2.0.5 questions

Bookmark this page

Learning PyMOL video 5: Q1

1/1 point (ungraded)

Check the THREE options necessary below to get the best quality images from PyMOL:

- [x] Display → Quality → Maximum Quality
- [ ] Display → Color Space → RGB
- [x] Scene → Cache → Optimize
- [x] Antialiasing
- [ ] Scene → Buttons

For the best quality images, Antialiasing and Ray Tracing should be used and the Display quality should be set to Maximum Quality. Also, optimizing the cache will store displays like surfaces in the cache, making for smoother transitions between scenes. You can find out more about each of these items on the PyMOL wiki.

Submit You have used 2 of 2 attempts Show answer

Answers are displayed within the problem

Learning PyMOL video 5: Q2

1/1 point (ungraded)

What command should you enter in the command line to change the background color to grey ?

bg_color grey **Answer:** bg_color grey **or** bg grey

The 'bg_color' command is useful to change the background color. Similarly, the 'color' command can be used to color objects and selections as in "color blue, chain A".

Submit You have used 1 of 3 attempts Save Show answer

Answers are displayed within the problem

Learning PyMOL video 5: Q3

1/1 point (ungraded)

Earlier in the PyMOL tutorial, we explored the structure of human deoxy-hemoglobin. Here we will compare deoxy-hemoglobin and oxy-myoglobin, two globin-fold proteins that use heme to bind oxygen. Be sure to save your work periodically as you progress, so you can return if you make a mistake.

Preparing the two files for comparison.

Open a new PyMOL session and fetch the structure of oxy-myoglobin. The PDB code for oxy-myoglobin is 1MBO.

Deoxy-hemoglobin is 2DN2.

Display both structures as ribbon. This is a good representation for looking at superpositions of different proteins, which is what we will do here. Color each protein a different color. For hemoglobin, display only chain A – this is the one we will use for superposition. This would be a good time to save a scene, and save your session!

Click on "(all) | A" and choose "center" select. This centers based on both objects. An alternative, which isn't quite the same, is to type "center visible". This will center only on atoms currently displayed. Try them both!

Type "translate [-20,0,0], 2DN2". Note: this permanently changes the x,y,z coordinates of your object. Here, moving 2DN2 20 Å along the x-axis in your display window. Type "translate [0,20,0], 1MBO". If you have not changed your camera view, you can return to the original coordinates, by typing "translate [20,0,0], 2DN2; translate [0,-20,0], 1MBO". Note that the absolute coordinates are not important for the continuation of this exercise.

PyMOL has several ways of superimposing structures. We are interested in the root mean square deviation (RMSD), which is a measure of how similar two structures are. RMSD provides the average distance between equivalent pairs of atoms, in Å.

To align myoglobin onto chain A in hemoglobin, type "align 1MBO, chain A in 2DN2" at the command line. (Hint: use "help align" to better understand how this works.) Note that this "align" command also permanently modifies the x,y,z coordinates of the mobile object.

What is the RMSD from this alignment?

1.375 **Answer:** 1.375

1.375

The RMSD between deoxy-hemoglobin and oxy-myoglobin in 1.375 angstroms. You can see this in the top window of PyMOL. A proper alignment of 2 or more protein structures is typically the first step in identifying structural differences between models.

Submit You have used 1 of 2 attempts Save Show answer

Answers are displayed within the problem

Learning PyMOL video 5: Q4

2/2 points (ungraded)

One small but significant difference between the aligned deoxy-hemoglobin and oxy-myoglobin structures can be seen in the heme cofactor. Locate the heme in the aligned structures. You will probably need to display the hemes one at a time to answer this question.

What is the ND-FE-NB angle of the heme in chain a of hemoglobin?

158.4 **Answer:** 158.4

158.4

What is the ND-FE-NB angle of the heme in myoglobin?

174.5 **Answer:** 174.5

174.5

To find this answer, select one heme (remember, you can select Display→ Sequence On and then navigate the sequence to find and select HEM). Show the heme as sticks, and label the atoms. Zoom in on the heme, then use the measurement tool in the 'wizard' menu to click each atom to measure their angle.

The ND-FE-NB angle for the 2DN2 heme is 158.4.

The ND-FE-NB angle for the 1MBO heme is 174.5.

Submit You have used 1 of 2 attempts Save Show answer

Answers are displayed within the problem

© All Rights Reserved

edX
About
Affiliates
edX for Business
Open edX
Careers
News

Legal
Terms of Service & Honor Code
Privacy Policy
Accessibility Policy
Trademark Policy
Sitemap

Connect
Blog
Contact Us
Help Center
Media Kit
Donate

© 2021 edX Inc. All rights reserved.
深圳市恒宇博科技有限公司 粤ICP备17044299号-2