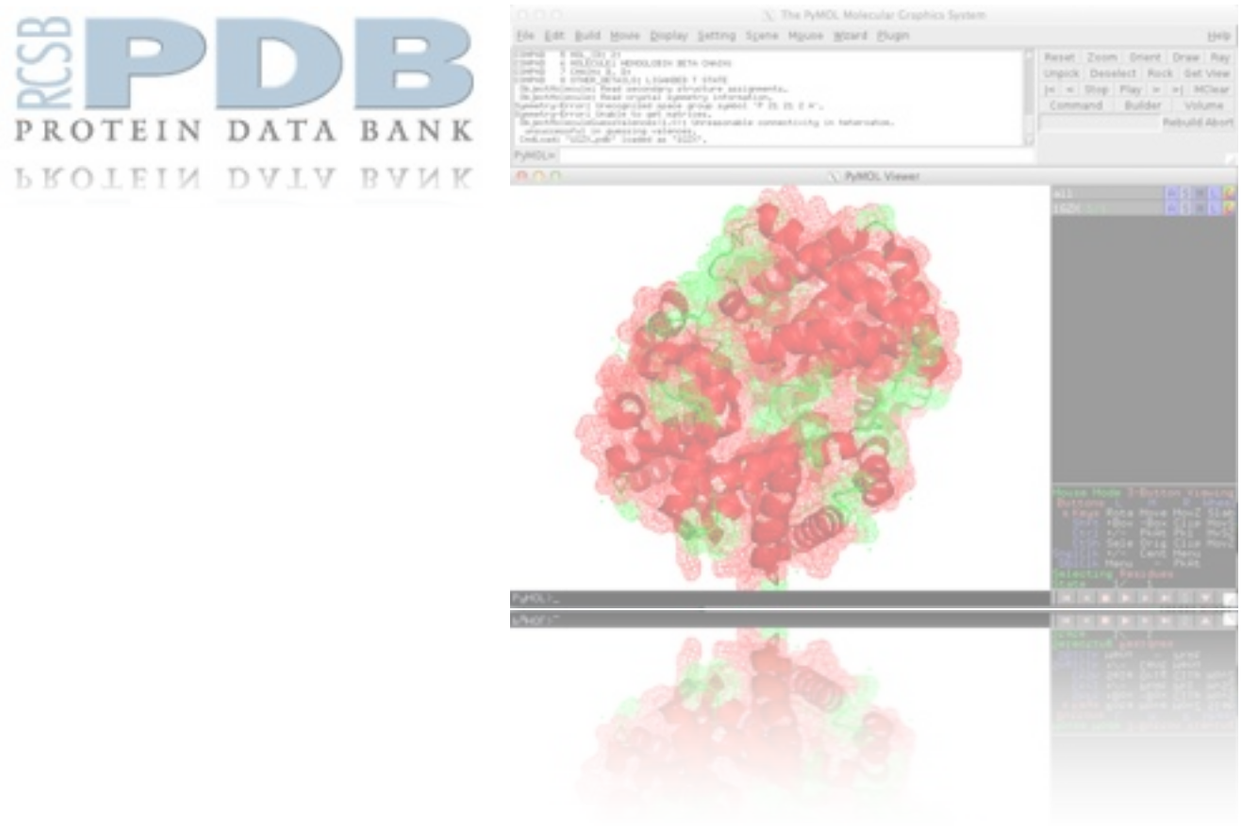
Structural Genomics

Protein data bases and viewers



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http://sgu.bioinfo.cipf.es

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Outline

- PDB: the Protein Data Bank
- How to use the PDB
- PyMOL model viewer introduction
- PyMOL example

PDB

Protein Data Bank

The Protein Data Bank (PDB) is a repository for the three-dimensional structural data of large biological molecules, such as proteins and nucleic acids.

The data, typically obtained by X-ray crystallography or NMR spectroscopy and submitted by biologists and biochemists from around the world, are freely accessible.

The PDB is a key resource in areas of structural biology, such as structural genomics.

The primary information stored in the PDB archive consists of coordinate files for biological molecules.

In a typical entry, you will find a diverse mixture of biological molecules, small molecules, ions, and water.

PDB

Yearly growth

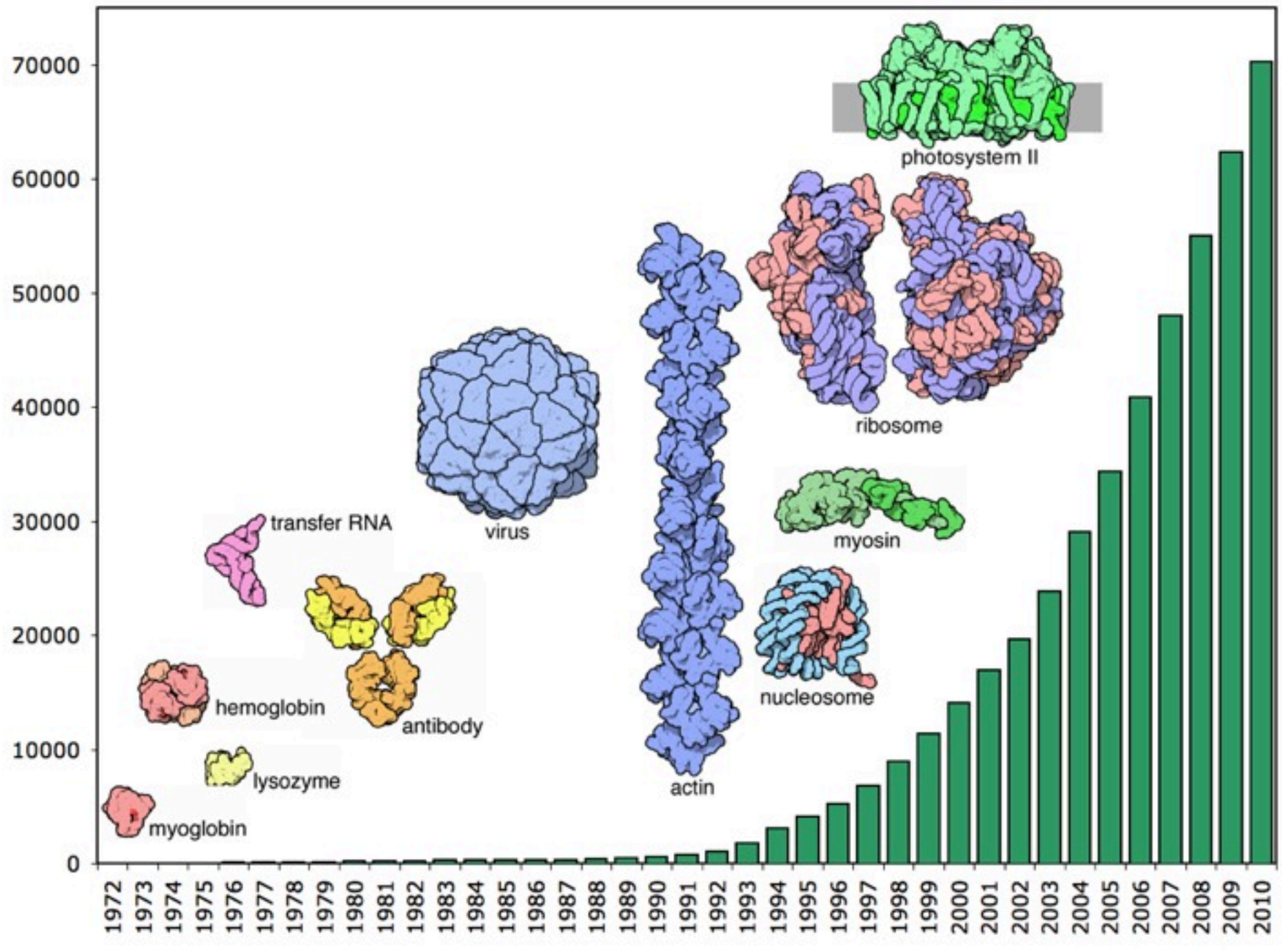


Image credits: http://www.pdb.org

PDB

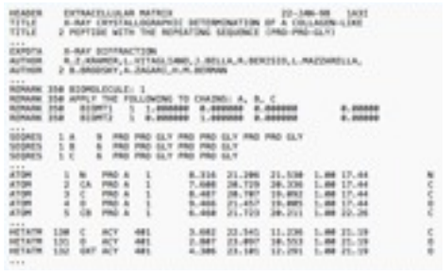
Current status

Exp. Method	Proteins	Nucleic Acids	Protein/NA Complexes	Other	Total
X-RAY	61683	1308	2985	3	65979
NMR	7898	957	179	7	9039
Electron Microscopy	258	22	96	0	376
Hybrid	40	3	1	1	45
Other	133	4	5	13	155
Total	**70010**	2294	3266	24	**75594**

PDB

File format

```
HEADER    EXTRACELLULAR MATRIX                      22-JAN-98   1A3I
TITLE     X-RAY CRYSTALLOGRAPHIC DETERMINATION OF A COLLAGEN-LIKE
TITLE    2 PEPTIDE WITH THE REPEATING SEQUENCE (PRO-PRO-GLY)
...
EXPDTA    X-RAY DIFFRACTION
AUTHOR    R.Z.KRAMER,L.VITAGLIANO,J.BELLA,R.BERISIO,L.MAZZARELLA,
AUTHOR   2 B.BRODSKY,A.ZAGARI,H.M.BERMAN
...
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
...
SEQRES   1 A    9  PRO PRO GLY PRO PRO GLY PRO PRO GLY
SEQRES   1 B    6  PRO PRO GLY PRO PRO GLY
SEQRES   1 C    6  PRO PRO GLY PRO PRO GLY
...
ATOM      1  N   PRO A   1       8.316  21.206  21.530  1.00 17.44           N
ATOM      2  CA  PRO A   1       7.608  20.729  20.336  1.00 17.44           C
ATOM      3  C   PRO A   1       8.487  20.707  19.092  1.00 17.44           C
ATOM      4  O   PRO A   1       9.466  21.457  19.005  1.00 17.44           O
ATOM      5  CB  PRO A   1       6.460  21.723  20.211  1.00 22.26           C
...
HETATM  130  C   ACY   401       3.682  22.541  11.236  1.00 21.19           C
HETATM  131  O   ACY   401       2.807  23.097  10.553  1.00 21.19           O
HETATM  132  OXT ACY   401       4.306  23.101  12.291  1.00 21.19           O
...
```



PDB

File format

HEADER, TITLE and AUTHOR
Respectively: first line of the entry, contains PDB ID code, classification, and date of deposition; list of contributors; description of the experiment represented in the entry.

REMARK
General remarks about the data.

SEQRES
The primary structure (sequences) of the protein or DNA/RNA.

ATOM
Atomic the coordinates of the protein residues. Each line reports the atom number, name, amino acid, chain sequence number, coordinates, occupancy (1.0), B-factor (flexibility), and the element name.

HETATM
Atomic coordinates of small molecules, that is those non-standard atoms which are not part of the protein molecule.

Summary

The Protein Data Bank (PDB) is a repository for the three-dimensional structural data of large biological molecules, such as proteins and nucleic acids.

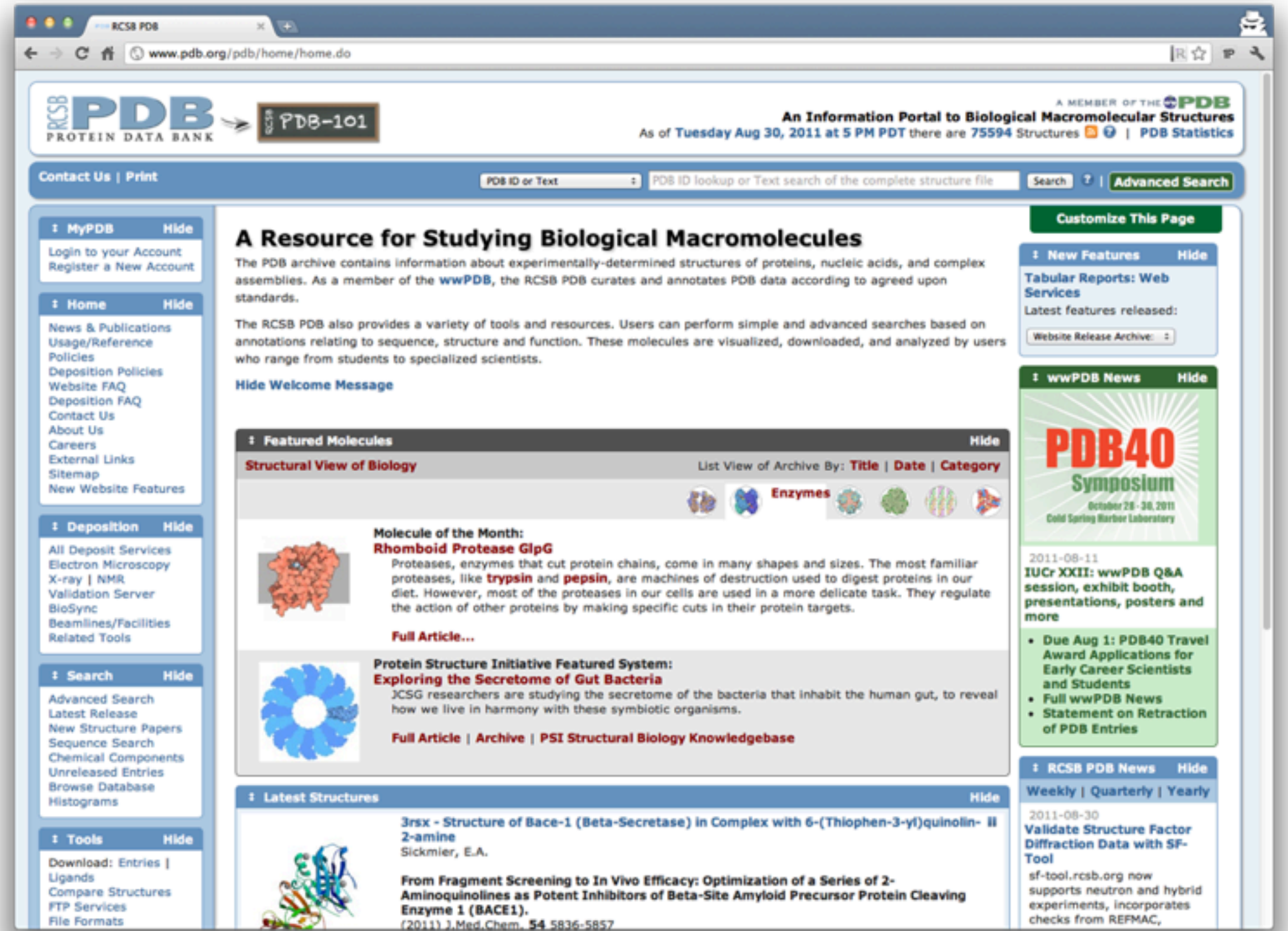
The data contained in the archive include atomic coordinates and experimental data.

Over 75000 structures deposited.

Freely accessible.

PDB Website

http://www.pdb.org



PDB Website

http://www.pdb.org

1. Go to www.pdb.org in your web browser
2. Search for PDB ID **1T46**
3. Navigate the **Summary** and **Sequence** tabs (top menu)
4. Display the **FASTA** sequence and **PDB file** (top-right menu)
5. Download the PDB file in text format (top-right menu)
6. From the Summary tab, select the first PDB related entry (**1PKG**) and download it

PyMOL

http://www.pymol.org

PyMOL is an open-source, multi-platform program to visualize molecules and is available from the web.

The PyMOL GUI allows for an easy usage with no need to use the command line.

PyMOL allows to create high-quality images from 3D structures and to manipulate them. Some basic functions to analyze their chemical properties are also available.

The user has the possibility to write his/her own scripts and plugins.

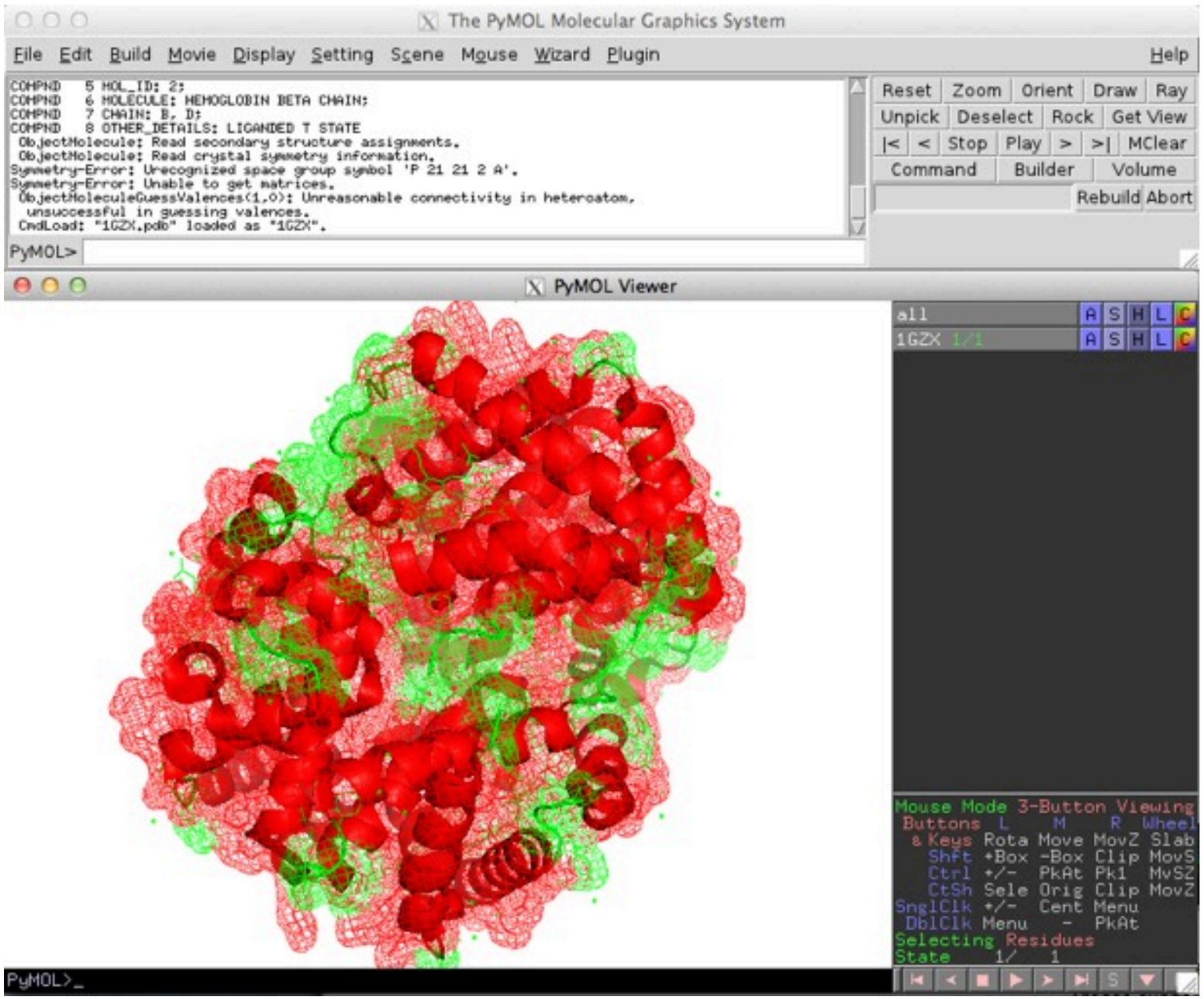
PyMOL

The graphical user interface (GUI)

PyMOL viewer: 3D molecules appear here.

External GUI: menu bar (File, Edit, etc), shortcut buttons, and the command line.

Object list: loaded molecules and user-defined selections.



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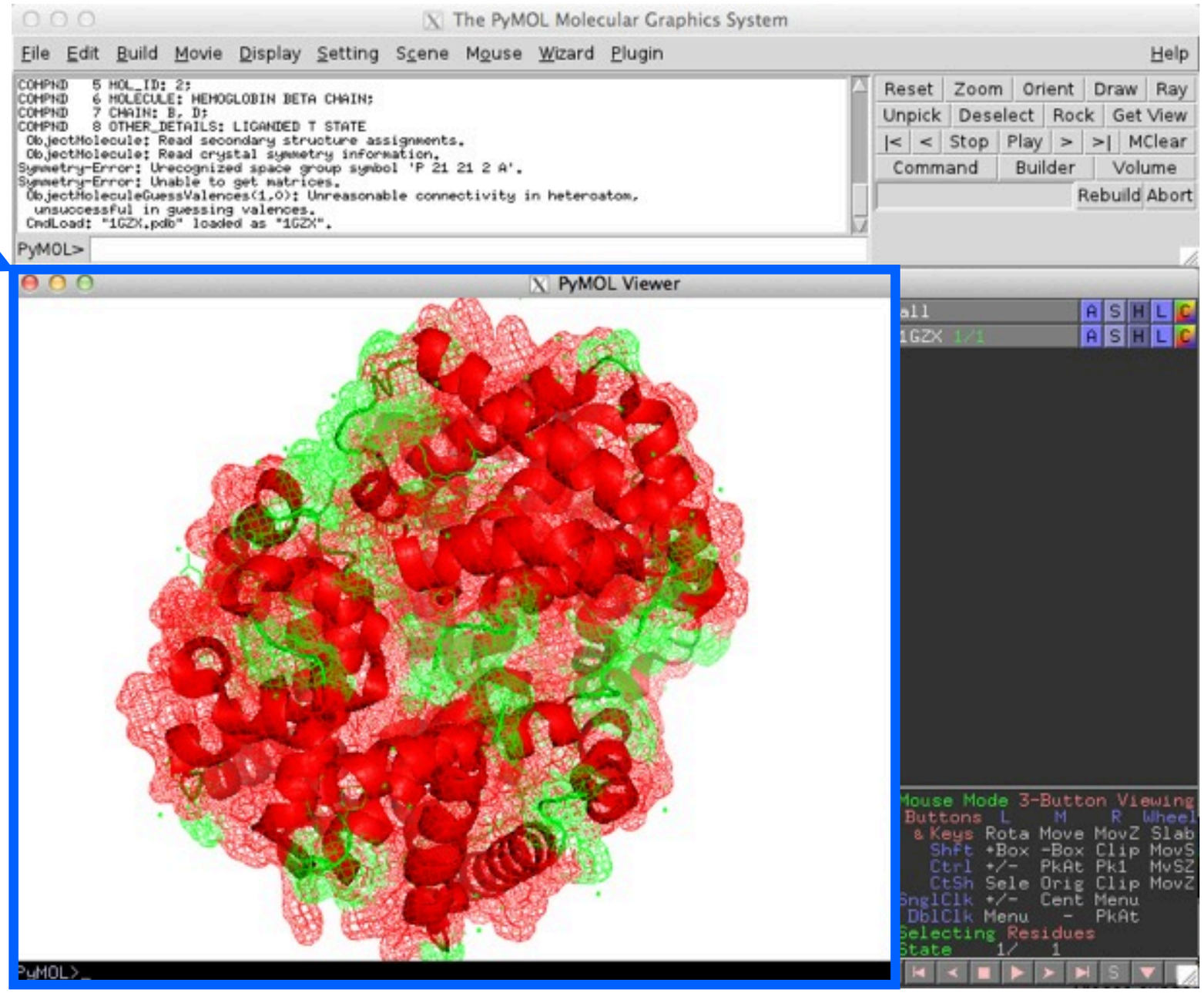

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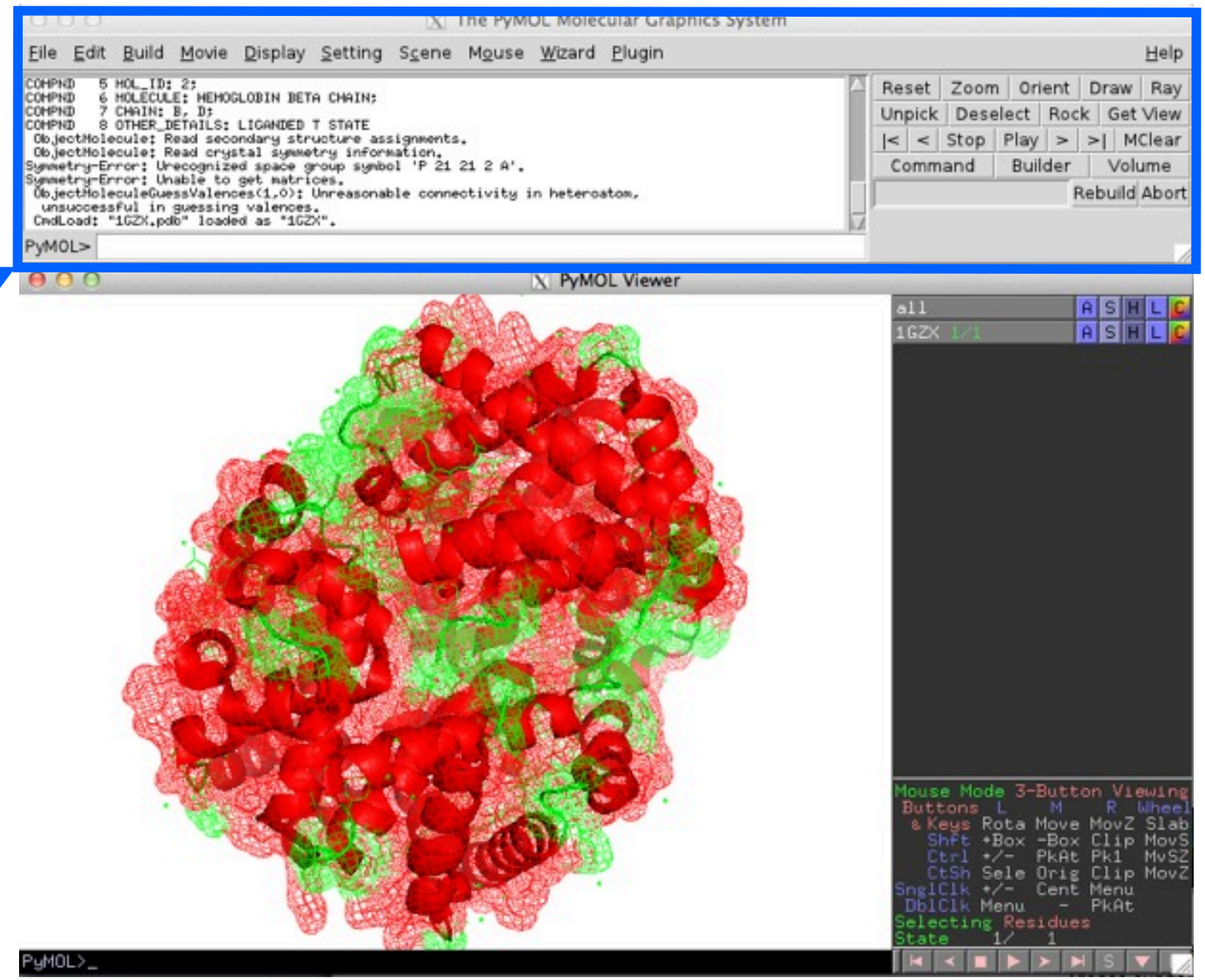

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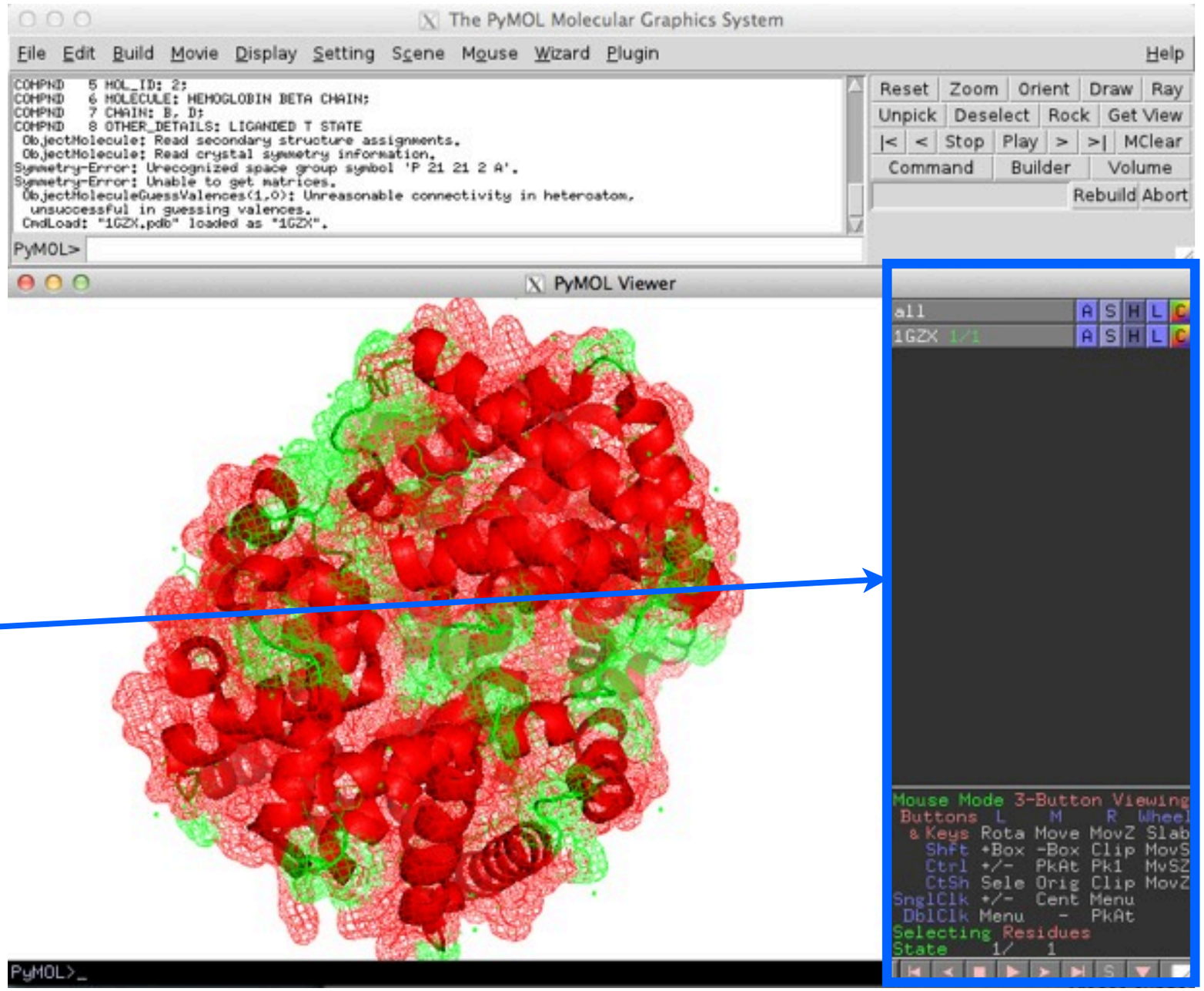

PyMOL

The graphical user interface (GUI)

In the object list, after each object name there is a set of command buttons which control the object:

A - *Actions*: Rename, duplicate, remove, apply presets (like "ball-and-stick" or "publication"), perform computations

S - *Show*: Change the way things appear, eg change to stick or cartoon view.

H - *Hide*: Things that are shown using **S** accumulate, and don't automatically replace the last view. **H** is the opposite of **S** and hides unwanted representations.

L - *Label*: Label atoms, residues, etc.

C - *Color*: Change the color of atoms and groups.

PyMOL

Tutorial

Run PyMOL from the main menu:

1. Application ⇒ Science ⇒ PyMOL

Open a protein from the PyMOL menu:

2. File ⇒ open (select the previously downloaded 1T46)
3. Use the mouse buttons to **rotate** (left), **move** (center) and **zoom** (right) the loaded structure.
4. *A (action)* ⇒ preset ⇒ ligands
5. 1T46_pol_conts: *S (show)* ⇒ labels
6. 1T46: *A (action)* ⇒ preset ⇒ default
7. Wizard ⇒ measurements

PyMOL

Tutorial

Open a protein from the PyMOL menu:

8. File ⇒ open (select the previously downloaded **1PKG**)

Now we have two proteins loaded!

9. **1T46: A** *(action)* ⇒ align ⇒ to molecule ⇒ **1PKG**

10. **1T46** and **1PKG: A** *(action)* ⇒ align ⇒ preset ⇒ publication

11. From the command line: **ray**

12. File ⇒ Save image as ⇒ PNG

Summary

PyMOL is an open-source, multi-platform program to visualize molecules and is available from the web:

http://www.pymol.org

The PyMOL GUI allows for an easy usage with no need to use the command line.

There are many other resources available online. A good one is the PyMOL wiki:

http://www.pymolwiki.org

Questions?
(and coffee break!)