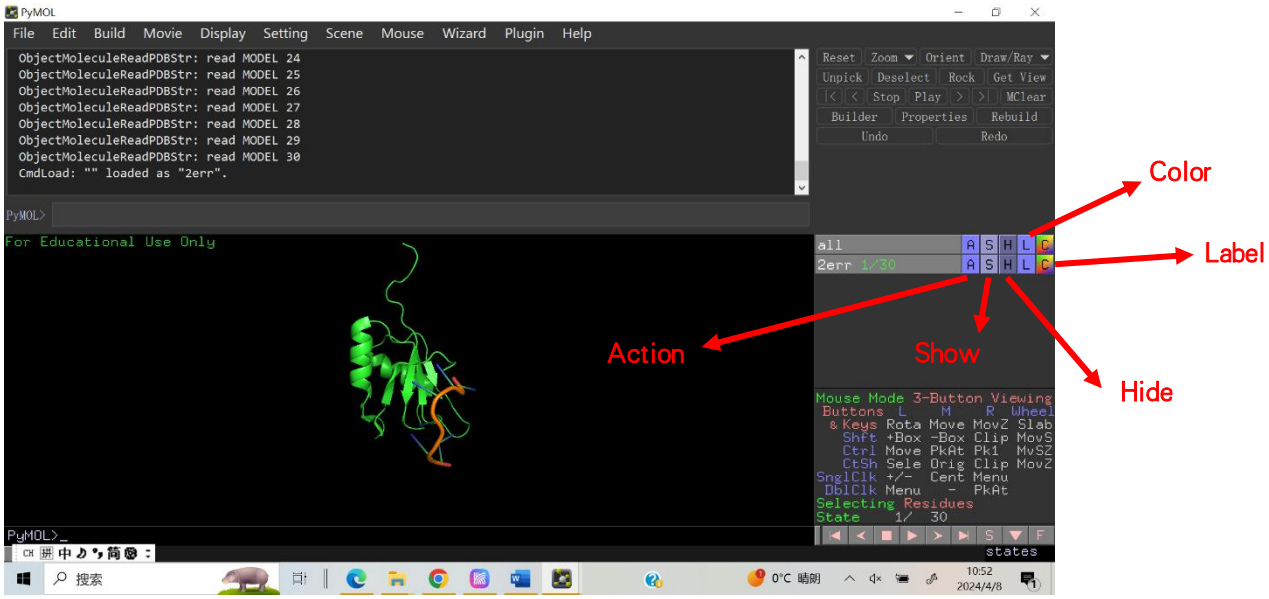
Contents

1.Protein or RNA display form

In the object list window, we can see that there are now 2 object names,

One is “all”, “all” is not a real object, it represents all objects. The other is “2err”, “2err” is the complex we just loaded. Each object has a corresponding A S H L C operation, as shown in the following figure:



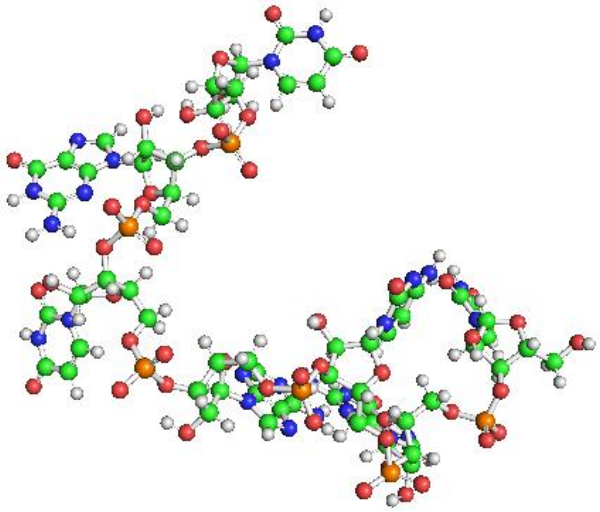
Action mainly includes a collection of common operations on objects, such as copying, deleting objects, hydrogenating objects, displaying objects, etc.

Part 1: Common display operations

Click A->preset->simple to display the simple form of the protein

Click A->preset->ball and stick to display the ball and stick model

Results as shown in the following figure:



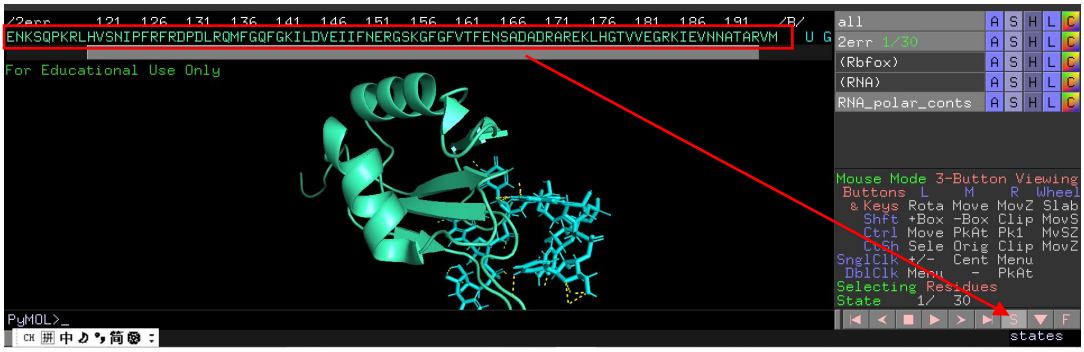
Click A->preset->b-factor putty to display the flexibility of the protein based on the bfactor value.

Click A->preset->publication high-quality publishing standards.

Part 2 :Object Operations

2.1 View the sequence of the structure (Sequence)

Click the S in the lower left corner to display the sequence information of the protein, as shown in the figure. Click the S again to hide the sequence information. S is the abbreviation of the word Sequence.



Some complexes contain water molecules:

Delete water molecules A->remove waters

This operation is a red warning operation and is irreversible. Once a water molecule is deleted, it cannot be undone via Ctrl-Z.

Add and delete hydrogen atoms:

H atoms can be seen in line and stick modes, but not in cartoon mode. Therefore, in line or stick mode, perform the following operations.

A->Hydrogens->remove deletes all hydrogen atoms;

A->Hydrogens->add adds all hydrogen atoms;

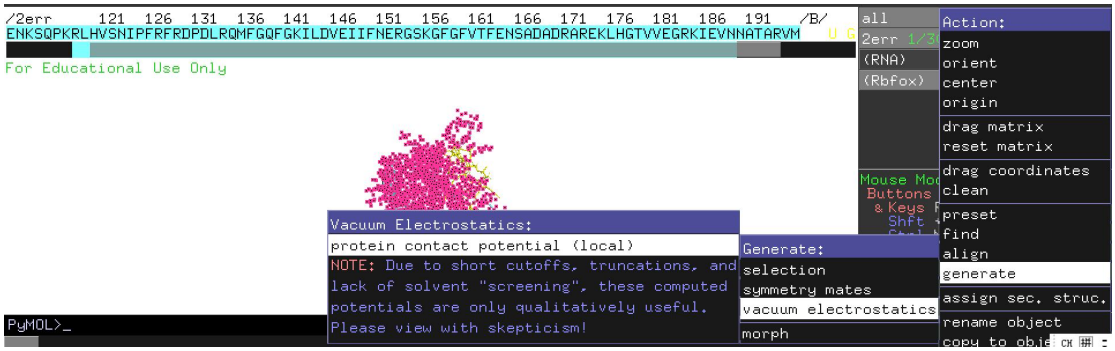
A->Hydrogens->remove non polar deletes all non-polar hydrogen atoms, we can see that all hydrogen atoms on C are deleted;

A->Hydrogens->remove deletes all hydrogen atoms again;

A->Hydrogens->add polar adds polar hydrogen atoms.

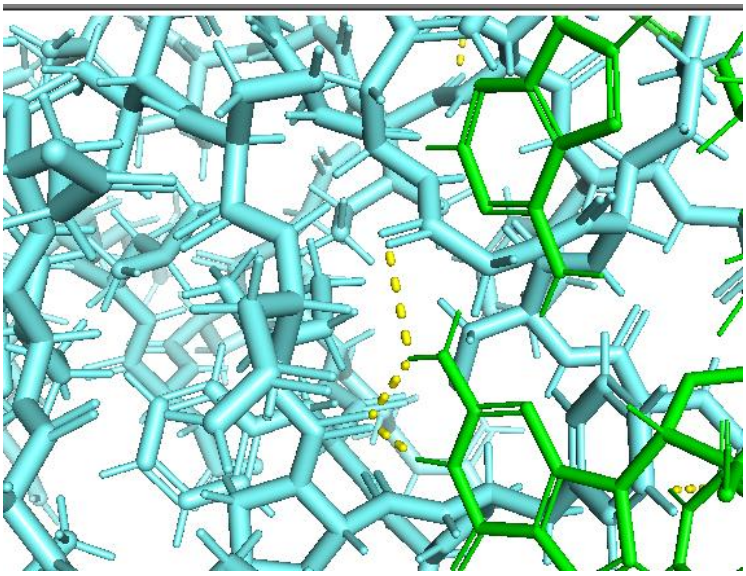
Part 3 :Action->generate operation

Display the electrostatic potential diagram of the protein Action->generate->vacuum_electrostatics->protein contact potential



Part 4:View polar interactions between protein and RNA

Select the RNA with the mouse, and the "sele" object will appear, then click action->find polar contacts->to other atom in object.

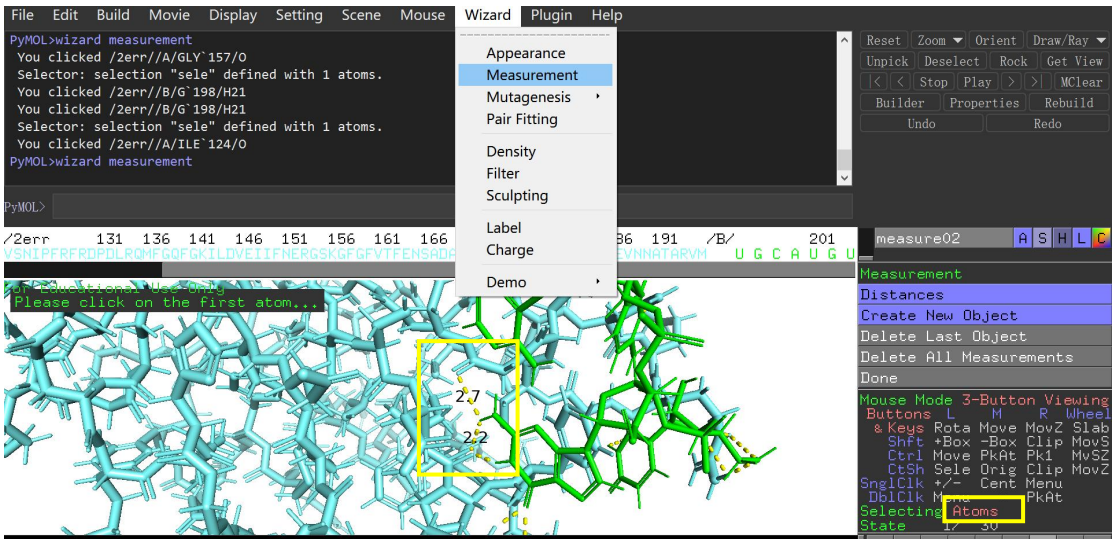


to other atom in object: Interactions between protein and RNA

to any atom: Consider both the interaction between the protein and the RNA, as well as the polar interaction within the RNA.

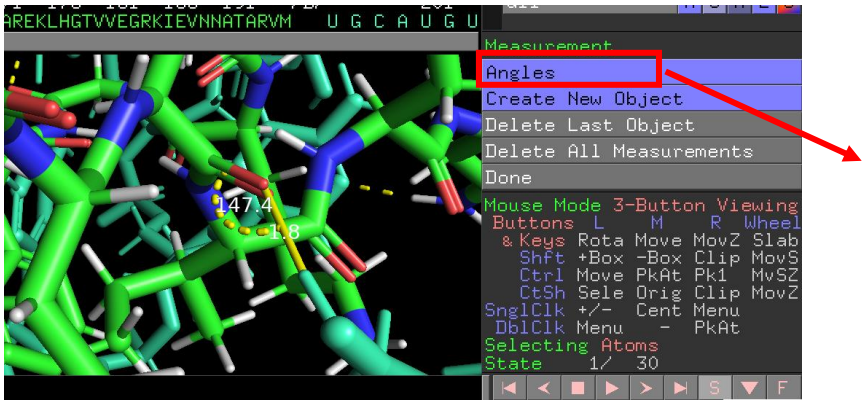
4.1 Measuring polar bonds distance

check the distance and angle to further determine the rationality and strength of the polar bonds.



4.2 Measure angle

Click Wizard->Measurement in the menu bar to open the measurement panel. The default mode is distance measurement. Click the Distances button in the Measuremnet panel to switch the Measurement Mode from Distances mode to Angles mode. Then select 3 atoms in sequence, such as ABC, then you can measure the angle <ABC.



After the measurement is completed, click done in the Measurement panel. Adjust the position of the Label and save the picture.

4.3 Measure the dihedral angle

The same operation as measuring distance and angle only needs to switch the measurement mode to Dihedrals.

4.4 Measure the distance of the ring

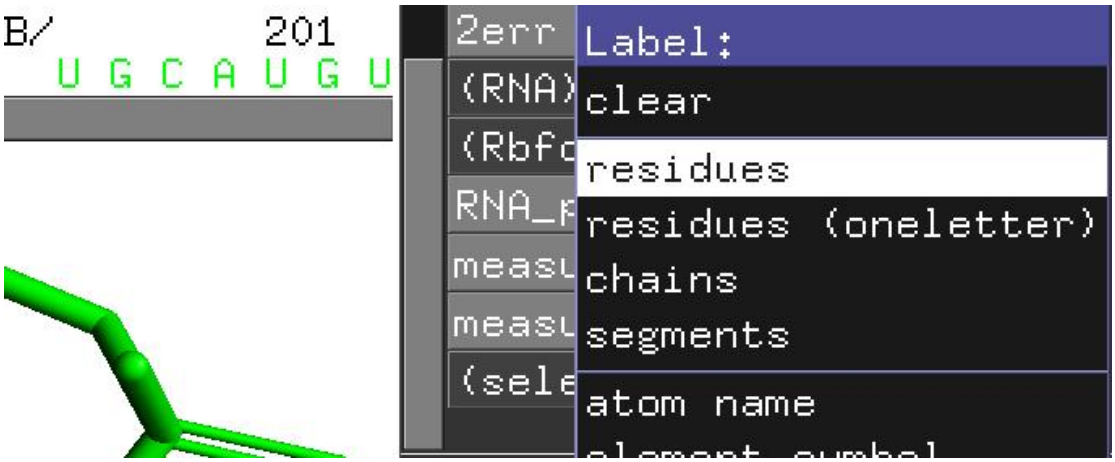
The same operation as measuring distance and angle only needs to switch the measurement mode to Dihedrals.

This mode is used to measure the distance between the centers of two rings, so the two selected atoms must be located on the ring, such as benzene ring, cyclohexane, N heterocyclic ring, etc. Otherwise it will be processed according to Distances mode.

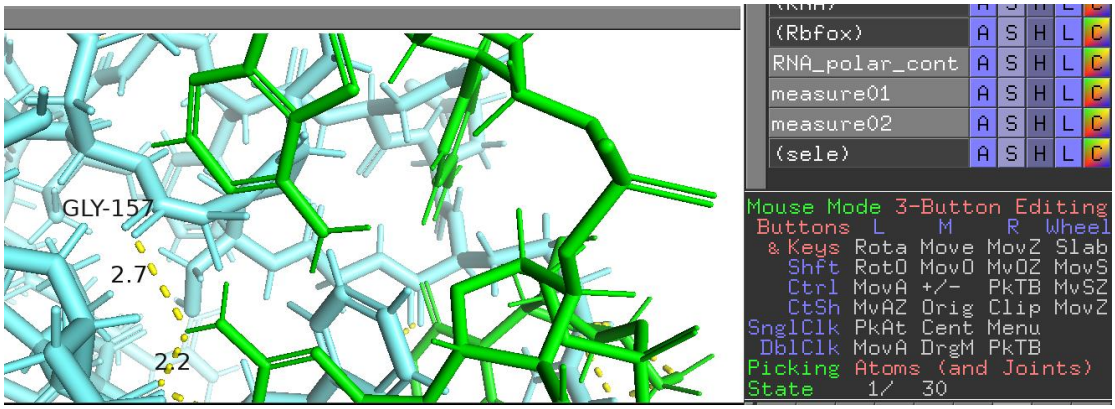
4.5 Shows the amino acid residues that form polar bonds

Click to select these residues respectively, note that the selection should be residues instead of atoms.

Select L->residues to display amino acids:

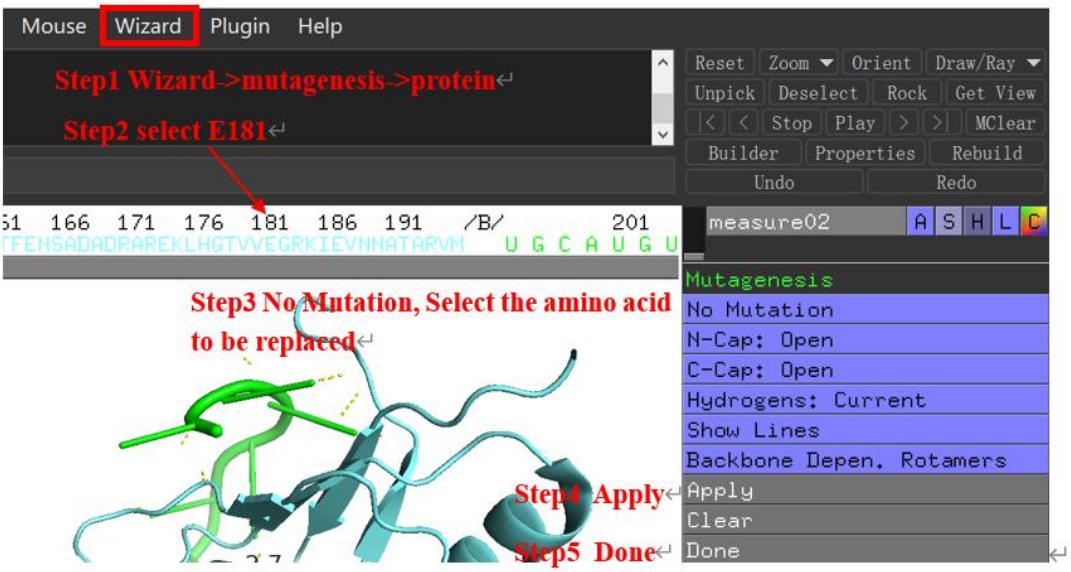


The results are shown :



2.Mutated amino acid residues

Click wizard->mutagenesis->protein in the menu

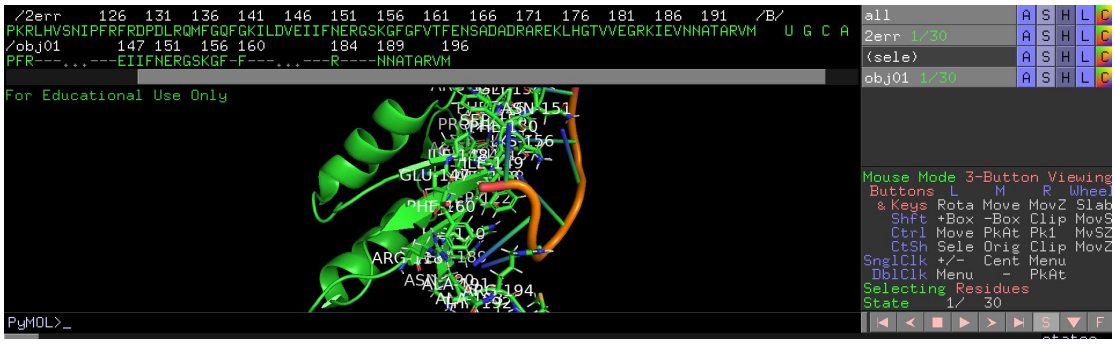


3. Amino acids near RNA

When the mode is residues mode, select the RNA.

Click A->MODIFY->RESIDUES WITHIN 4Å on the RNA; then click A->copy to object new.

After creating object, perform show as sticks and label residues on object1 to see the residues of nearby 4Å.



4. FAQs

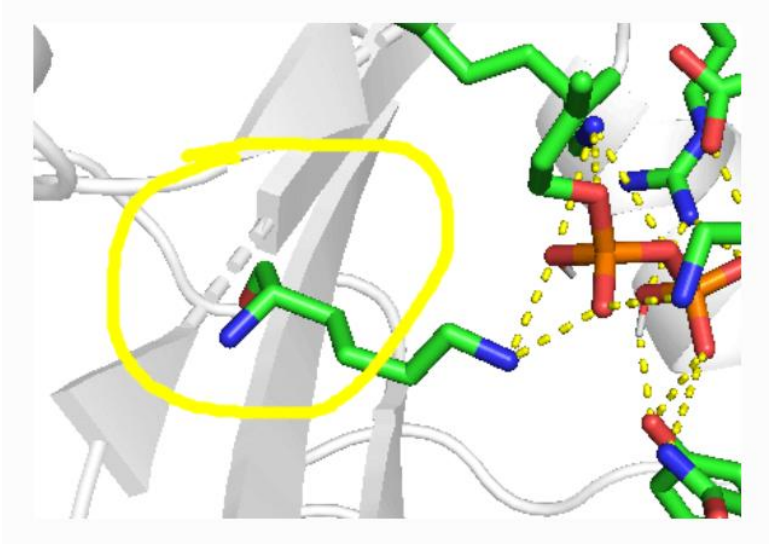
Q1. Dim interface

Q1. The structure opened in pymol is very dark, and reinstalling the software does not help. How to solve it?

The OpenGL module is not compatible. Turn off opengl in the rendering setting or reinstall the opengl driver. Or click File->reinitialize->original settings.

Q1. Protein fragmentation

Q1. When I use pymol to display interactions, show sticks, the beta fold of the protein is broken. How can I display it to make the protein look better and not break?



The main difference is show and show as.

The following focuses on Show: show has two types of operation methods:

show as click S->as->cartoon and S->as->stick respectively,

We can observe that AS mode erases the original rendering mode and then re-renders

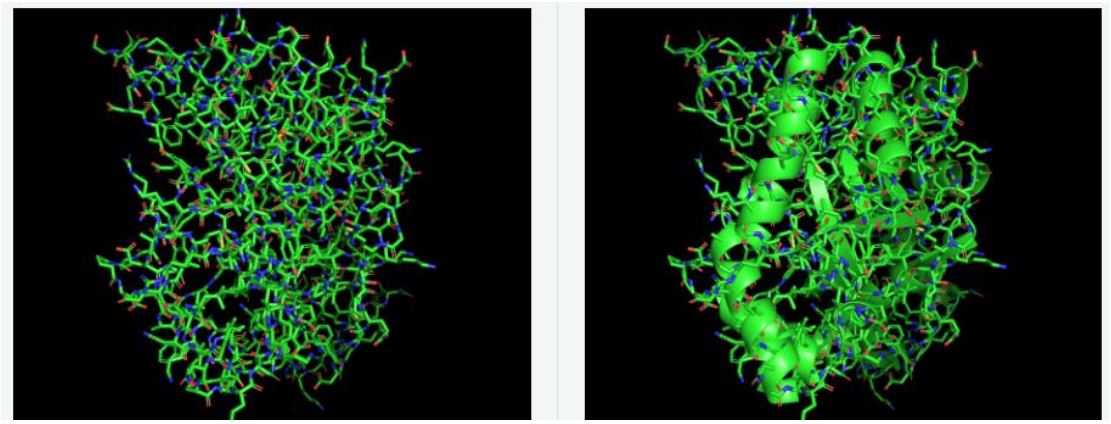
it. After the above operation, only the stick form is displayed.

show click S->as->cartoon and then click S->stick;

We can observe that the SHOW method retains the original rendering and then adds new rendering.

We first click S->as->cartoon on the 4hbk(PDBid) object, and then click S->as->stick, the effect is as shown in left picture;

We first click S->as->cartoon on the 4hbk object, and then click S->stick, the effect is as shown in right picture.



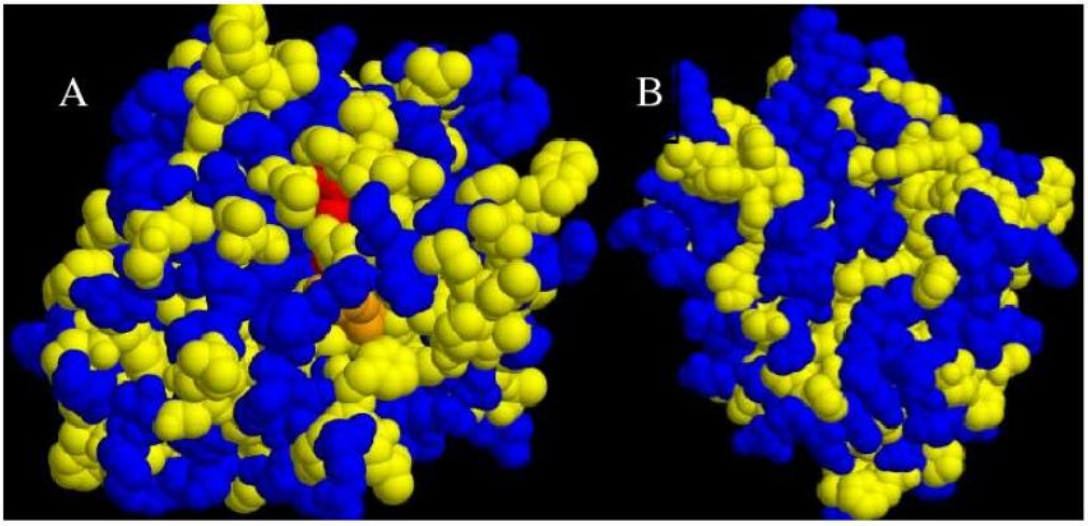
Q2. Eliminate dotted lines

Q2. How can pymol eliminate the dotted lines in automatic completion?

If an amino acid is missing or a section of seq has moved away from its original position, pymol will add a dotted line where it thinks the link is. If you want to hide the dotted line, just split it into two independent objects.

Q3. Hydrophobic amino acids and hydrophilic amino acids

Q3. How can I clearly display the hydrophilic amino acid residues and hydrophobic amino acid residue regions in pymol, as shown in the figure below?

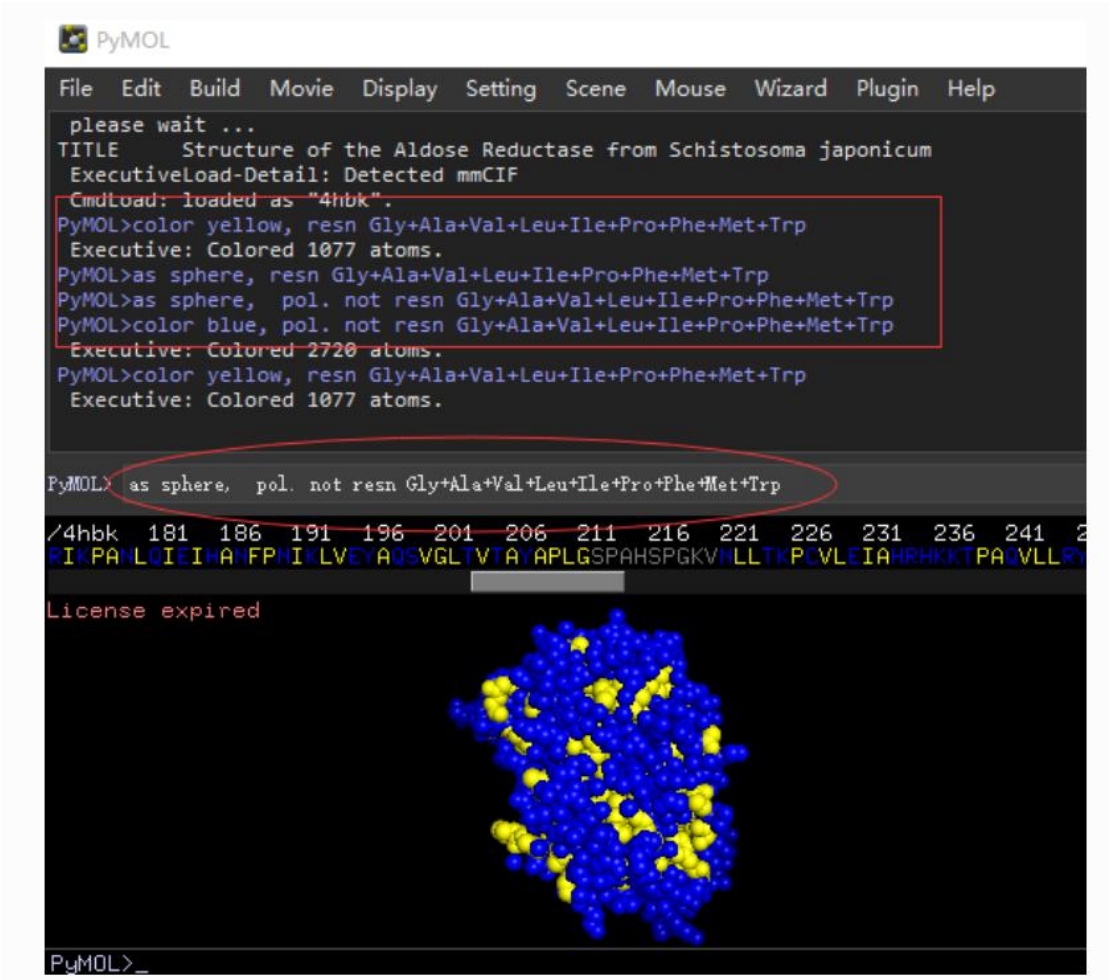


There are 9 hydrophobic amino acids: Gly, Ala, Val, Leu, Ile, Pro, Phe, Met, Trp. The nine amino acids that have hydrophobic side chains are glycine (Gly), alanine (Ala), valine (Val), leucine (Leu), isoleucine (Ile), proline (Pro), phenylalanine (Phe), methionine (Met), and tryptophan (Trp).

There are 6 non-electropolar (hydrophilic) amino acids: Ser, Thr, Cys, Asn, Gln, Tyr.

In the command line window, enter the following 4 commands:

```
color yellow, resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
as sphere, resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
as sphere,   resn Ser+Thr+Cys+Asn+Gln+Tyr+Asp+Glu+Arg+Lys+His
color blue,  resn Ser+Thr+Cys+Asn+Gln+Tyr+Asp+Glu+Arg+Lys+His
```


PyMOL
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
please wait ...
TITLE Structure of the Aldose Reductase from Schistosoma japonicum
ExecutiveLoad-Detail: Detected mmCIF
CmdLoad: loaded as "4hbk".
PyMOL>color yellow, resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
Executive: Colored 1077 atoms.
PyMOL>as sphere, resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
PyMOL>as sphere, pol. not resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
PyMOL>color blue, pol. not resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
Executive: Colored 2720 atoms.
PyMOL>color yellow, resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
Executive: Colored 1077 atoms.
PyMOL> as sphere, pol. not resn Gly+Ala+Val+Leu+Ile+Pro+Phe+Met+Trp
/4hbk 181 186 191 196 201 206 211 216 221 226 231 236 241
License expired
PyMOL>_