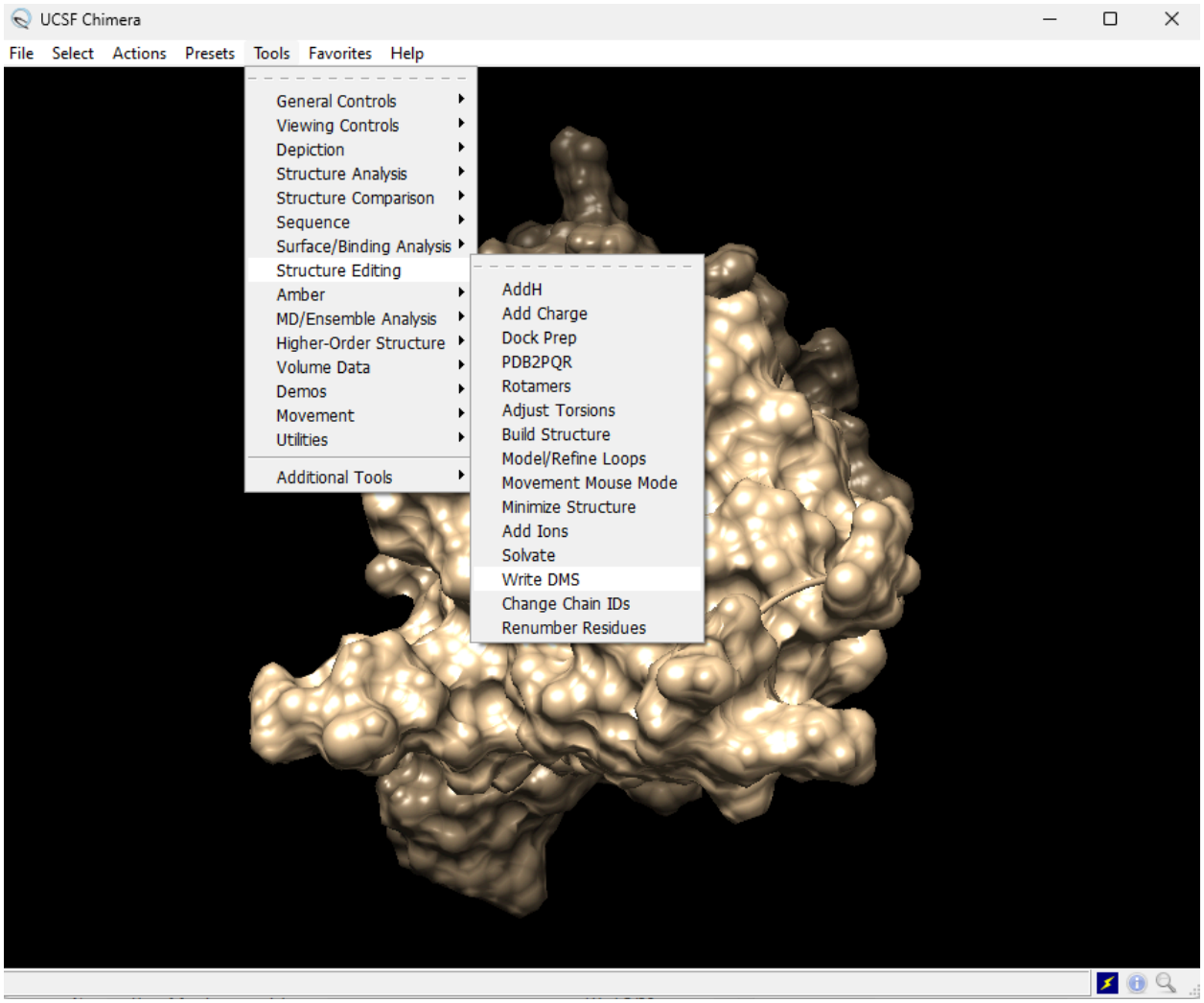
Make DMS of receptor:

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

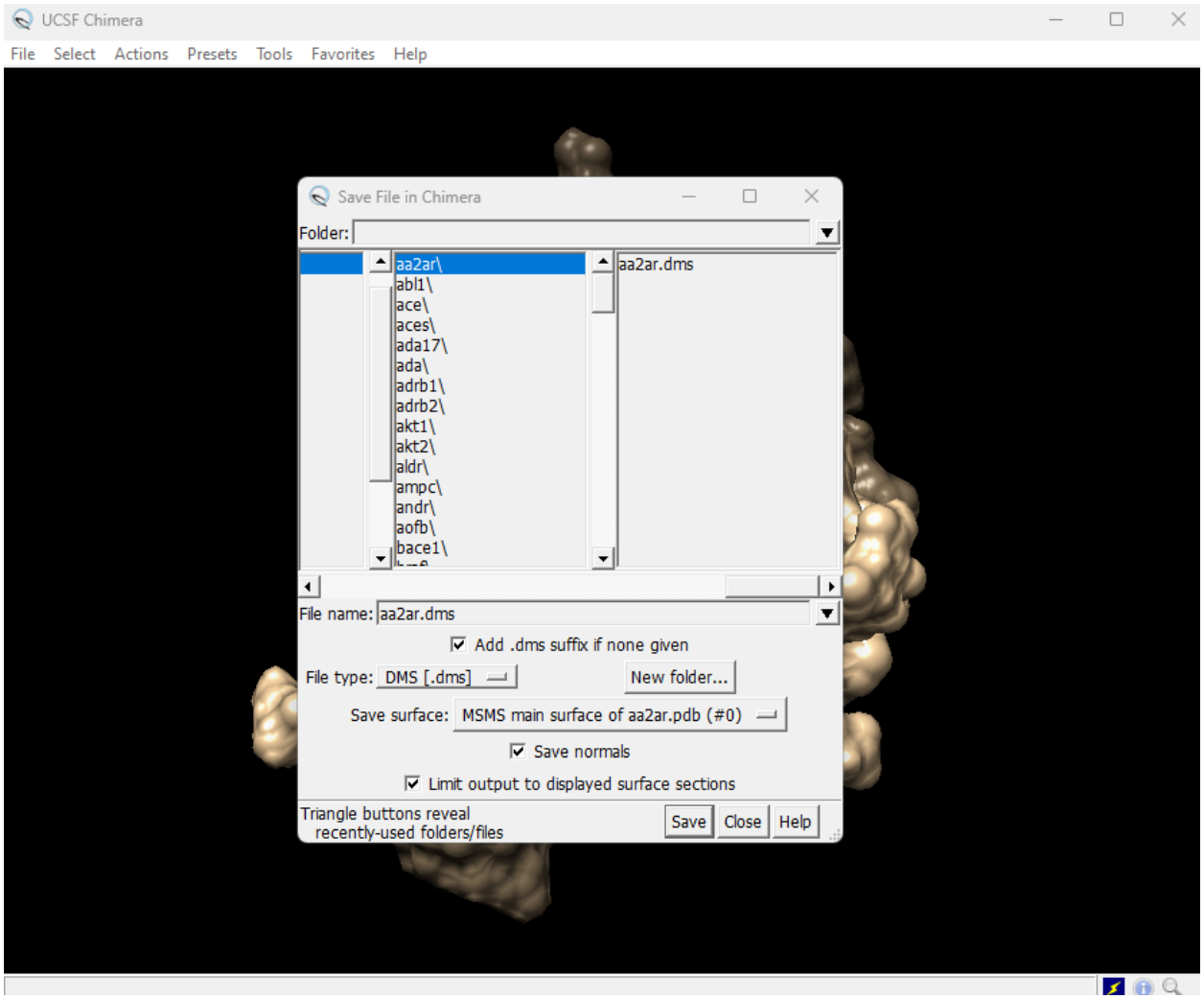

UCSF Chimera
File
Select
Actions
Presets
Tools
Favorites
Help
Atoms/Bonds
Ribbon
Surface
Color
Label
Focus
Set Pivot
Inspect
Write List...
Write PDB...
show
hide
solid
mesh
dot
transparency



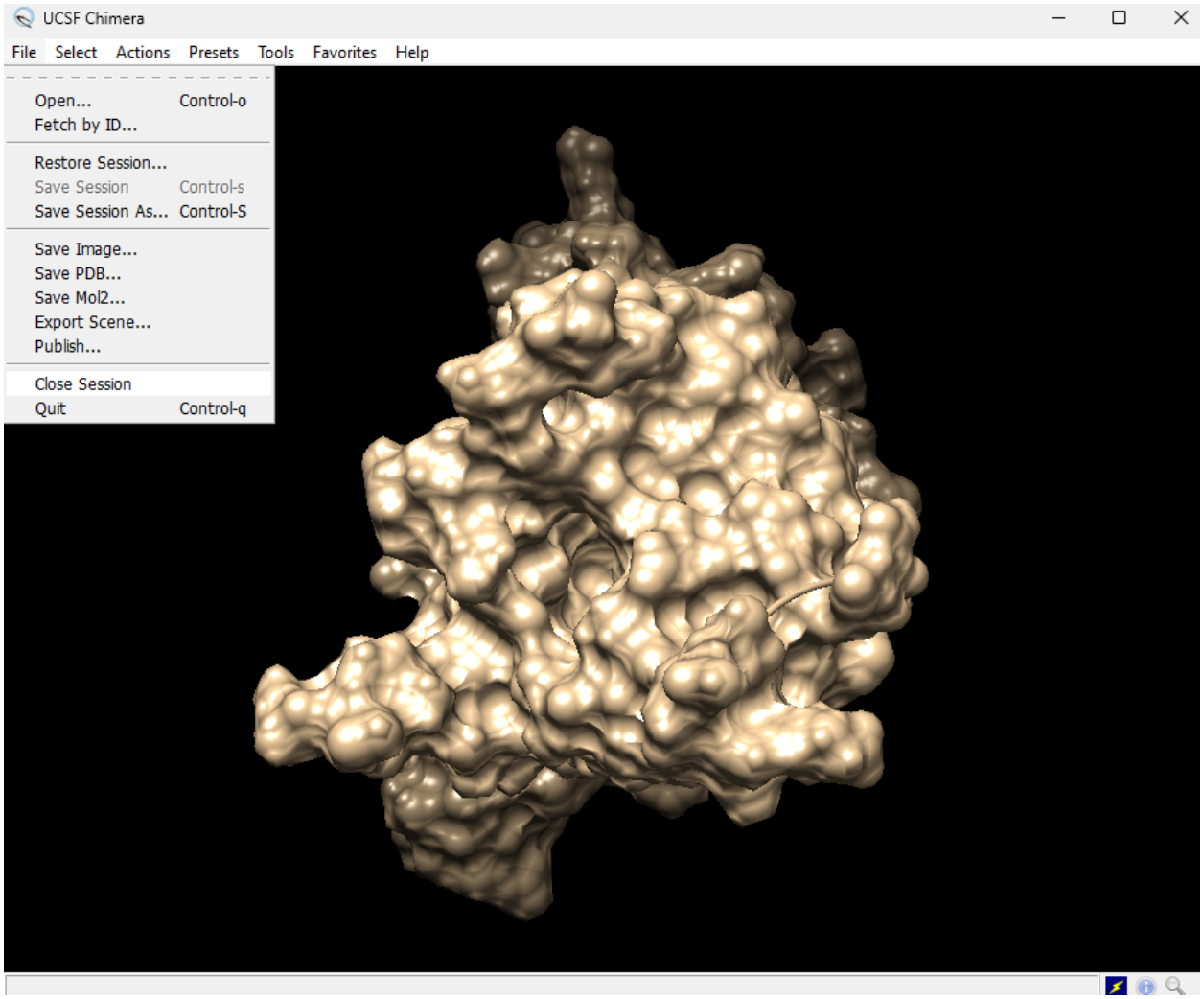
2. Write the surface to DMS: Tools->Structure Editing->Write DMS



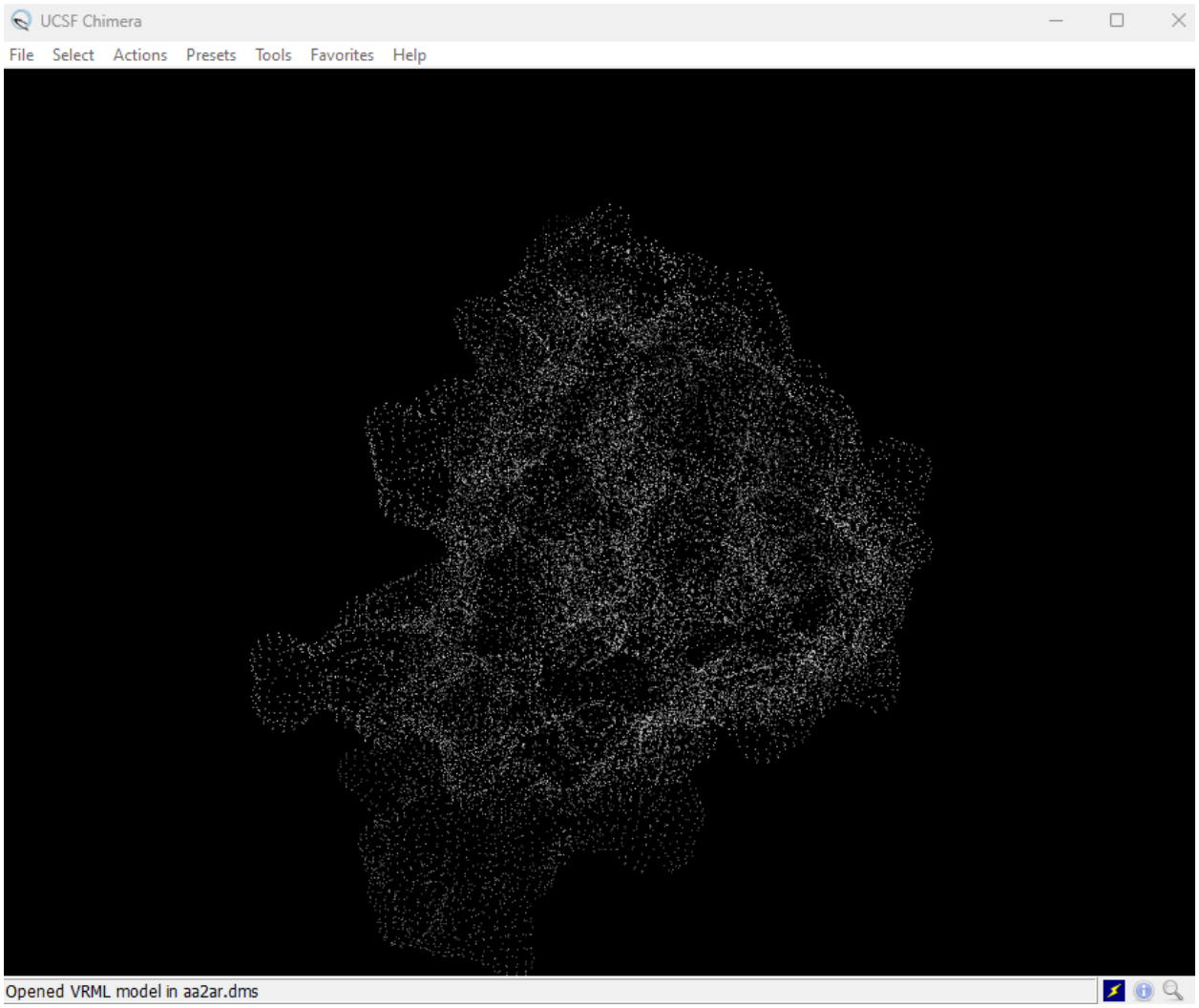
3. Save DMS file; i.e. aa2ar.dms



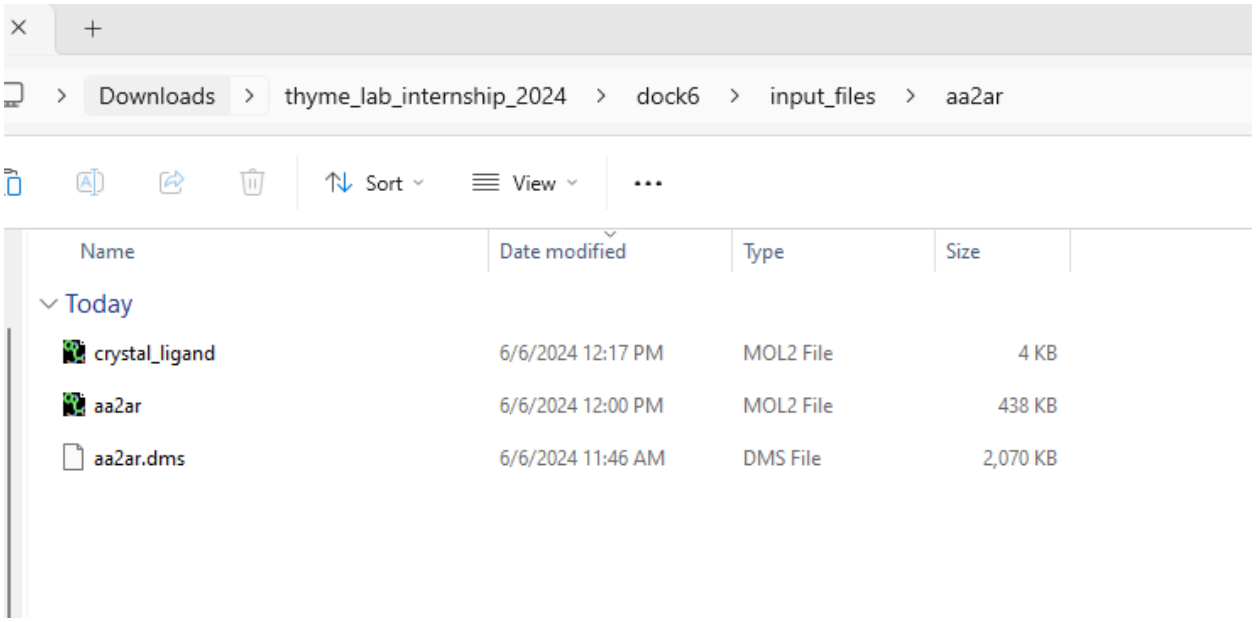
Close session with pdb file (not close entire chimera program to avoid startup): File->Close Session



(OPTIONAL) View dms file:



Receptor surface and mol2 locations:
Creating folders in the internship github repository to hold the input ligand (crystal-lig.mol2), receptor mol2, and receptor surface (dms). These are located at:
thyme_lab_internship_2024/dock6/input_files


Downloads
thyme_lab_internship_2024
dock6
input_files
aa2ar
Sort
View
Name
Date modified
Type
Size
Today
crystal_ligand
6/6/2024 12:17 PM
MOL2 File
4 KB
aa2ar
6/6/2024 12:00 PM
MOL2 File
438 KB
aa2ar.dms
6/6/2024 11:46 AM
DMS File
2,070 KB