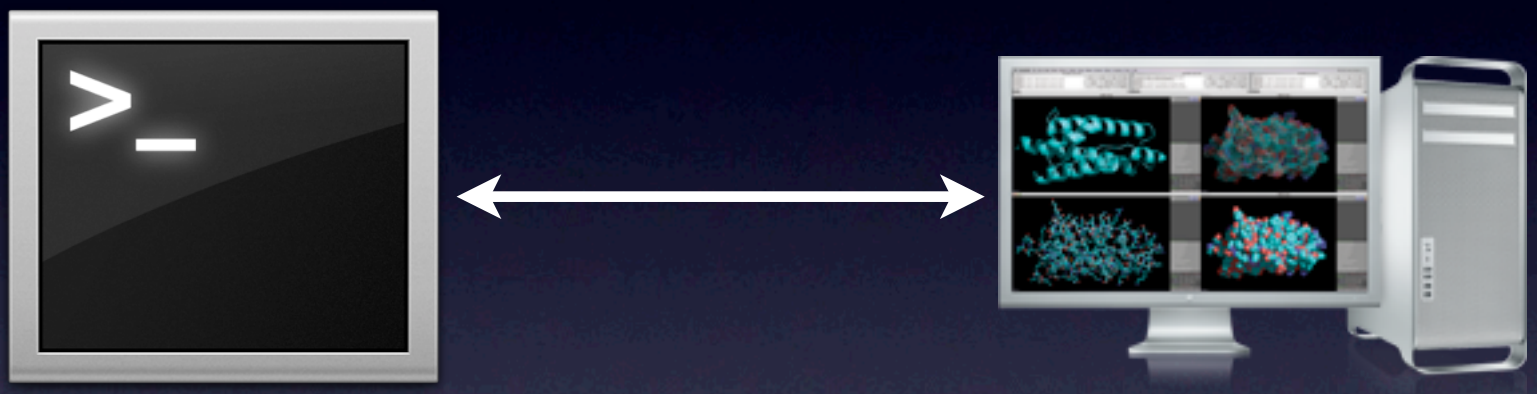
A “new” graphical interface for Rosetta



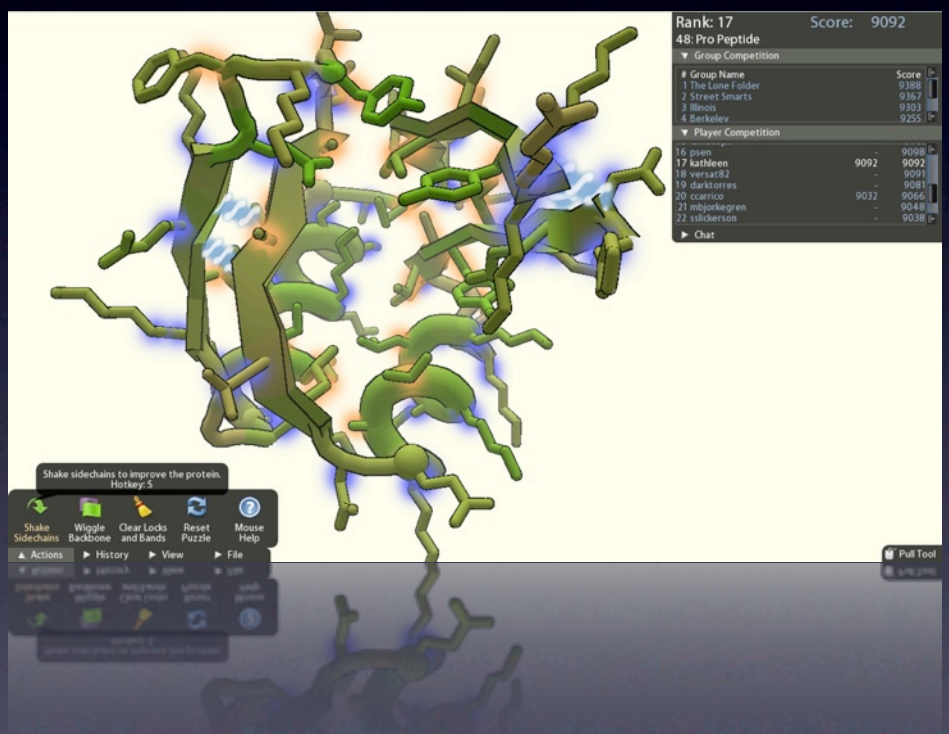
Evan Baugh, Sergey Lyskov, Brian Weitzner

RosettaCon 2010

My IP address: 192.168.20.106

http://pyrosetta.org/rosettacon2010.html

Foldit



Pros	Cons
• Attractive interface • Highly interactive • Great for end users	• Not meant for development use • Need to compile and install libraries • OS differences are problematic

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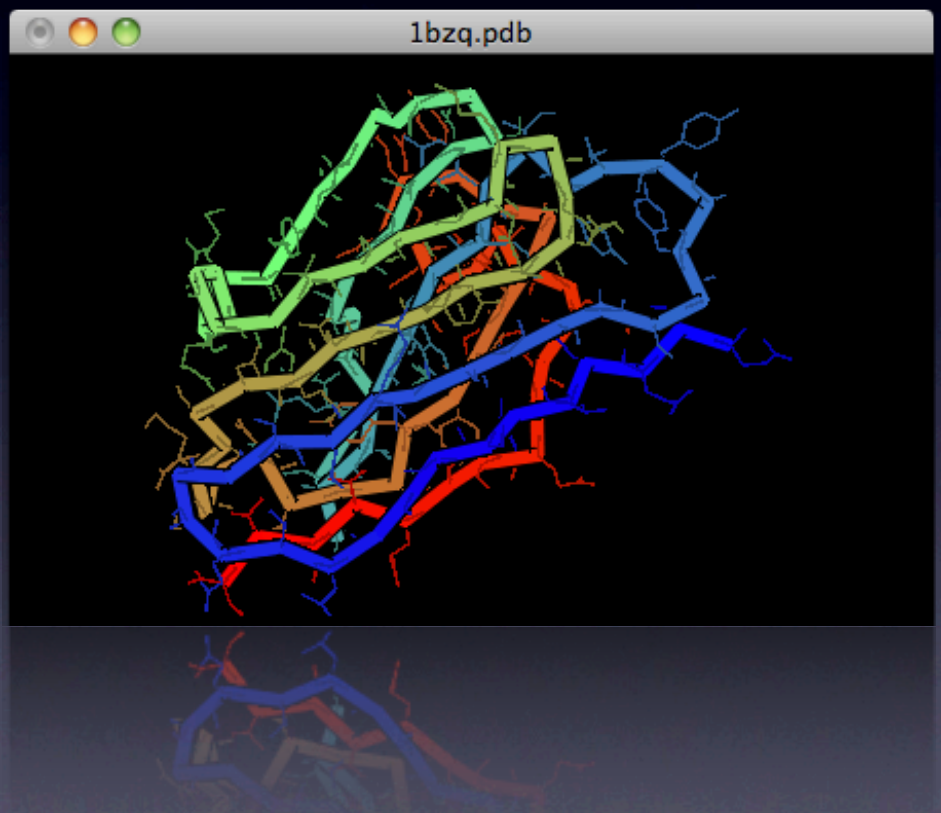
http://fold.it/portal/site_files/theme/science/competition.png

Rosetta Graphics Mode



Pros	Cons
• Built into mini	• Limited visualization
• Lightweight	• Need to compile specifically for graphics mode
	• Non-interactive

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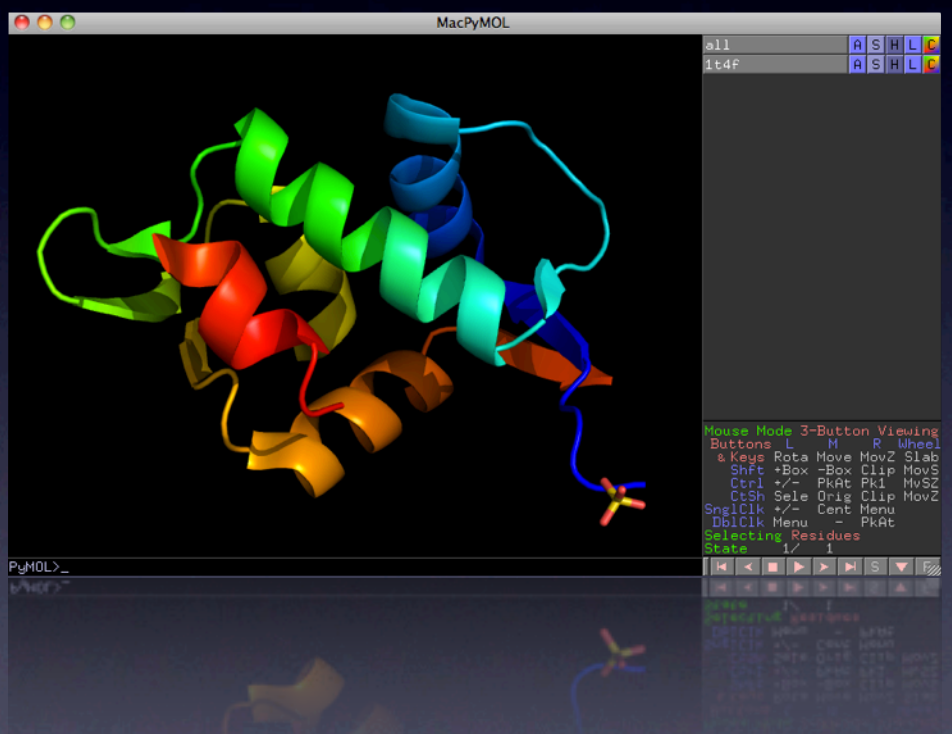
PyMOL



Pros	Cons
• Powerful • Cross platform • Familiar for most users & developers • Compatibility is not our responsibility	• Not integrated with Rosetta • Need to dump PDBs and load them • Tedious for development

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PDB accession code 1T4F

What makes an interface great?

- Useful for users to learn and to complete tasks
- Integration with PyRosetta
- Interactivity
- Intended to aid development
- Ease of use and maintenance
- Easy for developers!

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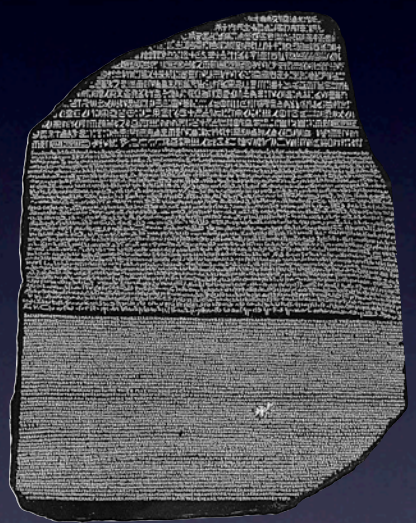
Structure of PyRosetta



Rosetta source code

Python bindings

Additional functions for Rosetta

Python scripting

User

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Advantages of PyRosetta

- Interactive use of PyRosetta has unique advantages
- New users learn the software quickly
- Development and testing of new, high-level protocols is significantly faster

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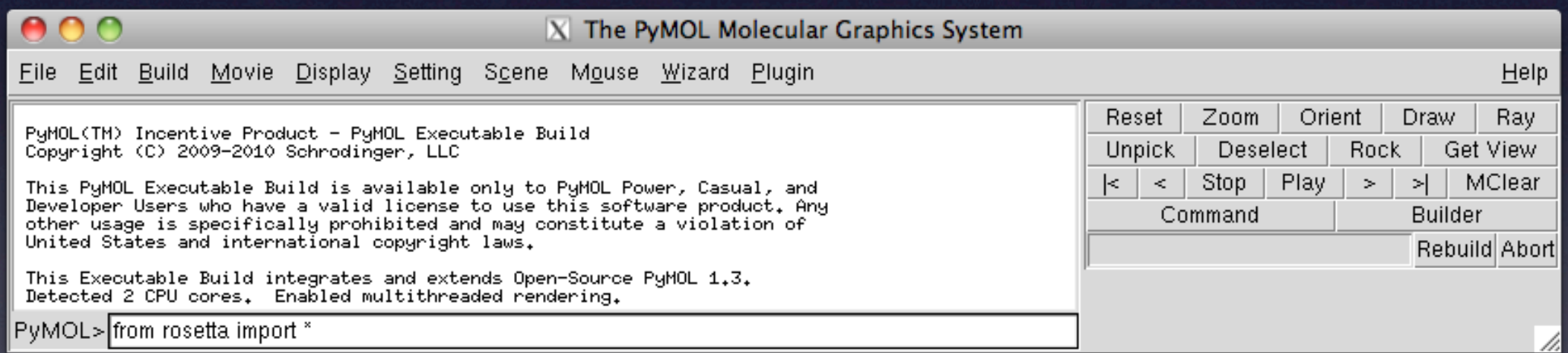
How can we run PyRosetta with PyMOL?

- Both are based on python
- PyMOL has a built-in python interpreter



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Attempt 1:
Direct PyMOL-PyRosetta Integration

This lead to many problems:

- No iPython (currently)
- The python version of PyMOL must match the version PyRosetta was linked against or it crashes - hard
  - Why is this such a big problem?
  - There are three major versions of python in the wild, each with a 32 and 64-bit version for each platform - this is unsustainable
- Potential licensing restrictions - Schrödinger owns PyMOL now and we would have to provide a custom distribution

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Postmortem:

What is the real problem?

- Does PyRosetta need to run within PyMOL to make it a functional interface?
- What is necessary to visualize a PyRosetta session?
- PyRosetta just needs to transmit data to PyMOL

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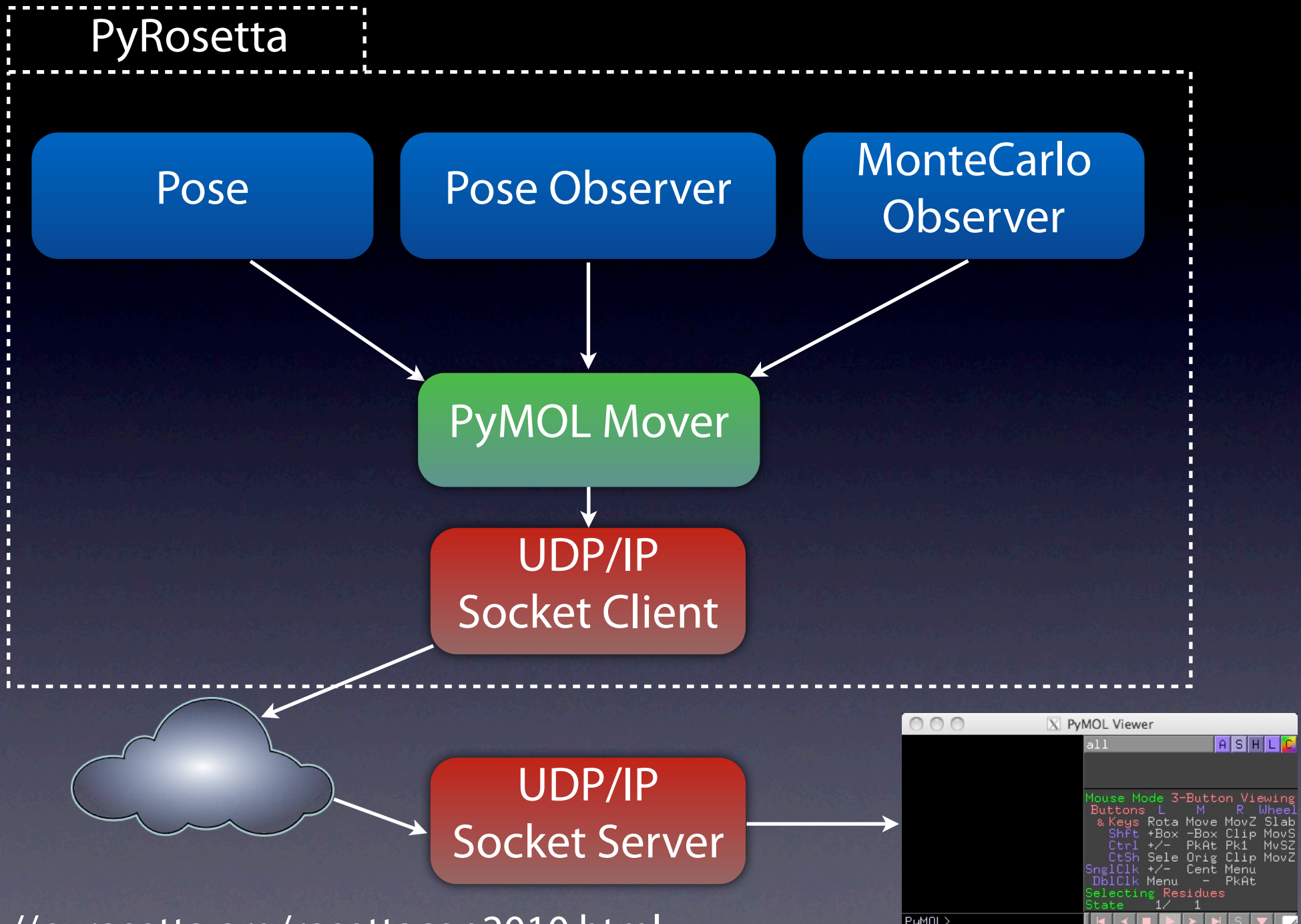

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Attempt 2:
Network socket communication

- Send data to PyMOL using a UDP network socket
- PyRosetta and PyMOL run as completely separate processes
  - PyRosetta performs the molecular simulation
  - PyMOL performs the visualization
- On demand, real-time visualization with no slow-downs
- Multiple instances of PyRosetta can send data to a single PyMOL process
  - This means these processes can be run on different computers, across different architectures, different operating systems and even in different buildings

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PyRosetta interface:

How do we use this?

```
from rosetta import *
init()
pose = Pose("1abc.pdb")
pymol = PyMOL_Mover()
pymol.apply(pose)
```

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Demo

You can even use it with mini!

- And all of this can be done with PyRosetta or even the mini C++ build
- To use the observer in C++, all you need to do is:

```
#include <protocols/moves/PyMolMover.hh>
core::protocols::moves::AddPyMolObserver(pose)
```

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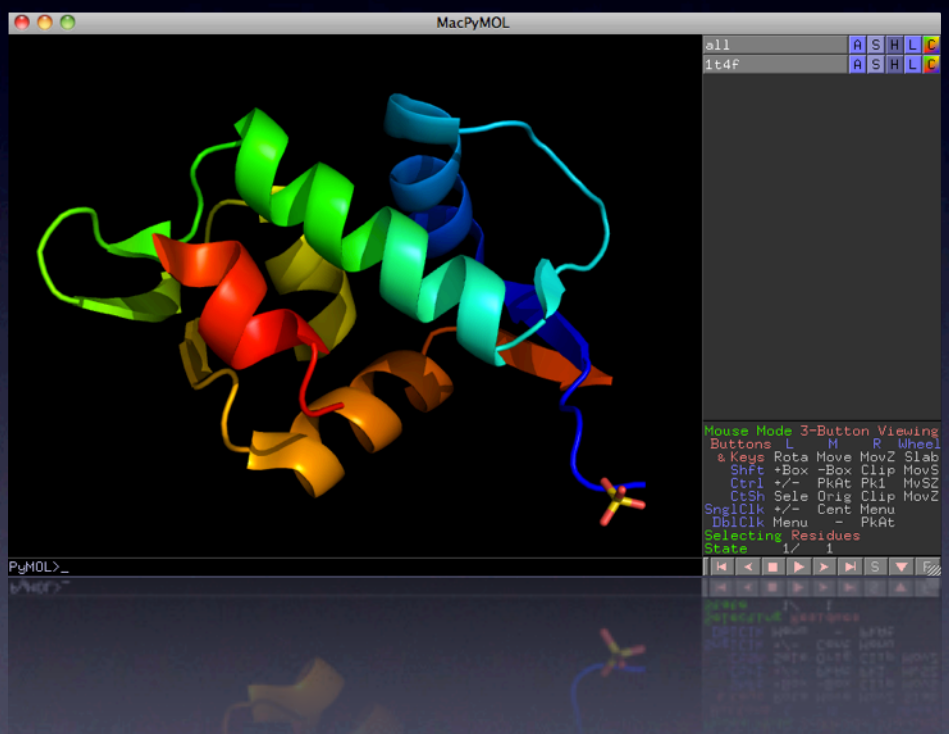
How did we do?



- ☑ Useful for users to learn and to complete tasks
- ☑ Integration with PyRosetta
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Future work

- Develop an interface for transmitting and interpreting additional data
- Add a "-pymol " flag to the protocol base class or jd2
- Allow specific tracer output to be displayed in the PyMOL interpreter
- Allow PyRosetta objects to be set up through PyMOL - movemaps, packer tasks, etc.

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How can you get in on the action?

- All of this code has already been checked in, so just build a new copy of mini and you can use the mover today.
- Developer versions of PyRosetta that support PyMOL integration are available at http://pyrosetta.org/download.html
- If you have any questions or requests, come talk to us! Or email us:

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