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PyMol Tutorial



Download the latest PyMOL version

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

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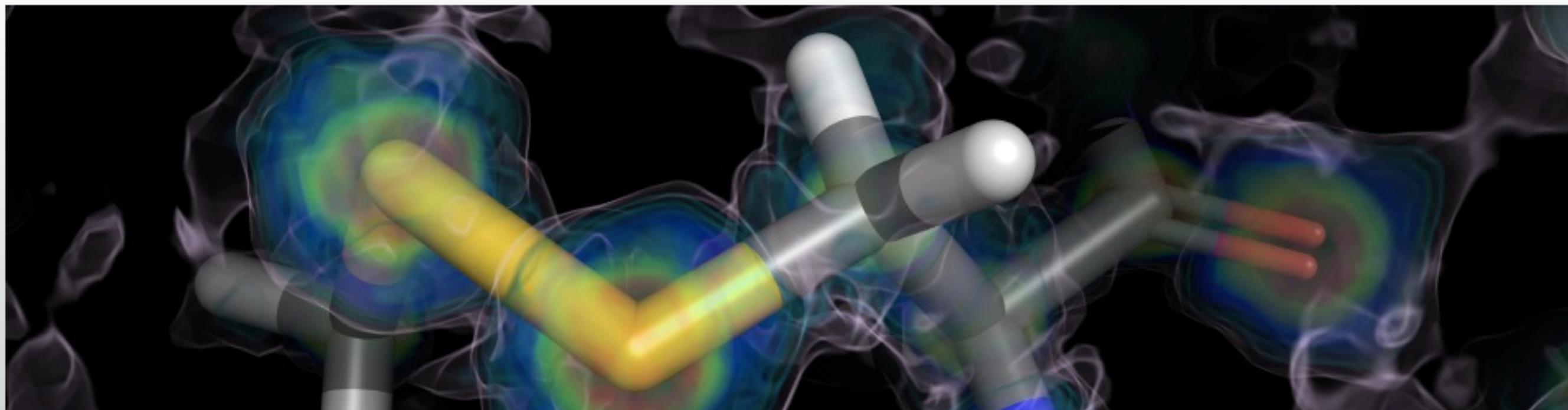
PyMOL

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

DOWNLOAD



PyMOL runs on



VIEW

3D Molecular Structures

RENDER

Figures Artistically

ANIMATE

Molecules Dynamically

EXPORT

Geometry Data

PRESENT

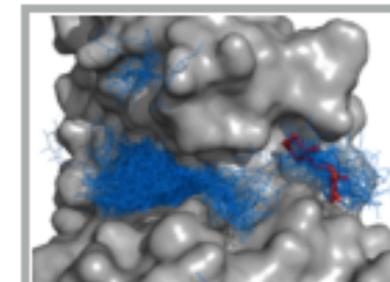
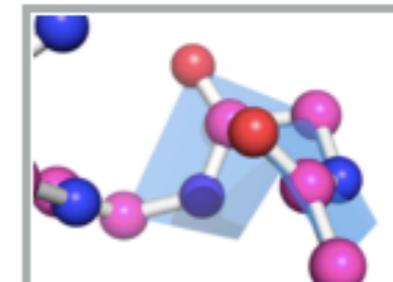
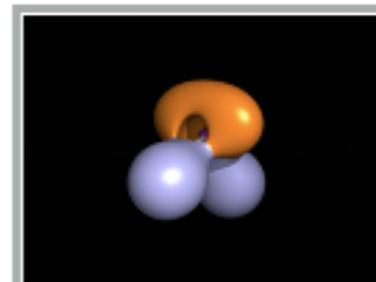
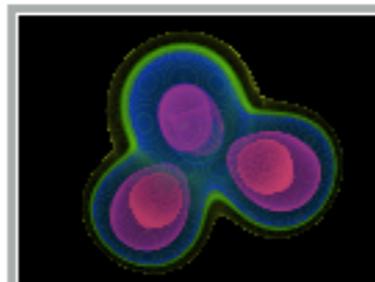
3D Data in PowerPoint

DEVELOP

Customized Visualizations

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:

MacPyMOL

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.

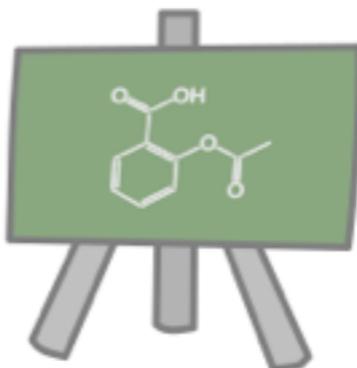
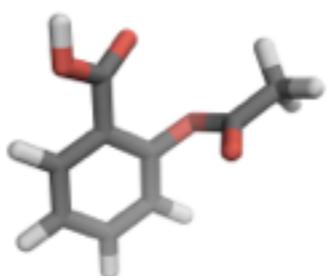
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
< << Stop Play >> |> MClear

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

SCHRÖDINGER.

all A S H L C

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	
Db1Clk	Menu	-	PkAt	

Selecting Residues
State 1/ 1

PyMOL>_



The interface

MacPyMOL

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. En

Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
< << Stop Play >> >| MClear

PyMOL>

For Educational Use Only

Edu PyMOL

<http://pymol.org/educational>
v1.74

Viewer

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SCHRÖDINGER.

all A S H L C

Mouse Mode 3-Button Viewing
Buttons L M R Whee
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip Mov9
Ctrl +/- PkAt Pk1 MvS2
CtSh Sele Orig Clip Mov2
SnglClk +/- Cent Menu
Db1Clk Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>_

Command line

Names Panel

Mouse actions



Mouse settings

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

The screenshot shows the PyMOL software interface. The top menu bar includes: MOL, File, Edit, Build, Movie, Display, Setting, Scene, **Mouse**, Wizard, Help. The 'Mouse' menu is open, displaying the following options:

- Selection Mode ▶ PyMOL
- 3 Button Motions
- 3 Button Editing
- 3 Button Viewing
- 3 Button Lights
- 3 Button All Modes
- 2 Button Editing
- 2 Button Viewing
- 2 Button Lights
- 1 Button Viewing
- Emulate ▶
- Virtual Trackball
- Show Mouse Grid
- Roving Origin

The main window displays a 3D molecular model of a protein structure, rendered in green, blue, and red stick representation. The left sidebar shows the command line with the following text:

```
1b01|  
Read secondary structure assignments.  
Read crystal symmetry information.  
Read 8 symmetry operators.  
1b01.pdb loaded as "1b01".
```

The right sidebar contains a toolbar with buttons: Reset, Zoom, Orient, Draw, Ray, Unpick, Deselect, Rock, Get View, and a navigation bar with buttons: |<, <, Stop, Play, >, >|, MClear.

The bottom right corner shows a status bar with the following text:

```
all A S H L C  
1b01 1/1 A S H L C  
Mouse Mode 3-Button Viewing  
Buttons L M R Whee  
& Keys Rota Move MovZ Slab  
ShFt +Box -Box Clip Mov
```



Loading a protein model – Option 1

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



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”

The screenshot shows the MacPyMOL application window. The title bar reads "MacPyMOL". The main window is divided into several sections:

- Command Log:** Displays the following text:

```
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".
```
- Control Panel:** Contains buttons for "Reset", "Zoom", "Orient", "Draw", "Ray", "Unpick", "Deselect", "Rock", "Get View", and a set of navigation buttons: "<|", "<", "Stop", "Play", ">", ">|", and "MClear".
- Command Line:** Shows the command "PyMOL> fetch 1b01".
- Object List:** A table on the right side of the interface:

all	A	S	H	L	C
1b01 1/1	A	S	H	L	C
- 3D View:** A large black area showing a complex protein structure rendered in stick representation. The atoms are colored in green, blue, and red.



Actions

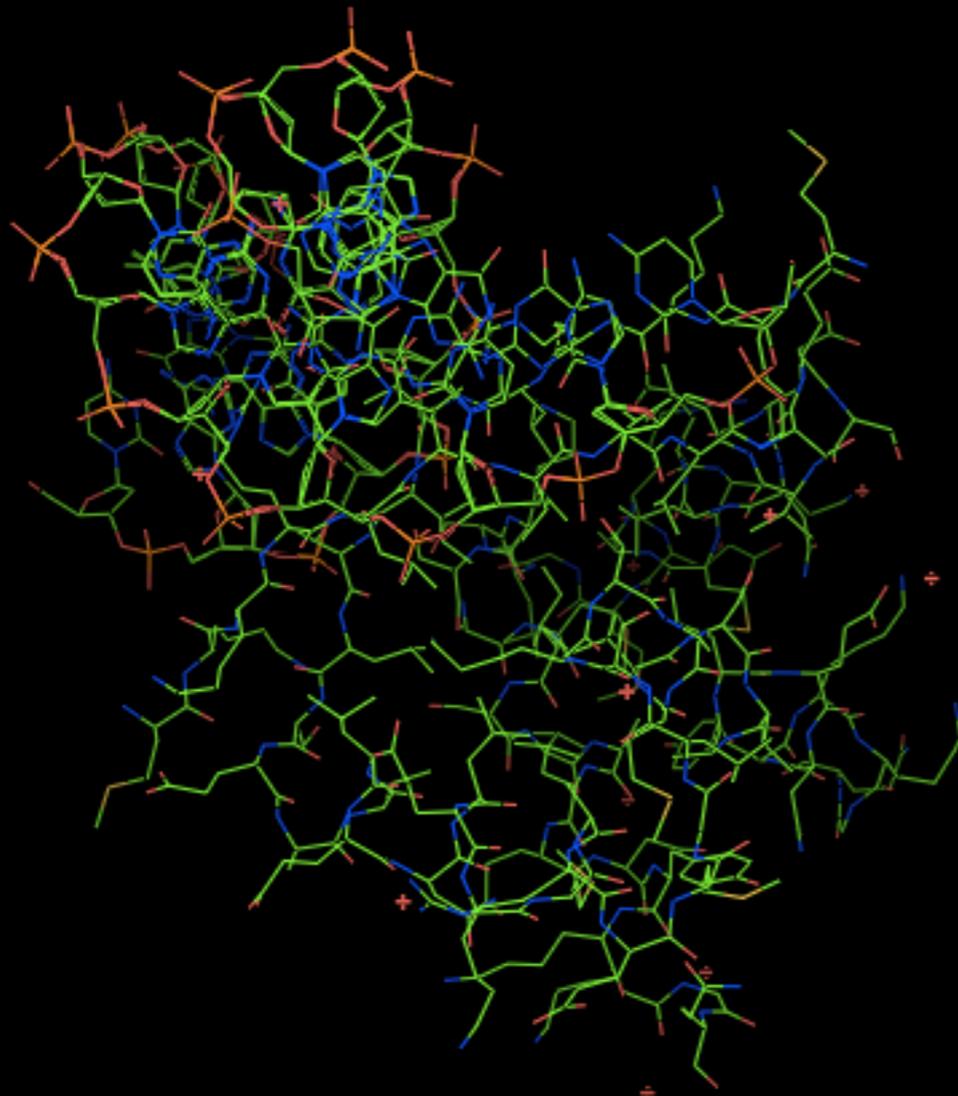
MacPyMOL

```
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".
```

Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear

PyMOL> fetch 1b01

or Educational Use Only



all	A	S	H	L	C
1b01 1/1	A	S	H	L	C

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

```
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
```



Pretty cartoon view

MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help Thu 21 Apr 07:57

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

For Educational Use Only

all 1b01 1/1

Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
< < Stop Play > >| MClear

1b01 Action:
zoom
orient
center
origin
drag matrix
reset matrix
drag coordinates
clean

Preset:
simple
simple (no solvent)
ball and stick
b factor putty
technical
ligands
ligand sites
pretty
pretty (with solvent)
publication
publication (with solvent)
default

preset
find
align
generate
assign sec. struc.
rename object
duplicate object
delete object
hydrogens
remove waters
state
masking
sequence
movement
compute

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
Db1Clk Menu - PkAt

Selecting Residues
State 1/ 1



Subset selection

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

The screenshot shows the MacPyMOL application window. The menu bar includes: MacPyMOL, File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Help. The 'Display' menu is open, showing options: Sequence On (highlighted), Sequence Mode, Stereo On, Stereo, Zoom, Clip, Background, Color Space, Quality, Grid, Orthoscopic View, Show Valences, Smooth Lines, Depth Cue, Two Sided Lighting, Specular Reflections, Use Display Lists, Texture Fonts, Animations, and Roving Detail. The main 3D view shows a protein structure with a ribbon representation. The command line at the bottom left shows: PyMOL> fetch 1b01. The status bar at the bottom right shows: State 1/1.



Save this object sub set

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

The screenshot displays the MacPyMOL application window. The title bar reads "MacPyMOL" and the system tray shows the date and time as "Thu 21 Apr 07:58". The main window contains a 3D molecular model of a protein structure with a DNA fragment highlighted in blue. A context menu is open over the DNA, with the following options: "Action:", "delete selection", "rename selection", "zoom", "orient", "center", "origin", "drag coordinates", "clean", "modify", "preset", "find", "align", "remove atoms", "hydrogens", "duplicate", "copy to object", "extract object", "masking", "movement", and "compute". The "rename selection" option is highlighted in blue. The command line at the bottom shows "PyMOL> fetch 1b01". The sequence viewer at the top shows the sequence "MKKRLTITLSESVLENLEK" with residues 101, 106, 111, and 116 highlighted in green. The mouse control panel at the bottom right shows "Mouse Mode 3-Button Viewing" and "Buttons L M R Wheel".



Now you can modify this part

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

MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

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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Hide:
everything
lines
sticks
ribbon

label
cell
nonbonded
dots
spheres
nb_spheres
mesh
surface
main chain
side chain
waters
hydrogens
unselected
valence

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
Db1Clk Menu - PkAt

Selecting Residues
State 1/ 1

PyMOL>_



The DNA part is now gone

MacPyMOL File Edit Build Movie Display Setting Scene Mouse Wizard Help

MacPyMOL

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      all
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
```

For Educational Use Only



1b01 1/1
(DNA)

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
Db1Clk Menu - PkAt

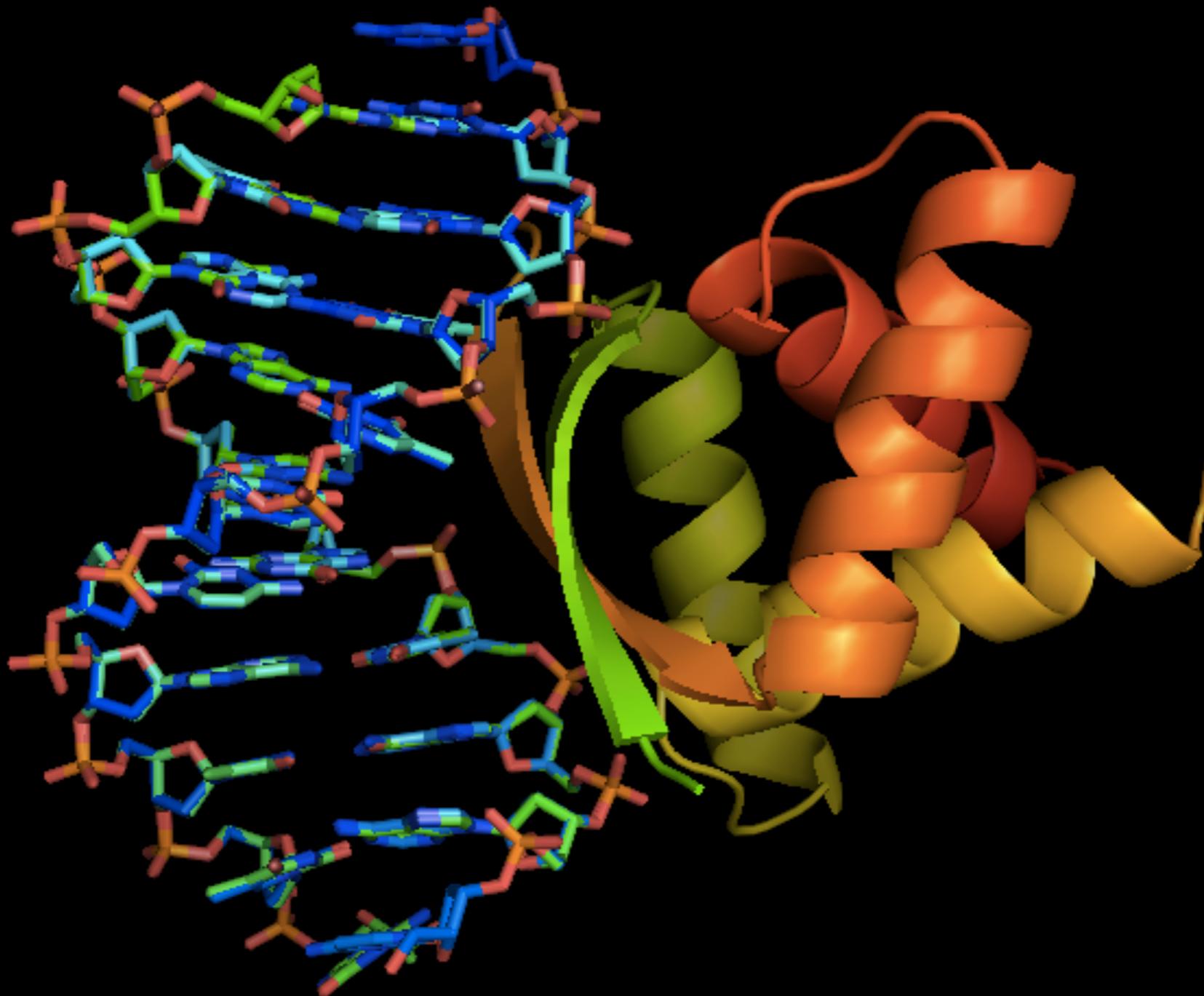
Selecting Residues
State 1/ 1

PyMOL>_



Or Show DNA as Sticks

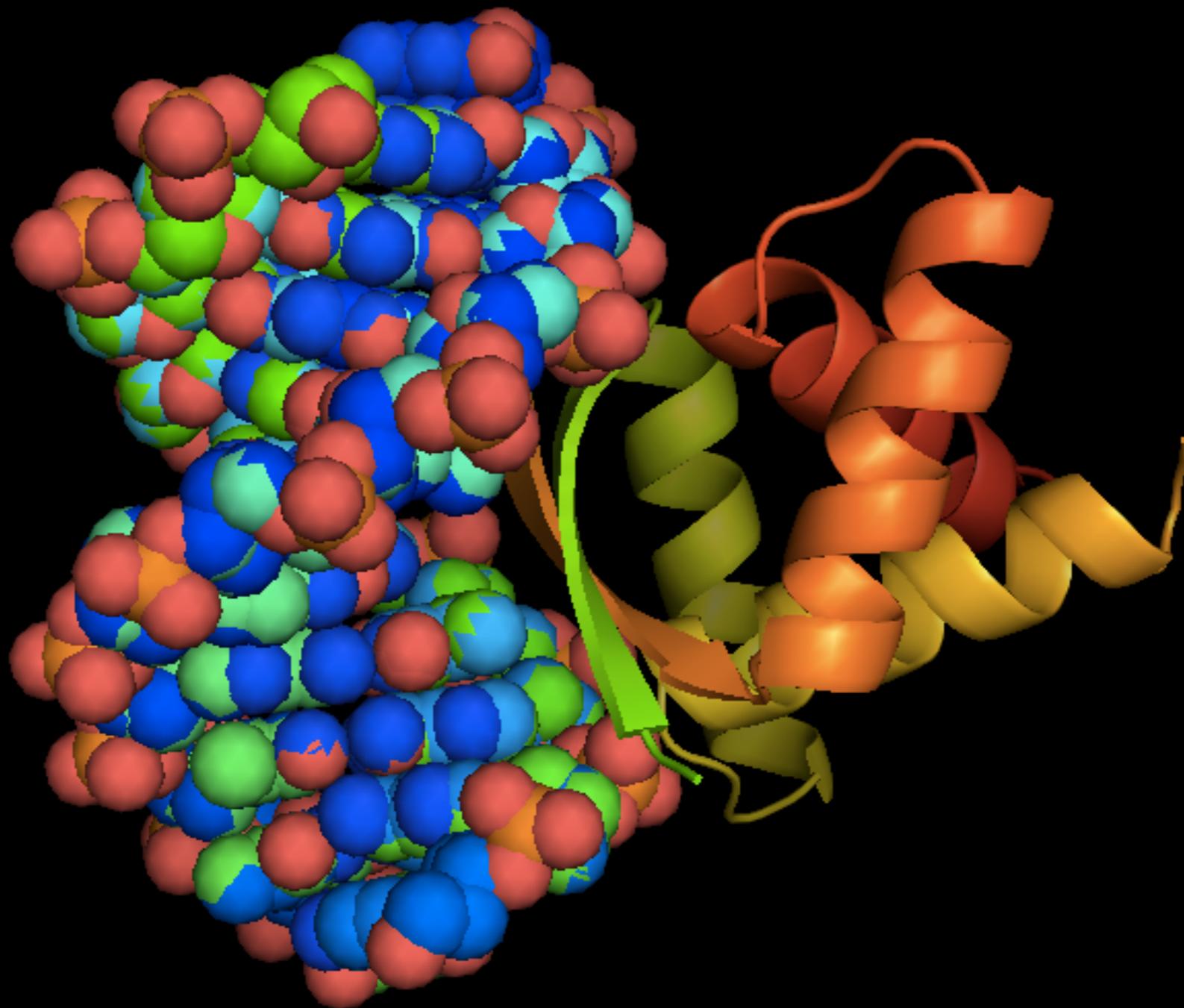
Click on S -> as: -> sticks





Or Show as Spheres

Click on S -> as: -> spheres





Save an image

File -> Save Image As -> PNG

The screenshot shows the MacPyMOL application window. The menu bar at the top includes: MacPyMOL, File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Help. The 'File' menu is open, showing options: Open... (⌘O), Save Session (⌘S), Save Session As..., Save Molecule..., Save Image As (highlighted), Save Movie As, Log..., Resume..., Append..., Close Log, Run..., Quit, Reinitialize, Close (⌘W). The 'Save Image As' submenu is open, showing: PNG... (highlighted), VRML 2..., POV-Ray... The main window displays a 3D ribbon model of a protein structure. The ribbon is colored in a gradient from orange to yellow to green. The background is dark. The command line at the bottom shows: PyMOL> fetch 1b01. The sequence viewer at the bottom right shows the sequence: 1b01 1/1 MKKRLTITLSESVLENLEKM (DNA). The mouse control panel at the bottom right shows: 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.



some

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