

Molecular Modelling Course

November 17. 2025 – 19. 2025 | Dr. Birkan Emrem, Dr. Ferdinand Jamitzky, Dr. Plamen Dobrev, Dr. Prasanth Ganta
Leibniz Supercomputing Centre

Visualizing biomolecular structures



- PyMOL
- VESTA
- VMD

PyMOL

PyMOL by Schrödinger

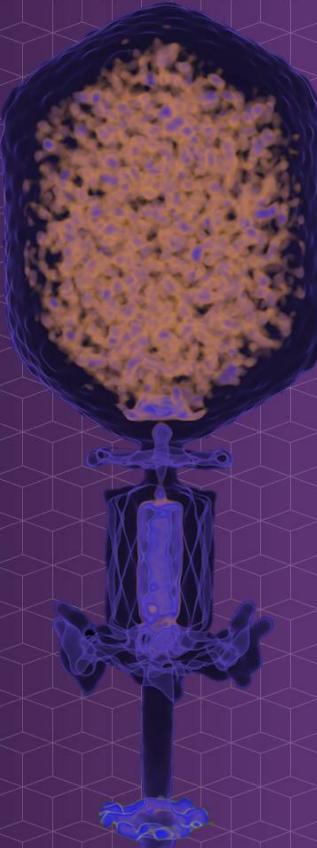
Introducing PyMOL 3.1

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

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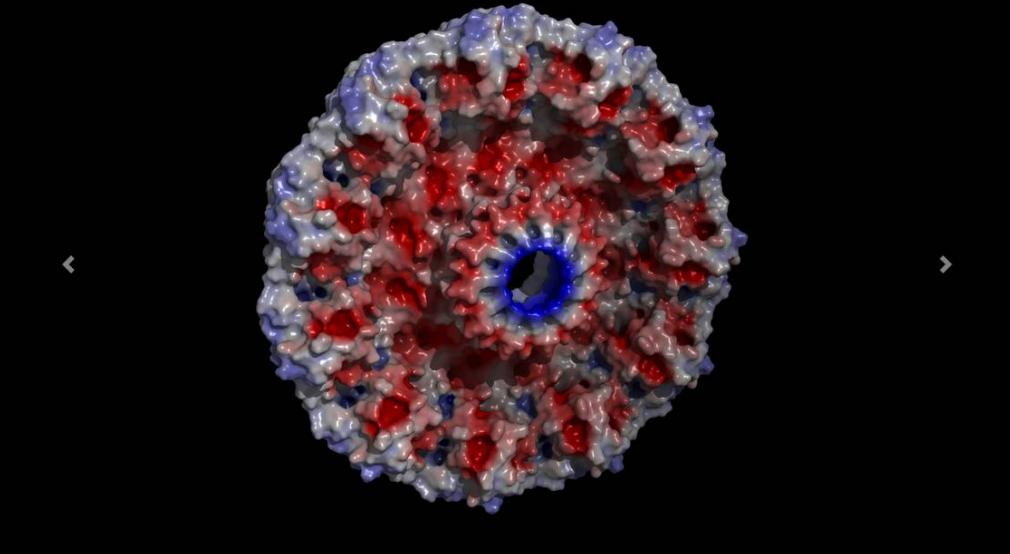
PYMOL 3 PRODUCT PAGE



PyMOL

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

PyMOL by Schrödinger DOWNLOAD SCREENSHOTS SUPPORT CONTACT

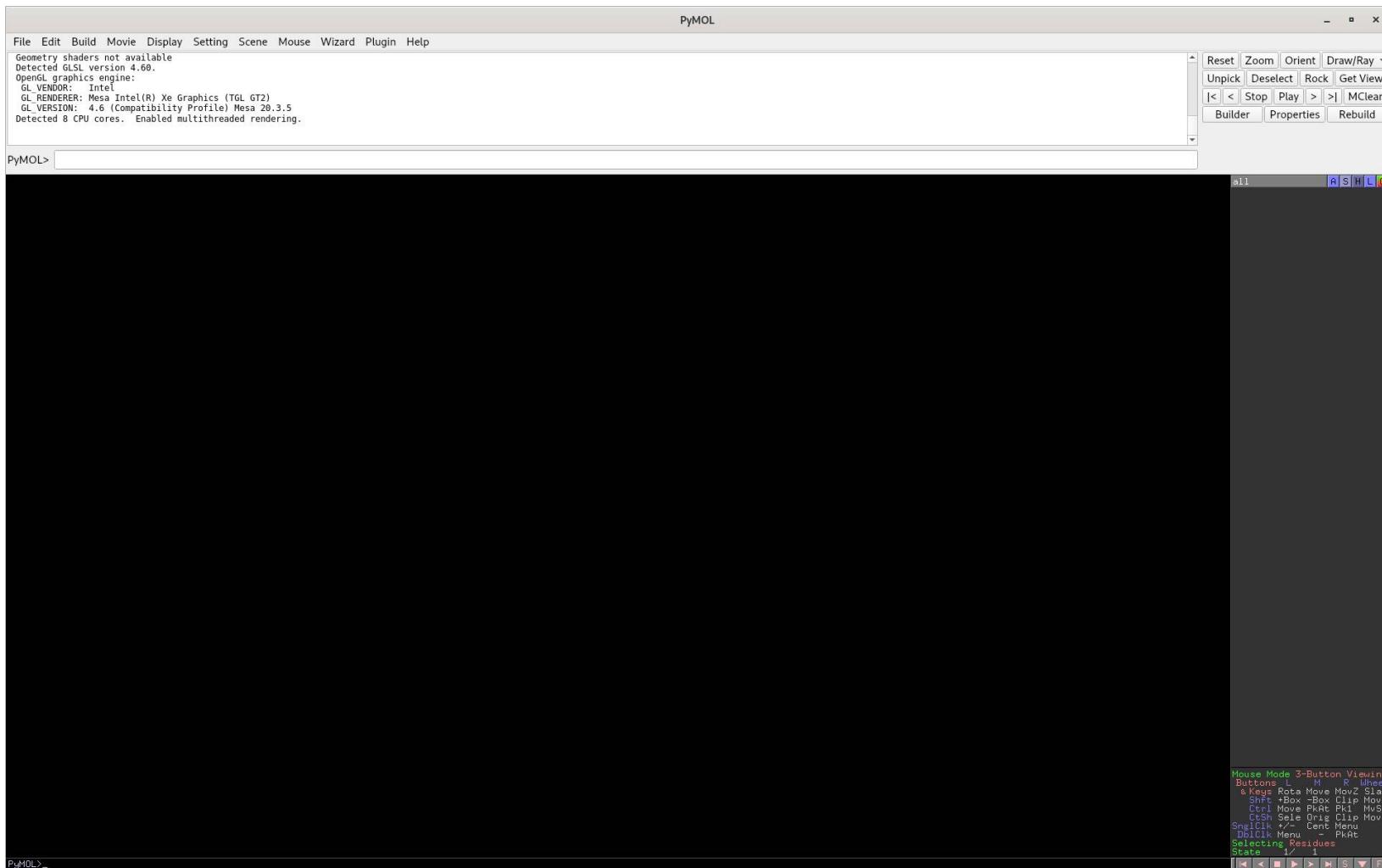


Open-Source Philosophy

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 MovS
Ctrl Move Pk1 MvS
(CtSh) Sel Orig Clip MovZ
Single Click +/- Cent Menu
DblClick Menu - PkAt
Selecting Residues
State 1/ 1
| < < > > S F

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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".

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

PyMOL>



all
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 Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1



PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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 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

all A S H L C
 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
 +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MvS2
 CtrSh Sele Orig Clip MovZ
 SnellClik +/- Cent Menu
 DblClik Menu - PkAt
 Selecting Residues
 State 1/ 1

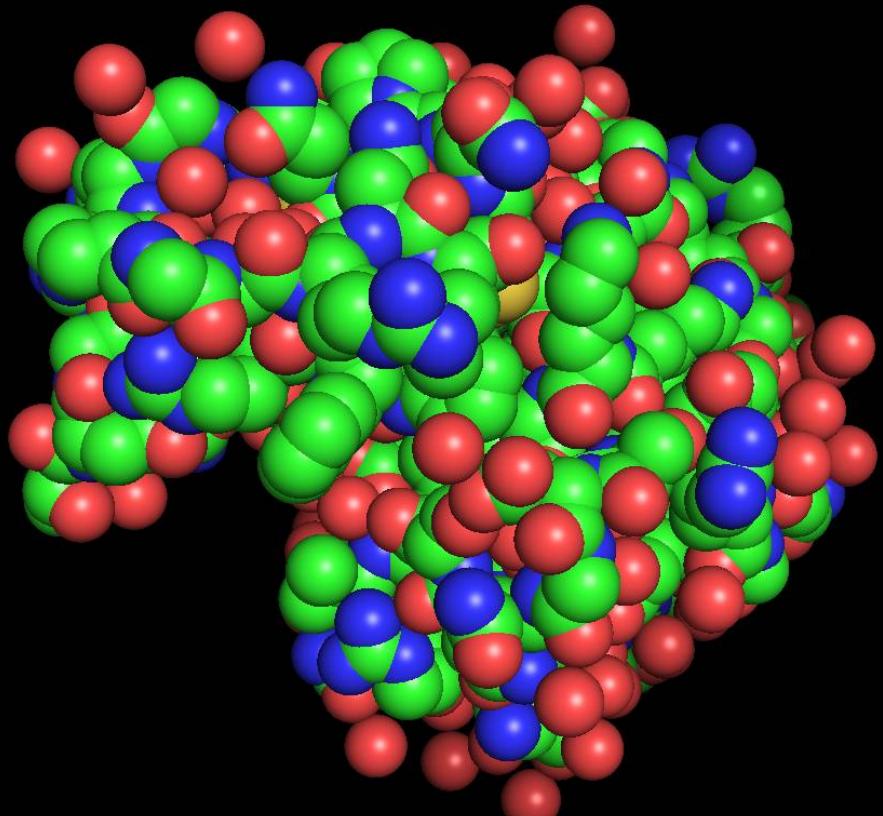


File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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/
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 MvSz
Ctrl Sh Sele Drag Clip MovZ
Single +/- Cent Menu
Double Click Menu - PkHt
Selecting Residues
State 1/ 1

|◀◀◀▶▶▶▶| S ▾ F

PyMOL>_

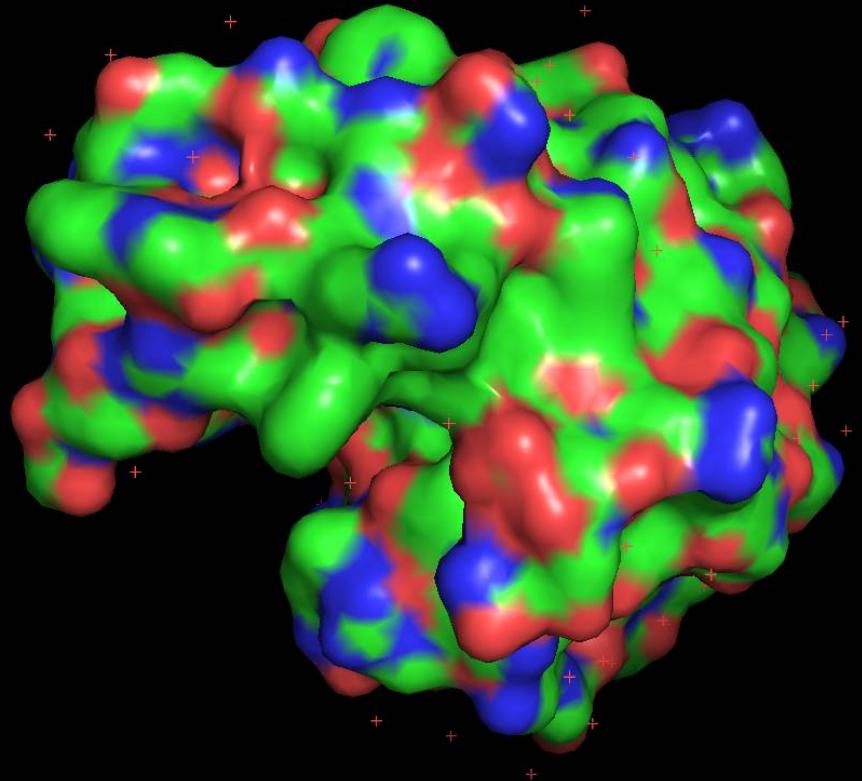
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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

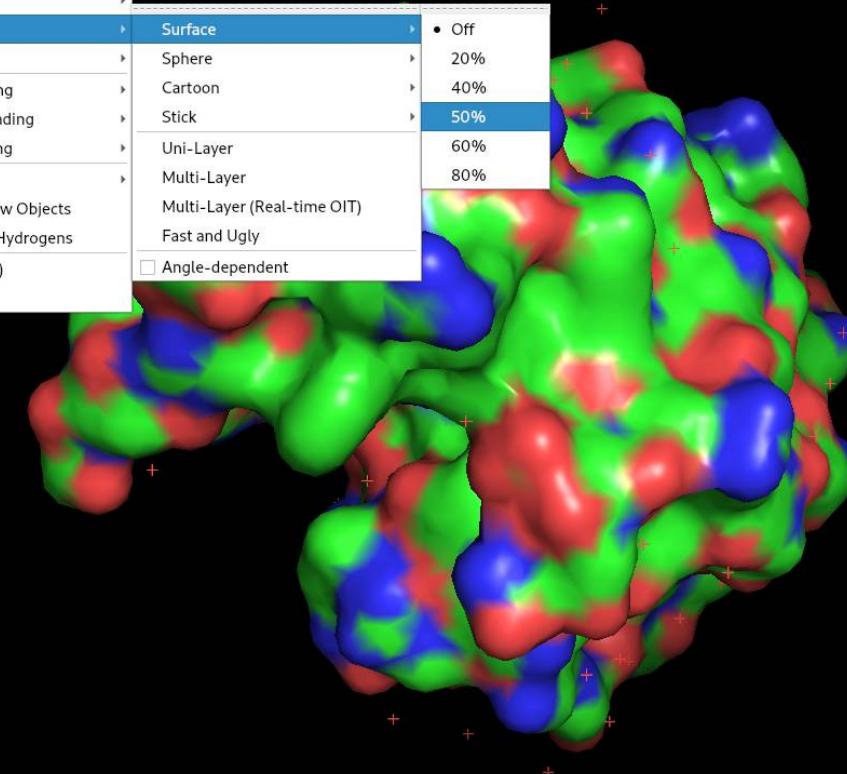
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
(tSh Sele Orig Clip MovZ
SigMov / Cent Menu
DblClick Menu PkAt
Selecting Residues
State 1/ 1
|◀◀◀▶▶▶| S ▾ F

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**
- Rendering
- PDB File Loading
- mmCIF File Loading
- Map File Loading
- Auto-Show ...
- Auto-Zoom New Objects
- Auto-Remove Hydrogens
- Show Text (Esc)
- Overlay Text



- Off
- 20%
- 40%
- 50%**
- 60%
- 80%

- 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 I M R Wheel
 & Keys Rota Move MovZ Slab
 Shft +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MvSZ
 CtSh Sele Orig Clip MovZ
 SnglClick +/- Cent Menu
 DblClick Menu - PkAt
 Selecting Residues
 State 1/1



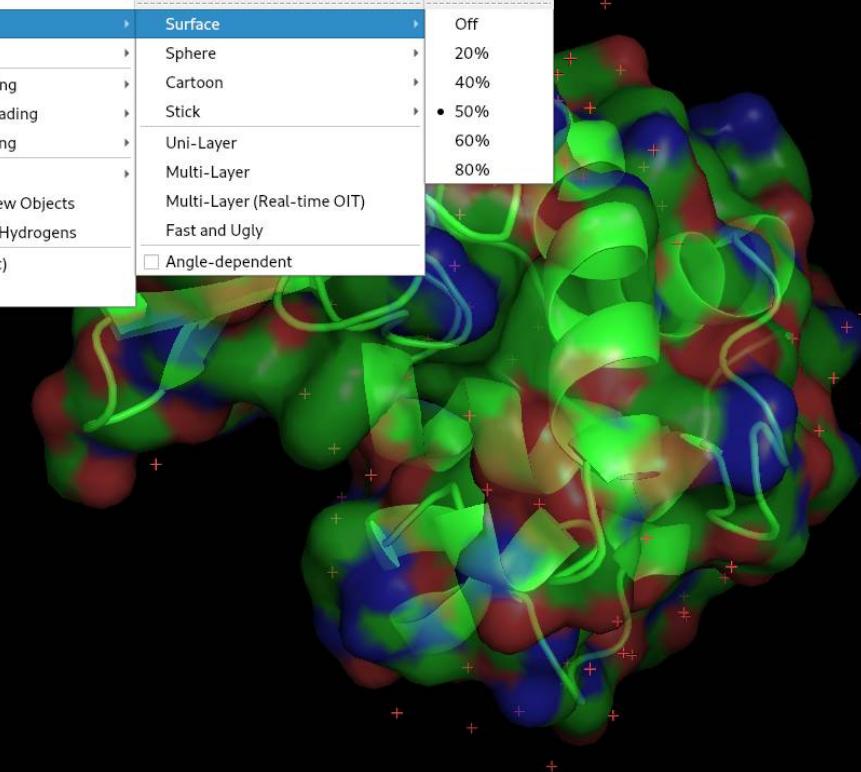
PyMOL>_

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

GL_RENDERER: Mesa Intel(R) Xe Graphics
 GL_VERSION: 4.6 (Compatibility Profile)
 Detected 8 CPU cores. Enabled multithreading.
 TITLE LYSOZYME C
 ObjectMolecule: Read crystal symmetry
 CmdLoad: "" loaded as "centered".
 Dragging whole object "centered".
 Setting: transparency set to 0.500

Edit All...
 Keyboard Shortcuts...
 Colors...
 Label
 Lines & Sticks
 Cartoon
 Ribbon
 Surface
 Volume

Transparency
 Rendering
 PDB File Loading
 mmCIF File Loading
 Map File Loading
 Auto-Show ...
 Auto-Zoom New Objects
 Auto-Remove Hydrogens
 Show Text (Esc)
 Overlay Text



Surface
 Off
 Sphere
 Cartoon
 Stick
 Uni-Layer
 Multi-Layer
 Multi-Layer (Real-time OIT)
 Fast and Ugly
 Angle-dependent

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

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

Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shft +Box =Box Clip MovS
 Ctrl Move PkAt Ph1 MvS2
 CtrSh Sele Drag Tab MovZ
 Single Click Cent Menu
 DblClick Menu PkAt
 Selecting Residues
 State 1/ 1



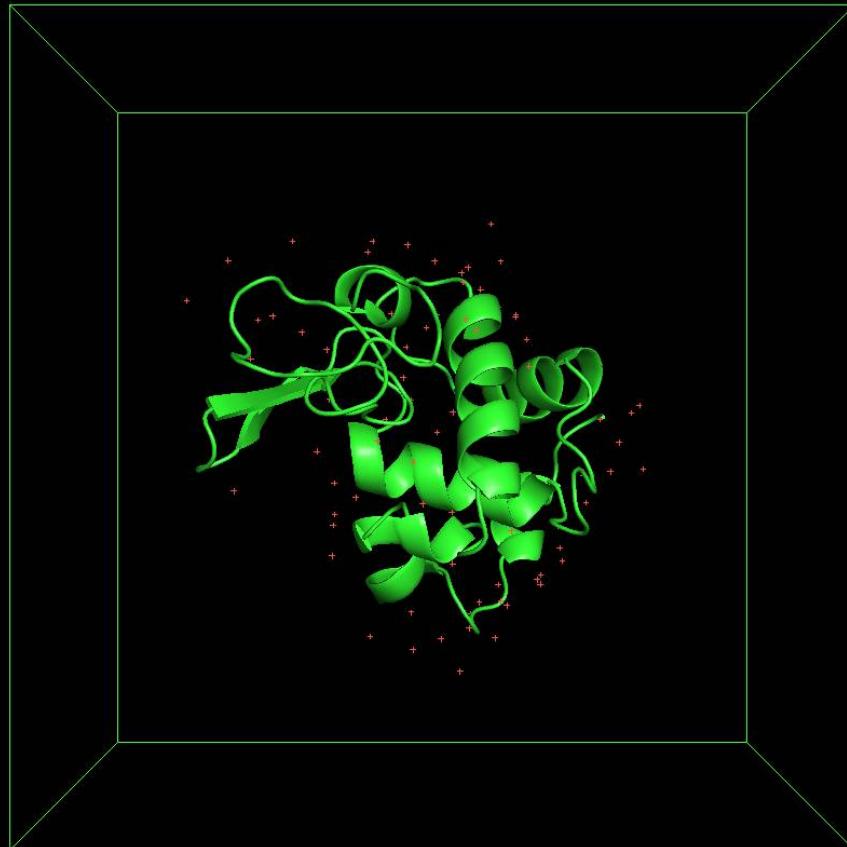
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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 GetView
< < 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 Move Clip MovS
Ctrl Move PkAt Ph1 MvZ
Ctrl Shift Selc Drag Tab MovZ
Single Click Cent Men
DoubleClick Menu PkAt
Selecting Residues
State 1/ 1

< < Stop Play > > S F

PyMOL>_

PyMOL

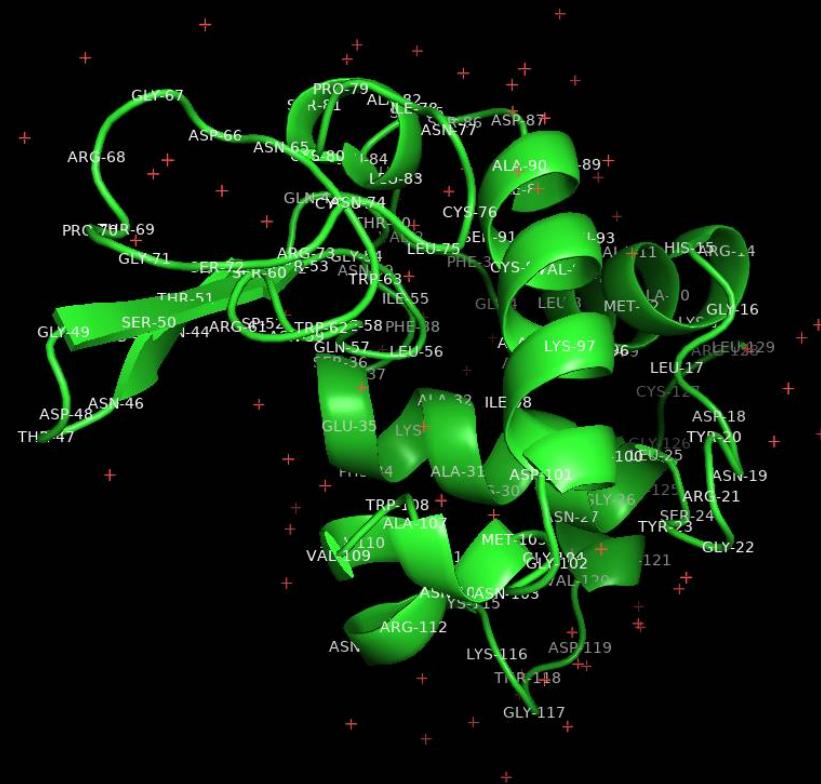
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
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.
```

A screenshot of the MeshLab toolbar, which includes buttons for Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rock, Get View, Stop, Play, MClear, Builder, Properties, and Rebuild.

all 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
    Shft +Box -Box Clip MovS
      Ctrl Move PkAt Pk1 MySz
        CtSh Ste Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/1
```



PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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 A S H L C
 centered 1/1 Color:
 by element
 By Secondary Structure: by chain
 Helix Sheet Loop by ss
 Helix Sheet Loop by rep
 Helix Sheet Loop spectr m
 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 MovS
 Ctrl Move PkAt Pk1 MvSZ
 AltSh Sele Orig Clip MovZ
 ShiftR /> Cent Menu
 DelIClr Menu PRht
 Selecting Residues
 State 1/1

[< < Stop Play > > S F]

PyMOL>_

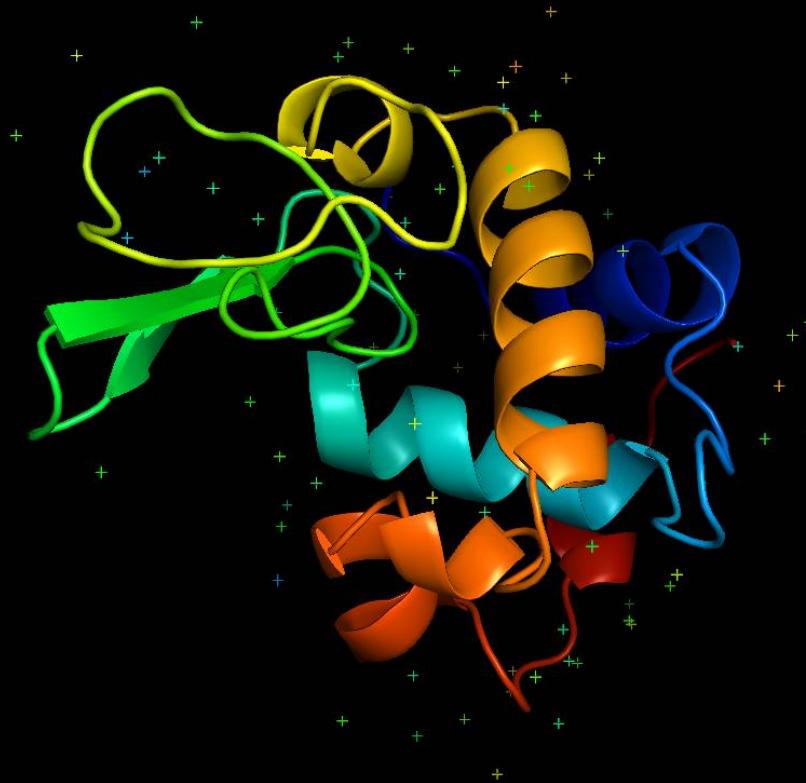
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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>



	A	S	H	L	C
all					
centered 1/1					
Color:					
by element					
by chain					
by ss					
by rep					
Spectrum:					
rainbow(elem C)					
rainbow(*/CA)					
rainbow					
auto					
reds					
greens					
blues					
yellows					
magentas					
cyanas					
oranges					
tints					
grays					

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

| < < Stop Play > | MClear

PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
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>



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

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
 Alt Sh Sele Orig Clip MovZ
 SighLk F2 Cent Menu
 Double Click Menu PRH
 Selecting Residues
 State 1/1

< < Stop Play > > S ▼ F

PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shift +Box =Box Clip MovS
Ctrl Move PkAt All MvSz
Alt Sh Sele Drig Clip MovZ
Single Click Cent Menu
DoubleClick Menu PkAt
Selecting Residues
State 1/ 1
[< < Stop Play > > S F]

PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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
8 Keys Rota Move MovZ Slab
Shift +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
BrgLClick +/- Cent Menu
DBLCLICK Menu - PkAt
Selecting Residues
State 1/ 1

|< < Stop Play >| S ▾ F

PyMOL> _

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
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	1/4	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 MvS
 CtrSh SelE Orig Clip MovZ
 SnglClick +/- Cent Menu
 DblClick Menu - PkAt
 Selecting Residues
 State 1/ 1

PyMOL>_

| < < > > S F

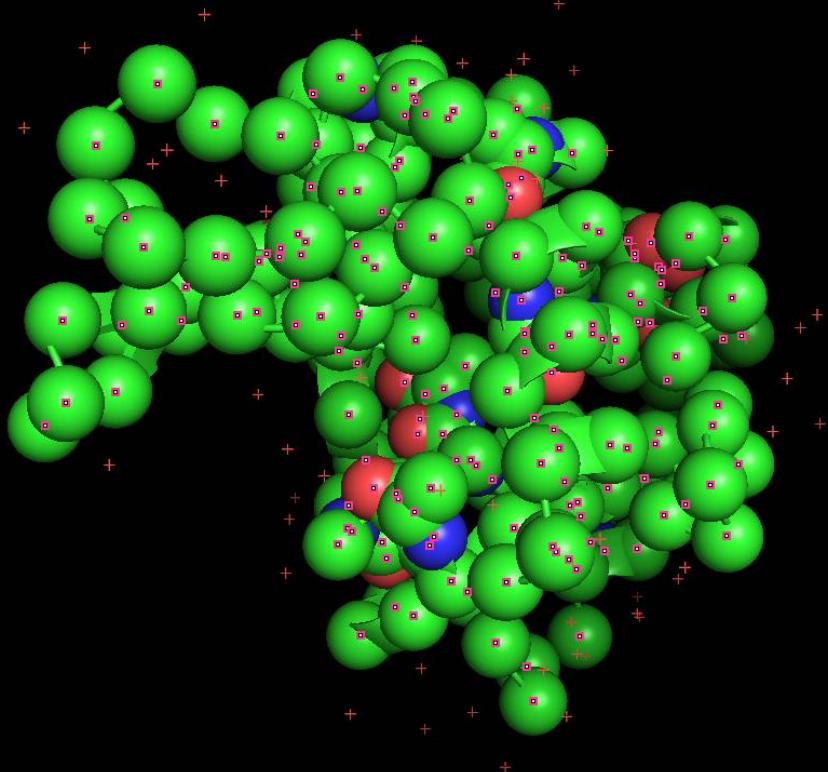
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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 "sel" 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	C
(sel)					
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 MvS2
 CtrSh Selc Orig Clip Mov2
 SnglClick +/- Cent Menu
 DblClick Menu - PkAt
 Selecting Residues
 State 1/ 1

|< < Stop Play >| S F

PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

Spectrum: range (17.45000 to 41.11000).

PyMOL>select resn ALA or name CA

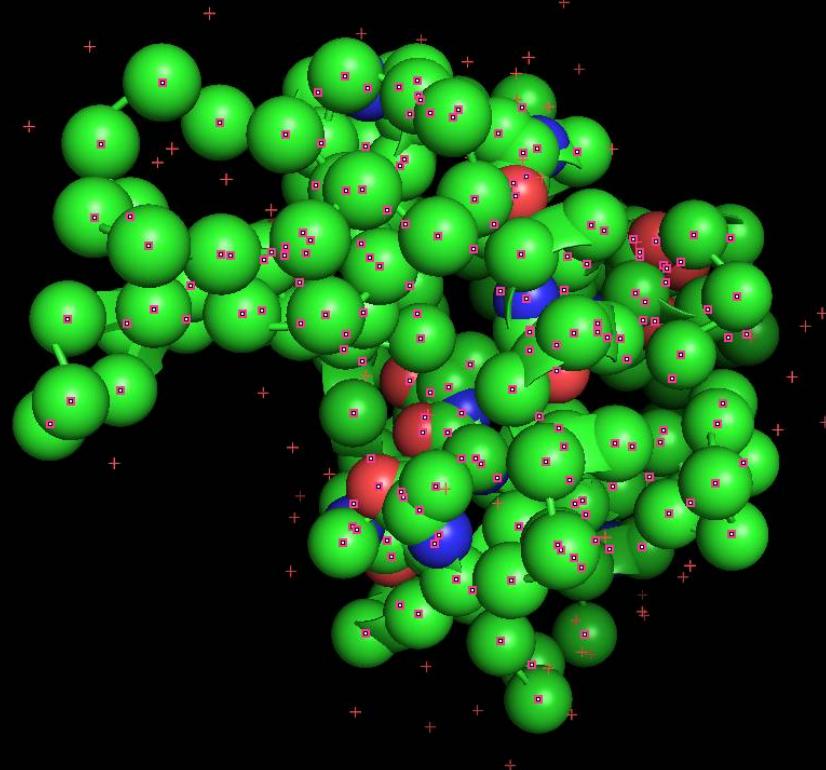
Selector: selection "sele" defined with 177 atoms.

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:
new duplicate
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 MvSz
CtSh Selz Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>_

[< < Stop Play > > S F]

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

Spectrum: range (17.45000 to 41.11000).

PyMOL>select resn ALA or name CA

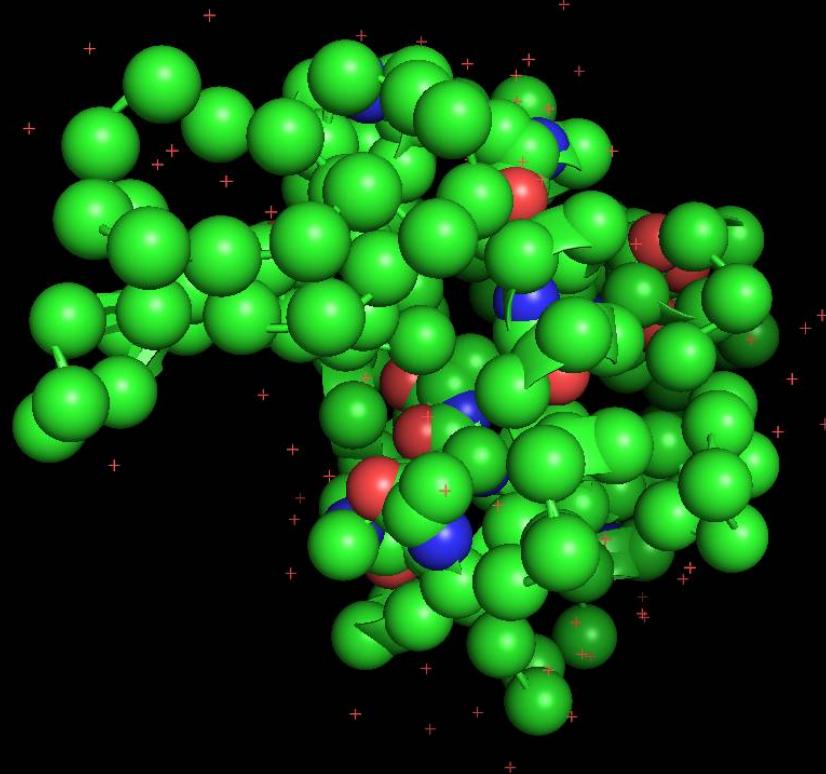
Selector: selection "sele" defined with 177 atoms.

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
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 MvS
CtSh Sale Orig Clip MovZ
SingleClick +/- Cent Menu
DoubleClick Menu -- PkAt
Selecting Residues
State 1/ 1

PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

Setting: bg_rgb set to black.

PyMOL>bg_rgb set to blue

File "toplevel", line 1

bg_rgb set to blue

SyntaxError: invalid syntax

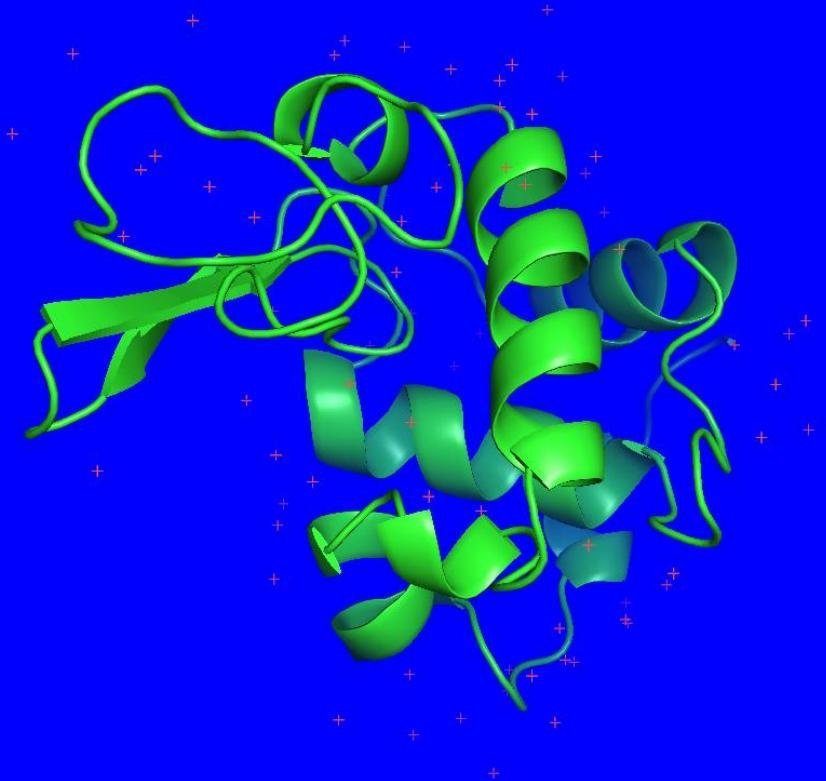
PyMOL>set bg_rgb, blue

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 Clip MovZ
Left Sh Sele Drag Clip MovZ
Single Click Cent Menu
Double Click Menu PkAt
Selecting Residues
State 1/ 1



PyMOL>_

PyMOL

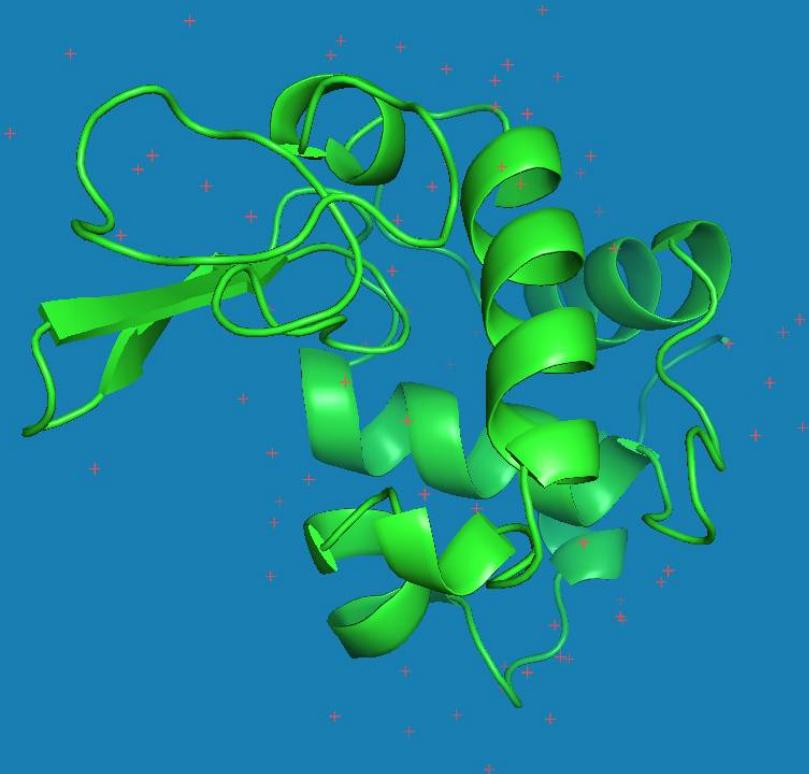
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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.
CndLoad: "" 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 Mov2 Slab
Shift +Box -Box Clip Movs
Ctrl Move PkAt PkC MvS3
PtkSh Move Ori Clip MovZ
Single Click +/- Cent Menu
Double Click Menu - PkAt
Selecting Residues
State 1/ 1
|◀◀◀▶▶▶| S ▼ F

PyMOL>

```
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
```

PyMOL>

Please click on the first atom...

- Appearance
- Measurement**
- Mutagenesis >
- Pair Fitting
- Density
- Filter
- Sculpting
- Label
- Charge
- Demo >



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

all [ASHL]C
centered 1/1 [ASHL]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 MovS
Ctrl Move PkAt Pk1 MvS
CtSh Sele Drag Clip MovZ
SnglClick +/- - Cent Menu
DblClick Menu - PkAt
Selecting Atoms
State 1/ 1

PyMOL>_

PyMOL

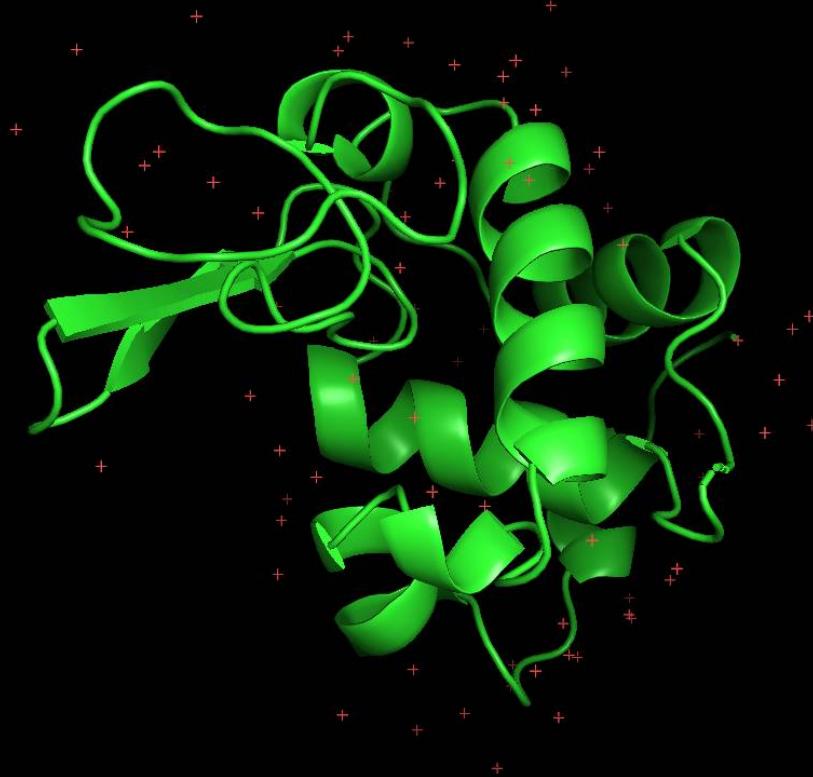
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
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
Del Dihedrals
Mouse Polar Neighbors
Build Heavy Neighbors
& Neighbors
Polar Contacts
Lasso Selection Loop MoveZ
Single Click +/- Cent Menu
Double Click Menu - PkAt
Selecting Atoms
State 1/ 1

PyMOL>_

| < < Stop Play > | S V F

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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
Sele					
measure01					

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 MvS2
 Ctrh Sele Orig Clip MovZ
 SnglClik +/- Cent Menu
 DblClik Menu - PkAt
 Selecting Atoms
 State 1/ 1

| < < > > S F

PyMOL>_

PyMOL

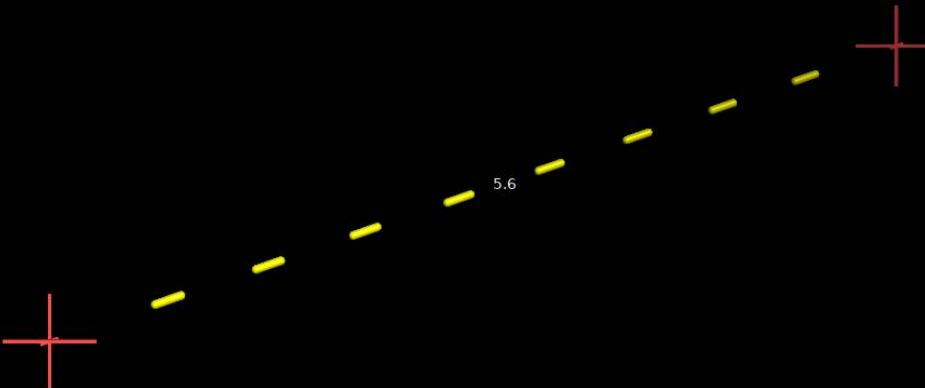
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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: L C
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 MvS2
 CtrSh Sel Orig Clip MovZ
 SingleClick +/- Cent Menu
 DoubleClick Menu - PkAt
 Selecting Atoms
 State 1/ 1

PyMOL>_

| < < Stop Play >| MClear
 Builder Properties Rebuild

PyMOL

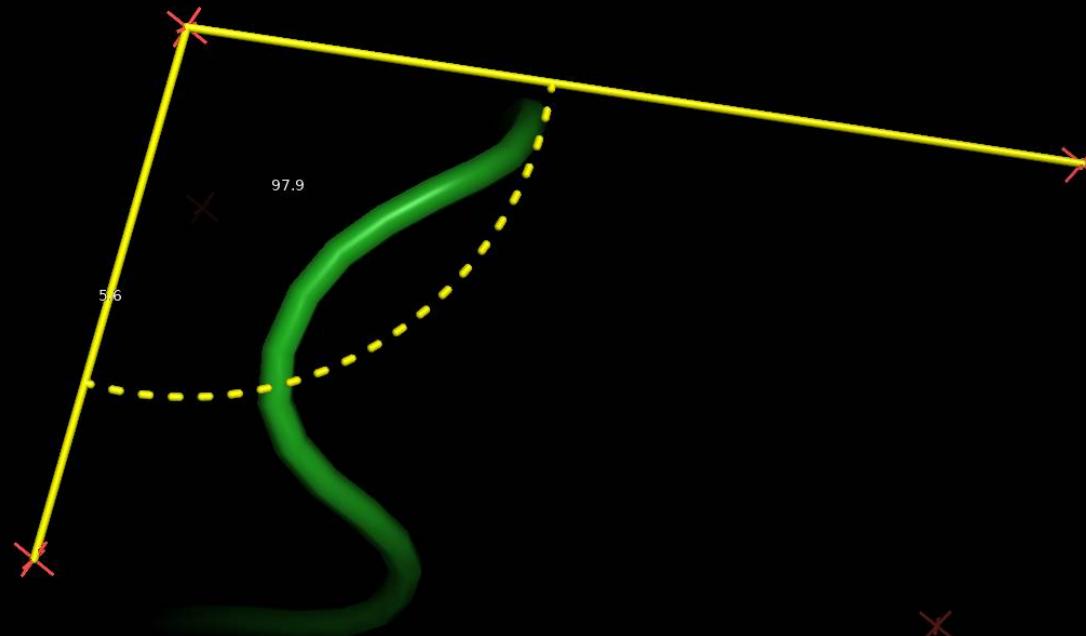
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
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	>
Builder	Properties	Rebuild	

PyMOL>

Please click on the first atom...



all	A	S	H	L	C	
centered	1/4	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 MvS
CtSh Sel Orig Clip MovZ
SnglClik +/- Cent Menu
DblClik Menu - PkAt
Selecting Atoms
State 1/ 1

PyMOL>_

◀ ▶ □ ▢ ▤ ▦ ▧ ▨ ▩ ▪ ▫ ▬ ▭ ▮ ▯ ▯ ▯

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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
& Shft +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvS
CtSh Sele Drig Clip MovZ
SnglClik +/- Cent Menu
DblClik Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>_

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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>

Reset Zoom Orient Draw/Ray

Save Image to File

Copy Image to Clipboard

< Back



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



PyMOL>_

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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>

PyMOL>

Setting menu open, showing:

- Edit All...
- Keyboard Shortcuts...
- Colors...
- Label
- Lines & Sticks
- Cartoon
- Ribbon
- Surface
- Volume
- Transparency
- Rendering** (selected)
- PDB File Loading
- mmCIF File Loading
- Map File Loading
- Auto-Show ...
- Auto-Zoom New Objects
- Auto-Remove Hydrogens
- Show Text (Esc)
- Overlay Text

Rendering submenu open, showing:

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

3D view showing a green ribbon model of a protein structure with red cross markers.

Right-click context menu open, showing:

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

Color palette on the right:

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

Bottom status bar:

Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 & Shift +Box -Box Clip MovS
 Ctrl Move PkAt Pk1 MvS2
 CtrSh SelE Orig Clip Mov2
 SnglClick +/- Cent Menu
 DblClick Menu - PkAt
 Selecting Residues
 State 1/ 1

Navigation icons at the bottom:

PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

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 28.79cm

Height 13.58cm

Lock aspect ratio

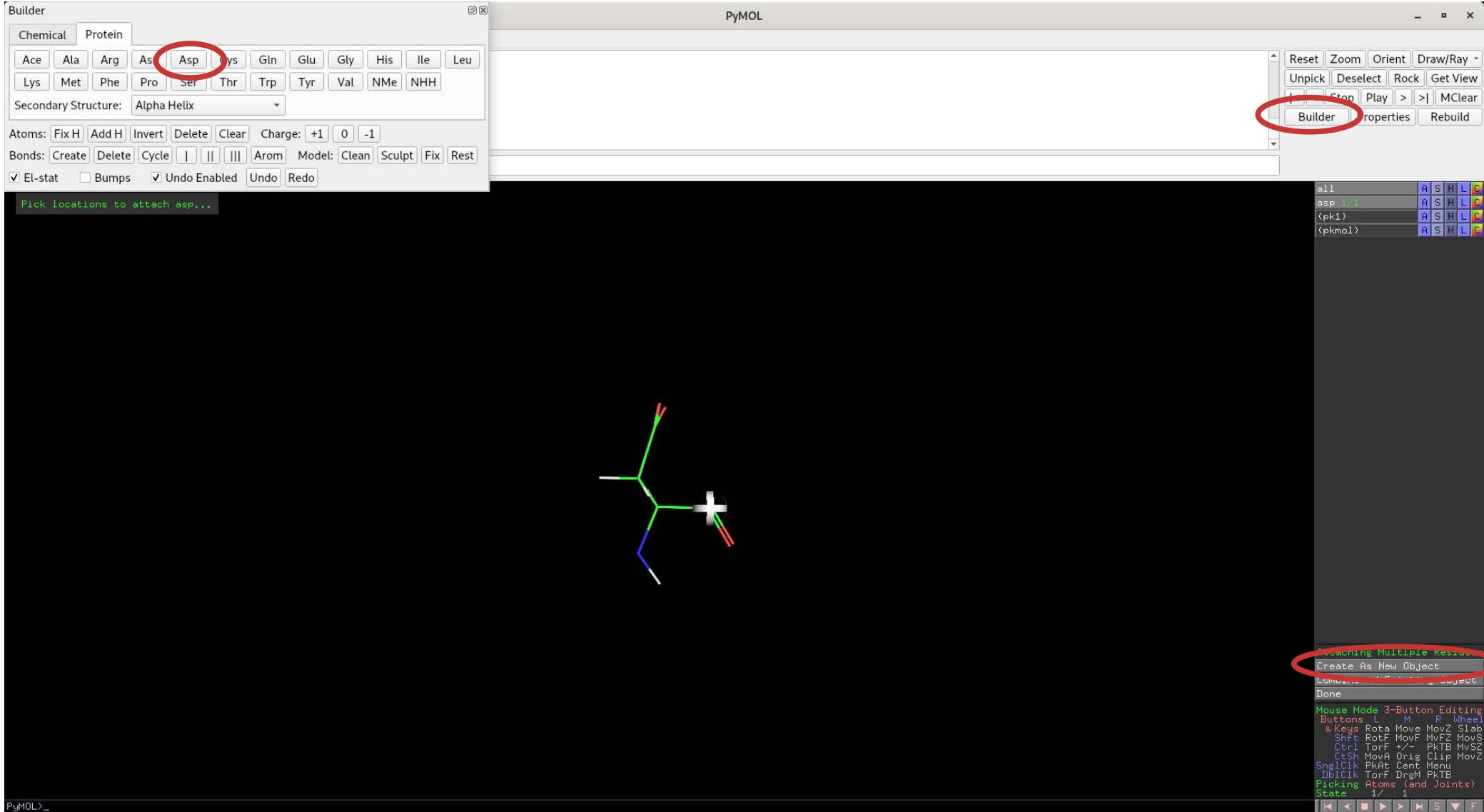
Units at DPI

transparent background ("Ray" only)

- or -

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 Mov2 Slab
 Shift +Box -Box Clip Mov3
 Ctrl Move PkAt PkC MvS3
 CtrSh Move Orig Clip MovZ
 SnglClick +/- Center Menu
 DblClick Menu - PkAt
 Selecting Residues
 State 1/ 1



Builder

Chemical Protein

Ace	Ala	Arg	Asn	Asp	Cys	Gln	Glu	Gly	His	Ile	Leu
Lys	Met	Phe	Pro	Ser	Thr	Trp	Tyr	Val	NMe	NHH	

Secondary Structure: Alpha Helix

Atoms: Fix H Add H Invert Delete Clear Charge: +1 0 -1

Bonds: Create Delete Cycle I II III Arom Model: Clean Sculpt Fix Rest

 El-stat Bumps Undo Enabled Undo Redo

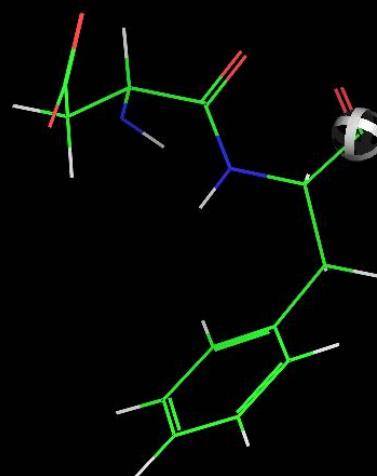
Pick locations to attach asp...

PyMOL

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

Builder	Properties	Rebuild
---------	------------	---------

all	A	S	H	L	C
asp 1/1	A	S	H	L	C
(pk1)	A	S	H	L	C
(pkmol)	A	S	H	L	C



Attaching Multiple Residues
 Create As New Object
 Combine w/ Existing Object
 Done

Mouse Mode 3-Button Editing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 Shft RotF MovF MovZ MovS
 Ctrl TorF +/- PkTB MovS
 CtrSh MovA Drig Clip MovZ
 SnglClik PkAt Cent Menu
 DblClik TorF Drag PkTB
 Picking Atoms (and Joints)
 State 1/ 1

