

MOLPLAY UNITYMOLCHEATSHEET

Main menu

Input

Load PDBID... Fetch mmCIF Read HET Bio Assembly

Utils View Effects IMD Raytracing Global Selections Annotations Tour Loaded Molecules (1)

model (6184) + ⌂ X (102) + ⌂ X

all_model

model_protein_or_nucleic

Cartoon Hyperball

model_water

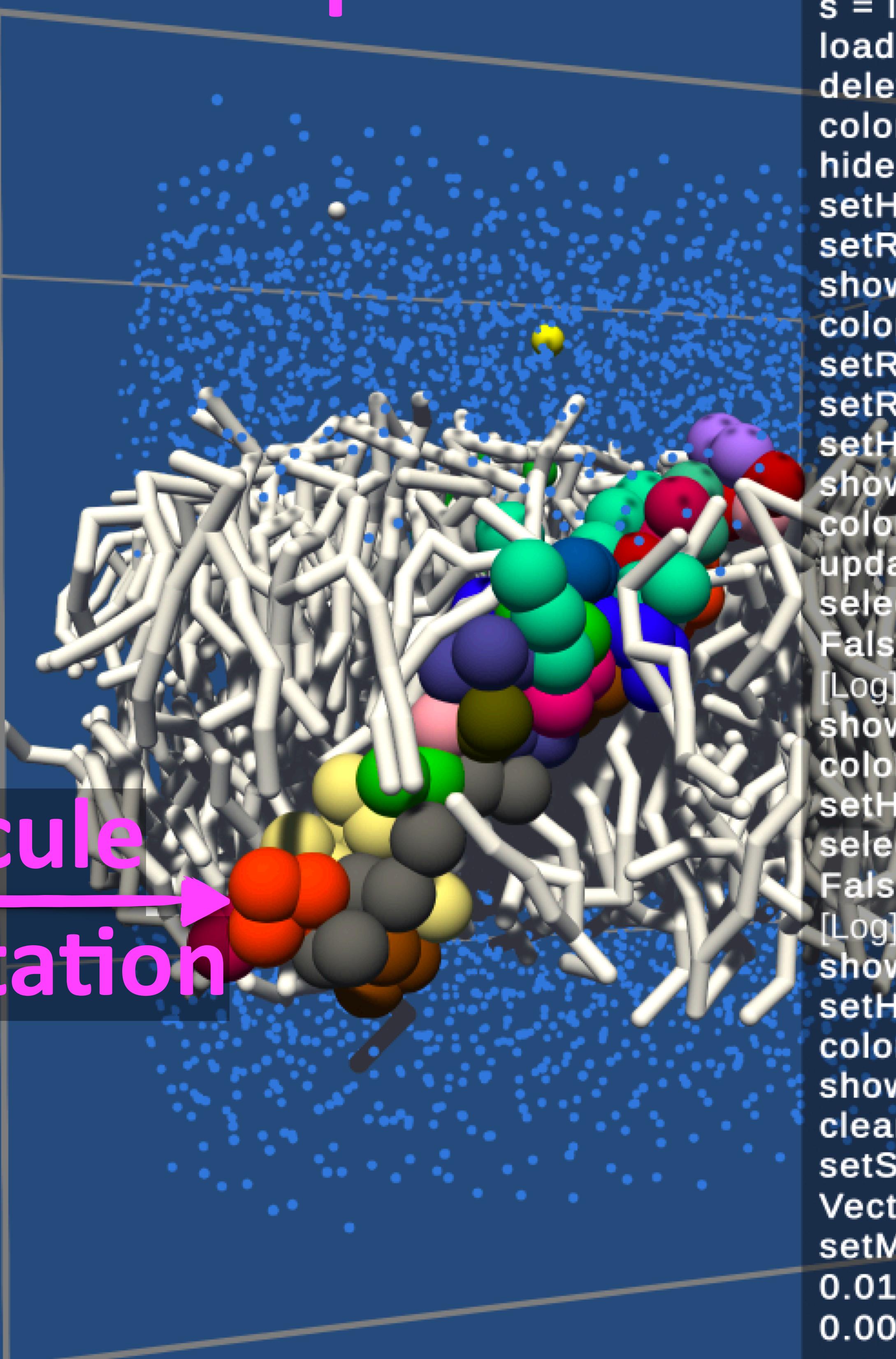
Point (3068) + ⌂ X (3068) + ⌂ X

model_not_protein

Hide/ show representations

Hyperball (12) ⌂ X

Hide/show side panels



a molecule representation

Python Console

```
def q():
    Application.Quit()

s = load("model.gro")
loadMartiniITP("model", "protein-cg.itp")
deleteSelection("model_MartiniElasticBonds")
colorByResidue("model_protein_or_nucleic", "hb")
hideSelection("model_protein_or_nucleic", "c")
setHyperBallMetaphore("model_protein_or_nucleic", "vdw", True)
setRepSize("model_protein_or_nucleic", "hb", 4.50)
showSelection("model_water", "p")
colorSelection("model_water", "p", RGBA(0.262, 0.482, 0.843, 1.000))
setRepSize("model_water", "p", 0.005)
setRepSize("model_unrecognized_atoms", "hb", 1.30)
setHyperballShrink("model_unrecognized_atoms", 0.01)
showSelection("model_unrecognized_atoms", "hb")
colorByHydrophobicity("model_unrecognized_atoms", "hb")
updateRepresentations("model_unrecognized_atoms")
select("model and chain A and resid 114", "ion", True, True, True, False, False, True)
[Log] Selection of 12 atoms, named '1lipid' (model and chain A and resid 114)
showSelection("1lipid", "hb")
colorSelection("1lipid", "hb", RGBA(0.951, 0.322, 0.247, 1.000))
setHyperBallMetaphore("1lipid", "Vdw", True)
select("model and chain A and resid 3316", "ion", True, True, True, False, False, True)
[Log] Selection of 1 atoms, named 'ion' (model and chain A and resid 3316)
showSelection("ion", "hb")
setHyperBallMetaphore("ion", "VdW", True)
colorSelection("ion", "hb", RGBA(1.000, 0.989, 0.000, 1.000))
showBoundingBox("model")
clearSelections()
setStructurePositionRotation("model", Vector3(0.0000, 0.0000, 0.0000), Vector3(0.0000, 0.0000, 0.0000))
setMolParentTransform( Vector3(0.6078, -0.5048, -1.2271), Vector3(0.0109, 0.0109, 0.0109), Vector3(356.6104, 342.1224, 0.3940), Vector3(0.0000, 0.0000, -0.9253) )
connectIMD("model", "127.0.0.1", 8888)
[Log] True
last().mddriverM.appliedForceFactor = 0.0001
setMouseMoveSpeed(5)
```

Command line

Exit the software:
CTRL+X