Pymol 使用简介

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Pymol： Python + Molecule

- 适用于创作高品质的小分子或是生物大分子（特别是蛋白质）的三维结构图像。
- 少数可以用在结构生物学领域的开放源代码视觉化工具。
- 由Warren Lyford DeLano编写，并且由DeLano Scientific LLC将它商业化。

Https://pymol.org/2/

Https://pymolwiki.org/index.php/

Pymol 安装方法

- 官网安装Education版本
- UCI大学对PyMOL 源码进行了预编译，并免费提供PyMOL的相关wheel文件

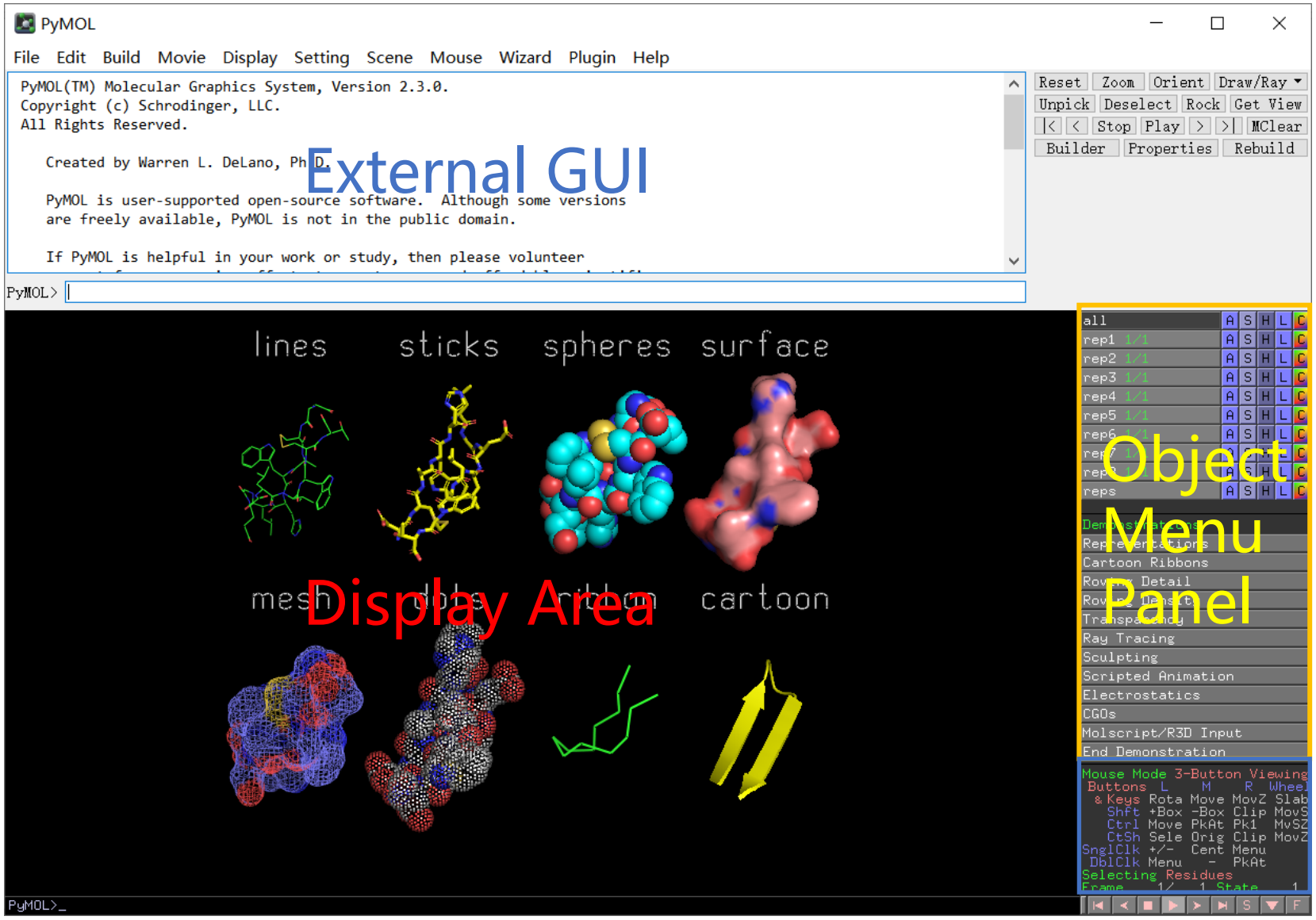
  安装Python，建议使用Anaconda， “Add Python 3.7 to PATH”

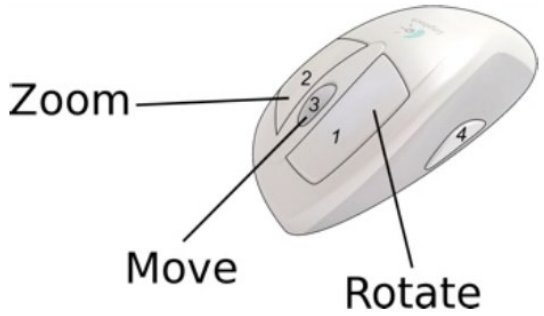
  到uci wheel官网下载相应的whl文件

  在下载了whl文件的文件夹中打开powershell窗口，通过 pip install 命令安装

```
> pip install pymol-2.3.0-cp37-cp37m-win_amd64.whl
```

Pymol 简介





Mouse Controls

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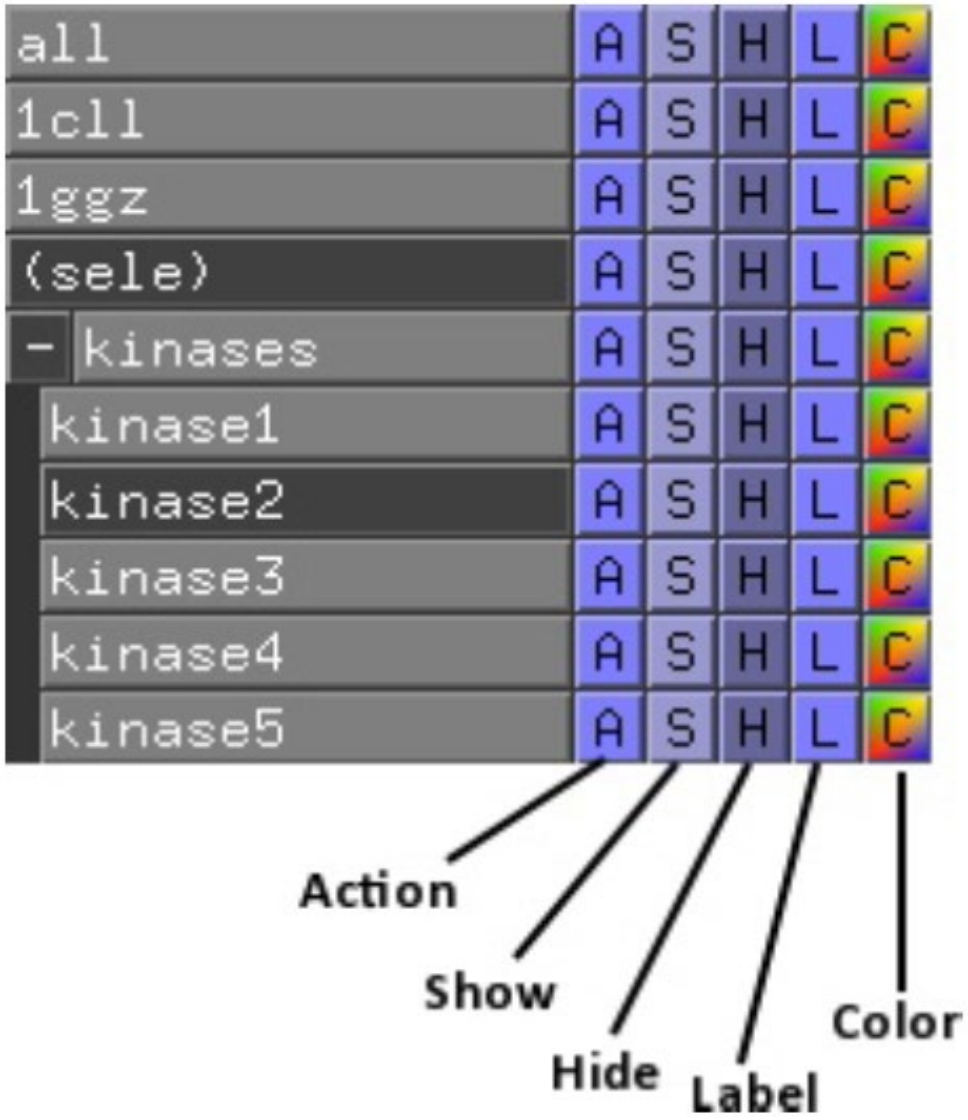
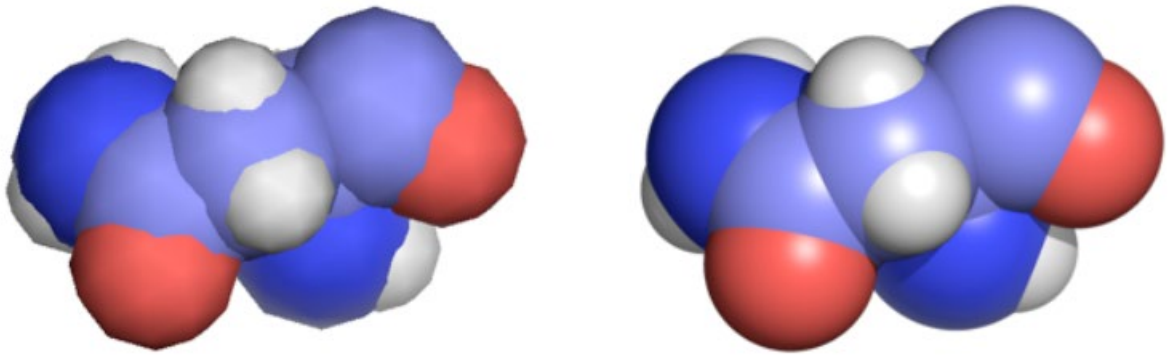

all A S H L C
1cll A S H L C
1ggz A S H L C
(sele) A S H L C
- kinases A S H L C
kinase1 A S H L C
kinase2 A S H L C
kinase3 A S H L C
kinase4 A S H L C
kinase5 A S H L C
Action
Show
Hide
Label
Color




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 Molecules
State 1/ 1 0.1 Hz
S
F

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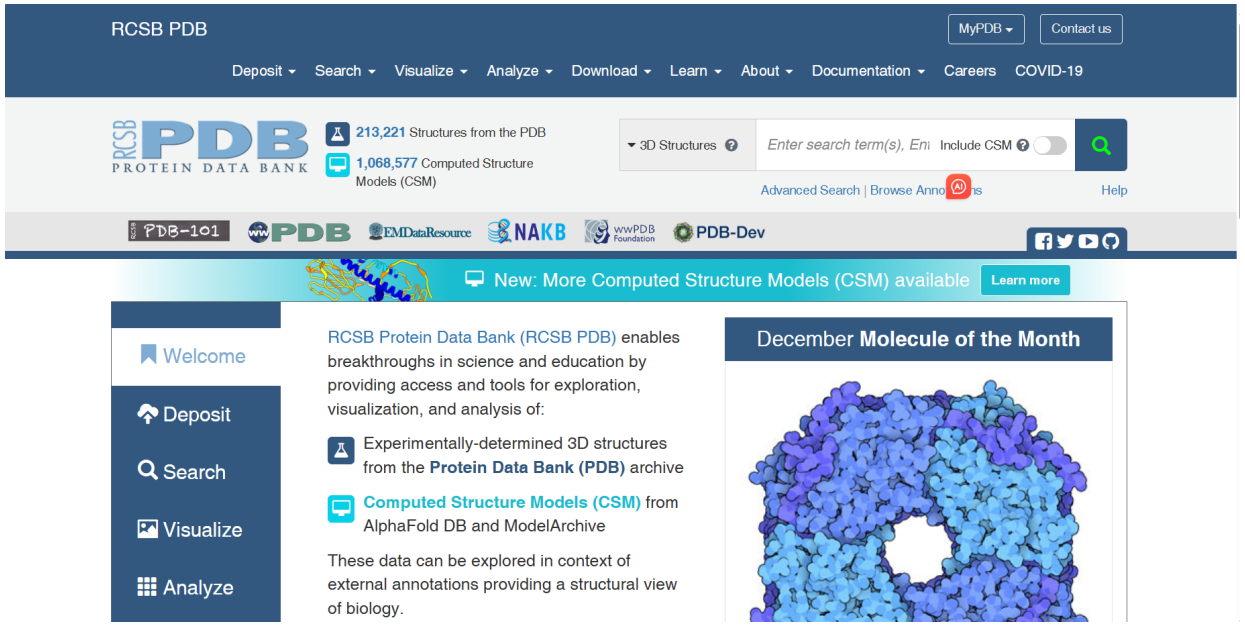
- 只要蛋白质的三维原子坐标被测定（低温冷冻电镜、X射线晶体衍射、核磁共振），它们即可以被编写成特定格式（例如PDB），从而用PyMOL等软件进行可视化。
- PDB: Protein Data Bank
- Research Collaboratory for Structural Bioinformatics (RCSB): 保存PDB文件的数据库



- PDB 中的每个数据库条目都有一个特定的四字符编号，用于识别特定结构

  - 可直接从RCSB数据库搜索并下载PDB文件用PyMOL打开
  - 若知道四字符编号，可直接通过PyMOL软件进行下载 （演示1CRN）

- Introduction to Protein Data Bank Format （蛋白质结构标准格式）

1CRN.pdb

```
SEQRES   1 A   46  THR THR CYS CYS PRO SER ILE VAL ALA ARG SER ASN PHE
SEQRES   2 A   46  ASN VAL CYS ARG LEU PRO GLY THR PRO GLU ALA ILE CYS
SEQRES   3 A   46  ALA THR TYR THR GLY CYS ILE ILE PRO GLY ALA THR
SEQRES   4 A   46  CYS PRO GLY ASP TYR ALA ASN
HELIX    1  H1 ILE A    7  PRO A   19  13/10 CONFORMATION RES 17,19      13
HELIX    2  H2 GLU A   23  THR A   30  1DISTORTED 3/10 AT RES 30         8
SHEET    1  S1 2 THR A   1  CYS A   4  0
SHEET    2  S1 2 CYS A  32  ILE A  35 -1
SSBOND   1 CYS A    3    CYS A   40                      1555   1555  2.00
SSBOND   2 CYS A    4    CYS A   32                      1555   1555  2.04
SSBOND   3 CYS A   16    CYS A   26                       1555   1555  2.05
```

SEQRES: 蛋白质一级序列信息

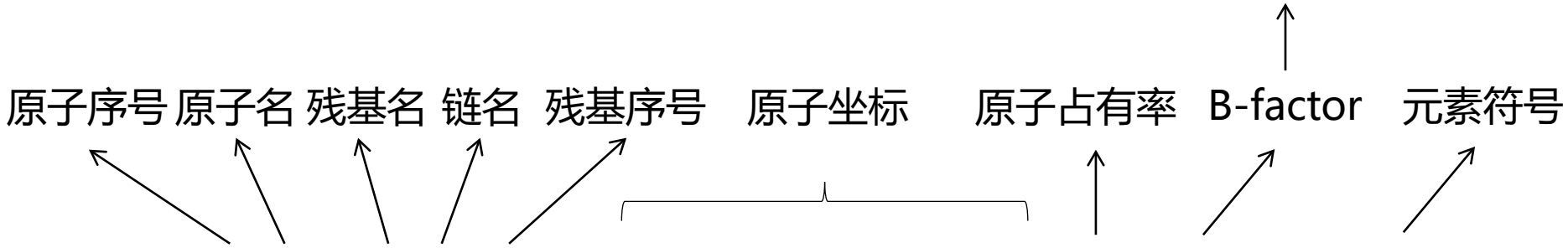
HELIX and SHEET: 蛋白质二级结构信息

SSBOND: 蛋白质中二硫键信息

- Introduction to Protein Data Bank Format （蛋白质结构标准格式）

1CRN.pdb

衡量原子位置不确定性的一种方法，体现了晶体中原子电子密度的“模糊度”（>60，无序，则结构不可靠）



ATOM	1	N	THR	A	1	17.047	14.099	3.625	1.00 13.79	N
ATOM	2	CA	THR	A	1	16.967	12.784	4.338	1.00 10.80	C
ATOM	3	C	THR	A	1	15.685	12.755	5.133	1.00 9.19	C
ATOM	4	O	THR	A	1	15.268	13.825	5.594	1.00 9.85	O
ATOM	5	CB	THR	A	1	18.170	12.703	5.337	1.00 13.02	C
ATOM	6	OG1	THR	A	1	19.334	12.829	4.463	1.00 15.06	O
ATOM	7	CG2	THR	A	1	18.150	11.546	6.304	1.00 14.23	C
ATOM	8	N	THR	A	2	15.115	11.555	5.265	1.00 7.81	N
ATOM	9	CA	THR	A	2	13.856	11.469	6.066	1.00 8.31	C
ATOM	10	C	THR	A	2	14.164	10.785	7.379	1.00 5.80	C

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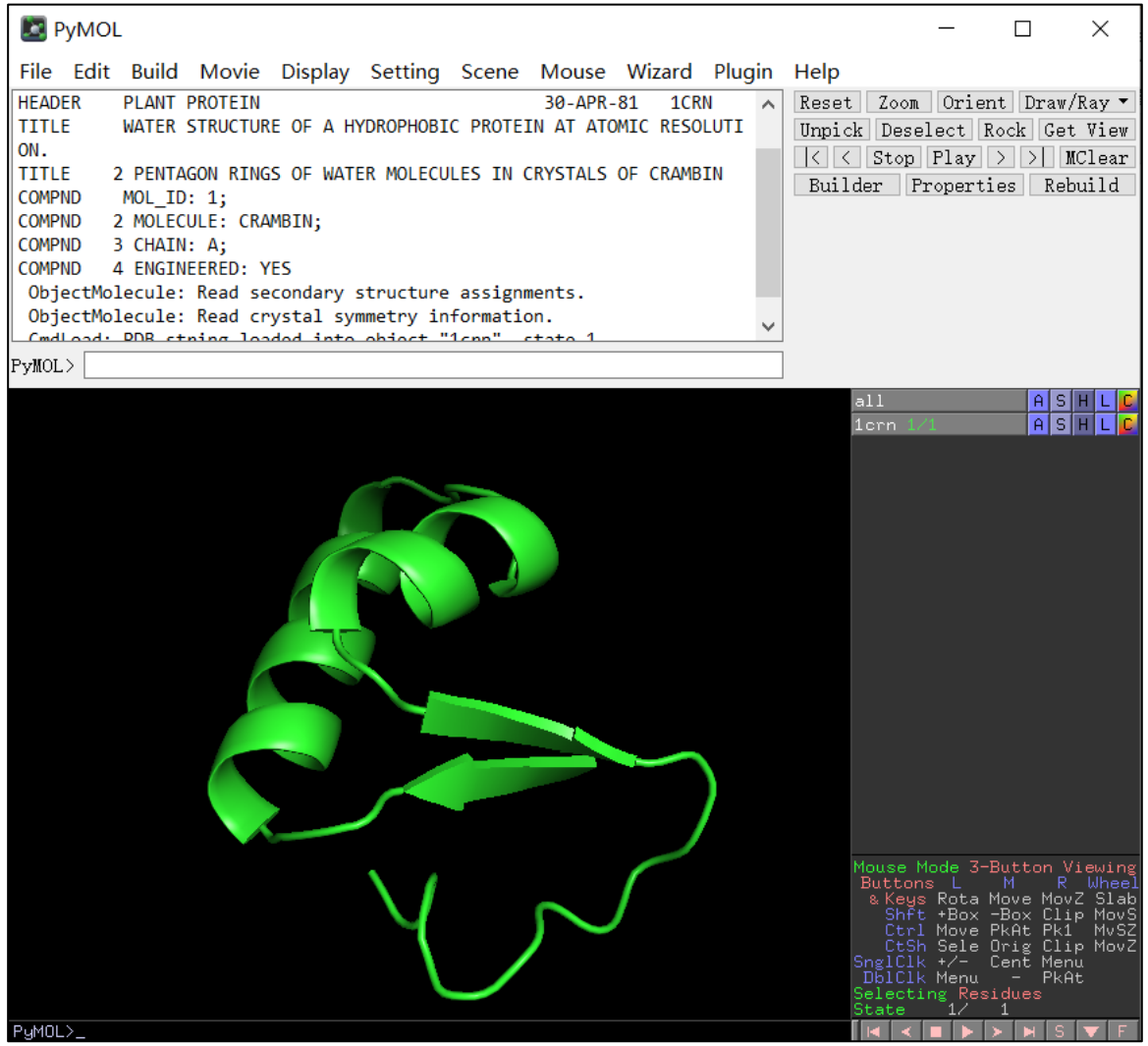
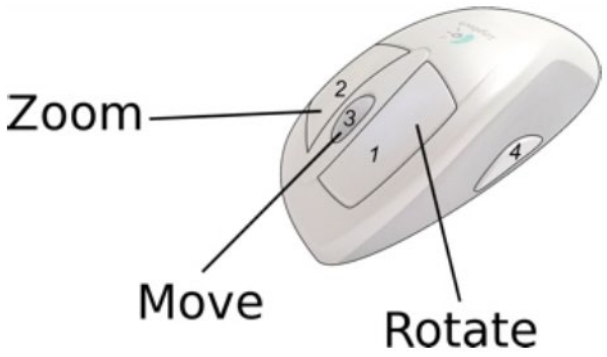
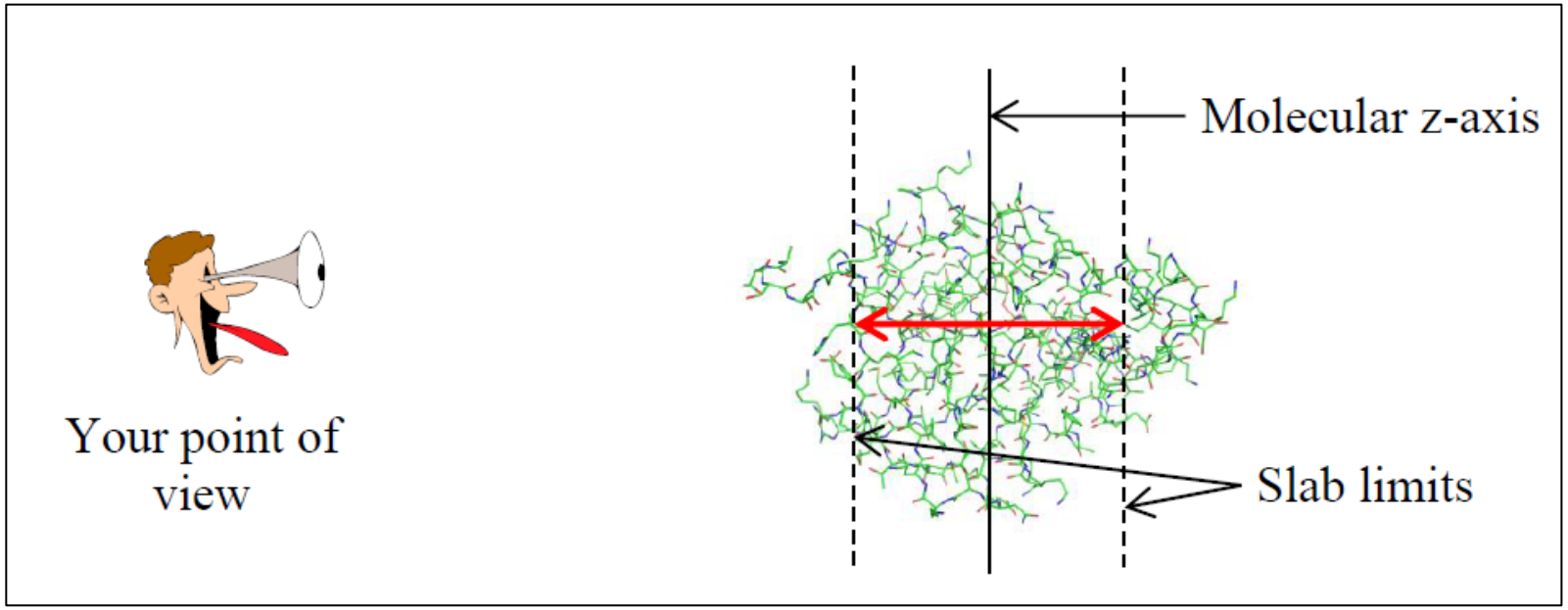


- 默认状态下，只有主链被显示出来，二级结构区用Cartoon模式显示。
- 熟悉鼠标操作，调整视图（演示）



➢ Slab tool



- 有时候，感兴趣的区域位于蛋白质的中心，会被表面的原子所遮挡，调整Slab limits可以更好地展示结构。
- 在Slab limits外的结构都会被隐藏。

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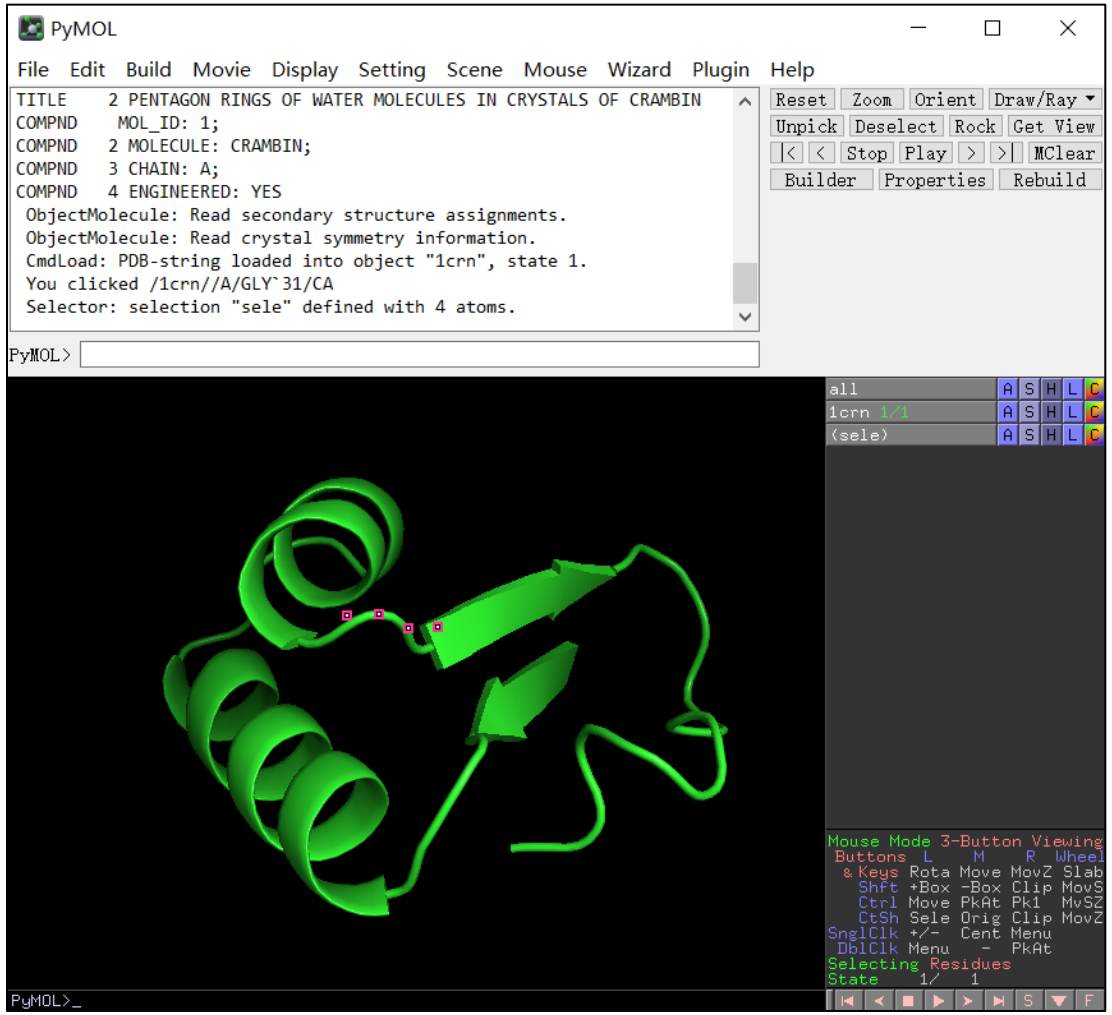
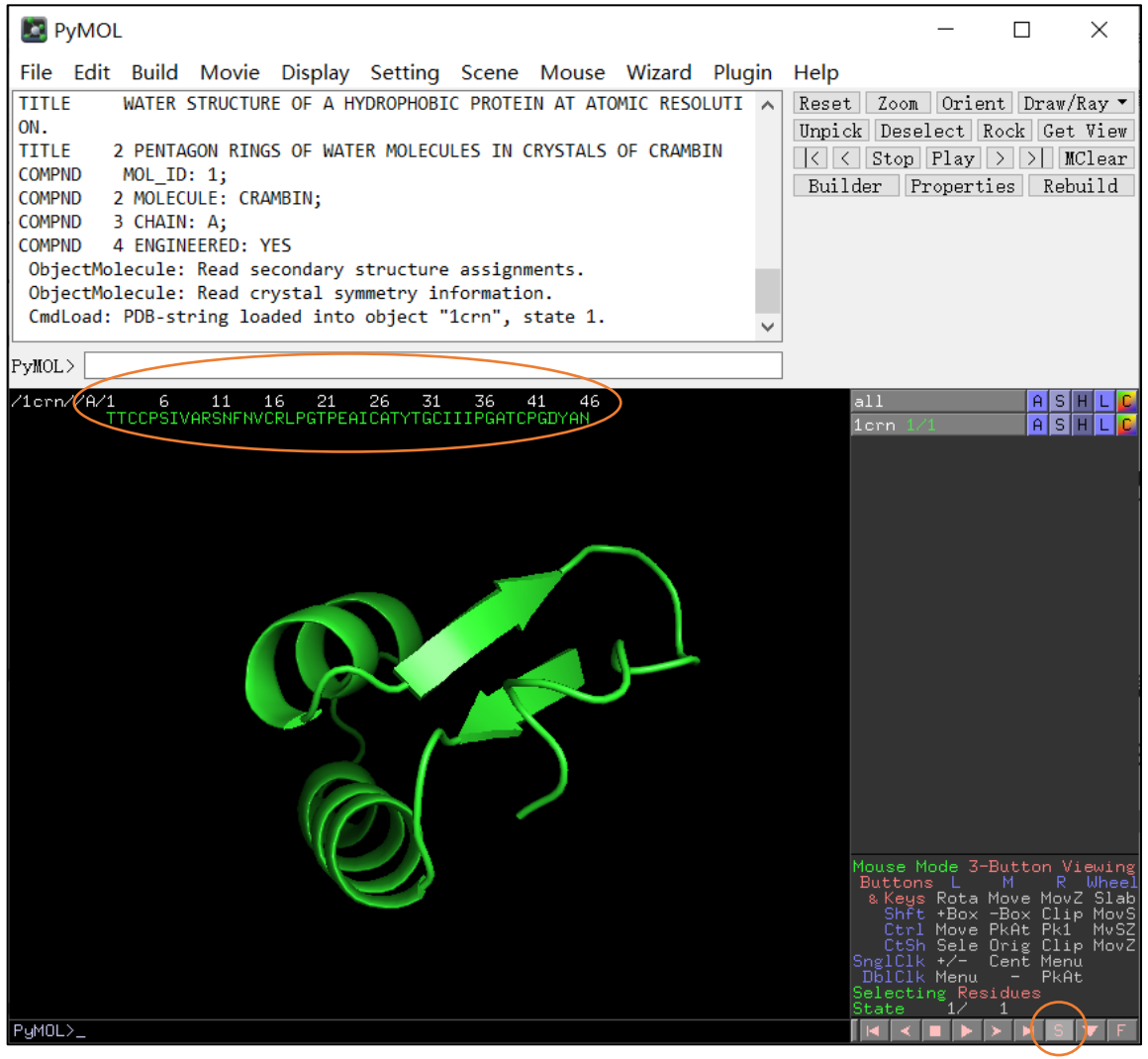
➢ 选择残基或者原子



- 直接点击蛋白质，所选残基中的原子会以粉色方框突出显示。
- 若选择模式为Residues模式，则只能选中某个残基，可根据需要调整选择模式。
- 其它模式： Objects, Segments, Chains, Molecules, Residues, Atoms, and C-alpha atoms

Pymol 简介

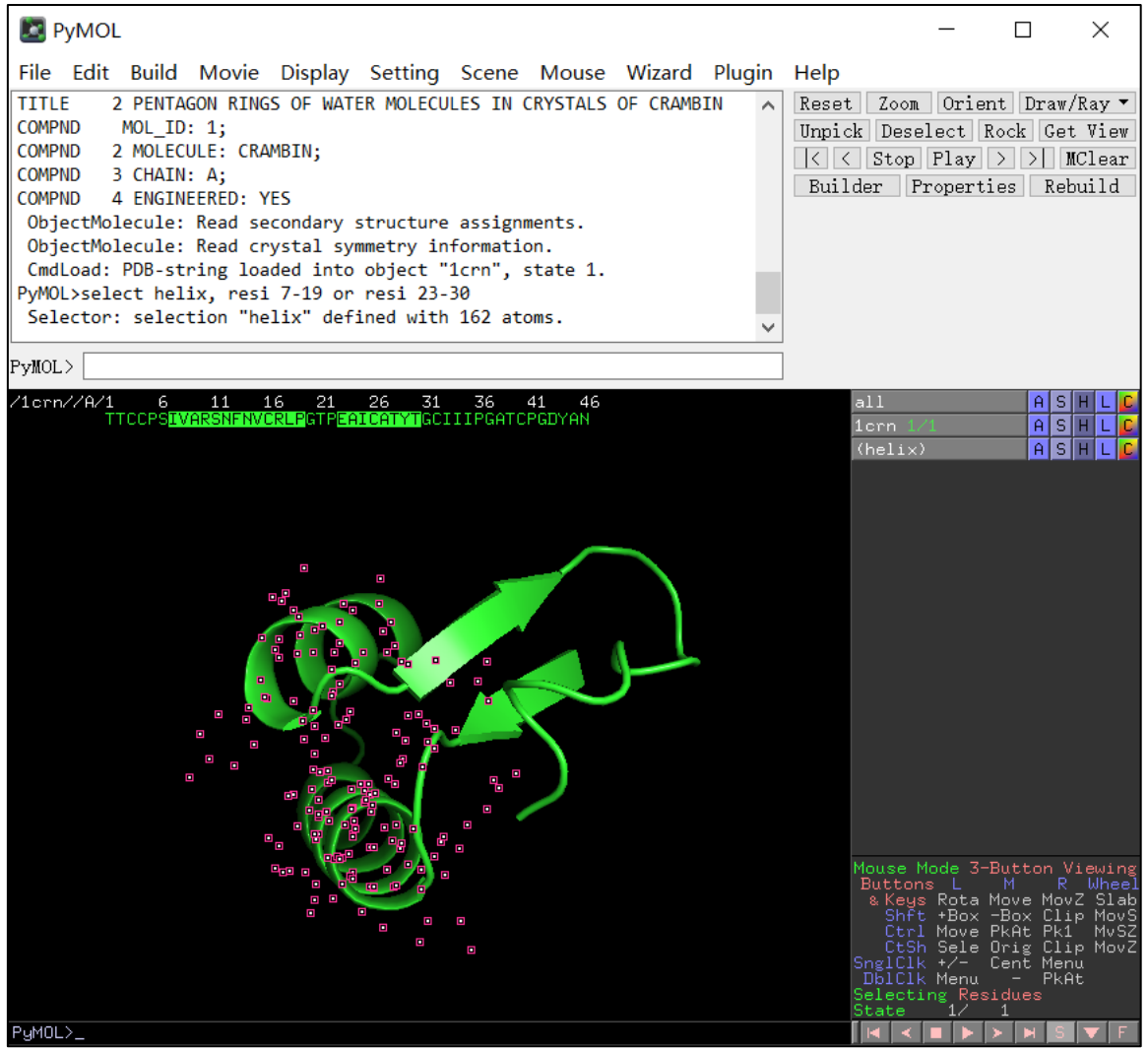
➢ 选择残基或者原子



- 打开Sequence功能，使用右下角S按钮
- 或者使用External GUI > Display > sequence
- 可根据不同需求选择Sequence Mode
- 然后可以根据序列选择感兴趣的残基或者原子，不用在结构中进行寻找了

Pymol 简介

➢ 选择残基或者原子（命令行操作）



- 按照残基序号选择α螺旋区域

  select helix, resi 7-19 or resi 23-30 （演示）

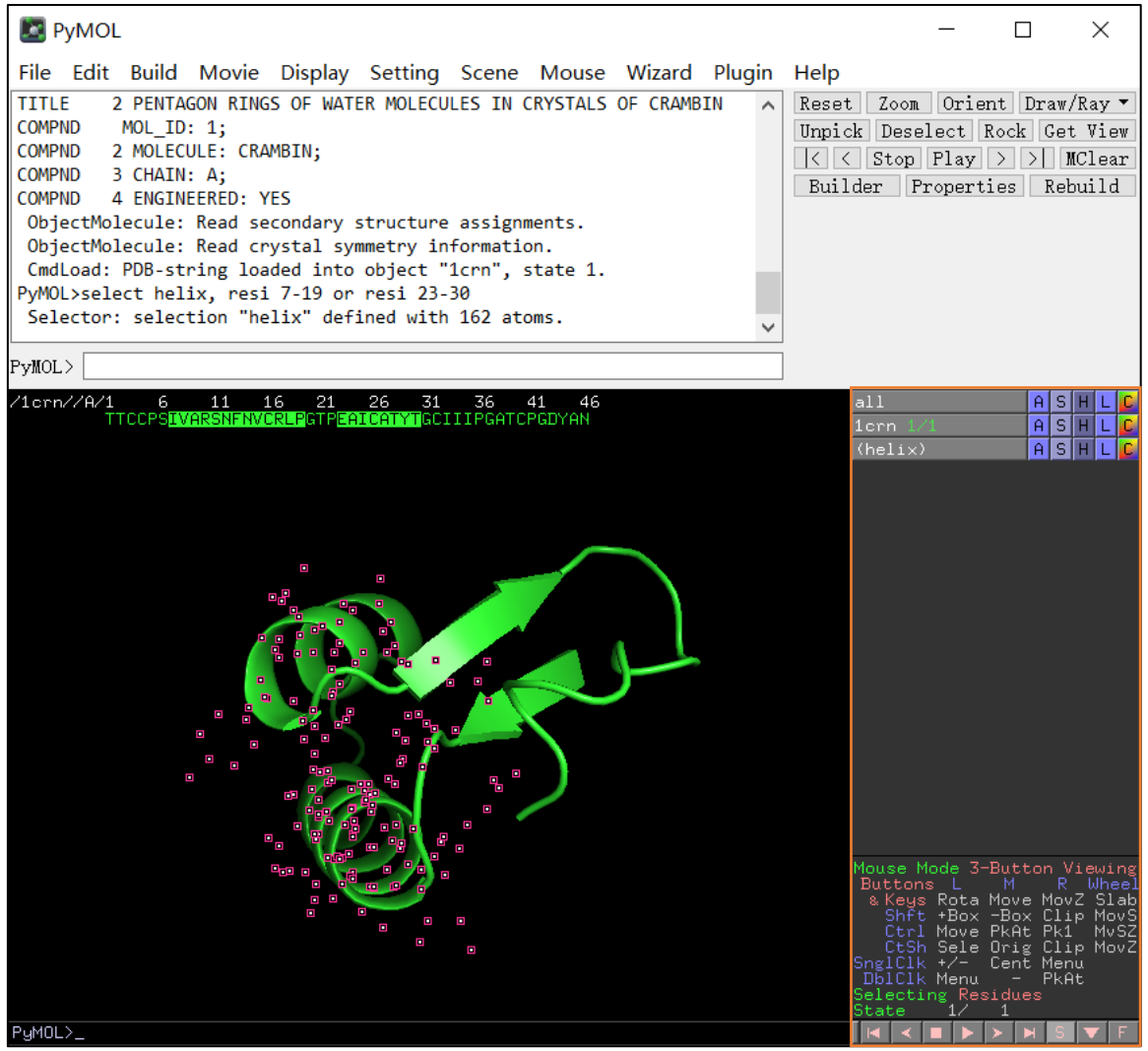
- resn： 选择特定残基名

  select negative, resn asp+glu

- elem：选择特定元素名
- 可用and, or, not进行组合使用

Pymol 简介

➢ Object Menu Panel

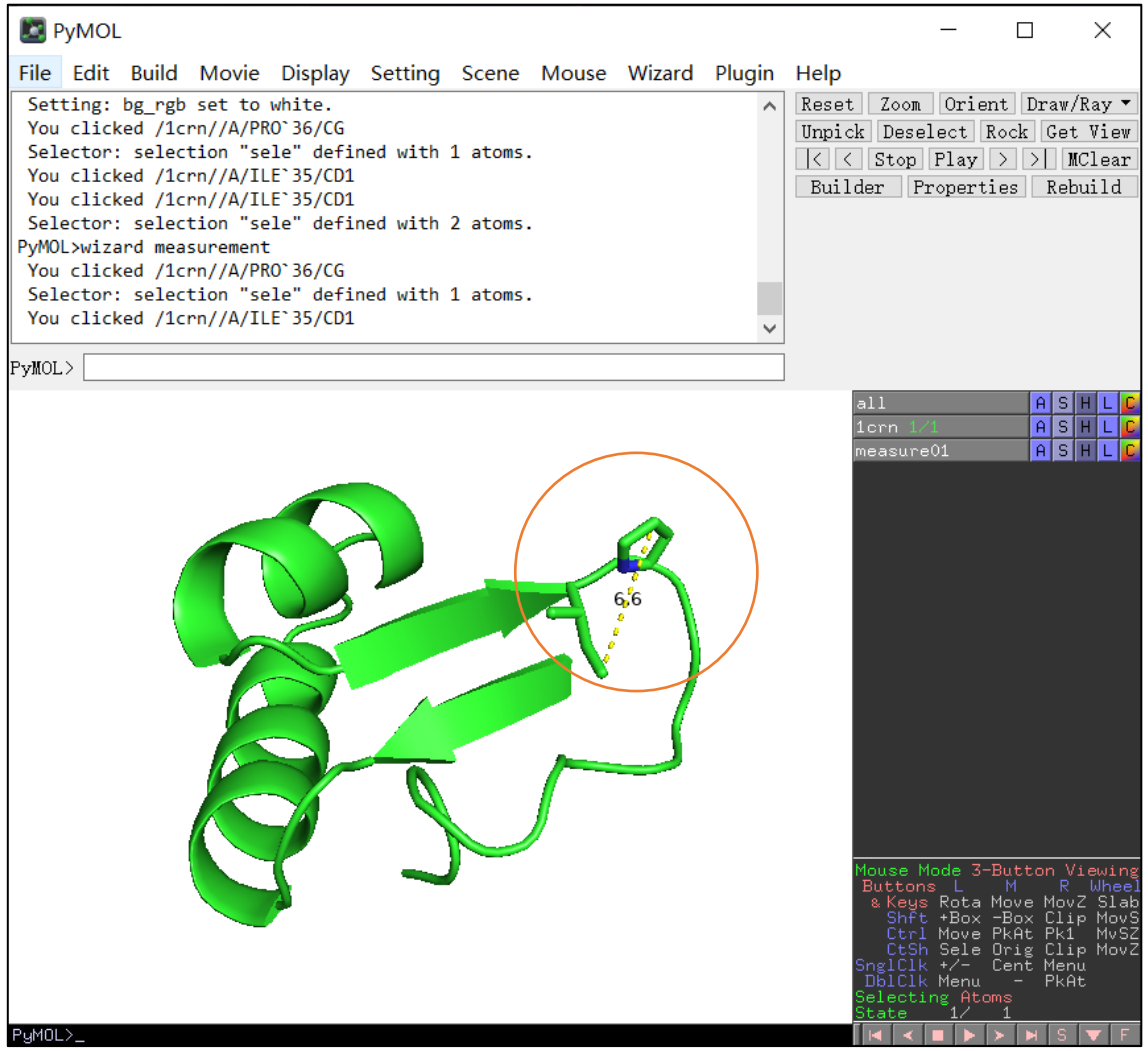


(演示)

- A (actions)：对该对象进行操作，例如调整视图，拖动，叠合，计算静电势等等。
- S (show)：更改该对象的显示方式，例如Sticks，Lines，Spheres，Cartoons
- H (hide)：隐藏该对象
- L (label)：显示或删除特定的标签
- C (color)：调整该对象的颜色

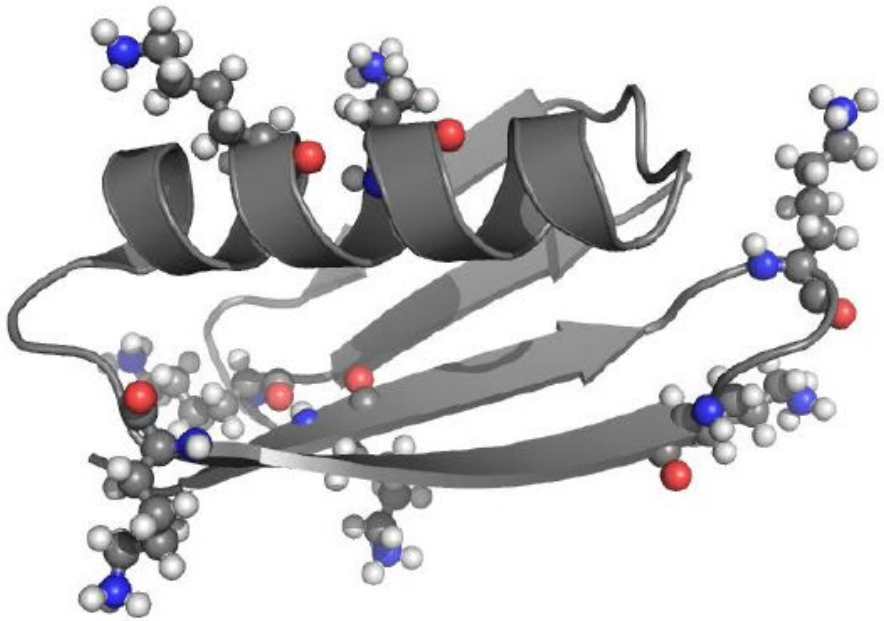
Pymol 简介

➢ 结构分析（测量原子间距离）

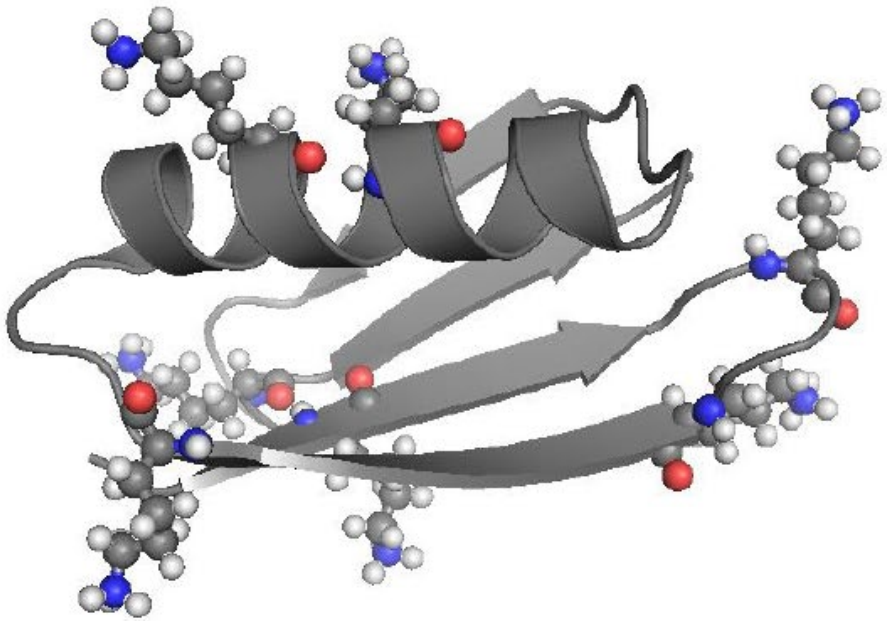


- Wizard > Measurement
- 按照提示选择两个原子，直接显示距离

- 保存高质量图片
  - 作为发表用途，图片背景最好是白色的，Display > Background > White
  - ray：对分子进行光线追踪，生成更真实的图像 （演示）



Ray Traced Image



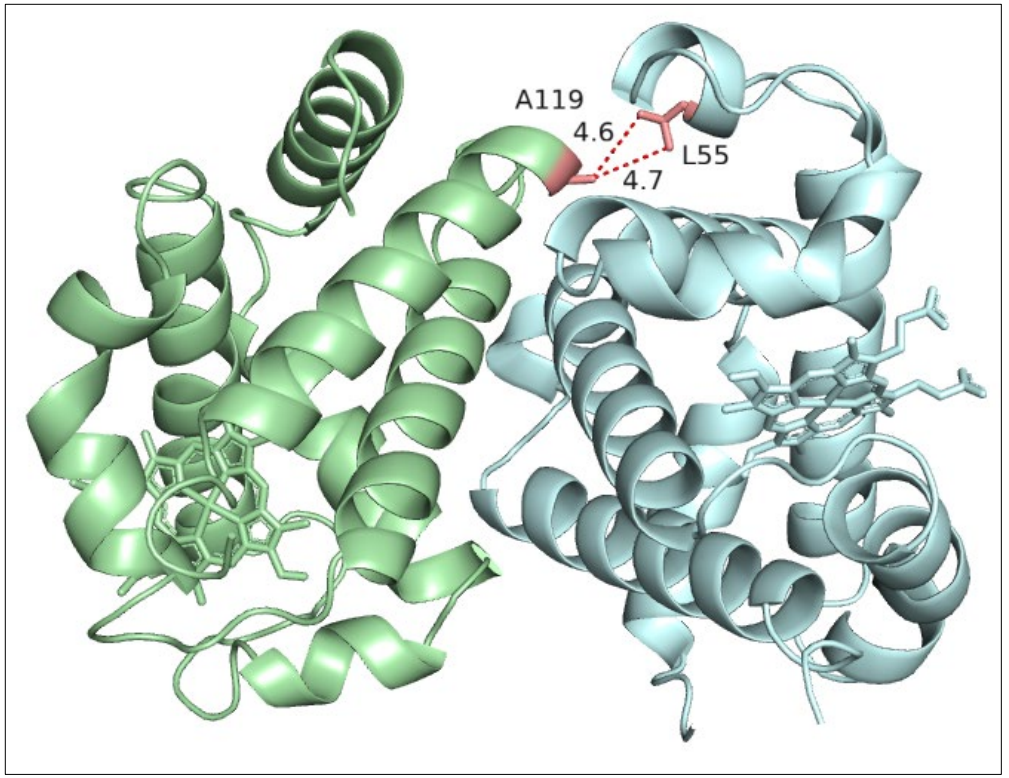
Standard Image

实例演示

- 血红蛋白比较分析：斑头雁 (1A4F) 与灰雁 (1FAW)

- 选择并保存灰雁氧合血红蛋白1FAW中四个亚基中的A链B链两个亚基选择A，B链存为新对象
- 将1A4F和1FAW的A,B链利用align命令进行结构叠合，计算RMSD
- 测量斑头雁(1A4F)A链119位丙氨酸侧链beta碳原子CB和B链55位亮氨酸侧链末端两个碳原子CD1和CD2之间的距离
- 测量灰雁(1FAW)A链119位脯氨酸侧链gamma碳原子CG和B链55位亮氨酸侧链末端两个碳原子CD1和CD2之间的距离
- 利用模拟突变的方法，将灰雁血红蛋白A链第119位脯氨酸突变成丙氨酸，测量突变后的A119CB和B55CD1、B55CD2之间的距离。

斑头雁(1A4F)



Pymol 简介

Pymol Reference Card

Modes

Pymol supports two modes of input: point and click mode, and command line mode. The point and click allows you to quickly rotate the molecule(s) zoom in and out and change the clipping planes. The command line mode where commands are entered into the external GUI window supports all of the commands in the point and click mode, but is more flexible and possibly useful for complex selection and command issuing. Commands entered on the command line are executed when you press the return key.

command help	`help` *keyword*

Loading Files

file loading	`load data/test/pept.pdb`
loading from terminal	`pymol data/test/pept.pdb`
toggle between text and graphics	*Esc*
toggle Y axis rocking	`rock`
stereo view	`stereo on/off`
stereo type	`stereo crosseye / walleye / quadbuffer`
undo action	`undo`
reset view	`reset`
reinitialize Pymol	`reinitialize`
quit (force, even if unsaved)	`quit`

Mouse Control

	L Rota	M Move	R MovZ	Wheel Slab
Shift	+Box	-Box	Clip	MovS
Ctrl	+/-	PkAt	Pk1	—
CtSh	Sele	Cent	Menu	—
DblClk	Menu	Cent	PkAt	—

set the center of rotation	`origin` *selection*

Atom Selection

object-name/segi-id/chain-id/resi-id/name-id

molecular system selection	`/pept`
molecule selection	`/pept/lig`
chain selection	`/pept/lig/a`
residue selection	`/pept/lig/a/10`
atom	`/pept/lig/a/10/ca`
ranges	`lig/a/10-12/ca`
ranges	`a/6+8/c+o`
missing selections	`/pept//a`
naming a selection	`select bb, name c+o+n+ca`
count atoms in a selection	`count_atoms bb`
remove atoms from a selection	`remove resi 5`
general	`all, none, hydro, hetatm, visible, present`
atoms not in a selection	`select sidechains, ! bb`
atoms with a vdW gap < 3 Å	`resi 6 around 3`
atom centers with a gap < 1.0 Å	`all near 1 of resi 6`
atom centers within < 4.0 Å	`all within 4 of resi 6`

Basic Commands

Some commands used with atoms selections. If you are unsure about the selection, click on the molecule part that you want in the viewing window and then look at the output line to see the selection.

fill viewer with selection	`zoom /pept//a`
center a selection	`center /pept//a`
colour a selection	`colour pink, /pept//a`
force Pymol to reapply colours	`recolor`
set background colour	`bg_color white`
vdW representation of selection	`show spheres, 156/ca`
stick representation of selection	`show sticks, a//`
line representation of selection	`show lines, /pept`
ribbon representation of selection	`show ribbon, /pept`
dot representation of selection	`show dots, /pept`
mesh representation of selection	`show mesh, /pept`
surface representation of selection	`show surface, /pept`
nonbonded representation of selection	`show nonbonded, /pept`
nonbonded sphere representation of selection	`show nb_spheres, /pept`
cartoon representation of selection	`show cartoon, a//`
clear all	`hide all`
rotate a selection	`rotate` *axis, angle, selection*
translate a selection	`translate [x,y,z],` *selection*

Cartoon Settings

Setting the value at the end to 0 forces the secondary structure to go though the CA position.

cylindrical helices	`set cartoon_cylindrical_helices,1`
fancy helices [tubular edge]	`set cartoon_fancy_helices,1`
flat sheets	`set cartoon_flat_sheets,1`
smooth loops	`set cartoon_smooth_loops,1`
find rings for cartoon	`set cartoon_ring_finder,[1,2,3,4]`
ring mode	`set cartoon_ring_mode,[1,2,3]`
nucleic acid mode	`set nucleic_acid_mode,[0,1,2,3,4]`
cartoon sidechains	`set cartoon_side_chain_helper; rebuild`
primary colour	`set cartoon_color,blue`
secondary colour	`set cartoon_highlight_color,grey`
limit colour to ss	`set cartoon_discrete_colors,on`
cartoon transparency	`set cartoon_transparency,0.5`
cartoon loop	`cartoon loop, a//`
cartoon loop	`cartoon loop, a//`
cartoon rectangular	`cartoon rect, a//`
cartoon oval	`cartoon oval, a//`
cartoon tubular	`cartoon tube, a//`
cartoon arrow	`cartoon arrow, a//`
cartoon dumbell	`cartoon dumbell, a//`
b-factor sausage	`cartoon putty, a//`

Image Output

low resolution	`ray`
high resolution	`ray 2000,2000`
ultra-high resolution	`ray 5000,5000`
change the default size [pts]	`viewport 640,480`
image shadow control	`set ray_shadow,0`
image fog control	`set ray_trace_fog,0`
image depth cue control	`set depth_cue,0`
image antialiasing control	`set antialias,1`
export image as .png	`png` *image*`.png`

Hydrogen Bonding

Draw bonds between atoms and label the residues that are involved.

draw a line between atoms	`distance 542/oe1,538/ne`
set the line dash gap	`set dash_gap,0.09`
set the line dash width	`set dash_width,3.0`
set the line dash radius	`set dash_radius,0.0`
set the line dash length	`set dash_length,0.15`
set round dash ends	`set dash_round_ends,on`
hide a label	`hide labels, dist01`
label a reside	`label (542/oe1), "%s" %("E542")`
set label font	`set label_font_id,4`
set label colour	`set label_color,white`

Electrostatics

There are a number of ways to apply electrostatics in Pymol. The user can use GRASP to generate a map and then import it. Alternatively the user can use the APBS Pymol plugin. Pymol also has a built in function that is quick and dirty.

generate electrostatic surface `action > generate>vacuum electrostatics > protein contact potential`

Pymol Movies (mac)

move the camera	`move x,10`
turn the camera	`turn x,90`
play the movie	`mplay`
stop the movie	`mstop`
writeout png files	`mpng` *prefix* `[, first [, last]]`
show a particular frame	`frame` *number*
move forward on frame	`forward`
move back one frame	`backwards`
go to the start of the movie	`rewind`
go to the middle of the movie	`middle`
go to the movie end	`ending`
determine the current frame	`get_frame`
clear the movie cache	`mclear`
execute a command in a frame	`mdo 1, turn x,5; turn y,5;`
dump current movie commands	`mdump`
reset the number of frames per second	`meter_reset`

脚本扩展

Https://pymolwiki.org/index.php/

参考资料

Https://pymol.org/2/

Https://pymolwiki.org/index.php/

Pymol Reference Card

A Beginner’s Guide to Molecular Visualization Using PyMOL

By Nicholas Fitzkee

THANKS !