

Molecular Modelling Course

November 18. 2025 – 20. 2025 | Dr. Birkan Emrem, Dr. Ferdinand Jamitzky, Dr. Plamen Dobrev, Dr. Prasanth Ganta, Dr. Elmira Birang
Leibniz Supercomputing Centre

Visualizing biomolecular structures



- PyMOL
- VESTA
- VMD

PyMOL

← → ⌂ https://www.pymol.org ☆ ☰

PyMOL by Schrödinger

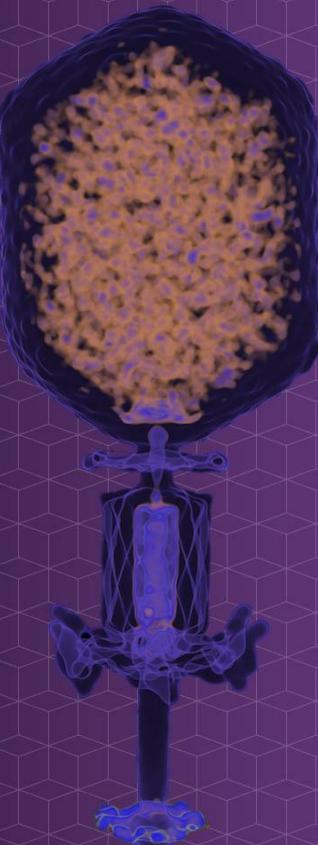
DOWNLOAD SCREENSHOTS SUPPORT CONTACT

Introducing PyMOL 3.1

PyMOL is a user-sponsored molecular visualization system on an [open-source foundation](#), maintained and distributed by Schrödinger.

[DOWNLOAD NOW](#) [BUY LICENSE](#)

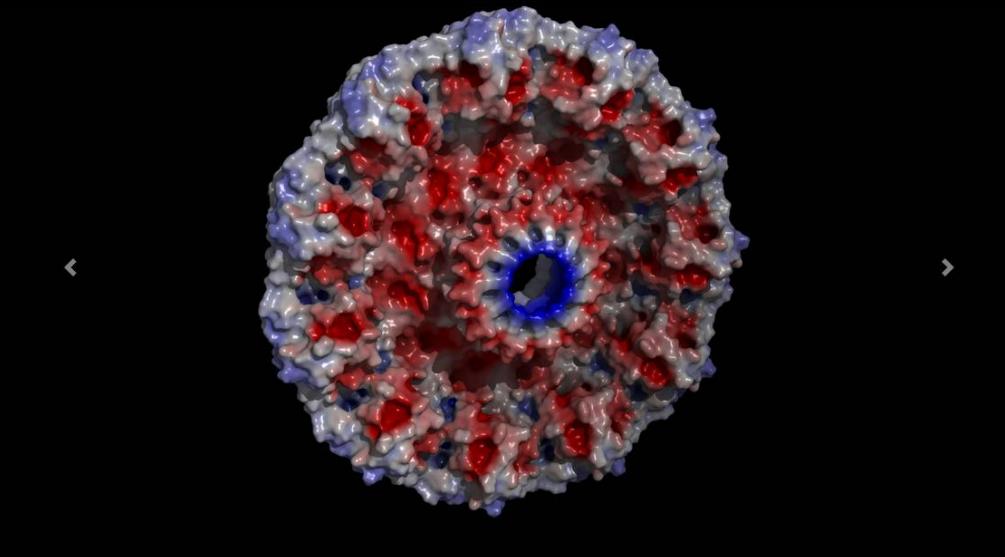
[PYMOL 3 PRODUCT PAGE](#)



PyMOL

← → ⌂ https://www.pymol.org ☆ ☰ ↴ ⌂ ⌂ ⌂ ⌂ ⌂ ⌂ ⌂

PyMOL by Schrödinger DOWNLOAD SCREENSHOTS SUPPORT CONTACT

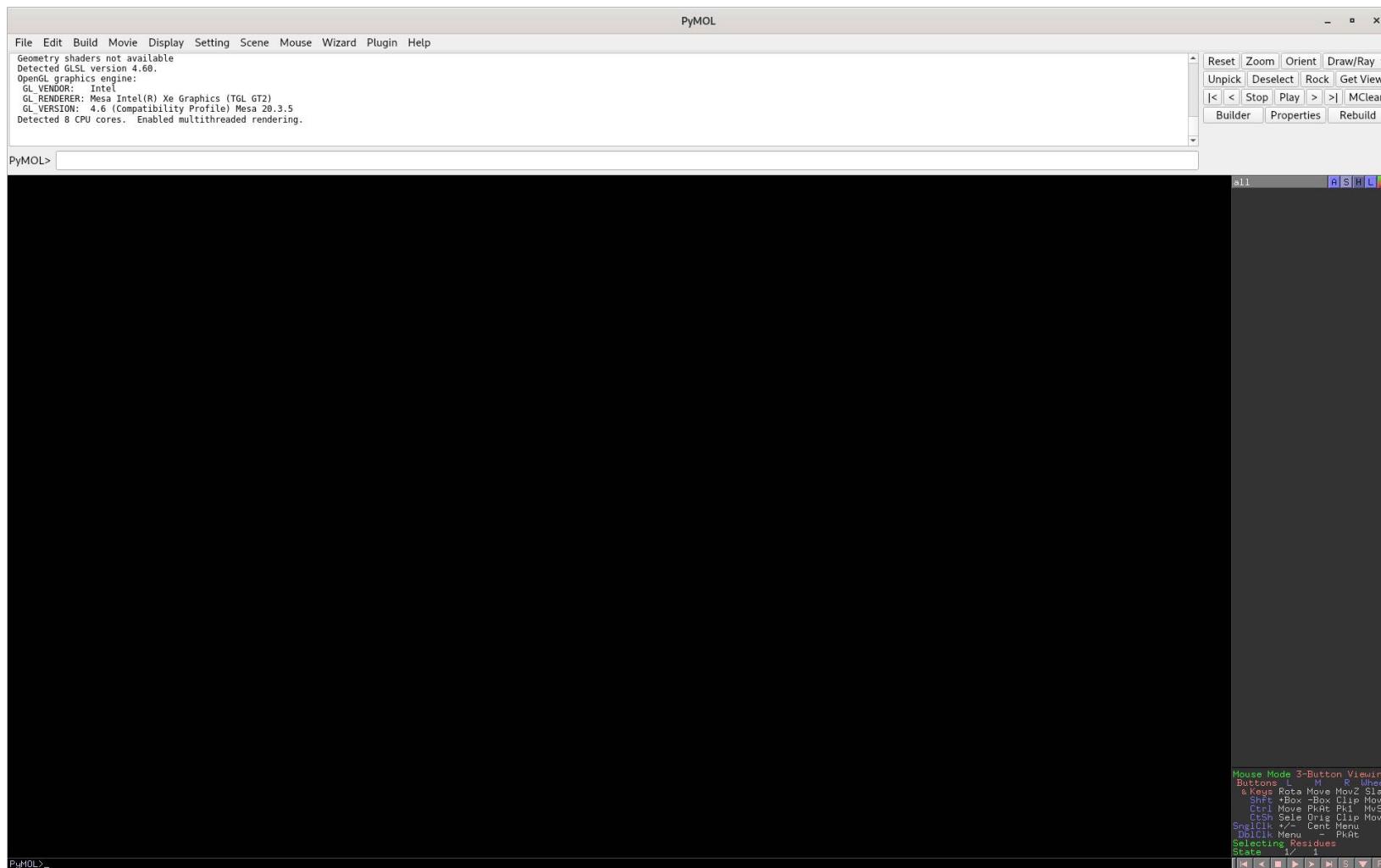


Open-Source Philosophy

PyMOL is a commercial product, but we make most of its source code freely available under a permissive license. The open source project is maintained by [Schrödinger](#) and ultimately funded by everyone who purchases a PyMOL license.

Open source enables open science.
This was the vision of the original PyMOL author Warren L. DeLano.

PyMOL



New PyMOL Window

Open...

Open Recent...

Get PDB...

Save Session

Save Session As...

Export Molecule...

Export Map...

Export Alignment...

Export Image As

Export Movie As

Log File

Run Script...

Working Directory

Edit pymolrc

Reinitialize

Quit

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

all A S H L C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
Keys Rota Move MovZ Slab
Shift +Box -Box Clip Slab
Ctrl Move PkAt Pk1 MvS
CtSh Sel Orig Clip MovZ
SinglClik +/- Cent Menu
DblClik Menu PkAt
Selecting Residues
State 1/ 1

OpenGL graphics engine:
GL_VENDOR: Intel
GL_RENDERER: Mesa Intel(R) Xe Graphics (TCL GT2)
GL_VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
Detected 8 CPU cores. Enabled multithreaded rendering.
TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".

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

PyMOL>



all
centered 1/
ASHLC

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
6 Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sale Orig Clip MovZ
SnglClik +/- Cent Menu
DblClik Menu - PkAt
Selecting Residues
State 1/ 1



OpenGL graphics engine:
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 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry information.
 CmdLoad: "" loaded as "centered".

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

PyMOL>



all centered Action:
 zoom orient center origin
 drag matrix reset matrix
 drag coordinates clean
 preset find align generate
 assign sec. struc.
 rename object copy to object group
 delete object hydrogens remove waters
 state masking sequence movement compute

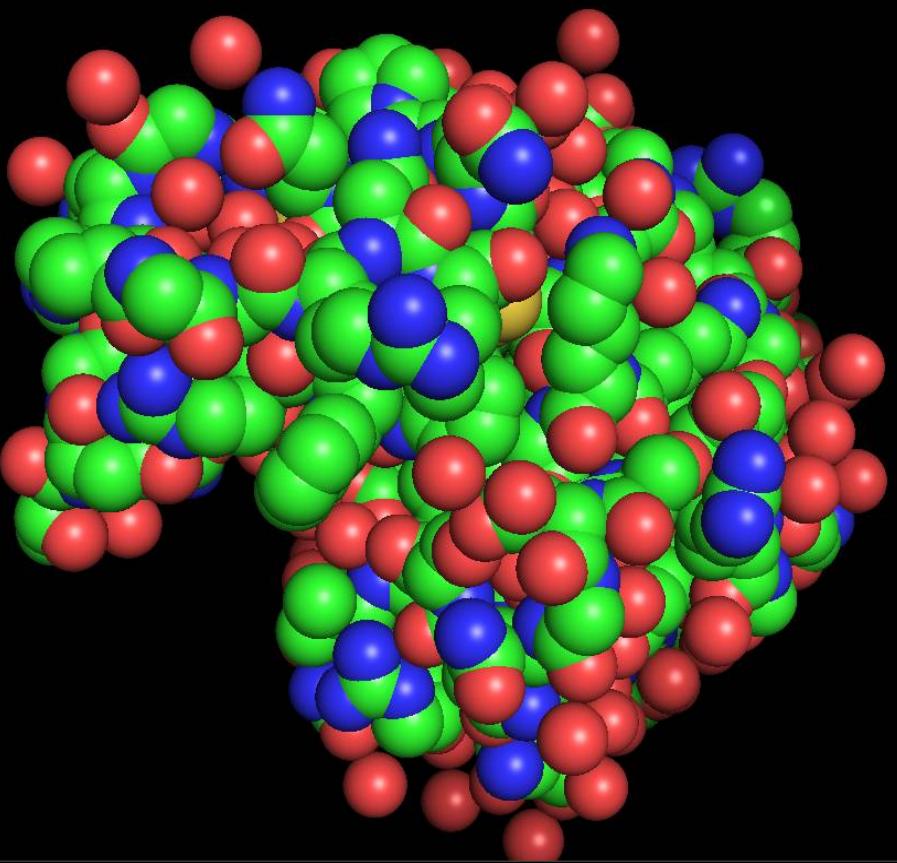
Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MovZ
 CtSh Sel Orig Clip MovZ
 SinglClik +/- Cent Menu
 DblClik Menu - PkAt
 Selecting Residues
 State 1/ 1

PyMOL>

GL_VENDOR: Intel
 GL_RENDERER: Mesa Intel(R) Xe Graphics (TGL GT2)
 GL_VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
 Detected 8 CPU cores. Enabled multithreaded rendering.
 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry information.
 CmdLoad: "" loaded as "centered".
 Dragging whole object "centered".

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

PyMOL>



all
 centered 1/1
 Show:
 as
 wire
 lines
 nonbonded
 licorice
 sticks
 nb_spheres
 ribbon
 cartoon
 label
 cell
 dots
 spheres
 mesh
 surface
 flag ignore
 organic
 main chain
 side chain
 disulfides
 valence

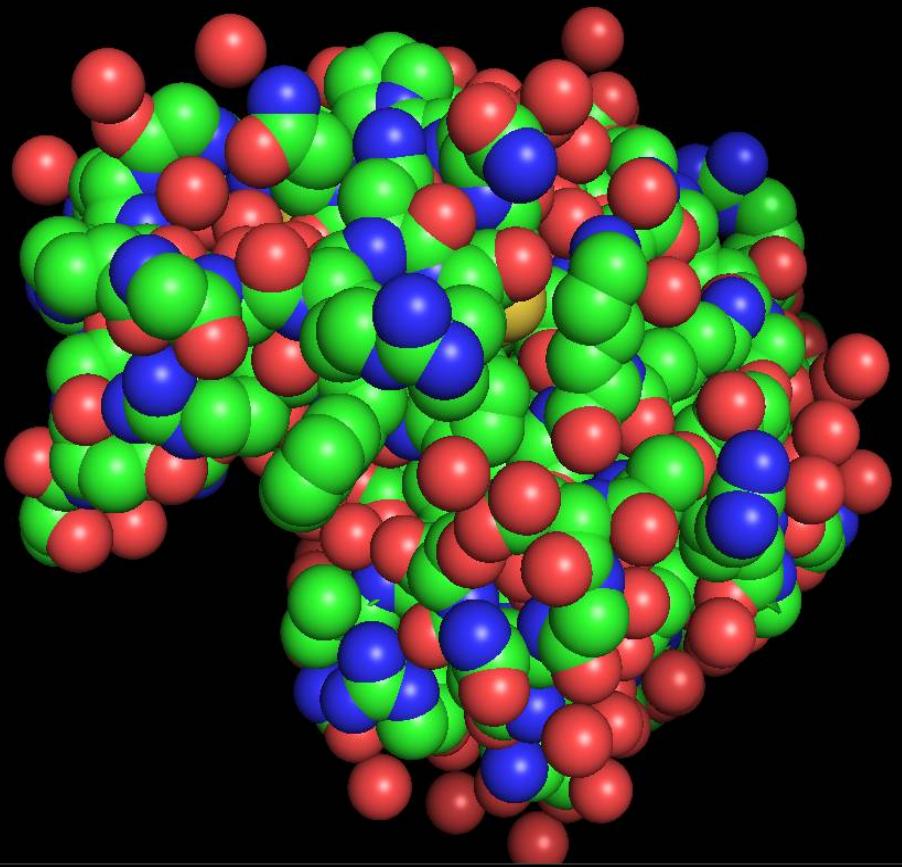
Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MovZ
 CtSh Sel Obj Clip MovZ
 SingleClick +/- Cent Menu
 DoubleClick Cent
 Selecting Residues
 State 1/ 1



```
COMPND 1 MOL_ID: 1;
COMPND 2 MOLECULE: LYSOZYME C;
COMPND 3 CHAIN: A;
COMPND 4 SYNONYM: 1,4-BETA-N-ACETYLMURAMIDASE C, ALLERGEN GAL D 4, GAL D IV;
COMPND 5 EC: 3.2.1.17
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "loaded as \"2YB\"".
```

A horizontal toolbar with the following buttons from left to right: Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rock, Get View, Stop, Play, >, MClear, Builder, Properties, and Rebuild.

PyMOL>



ASHLC
/ Hide:
everything
wire
lines
nonbonded
licorice
sticks
nb_spheres
ribbon
cartoon
label
cell
dots
spheres
mesh
surface
flag ignore
main chain
side chain
waters
hydrogens
unselected
valence

```

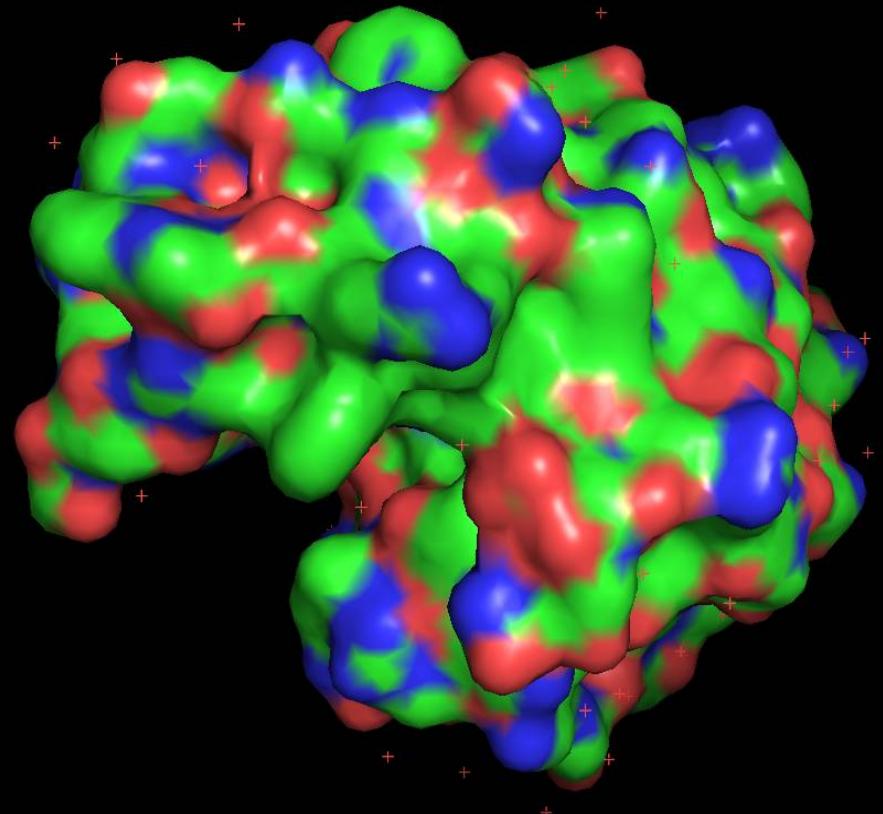
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSz
CtSh Sel Dirg Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1

```

GL_VENDOR: Intel
GL_RENDERER: Mesa Intel(R) Xe Graphics (TGL GT2)
GL_VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
Detected 8 CPU cores. Enabled multithreaded rendering.
TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".
Dragging whole object "centered".

Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
< < Stop Play > > I MClear
Builder Properties Rebuild

PyMOL>



all centered 1/1 Show:
as
wire
lines
nonbonded
licorice
sticks
nb_spheres
ribbon
cartoon
label
cell
dots
spheres
mesh
surface
flag ignore
organic
main chain
side chain
disulfides
valence

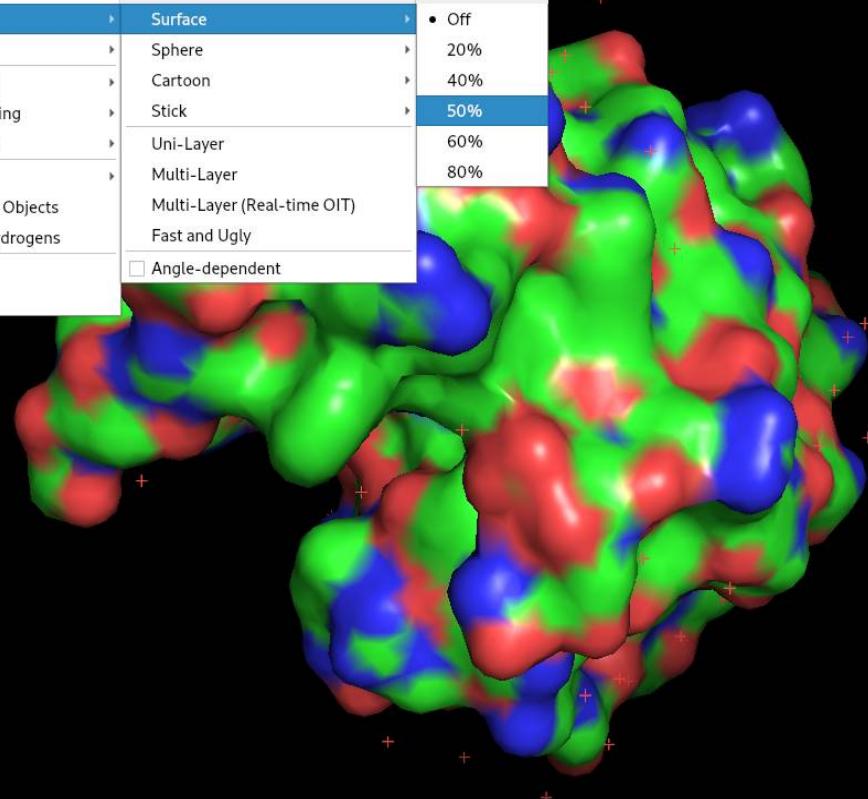
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Orig Clip MovZ
SnglClik +/- Cent Menu
DblClik Menu C PkAt
Selecting Residues
State 1/ 1

PyMOL>

GL_VENDOR: Intel
 GL_RENDERER: Mesa Intel(R) Xe Graphics
 GL_VERSION: 4.6 (Compatibility Profile)
 Detected 8 CPU cores. Enabled multi-threading.
 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry
 CmdLoad: "" loaded as "centered".
 Dragging whole object "centered".

PyMOL>

- [Edit All...](#)
- [Keyboard Shortcuts...](#)
- [Colors...](#)
- [Label](#)
- [Lines & Sticks](#)
- [Cartoon](#)
- [Ribbon](#)
- [Surface](#)
- [Volume](#)
- [Transparency](#) >
 - [Surface](#) >
 - Off
 - Sphere 20%
 - Cartoon 40%
 - Stick 50%
 - Uni-Layer 60%
 - Multi-Layer 80%
 - Multi-Layer (Real-time OIT)
 - Fast and Ugly
 - Angle-dependent
- [Rendering](#)
- [PDB File Loading](#)
- [mmcIF File Loading](#)
- [Map File Loading](#)
- [Auto-Show ...](#)
- Auto-Zoom New Objects
- Auto-Remove Hydrogens
- Show Text (Esc)
- Overlay Text

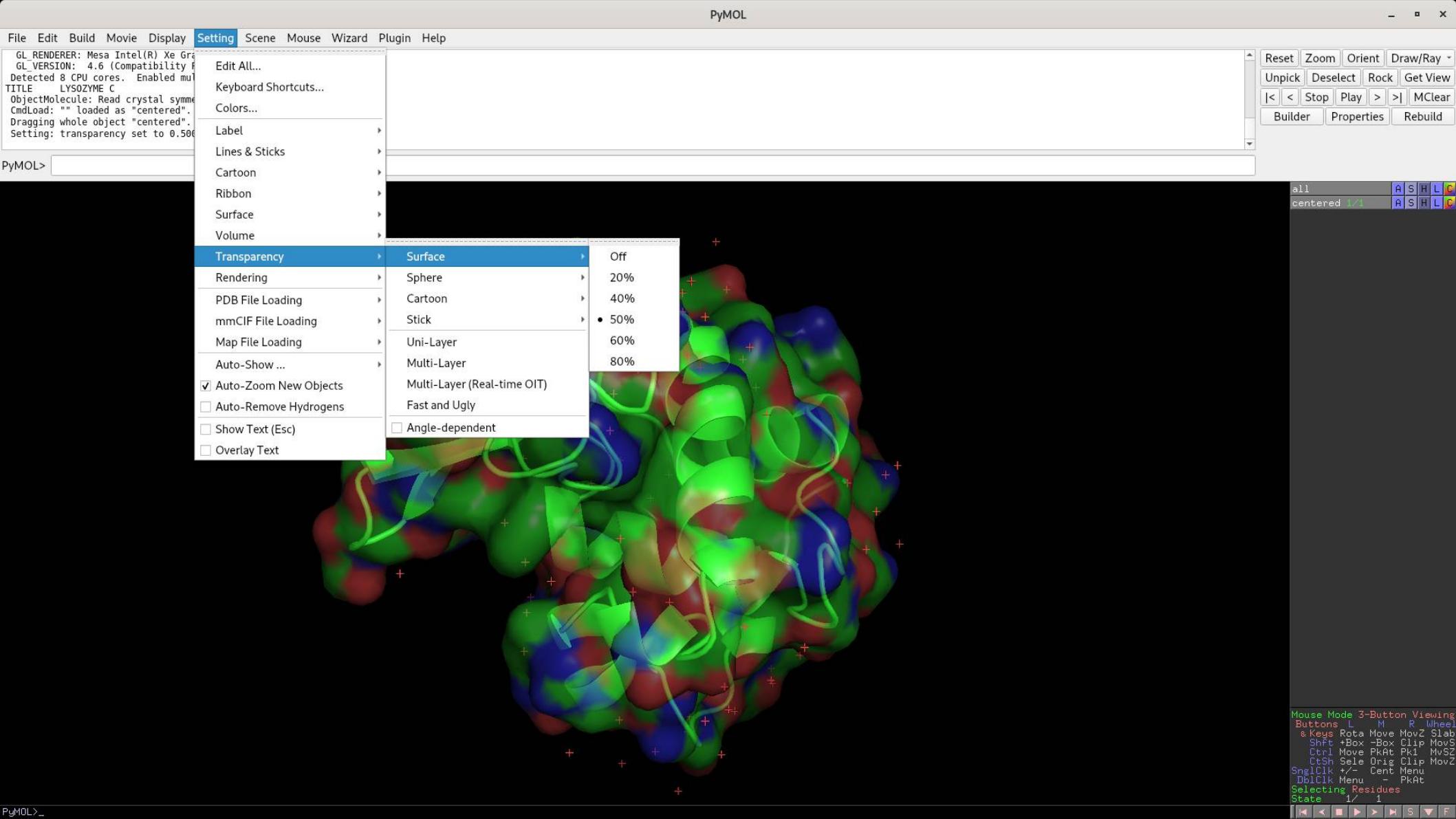


Reset	Zoom	Orient	Draw/Ray
Unpick	Deselect	Rock	Get View
<	<	Stop	Play >
>	>	MClear	
Builder		Properties	
		Rebuild	

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

Mouse Mode: 3-Button Viewing
 Buttons: L M R Wheel
 Keys: Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MovZ
 CtSh Sel Orig Clip MovZ
 SnglClick +/- Cent Menu
 DblClick Menu C PkAt
 Selecting Residues
 State 1/ 1

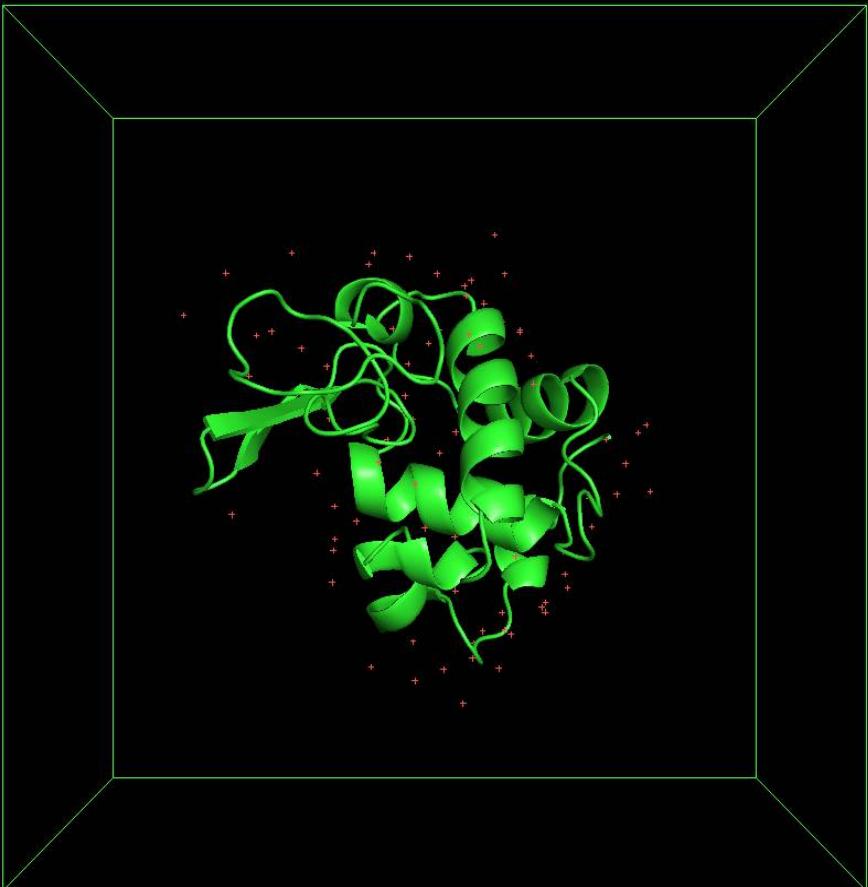
PyMOL>



TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".
Dragging whole object "centered".
Setting: transparency set to 0.50000.
Spectrum: range (15.29000 to 61.04000).
Executive: Colored 1082 atoms and 1 object.
Spectrum: range (17.45000 to 41.11000).

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

PyMOL>



all
centered 1/1
Show:
as
wire
lines
nonbonded
licorice
sticks
nb_spheres
ribbon
cartoon
label
cell
dots
spheres
mesh
surface
flag ignore
organic
main chain
side chain
disulfides
valence

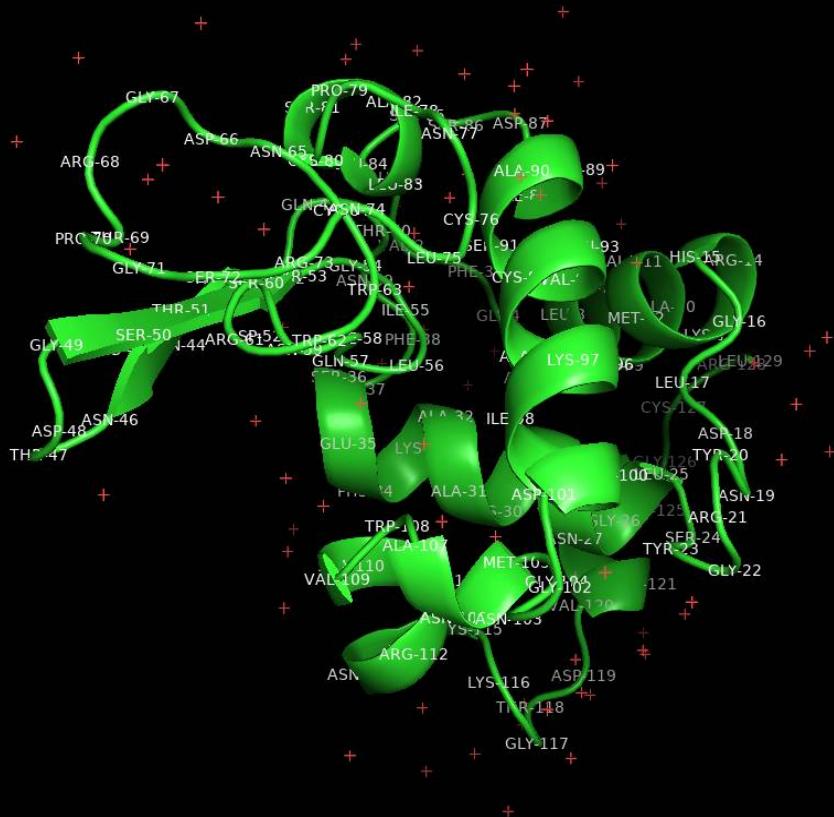
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Selz Selg Clip MovZ
SingleClick +/- Cent PkAt
DoubleClick Menu
Selecting Residues
State 1/ 1

R < > S ▽ F

GL RENDERER: Mesa Intel(R) Xe Graphics (TGL GT2)
 GL VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
 Detected 8 CPU cores. Enabled multithreaded rendering.
 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry information.
 CmdLoad: "" loaded as "centered".
 Dragging whole object "centered".
 Setting: transparency set to 0.50000.

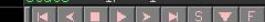
Reset Zoom Orient Draw/Ray
 Unpick Deselect Rock Get View
 |< < Stop Play > >| MClear
 Builder Properties Rebuild

PyMOL>



all A S H L C
 center Label:
 clear
 residues
 residues (oneletter)
 chains
 segments
 atom name
 element symbol
 residue name
 one letter code
 residue identifier
 chain identifier
 segment identifier
 b-factor
 occupancy
 vdw radius
 other properties
 atom identifiers

Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl Move PkAt PK1 MovZ
 CtSh Del Obj Clip MovZ
 SingleClick +/- Cent Menu
 DoubleClick Menu - PKAt
 Selecting Residues
 State 1 / 1



GL VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
Detected 8 CPU cores. Enabled multithreaded rendering.
TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".
Dragging whole object "centered".
Setting: transparency set to 0.50000.
Spectrum: range (15.29000 to 61.04000).

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

PyMOL>



all
centered 1/1
Color:
by element
Helix Sheet Loop
by ss
by rep
spectra
auto
reds
greens
blues
magentas
cyans
oranges
tints
grays

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
&Keys Rota Move MovZ Slab
Shift +Box -Box Clip MvsS
Ctrl Move PkAt Pk1 MvsZ
CtSh Sel Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Residues
State 1/ 1



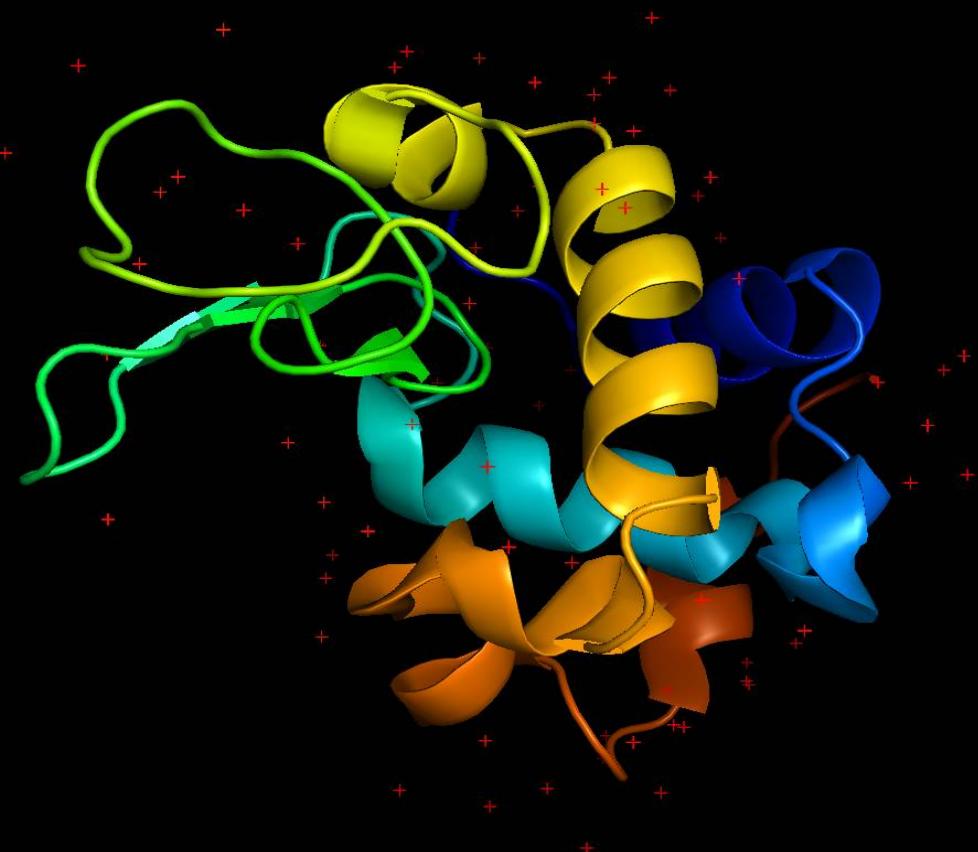
```

COMPND  MOL_ID: 1;
COMPND  2 MOLECULE: LYSOZYME C;
COMPND  3 CHAIN: A;
COMPND  4 SYNONYM: 1,4-BETA-N-ACETYLGLUCOSAMINIDASE C, ALLERGEN GAL D 4, GAL D IV;
COMPND  5 EC: 3.2.1.17
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "2YVB".

```

Reset Zoom Orient Draw/Ray
 Unpick Deselect Rock Get View
 < < Stop Play > > I MClear
 Builder Properties Rebuild

PyMOL>



	A	S	H	L	C
all					
2YVB 1/1					
Color:					
by element					
by chain					
by ss					
by rep					
Spectrum:					
rainbow (elem C)					
rainbow (*-/CA)					
rainbow					
b-factors					
b-factors(*-/CA)					
area (molecular)					
area (solvent)					
spectrum					
auto					
reds					
greens					
blues					
yellow					
magentas					
cilians					
oranges					
tints					
grays					

Mouse Mode 3-Button Viewing
 Buttons R Wheel
 & Keys Rota Move Mod Z Slab
 L Box -Box Clip Mod S
 Ctrl Move PkAt Pk1 MvZ
 Ctrh Sele Orig Clip Mod Z
 DblClick +/- Cent Menu
 DblClick - PkAt
 Selecting Residues
 State 1 / 1

TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".
Dragging whole object "centered".
Setting: transparency set to 0.50000.
Spectrum: range (15.29000 to 61.04000).
Executive: Colored 1082 atoms and 1 object.
Spectrum: range (17.45000 to 41.11000).

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

PyMOL>



all
centered 1/1
Color:
by element
by chain
by ss
by rep
Spectrum:
rainbow (elem C)
rainbow (*/CA)
rainbow
b-factors
b-factors (*/CA)
area (molecular)
area (solvent)
reds
greens
blues
yellows
magentas
cyans
oranges
tints
grays

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip Pk1 MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>

Detected 8 CPU cores. Enabled multithreaded rendering.
 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry information.
 CmdLoad: "" loaded as "centered".
 Dragging whole object "centered".
 Setting: transparency set to 0.50000.
 Spectrum: range (15.29000 to 61.04000).
 Executive: Colored 1082 atoms and 1 object.

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

PyMOL>



all
 centered 1/1
 Color:
 by element
 by chain
 by ss
 by rep
 spectrum
 Reds
 red
 tv_red
 raspberry
 darksalmon
 salmon
 deepsalmon
 warmpink
 Firebrick
 ruby
 chocolate
 brown
 auto
 reds
 greens
 blues
 yellows
 magentas
 cyans
 oranges
 tints
 grays

Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shift +Box -Box Clip MvsS
 Ctrl Move PkAt Pk1 MvsZ
 CtSh Sel Obj Clip MovZ
 SingleClick +/- Cent Menu
 DoubleClick Menu
 Selecting Residues
 State 1/ 1



bg_rgb set to blue

SyntaxError: invalid syntax

PyMOL> set bg_rgb, blue

Setting: bg_rgb set to blue.

Setting: bg_rgb set to black.

PyMOL> select chain A and resid 20

Selector: selection "sele" defined with 12 atoms.

Reset	Zoom	Orient	Draw/Ray
Unpick	Deselect	Rock	Get View
<	<	Stop	Play >
>	>	MClear	
Builder	Properties	Rebuild	

PyMOL> select chain A and resid 20|



all	A	S	H	L	C	
centered	1/1	A	S	H	L	C
(sele)	A	S	H	L	C	

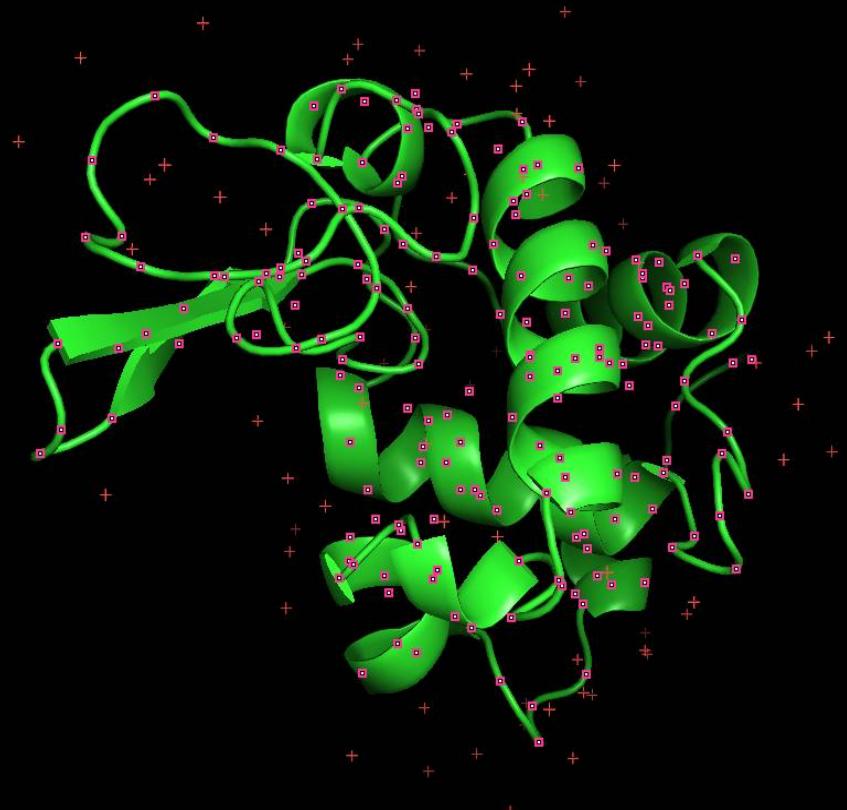
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Orig Clip MovZ
SinglClick +/- Cent Menu
DblClick Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>_

CmdLoad: "" loaded as "centered".
Dragging whole object "centered".
Setting: transparency set to 0.50000.
Spectrum: range (15.29000 to 61.04000).
Executive: Colored 1082 atoms and 1 object.
Spectrum: range (17.45000 to 41.11000).
PyMOL>select resn ALA or name CA
Selector: selection "sele" defined with 177 atoms.

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

PyMOL> select resn ALA or name CA



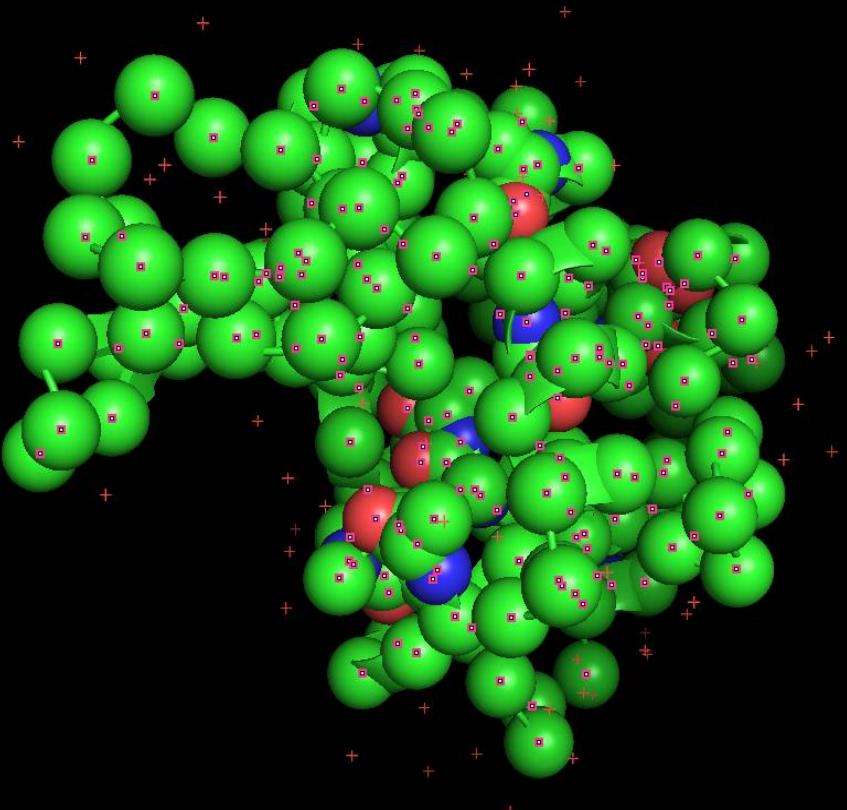
all	A	S	H	L	C	
centered	1/1	A	S	H	L	C
(sele)		A	S	H	L	C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Orig Clip MovZ
SinglClick +/- Cent Menu
DblClick Menu - PkAt
Selecting Residues
State 1/ 1

CmdLoad: "" loaded as "centered".
 Dragging whole object "centered".
 Setting: transparency set to 0.50000.
 Spectrum: range (15.29000 to 61.04000).
 Executive: Colored 1082 atoms and 1 object.
 Spectrum: range (17.45000 to 41.11000).
 PyMOL>select resn ALA or name CA
 Selector: selection "sele" defined with 177 atoms.

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

PyMOL>



all	A	S	H	L	C
centered 1/1	A	S	H	L	C
(sele)	Show:				

as
 wire
 lines
 nonbonded
 licorice
 sticks
 nb_spheres

ribbon
 cartoon

label
 cell

dots
 spheres

mesh
 surface

flag ignore

organic

main chain

side chain

disulfides

valence

Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shift +Box -Box Clip MvsS
 Ctrl Move PkAt Pk1 MvsZ
 CtSh Selz Orig Clip MovZ
 SnglClik +/- Ctr Menu
 DblClik Menu Ctr PkAt
 Selecting Residues
 State 1/ 1

PyMOL>

Spectrum: range (17.45000 to 41.11000).

PyMOL>select resn ALA or name CA

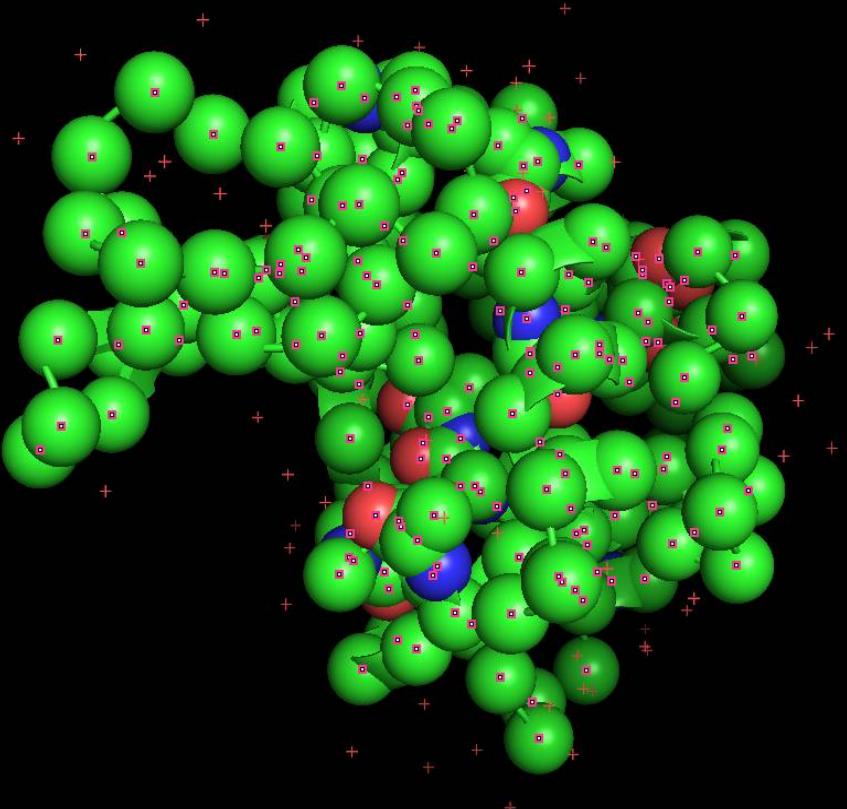
Selector: Selection "sele" defined with 177 atoms.

Incentive-Only-Error: "clean" is not available in Open-Source PyMOL

Please visit <http://pymol.org> if you are interested in the full featured "Incentive PyMOL" version.

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

PyMOL>



all A S H L C
centered 1/1 A S H L C
(sele) Action:
delete selection
rename selection
zoom
orient
center
origin
drag coordinates
clean
modify
preset
find
align
remove atoms
hydrogens
Copy To: duplicate
new copy to object
extract object
masking
movement
compute

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Selz Selg Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Residues
State 1/ 1

Spectrum: range (17.45000 to 41.11000).

PyMOL>select resn ALA or name CA

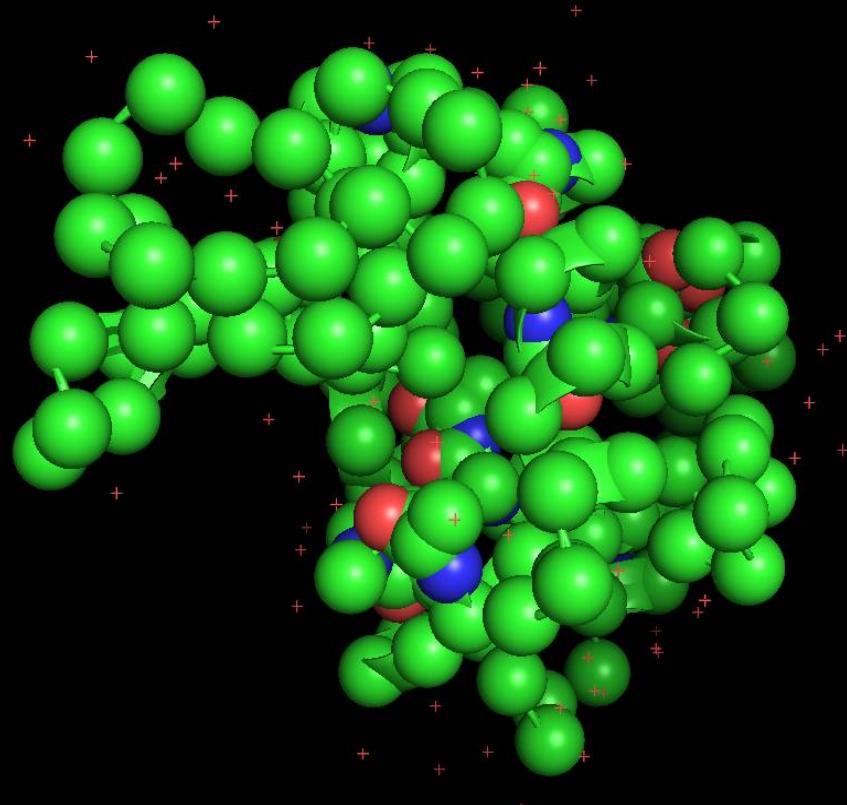
Selector: Selection "sele" defined with 177 atoms.

Incentive-Only-Error: "clean" is not available in Open-Source PyMOL

Please visit <http://pymol.org> if you are interested in the full featured "Incentive PyMOL" version.

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

PyMOL>



all A S H L C
centered 1/1 A S H L C
(sele) A S H L C
obj01 1/1 A S H L C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Obj Clip MovZ
SinglClik +/- Cent Menu
DblClik Menu
Selecting Residues
State 1/ 1

PyMOL>

PyMOL> select resn ALA or I
 Selector: selection "sel"

Incentive-Only-Error: "c"

Please visit <http://pymol.org/>

full featured "Incentive-Only-Error" mode.

Setting: bg_rgb set to white

PyMOL>

Stereo

Stereo Mode

Zoom

Clip

Background

Color Space

Quality

Grid

Orthoscopic View

Show Valences

Smooth Lines

Depth Cue (Fogging)

Two Sided Lighting

Specular Reflections

Animation

Roving Detail

External GUI

Sequence

Sequence Mode

Source PyMOL

in the

Internal GUI

Internal Prompt

Internal Feedback

Overlay

Stereo

Stereo Mode

Zoom

Clip

Background

Color Space

Quality

Grid

Orthoscopic View

Show Valences

Smooth Lines

Depth Cue (Fogging)

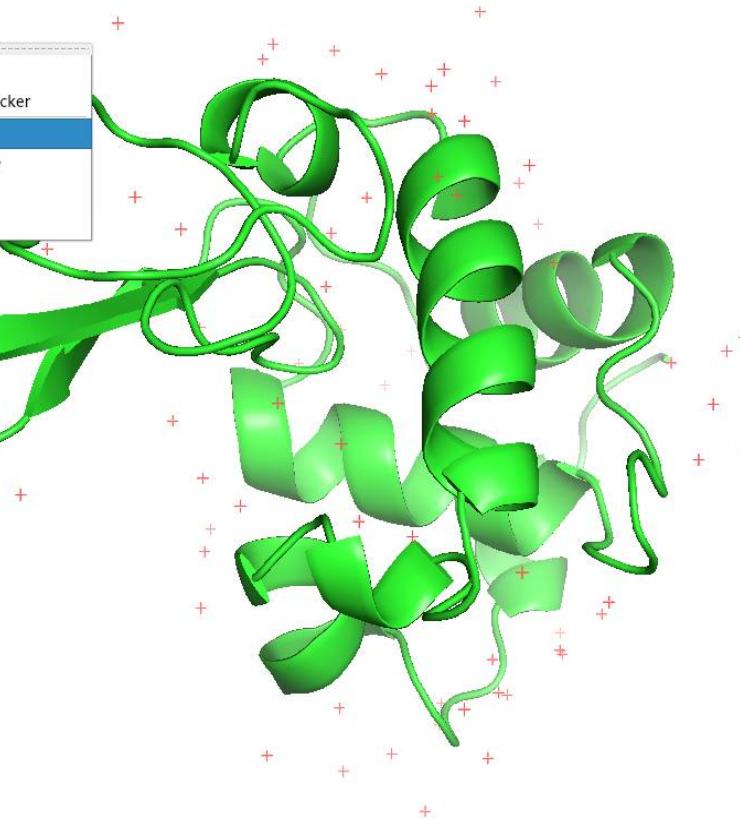
Two Sided Lighting

Specular Reflections

Animation

Roving Detail

External GUI



Opaque

Alpha Checker

• White

Light Grey

Grey

Black

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

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

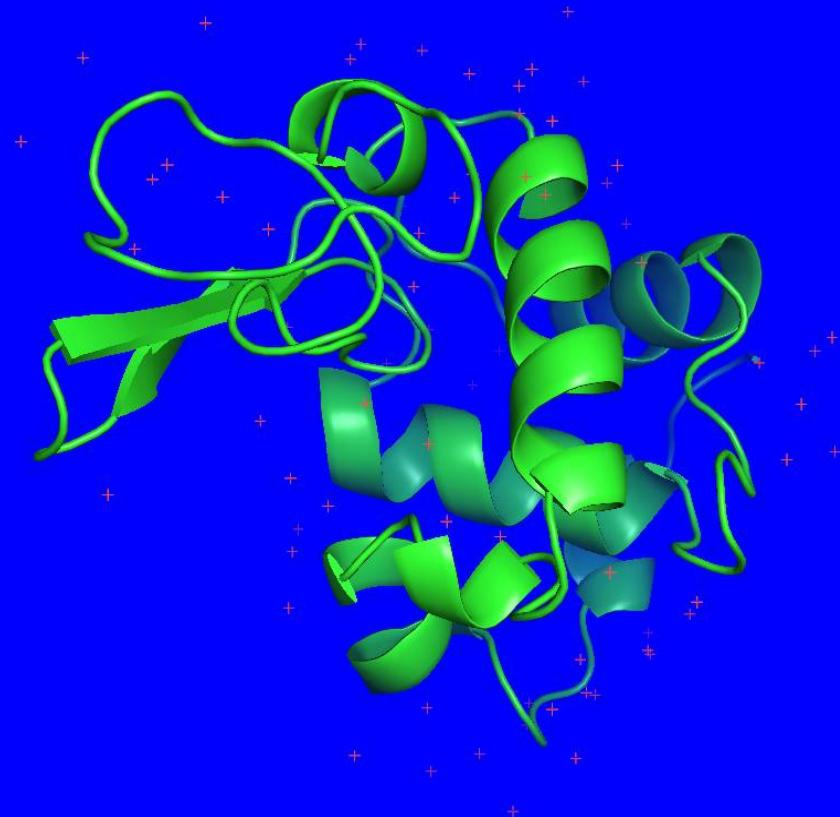
Mouse Mode: 3-Button Viewing
 Buttons: L M R Wheel
 & Keys: Rota Move MovZ Slab
 Shift +Box -Box Clip Move
 Ctrl Move PkAt Pk1 MvSz
 CtrSh Sel Orig Clip MovZ
 SinglClik +/- Cent Menu
 DblClik Menu
 Selecting Residues
 State 1/1

Setting: bg_rgb set to black.

PyMOL>bg_rgb set to blue
File "toplevel", line 1
bg_rgb
^SyntaxError: invalid syntax
PyMOL>set bg_rgb, blue
Setting: bg_rgb set to blue.

Reset	Zoom	Orient	Draw/Ray
Unpick	Deselect	Rock	Get View
<	<	Stop	Play >
>	>	MClear	
Builder	Properties	Rebuild	

PyMOL> set bg_rgb, blue|



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

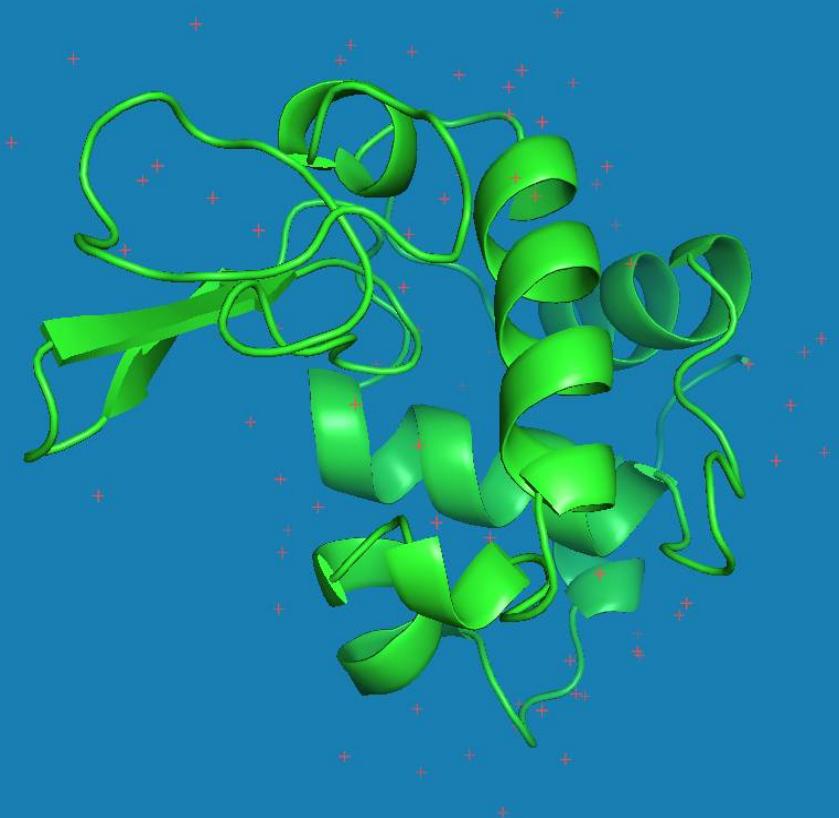
Mouse Mode: 3-Button Viewing
Buttons L M R Wheel
Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovS
CtSh Sel Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Residues
State 1/ 1

PyMOL>_

GL RENDERER: Mesa Intel(R) Xe Graphics (TGL GT2)
GL VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
Detected 8 CPU cores. Enabled multithreaded rendering.
TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".
PyMOL> set bg_rgb,[0.1,0.5,0.7]
Setting: bg_rgb set to 0x197fb2.

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

PyMOL> set bg_rgb,[0.1,0.5,0.7]

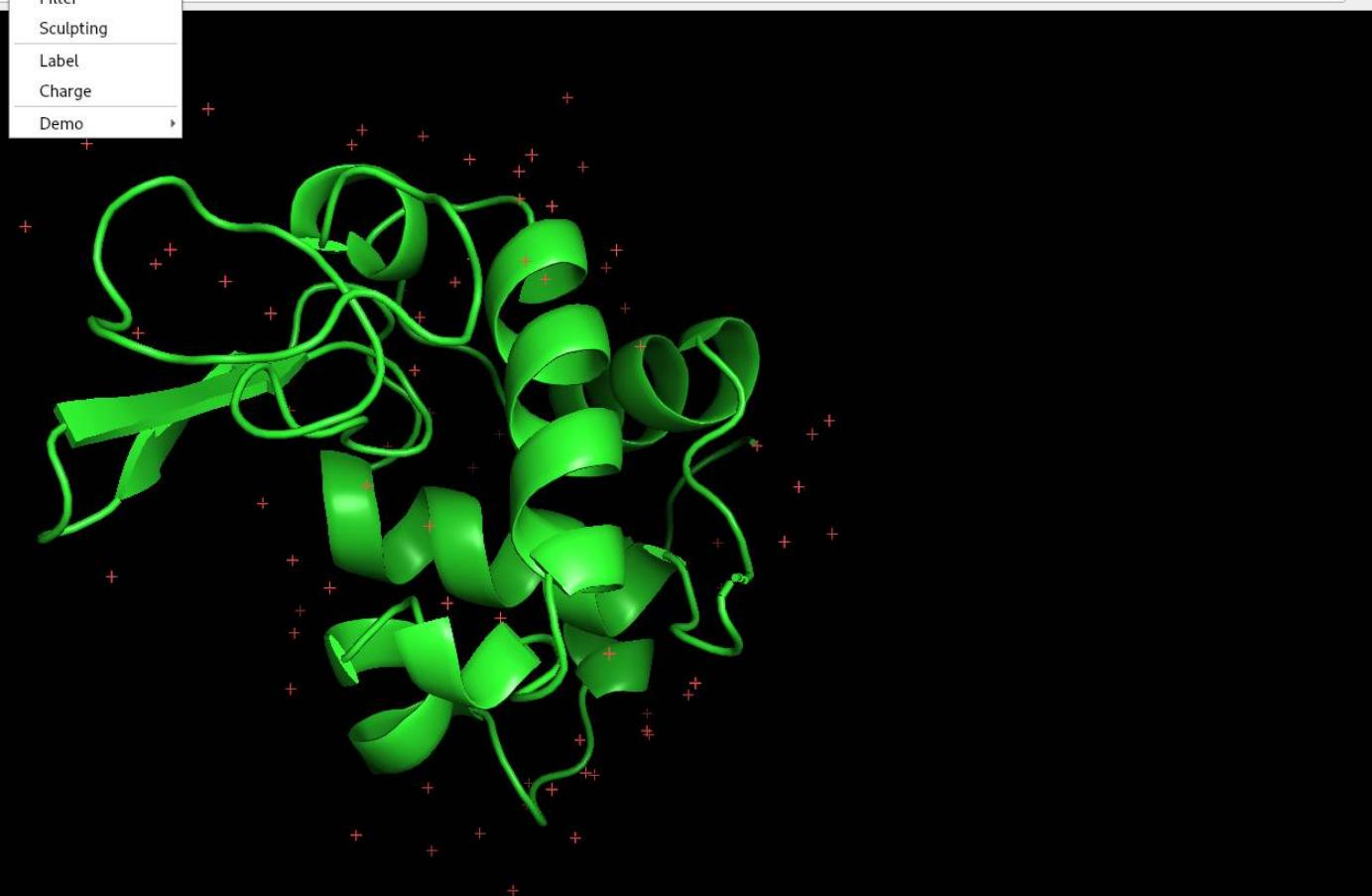
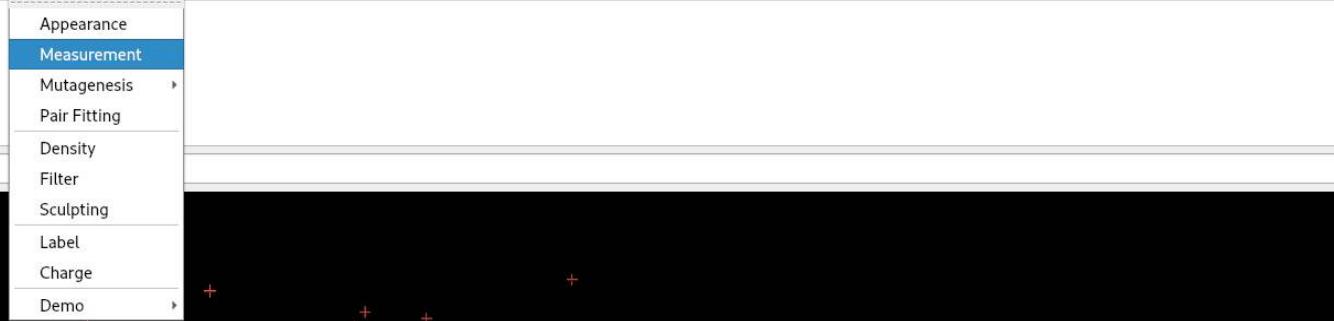


all A S H L C
centered 1/1 A S H L C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
&keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sale Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu PkAt
Selecting Residues
State 1/ 1

```
SyntaxError: invalid syntax
PyMOL>set bg_rgb, blue
  Setting: bg_rgb set to blue.
  Setting: bg_rg set to black.
PyMOL>select chain A and resid 20
  Selector: selection "sele" defined with 12 atoms.
PyMOL>wizard measurement
```

PyMOL>



```
Measurement
Distances
Create New Object
Delete Last Object
Delete All Measurements
Done

Mouse Mode 3-Button Viewing
Buttons L M R Whee
& Keys Rota Move MovZ Slal
Shft +Box -Box Clip MovX
Ctrl Move PkAt Prk MvS
Ctsh Sel Orig Clip MovY
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Atoms
State 1/ 1
```

```
SyntaxError: invalid syntax
PyMOL>set bg_rgb, blue
Setting: bg_rgb set to blue.
Setting: bg_rgb set to black.
PyMOL>select chain A and resid 20
Selector: selection "sele" defined with 12 atoms.
PyMOL>wizard measurement
```

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

PyMOL>

Please click on the first atom...



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

Measurement
Dis Measurement Mode
Cre Distances
Del Distances to Rings
Del Angles
Don Dihedrals
Mou Polar Neighbors
Bu Heavy Neighbors
N Neighbors
Polar Contacts
Lasso select using Lasso
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Atoms
State 1/ 1

Setting: bg_rgb set to blue.
Setting: bg_rgb set to black.
PyMOL>select chain A and resid 20
Selector: selection "sele" defined with 12 atoms.
PyMOL>wizard measurement
You clicked /centered//A/HOH'130/0
Selector: selection "sele" defined with 1 atoms.
You clicked /centered//A/HOH'204/0

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

PyMOL>

Please click on the first atom...



all A S H L C
measure01 A S H L C

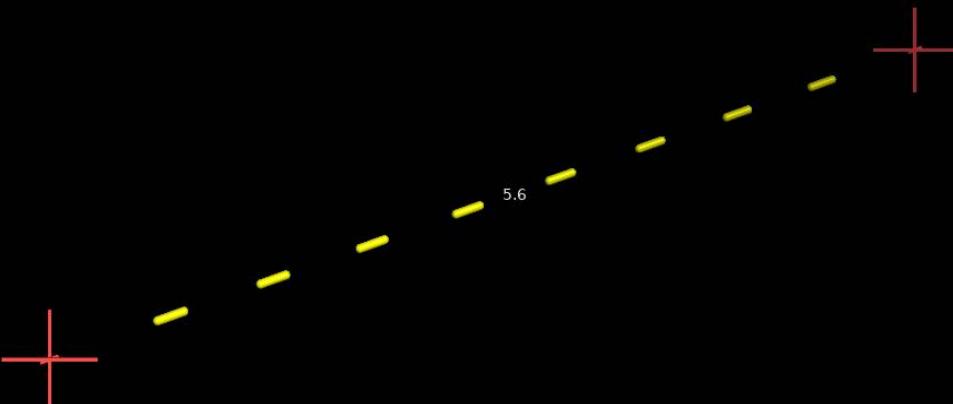
Measurement
Distances
Create New Object
Delete Last Object
Delete All Measurements
Done
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MwS
Ctrl Move PkAt Pk1 MwZ
CtSh Selc Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Atoms
State 1/ 1

Setting: bg_rgb set to blue.
 Setting: bg_rgb set to black.
 PyMOL>select chain A and resid 20
 Selector: selection "sele" defined with 12 atoms.
 PyMOL>wizard measurement
 You clicked /centered//A/HOH'130/0
 Selector: selection "sele" defined with 1 atoms.
 You clicked /centered//A/HOH'204/0

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

PyMOL>

Please click on the first atom...



all	A	S	H	L	C
centered 1/1	A	S	H	L	C
measure01	Action:				
	zoom				
	center				
	origin				
	drag				
	reset				
	rename				
	group				
	delete				

Measurement
 Distances
 Create New Object
 Delete Last Object
 Delete All Measurements
 Done

Mouse Mode: 3-Button Viewing
 Buttons L M R Wheel
 & Keys: Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MovZ
 CtrSh Selz Orig Clip MovZ
 SingleClick +/- Cent Menu
 DoubleClick Menu PkAt
 Selecting Atoms
 State 1/ 1

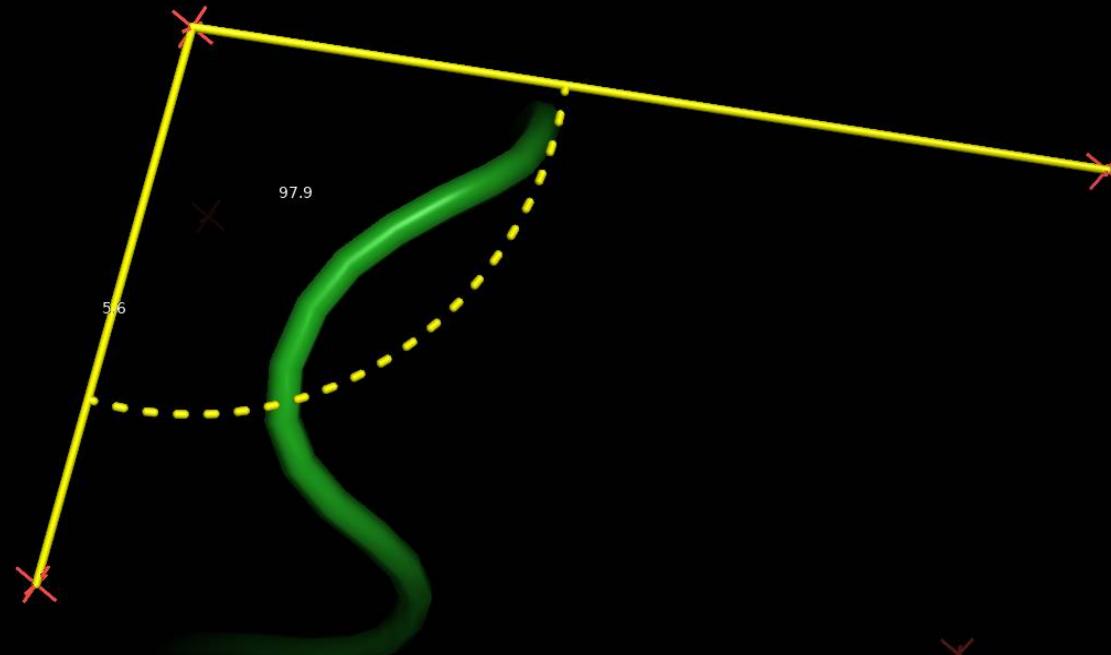
PyMOL>

```
PyMOL>wizard measurement
You clicked /centered//A/HOH`130/0
Selector: selection "sele" defined with 1 atoms.
You clicked /centered//A/HOH`204/0
You clicked /centered//A/HOH`166/0
Selector: selection "sele" defined with 1 atoms.
You clicked /centered//A/HOH`204/0
You clicked /centered//A/HOH`130/0
```

Reset	Zoom	Orient	Draw/Ray
Unpick	Deselect	Rock	Get View
<	<	Stop	Play >
<	<		>
MClear			
Builder	Properties	Rebuild	

PyMOL>

Please click on the first atom...



all	A	S	H	L	C
centered 1/1	A	S	H	L	C
measure01	A	S	H	L	C
measure02	A	S	H	L	C

Measurement
Angles
Create New Object
Delete Last Object
Delete All Measurements
Done
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Selz Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Atoms
State 1/ 1

PyMOL>

OpenGL graphics engine:
GL_VENDOR: Intel
GL_RENDERER: Mesa Intel(R) Xe Graphics (TGL GT2)
GL_VERSION: 4.6 (Compatibility Profile) Mesa 20.3.5
Detected 8 CPU cores. Enabled multithreaded rendering.
TITLE LYSOZYME C
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "centered".

PyMOL>

Reset Zoom Orient Draw/Ray

Width 1700px 28.79cm
Height 802px 13.58cm

Reset Lock aspect ratio

Units cm at 150 DPI
 transparent background ("Ray" only)

Draw (fast) - or - Ray (slow)

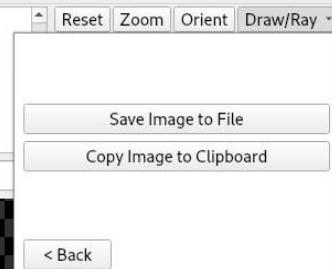


Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Obj Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Residues
State 1/ 1

PyMOL>

```
ObjectMolecule: Read crystal symmetry information.  
CmdLoad: "" loaded as "centered".  
PyMOL>ray 1700, 802, async=1  
Ray: render time: 0.37 sec. = 9620.8 frames/hour (0.37 sec. accum.).  
You clicked /centered//A/ASN'74/CA  
Selector: selection "sele" defined with 8 atoms.  
PyMOL>ray 1700, 802, async=1  
Ray: render time: 0.37 sec. = 9814.0 frames/hour (0.74 sec. accum.).
```

PyMOL>



Mouse Mode: 3-Button Viewing
Buttons L M R Wheel
& Keys: Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Obj Clip MovZ
SnglClick +/- Cent Menu
DblClick Menu PkAt
Selecting Residues
State 1/ 1

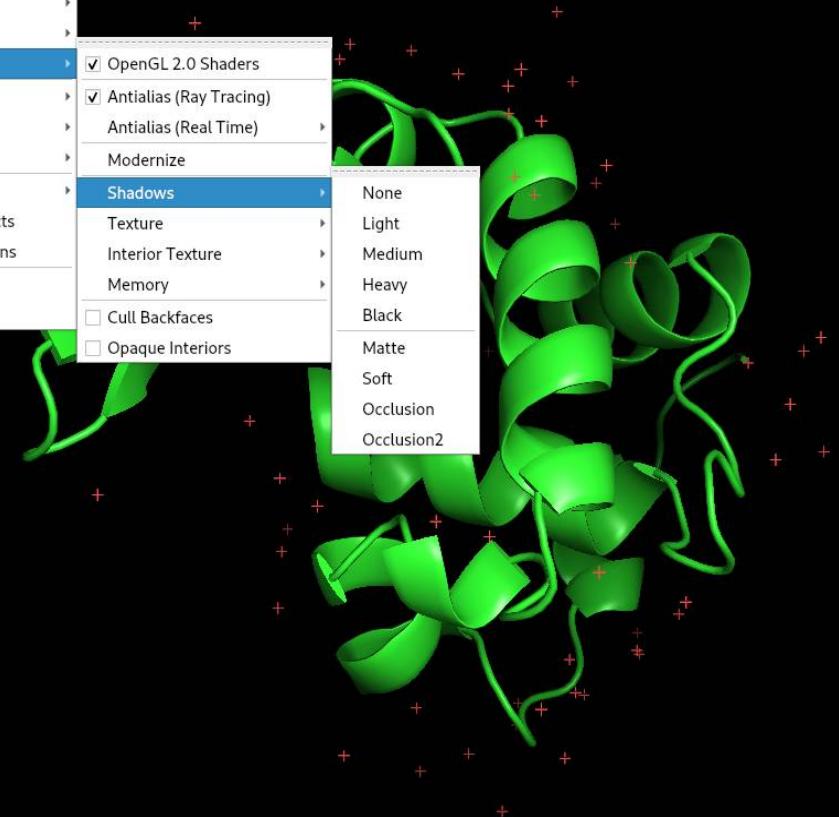
PyMOL>_

OpenGL graphics engine:
 GL_VENDOR: Intel
 GL_RENDERER: Mesa Intel(R) Xe Graphics
 GL_VERSION: 4.6 (Compatibility Profile)
 Detected 8 CPU cores. Enabled multi-threading.
 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry
 CmdLoad: "" loaded as "centered".

PyMOL>

Setting menu open, showing:

- OpenGL 2.0 Shaders (checked)
- Antialias (Ray Tracing) (checked)
- Antialias (Real Time)
- Modernize
- Shadows** (selected)
 - None
 - Light
 - Medium
 - Heavy
 - Black
 - Matte
 - Soft
 - Occlusion
 - Occlusion2
- Cull Backfaces
- Opaque Interiors



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

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

Mouse Mode: 3-Button Viewing
 Buttons: L M R Wheel
 & Keys: Rota Move MovZ Slab
 Shift +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MovZ
 CtSh Sel Orig Clip MovZ
 SnglClick +/- Cent Menu
 DblClick Menu C PkAt
 Selecting Residues
 State 1/ 1

PyMOL>

```
Setting: spec_count set to -1.  
Setting: shininess set to 90.00000.  
Setting: power set to 1.00000.  
Setting: specular_intensity set to 0.50000.  
Setting: spec_direct set to 0.00000.  
Setting: ray_shadow_decay_factor set to 0.00000.  
PyMOL>ray 1700, 802, async=1  
Ray: render time: 0.39 sec. = 9176.3 frames/hour (0.39 sec. accum.).
```

PyMOL>



Reset Zoom Orient Draw/Ray

Width 1700px 28.79cm
Height 802px 13.58cm

Reset Lock aspect ratio

Units cm at 150 DPI

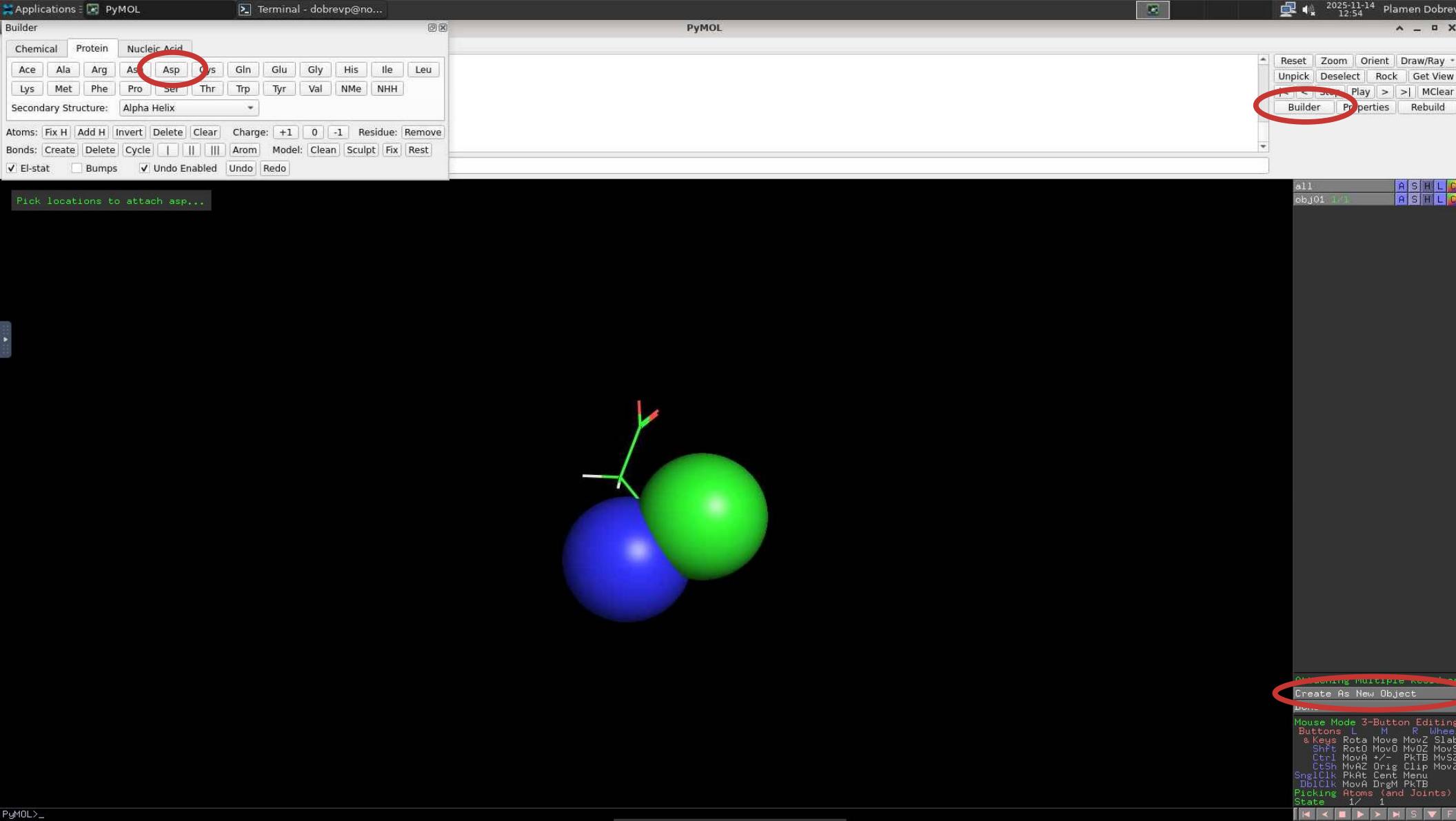
transparent background ("Ray" only)

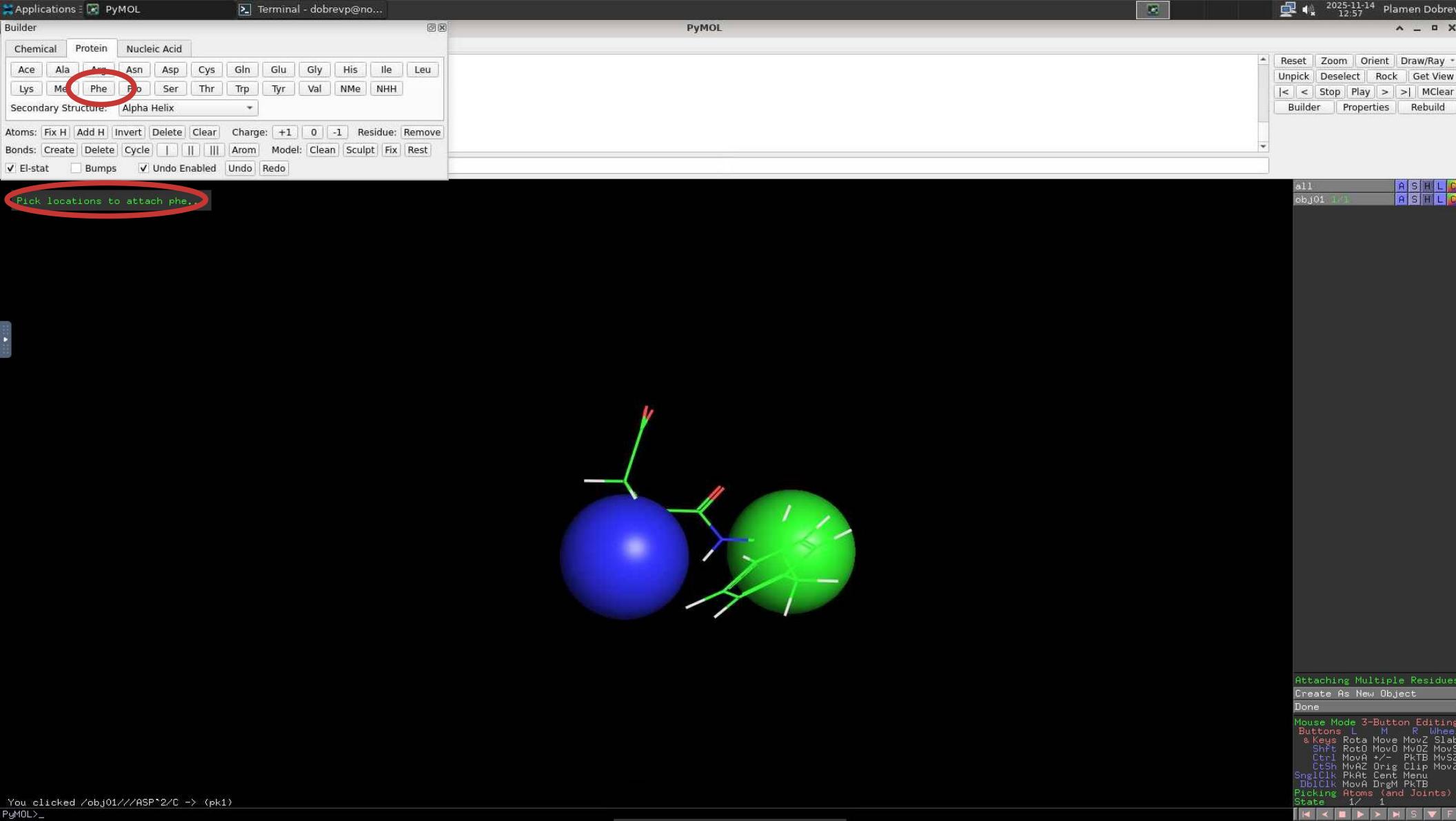
Draw (fast) - or - Ray (slow)

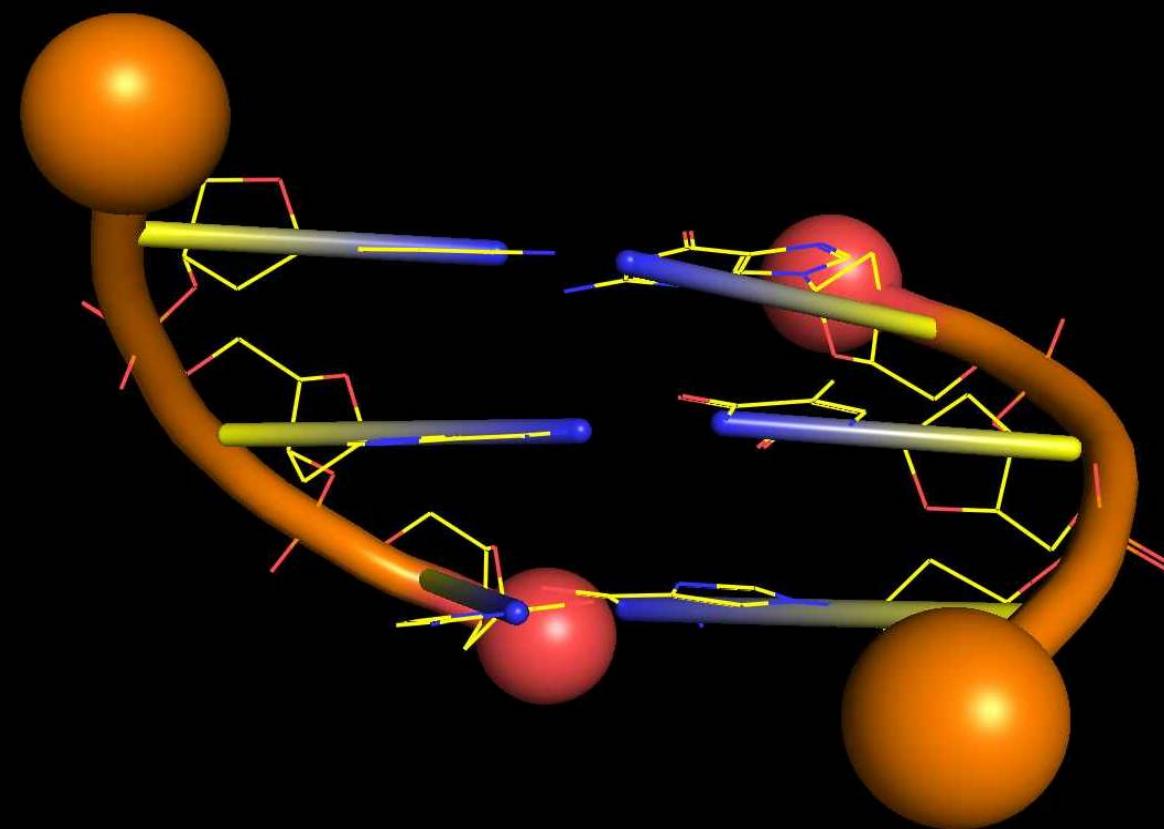
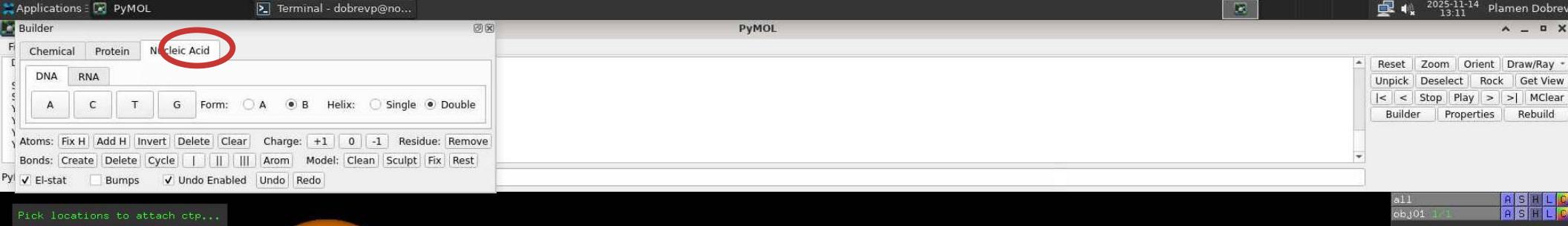
Use high-quality ray-tracing.
Supports optimal multi-layer transparency, shadows, and alpha-channel background.

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
&Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MovZ
CtSh Sel Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu
Selecting Residues
State 1/ 1

PyMOL>







Attaching Multiple Residues
Create As New Object
Done
Mouse Mode 3-Button Editing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift Rot0 Mov0 MovZ MovS
Ctrl MovA +/- PkTB MovZ
Lsh MovA Drig Clip MovZ
Single Click PkAt Cent Menu
Double Click MovA DrigM PkTB
Picking Atoms (and Joints)
State 1/1

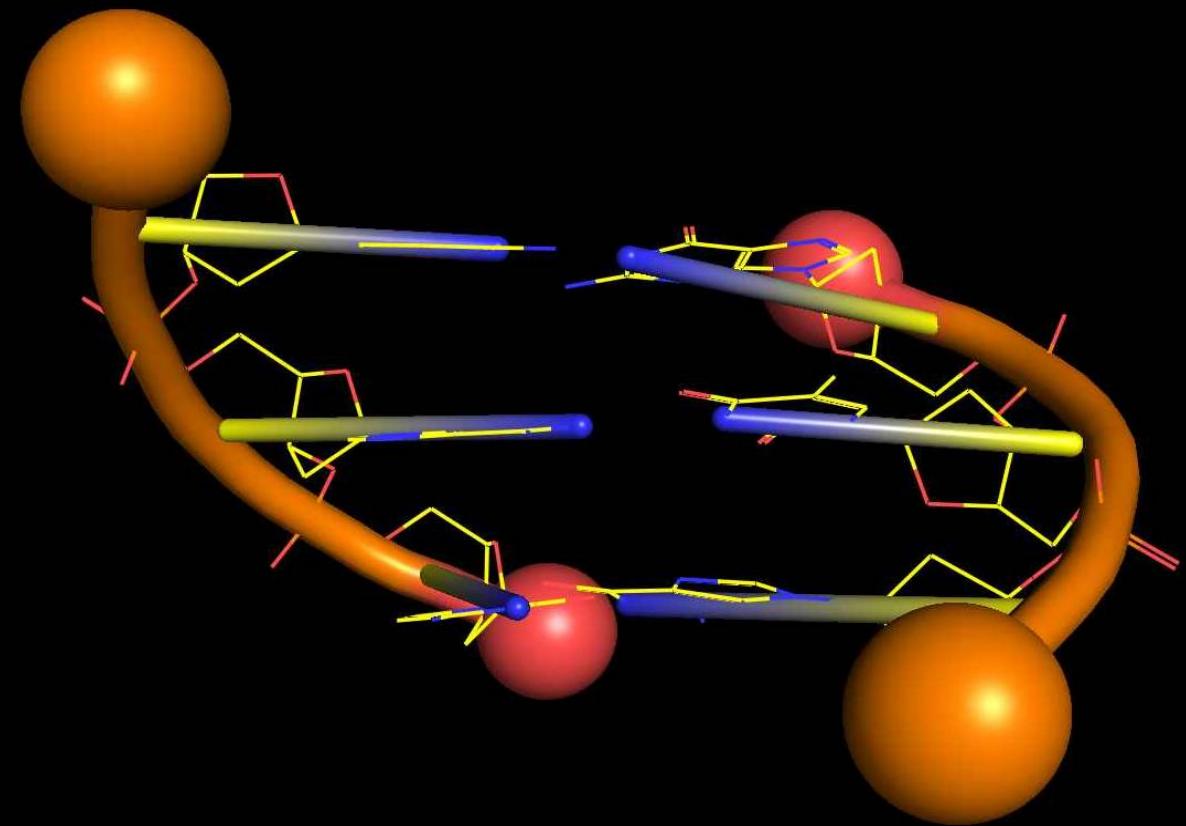
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

New PyMOL Window
Open...
Open Recent...
Get PDB...
Save Session
Save Session As...
Export Molecule...
Export Map...
Export Alignment...
Export Image As...
Export Movie As...
Log File
Run Script...
Working Directory
Edit pymolrc
Reinitialize
Quit

abled multithreaded rendering.
to off.
ndo is not supported in Open-Source version of PyMOL
> /N -> (pk1)
> /C -> (pk1)
> -1/P -> (pk1)
> 1/P -> (pk1)

Reset Zoom Orient Draw/Ray
Upick Deselect Rock Get View
< Stop Play > Mclear
Builder Properties Rebuild



all
obj01 1/1

A S H L C
A S H L C

Attaching Multiple Residues
Create As New Object
Done

Mouse Mode 3-Button Editing
Buttons L M R Wheel
6 Keys Rota Move MovZ Slab
Shft RotO MovO MovZ MovS
Ctrl MovA +/- PKTB MovZ
CTSH MovA Orig Clip MovZ
DblClick MovA DragM PKTB
SinglClick PKTB Cent Menu
Picking Atoms (and Joints)
State 1/ 1

