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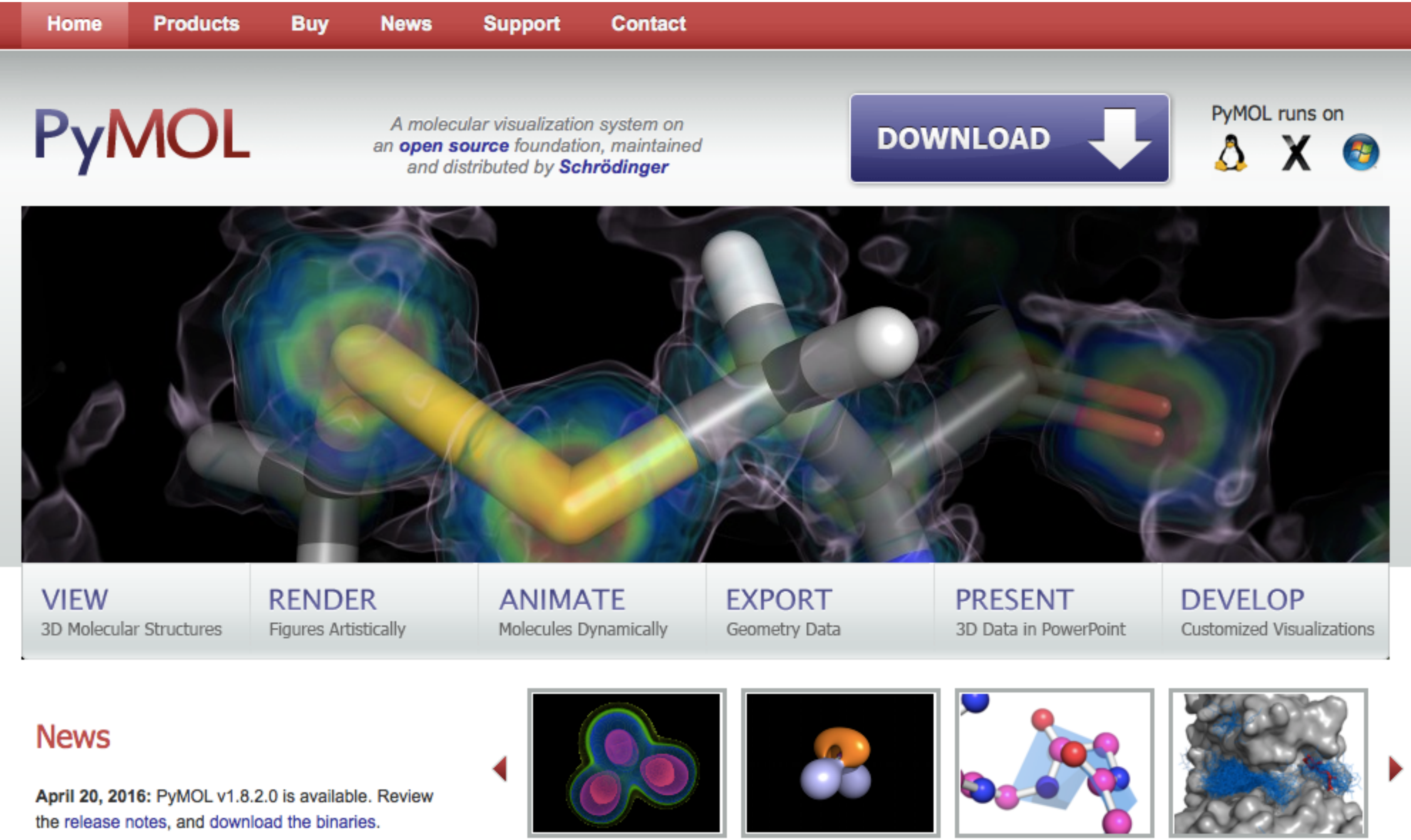
PyMol Tutorial

Download the latest PyMol version

Free educational license: http://pymol.org/edu/?q=educational/



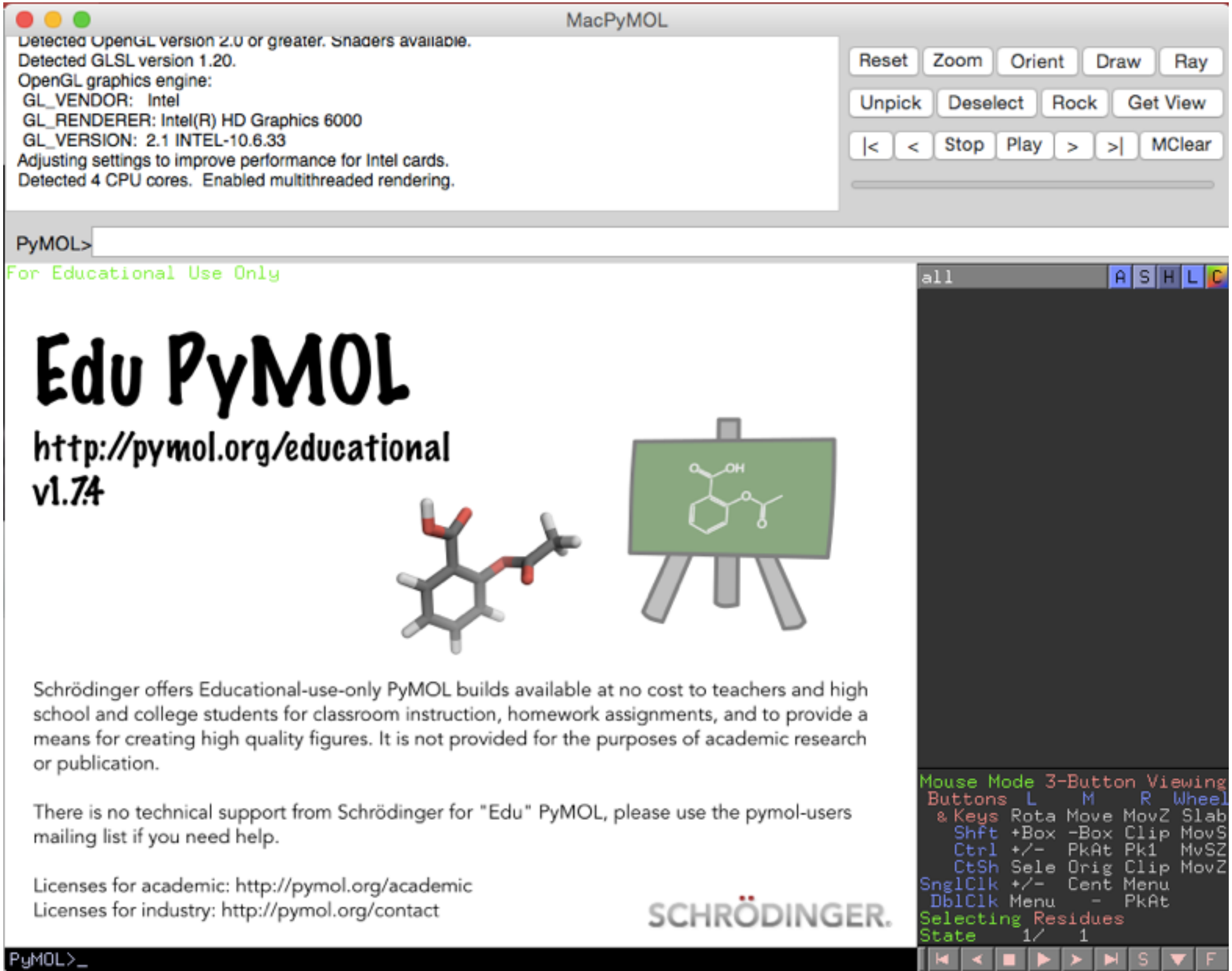
A molecular visualization system on an ***open source*** *foundation, maintained and distributed by* ***Schrödinger***

News

April 20, 2016: PyMOL v1.8.2.0 is available. Review the release notes, and download the binaries.

Start PyMol

I should more or less look like this:



```
Detected OpenGL version 2.0 or greater. Shaders available.
Detected GLSL version 1.20.
OpenGL graphics engine:
 GL_VENDOR:   Intel
 GL_RENDERER: Intel(R) HD Graphics 6000
 GL_VERSION:  2.1 INTEL-10.6.33
Adjusting settings to improve performance for Intel cards.
Detected 4 CPU cores.  Enabled multithreaded rendering.
PyMOL>
```

For Educational Use Only

Edu PyMOL

http://pymol.org/educational

v1.74

Schrödinger offers Educational-use-only PyMOL builds available at no cost to teachers and high school and college students for classroom instruction, homework assignments, and to provide a means for creating high quality figures. It is not provided for the purposes of academic research or publication.

There is no technical support from Schrödinger for "Edu" PyMOL, please use the pymol-users mailing list if you need help.

Licenses for academic: http://pymol.org/academic
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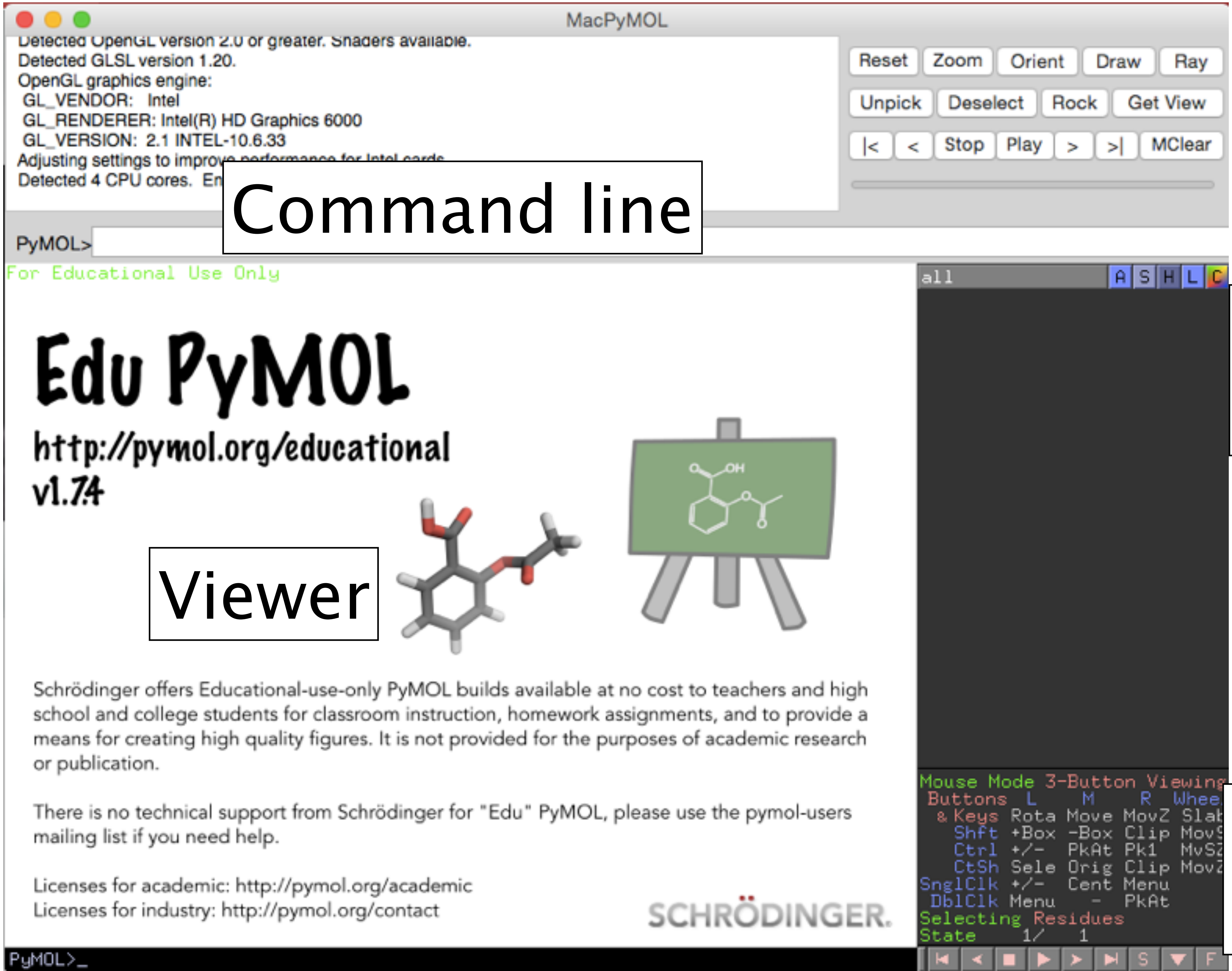
```
PyMOL>_
```

The interface



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PyMOL>
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Licenses for industry: http://pymol.org/contact

SCHRÖDINGER.

```
PyMOL>_
```

```
Mouse Mode 3-Button Viewing
 Buttons  L    M    R  Whee
  & Keys Rota Move MovZ Slab
    Shft +Box -Box Clip Mov
    Ctrl +/-  PkAt Pk1  MvS
    CtSh Sele Orig Clip Mov
SnglClk +/-  Cent Menu
 DblClk Menu  -   PkAt
Selecting Residues
State      1/   1
```

Command line

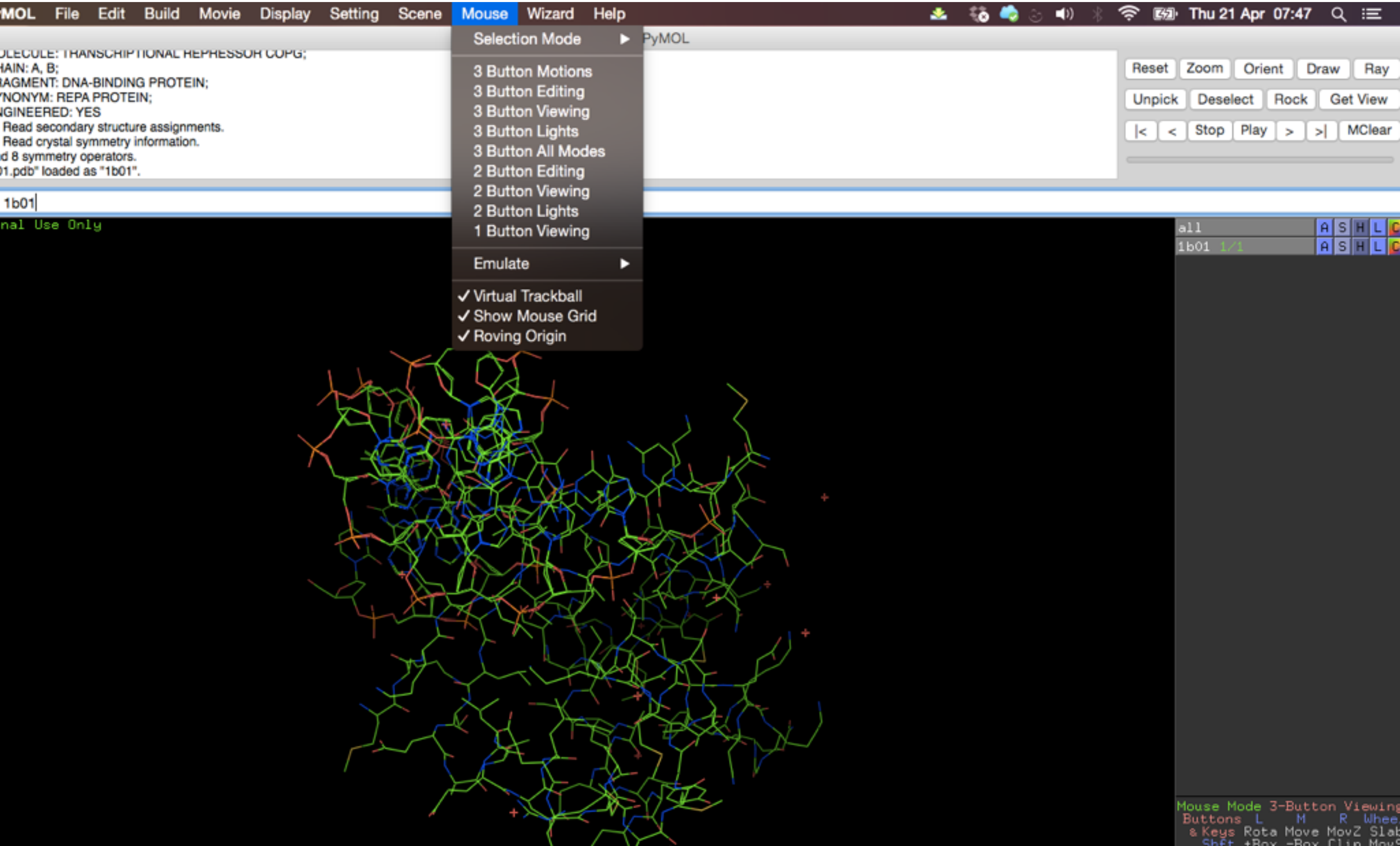
Viewer

Names Panel

Mouse actions

Mouse settings

Select the type of mouse you are using, on a laptop go for “1 button viewing”



```
OLECULE: TRANSCRIPTIONAL REPRESSOR COPG;
HAIN: A, B;
RAGMENT: DNA-BINDING PROTEIN;
YNONYM: REPA PROTEIN;
NGINEERED: YES
 Read secondary structure assignments.
 Read crystal symmetry information.
d 8 symmetry operators.
01.pdb" loaded as "1b01".
```

```
1b01
```

Loading a protein model – Option 1

- Download the model from a protein database
  - http://www.rcsb.org/pdb/home/home.do

An Information Portal to 118087 Biological Macromolecular Structures

1B01

TRANSCRIPTIONAL REPRESSOR COPG/DNA COMPLEX

DOI: 10.2210/pdb1b01/pdb **NDB:** PD0091

Classification: GENE REGULATION / DNA
Deposited: 1999-11-15 **Released:** 1999-11-19
Deposition author(s): Gomis-Rueth, F.X., Sola, M., Acebo, P., Parraga, A., Guasch, A., Eritja, R., Gonzalez, A., Espinosa, M., del Solar, G., Coll, M.
Organism: Streptococcus agalactiae
Expression System: Escherichia coli

Structural Biology Knowledgebase: 1B01 (>14 annotations)

Experimental Data Snapshot **wwPDB Validation**

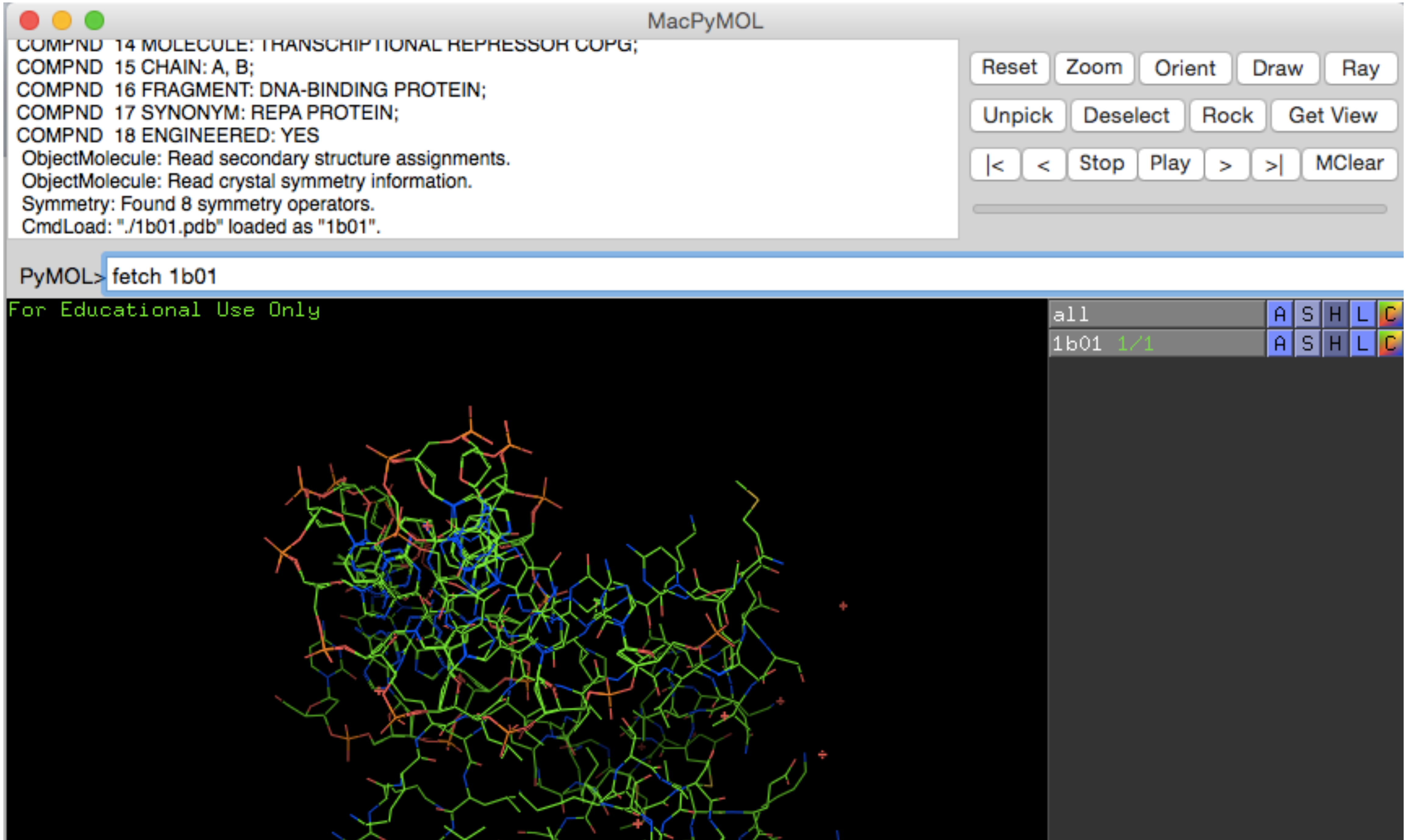
Search

Download PDB format

- Load into PyMol, via command line:
  - “cd desktop” in case your file is on your desktop
  - “load 1b01.pdb”

Loading a protein model – Option 2

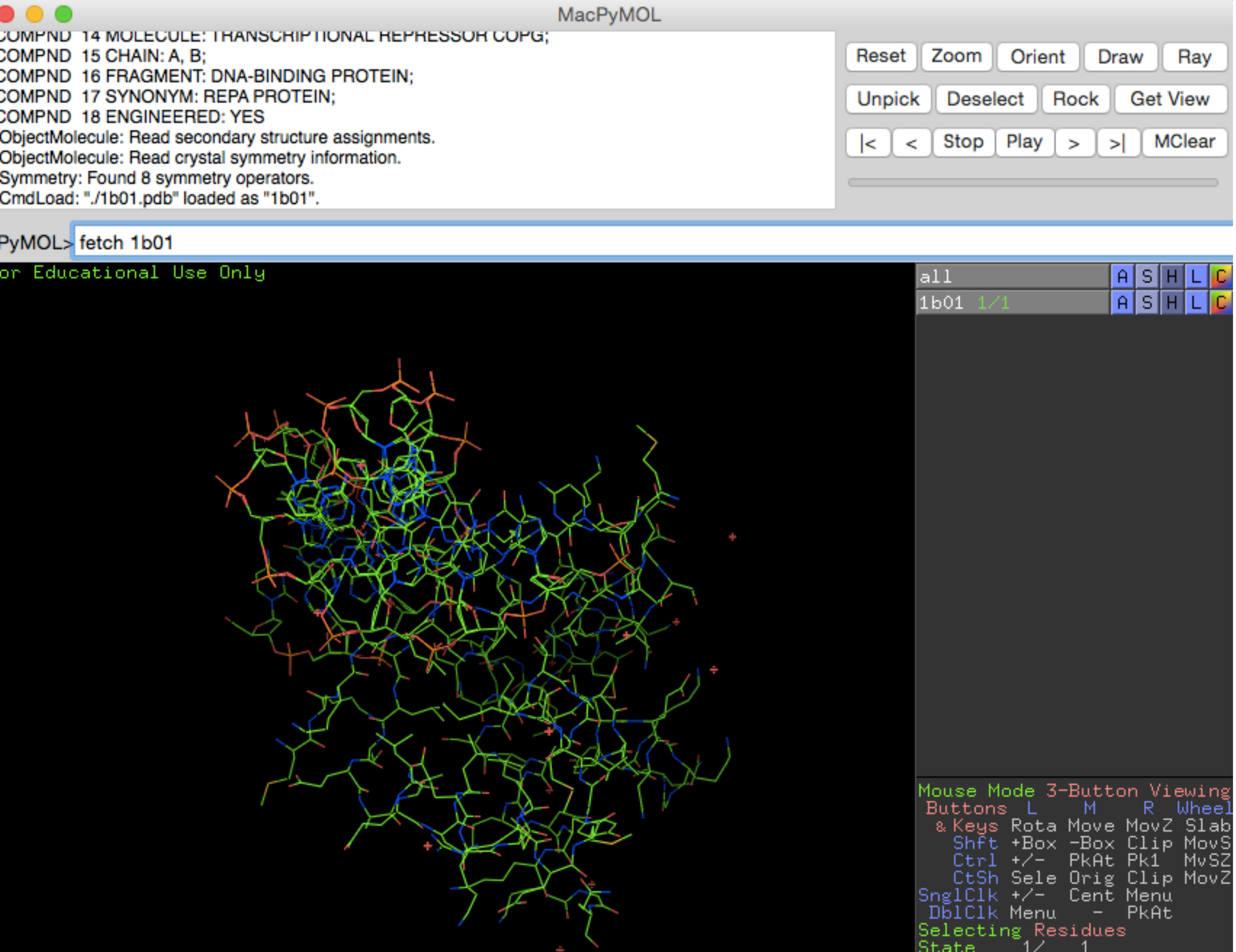
- Load straight into PyMol via command line
  - “fetch 1b01”



```
COMPND  14 MOLECULE: TRANSCRIPTIONAL REPRESSOR COPG;
COMPND  15 CHAIN: A, B;
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
COMPND  18 ENGINEERED: YES
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 8 symmetry operators.
 CmdLoad: "./1b01.pdb" loaded as "1b01".
```

```
PyMOL> fetch 1b01
```

Actions



```
COMPND  14 MOLECULE: TRANSCRIPTIONAL REPRESSOR COPG;
COMPND  15 CHAIN: A, B;
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
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ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 8 symmetry operators.
CmdLoad: "./1b01.pdb" loaded as "1b01".
```
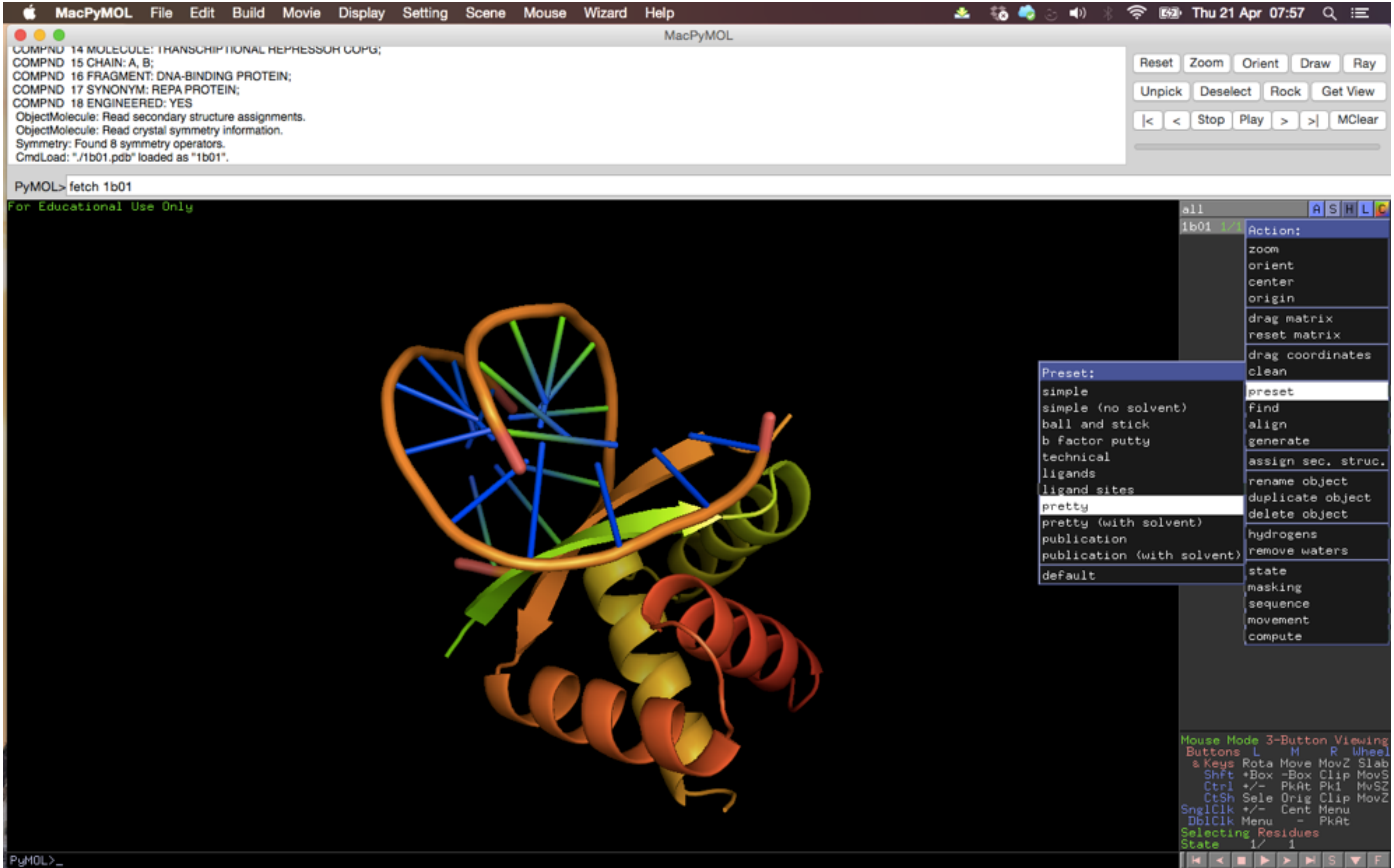

```
PyMOL> fetch 1b01
```

```
Mouse Mode 3-Button Viewing
 Buttons  L    M    R  Wheel
  & Keys Rota Move MovZ Slab
    Shft +Box -Box Clip MovS
    Ctrl +/-  PkAt Pk1  MvSZ
    CtSh Sele Orig Clip MovZ
 SnglClk +/-  Cent Menu
  DblClk Menu  -   PkAt
Selecting Residues
State      1/    1
```

A: Action
S: Show
H: Hide
L: Label
C: Color

Pretty cartoon view



```
COMPND  14 MOLECULE: TRANSCRIPTIONAL REPRESSOR COPG;
COMPND  15 CHAIN: A, B;
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
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 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 8 symmetry operators.
 CmdLoad: "./1b01.pdb" loaded as "1b01".
```
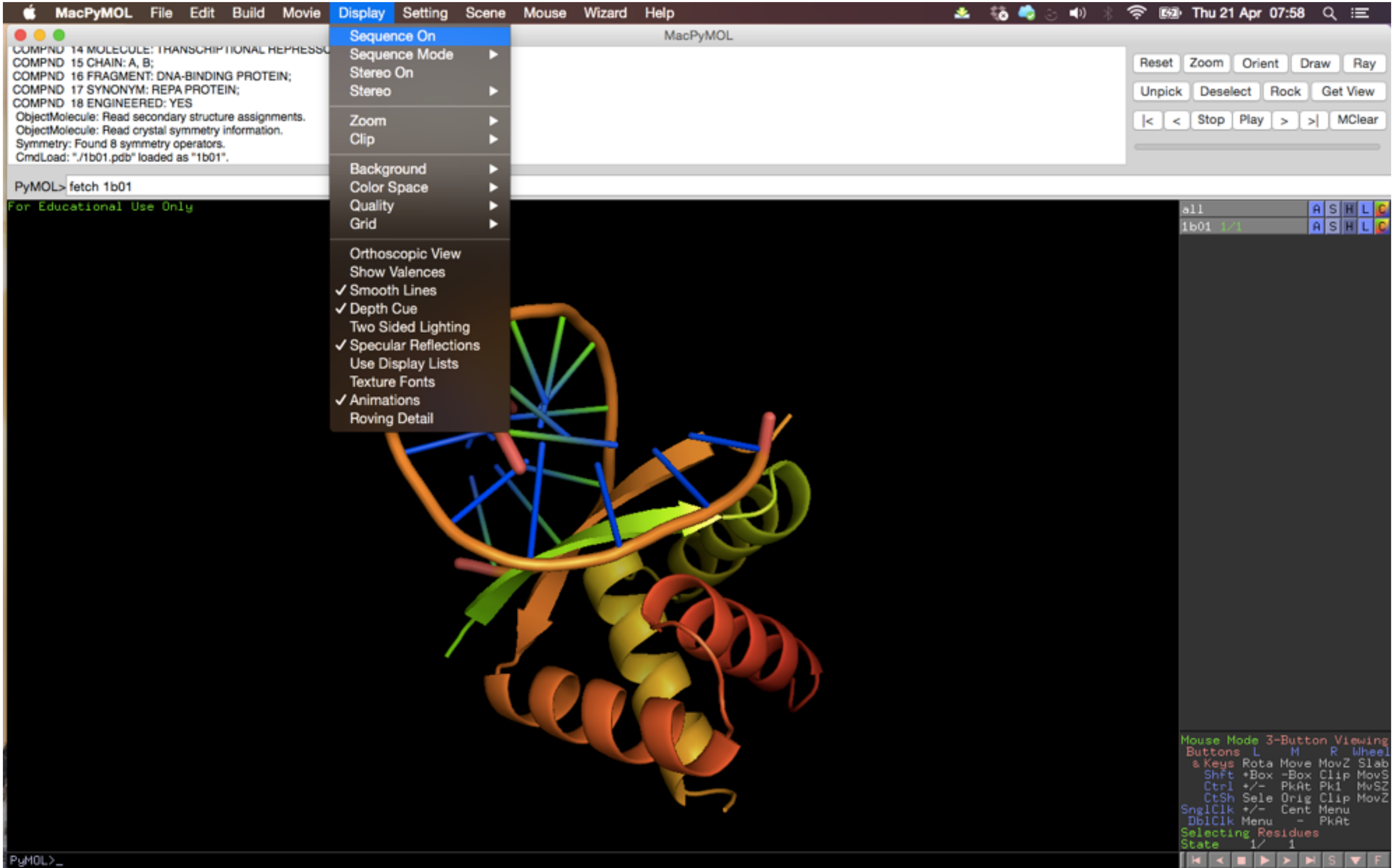

```
PyMOL> fetch 1b01
```

Subset selection

Display the sequence of your object: Display -> Sequence On



```
COMPND  14 MOLECULE: TRANSCRIPTIONAL REPRESS
COMPND  15 CHAIN: A, B;
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
COMPND  18 ENGINEERED: YES
 ObjectMolecule: Read secondary structure assignments.
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 CmdLoad: "./1b01.pdb" loaded as "1b01".
```

```
PyMOL> fetch 1b01
```

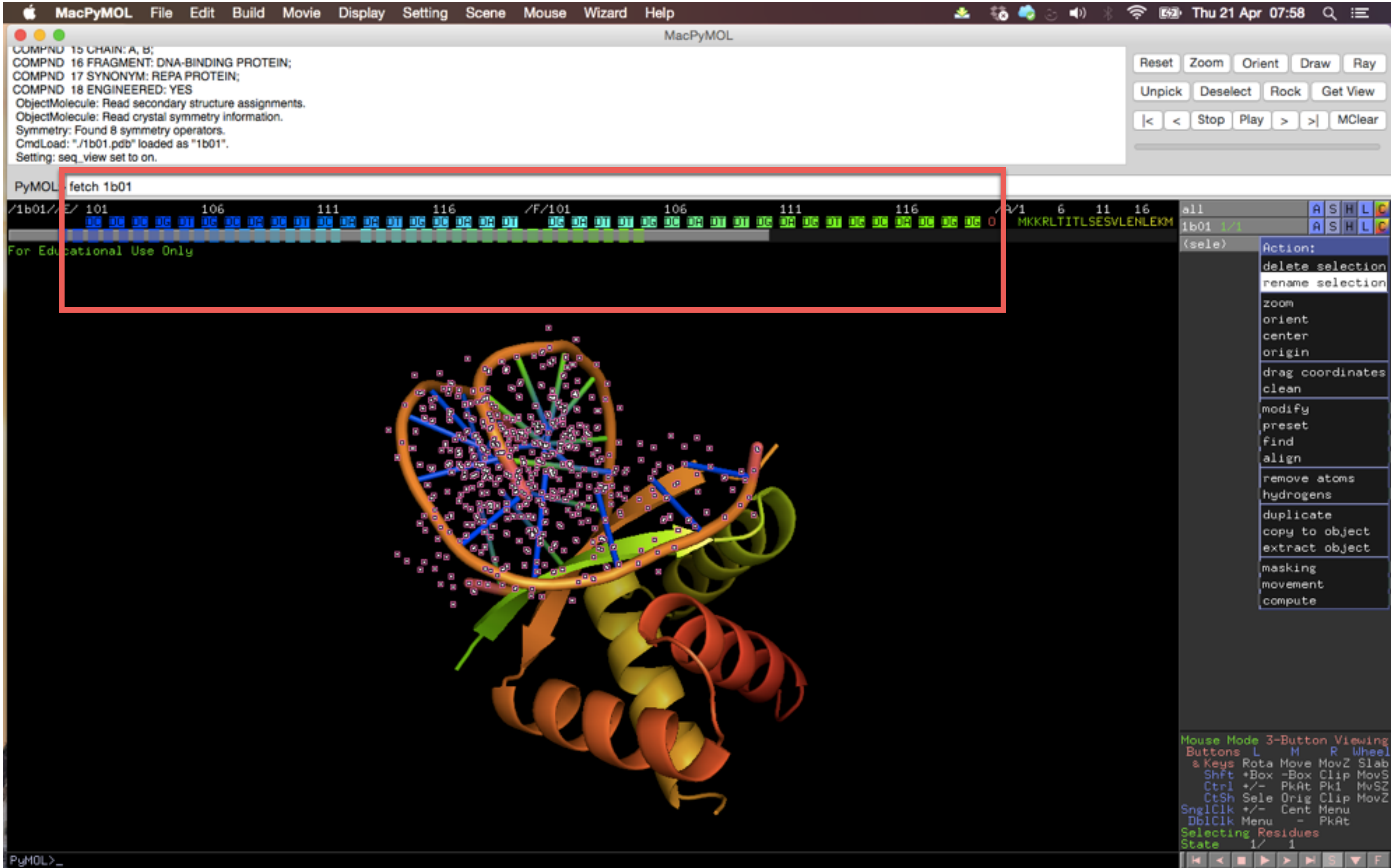
For Educational Use Only

```
Mouse Mode 3-Button Viewing
 Buttons  L    M    R  Wheel
  & Keys Rota Move MovZ Slab
    Shft +Box -Box Clip MovS
    Ctrl +/-  PkAt Pk1  MvSZ
    CtSh Sele Orig Clip MovZ
SnglClk +/-  Cent Menu
 DblClk Menu   -  PkAt
Selecting Residues
State      1/   1
```

```
PyMOL>_
```

Select all DNA residues

Click and drag in the Sequence Bar

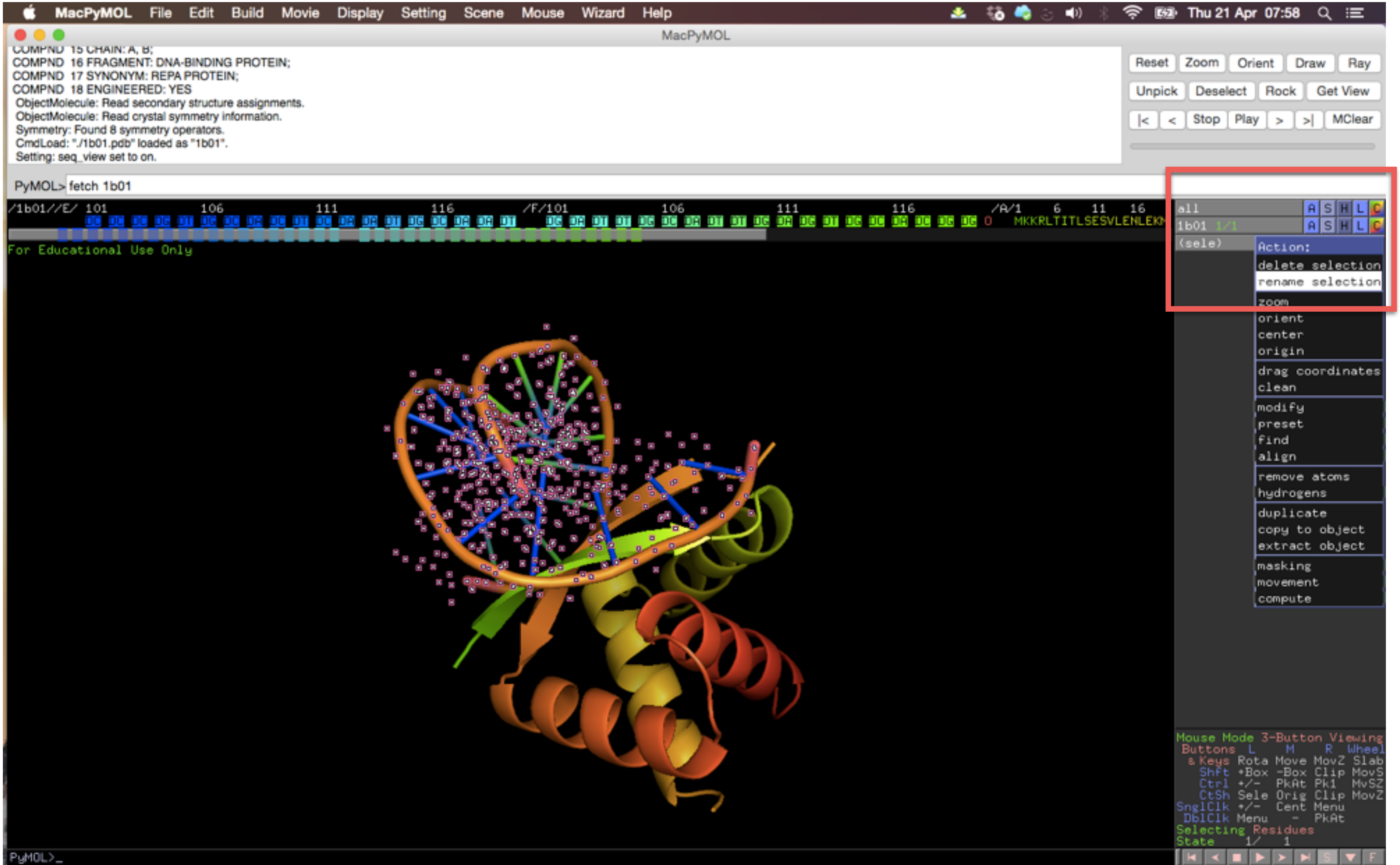


```
COMPND  15 CHAIN: A, B;
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
COMPND  18 ENGINEERED: YES
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 8 symmetry operators.
 CmdLoad: "./1b01.pdb" loaded as "1b01".
 Setting: seq_view set to on.
```

```
PyMOL> fetch 1b01
```

Save this object sub set

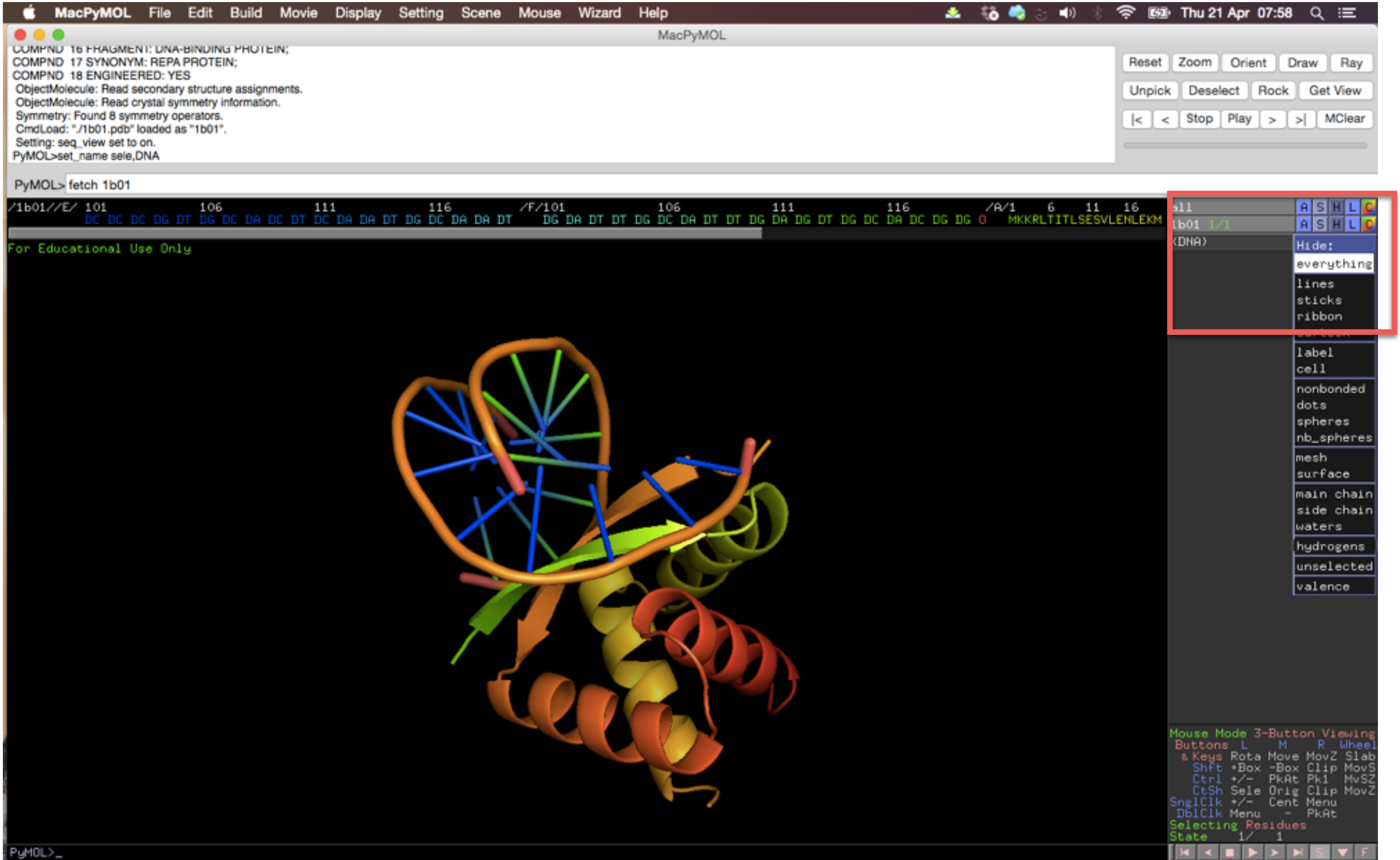
Click on A -> Rename Selection. Type DNA and press enter



```
COMPND  15 CHAIN: A, B;
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
COMPND  18 ENGINEERED: YES
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 8 symmetry operators.
 CmdLoad: "./1b01.pdb" loaded as "1b01".
 Setting: seq_view set to on.
PyMOL> fetch 1b01
```

Now you can modify this part

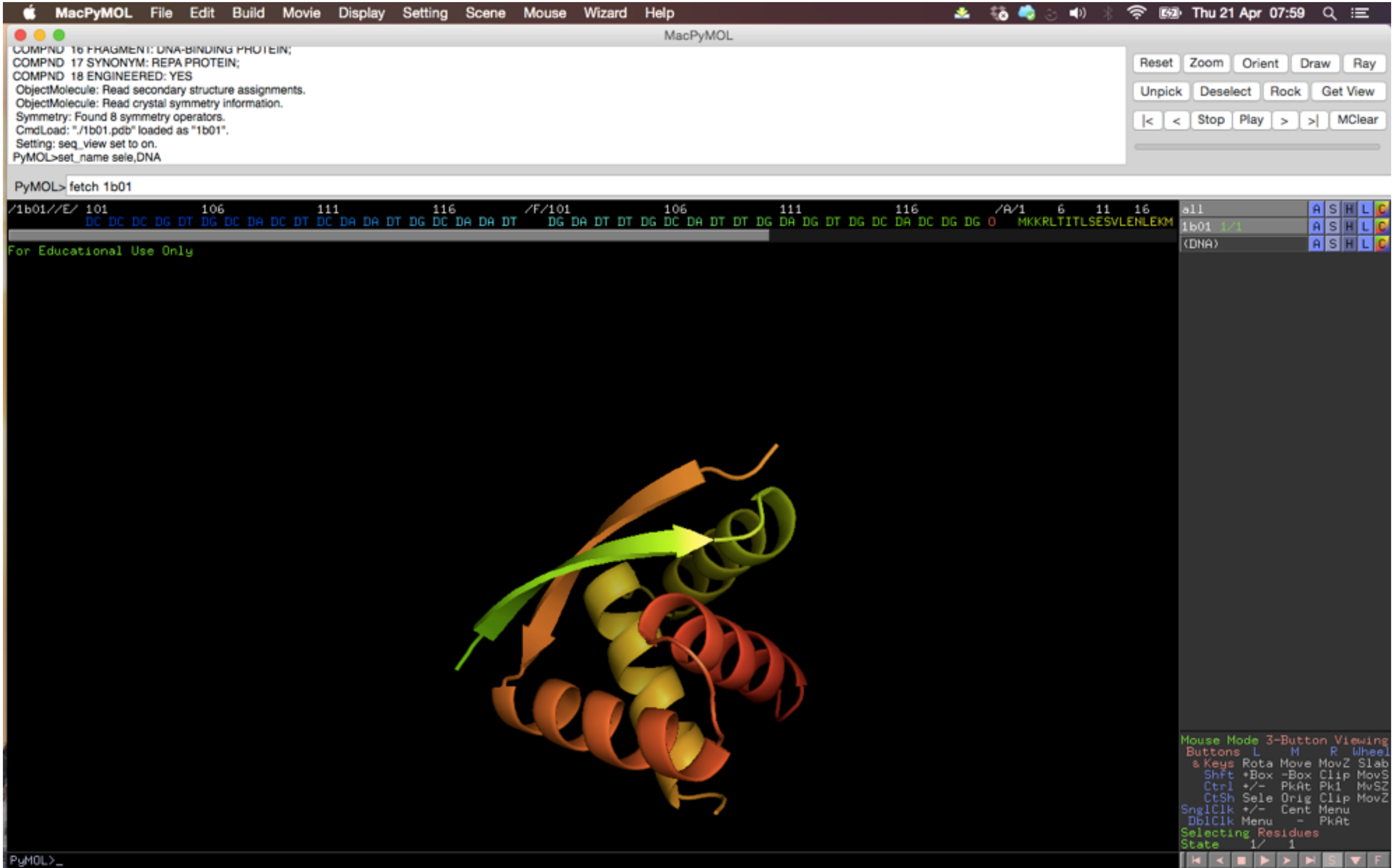
For example, hide the DNA strand: H -> everything



```
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
COMPND  18 ENGINEERED: YES
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 8 symmetry operators.
 CmdLoad: "./1b01.pdb" loaded as "1b01".
 Setting: seq_view set to on.
PyMOL>set_name sele,DNA
```

```
PyMOL> fetch 1b01
```

The DNA part is now gone



```
COMPND  16 FRAGMENT: DNA-BINDING PROTEIN;
COMPND  17 SYNONYM: REPA PROTEIN;
COMPND  18 ENGINEERED: YES
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 8 symmetry operators.
 CmdLoad: "./1b01.pdb" loaded as "1b01".
 Setting: seq_view set to on.
PyMOL>set_name sele,DNA
```

```
PyMOL> fetch 1b01
```

```
/1b01//E/ 101          106            111            116         /F/101          106            111            116          /A/1    6    11   16
          DC DC DC DG DT DG DC DA DC DT DC DA DA DT DG DC DA DA DT   DG DA DT DT DG DC DA DT DT DG DA DG DT DG DC DA DC DG DG O   MKKRLTITLSESVLENLEKM
```

```
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```
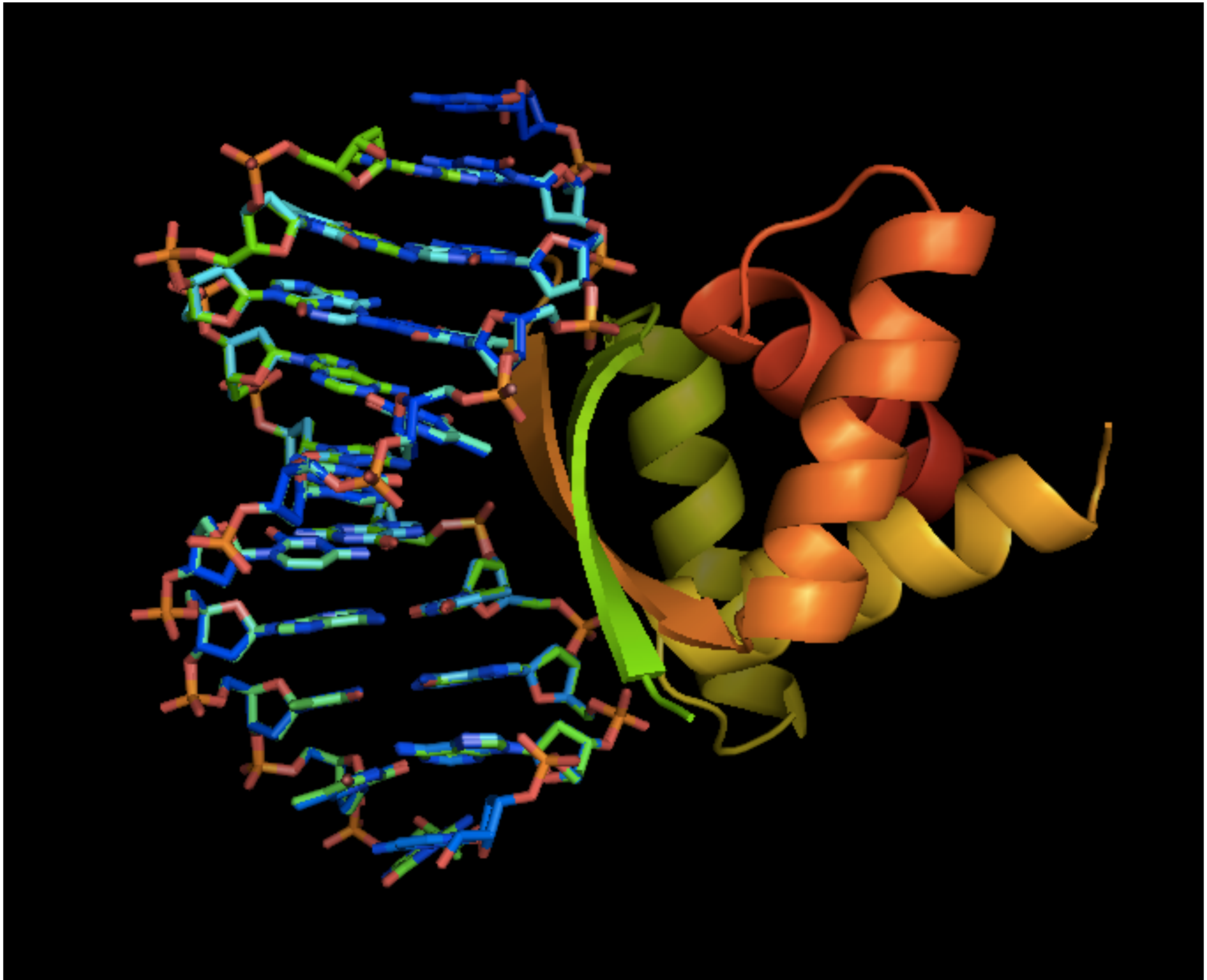

```
PyMOL>_
```

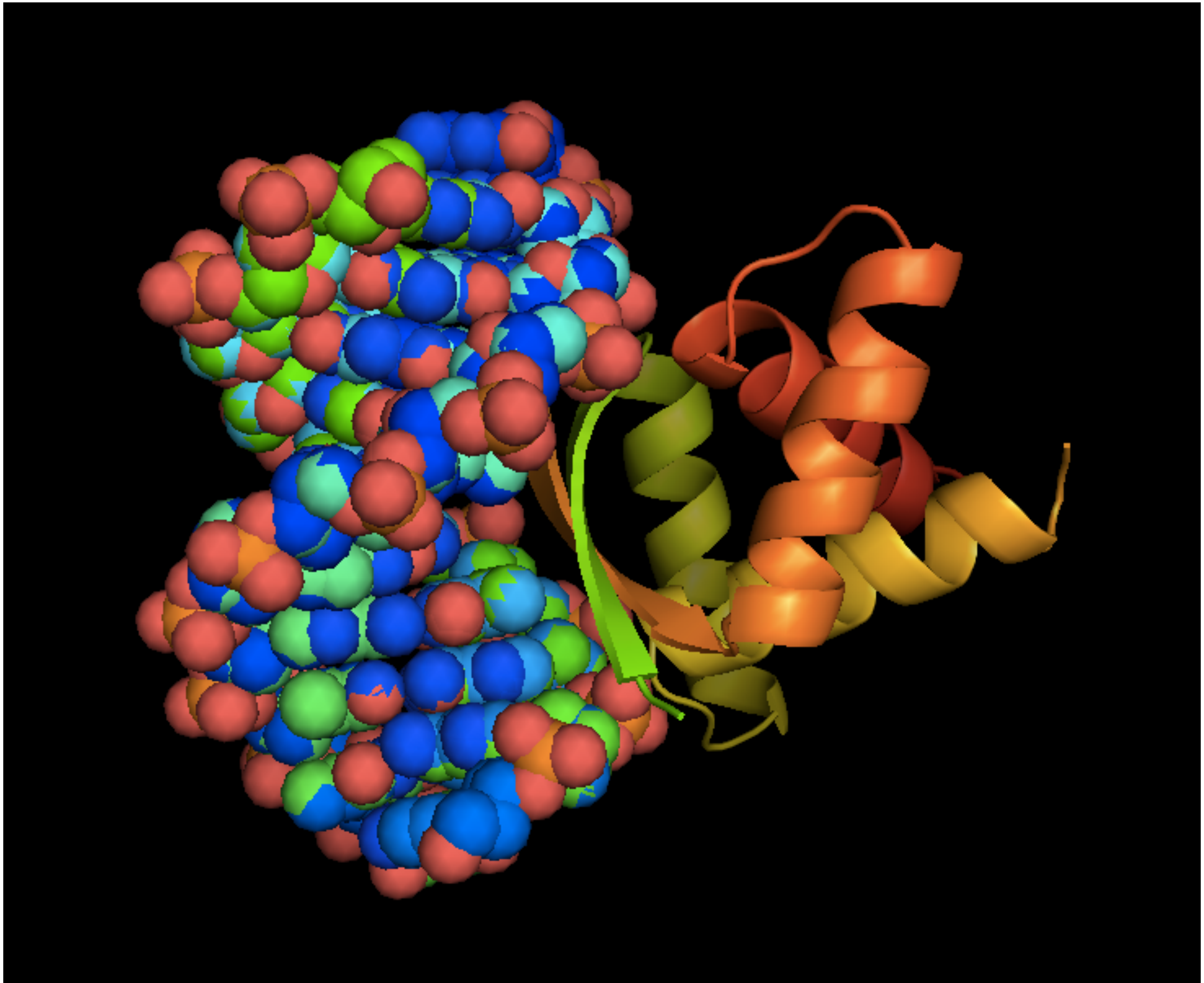
Or Show DNA as Sticks

Click on S -> as: -> sticks



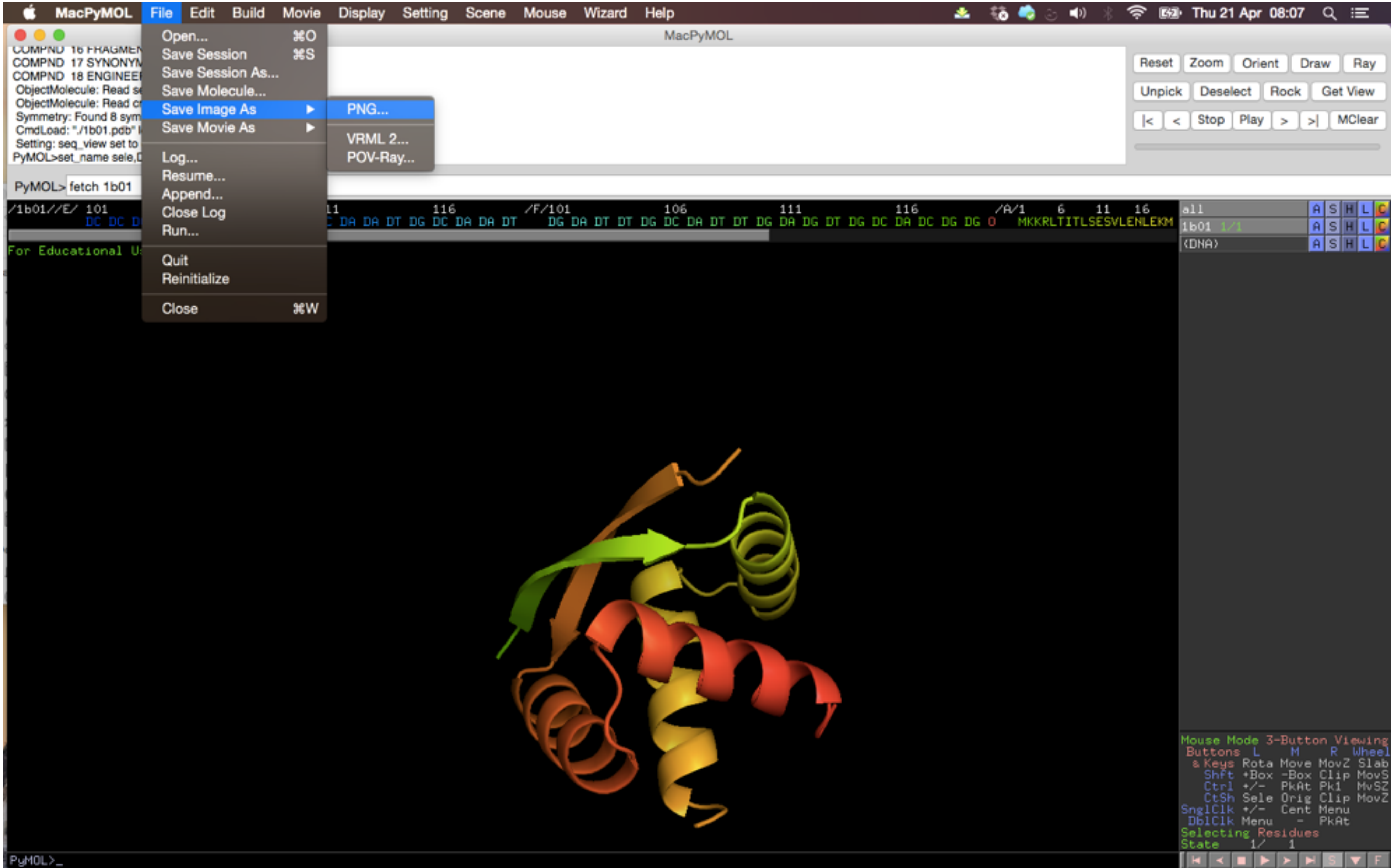
Or Show as Spheres

Click on S -> as: -> spheres



Save an image

File -> Save Image As -> PNG



```
COMPND  16 FRAGMEN
COMPND  17 SYNONYM
COMPND  18 ENGINEEI
 ObjectMolecule: Read se
 ObjectMolecule: Read cr
 Symmetry: Found 8 sym
 CmdLoad: "./1b01.pdb" l
 Setting: seq_view set to
PyMOL>set_name sele,D
```

```
PyMOL> fetch 1b01
```

```
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```


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