

PDB and Jmol Worksheet

1. Make a folder on your computer called "Molecular Modeling."
2. Go to the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) home page (<http://www.rcsb.org/>) and do the narrated tutorial if needed. Retrieve and place the following structure files in your "Molecular Modeling" folder: 1gcn and 1lcd (one-el-c-d).
3. Open the "Using Jmol" document in a separate window. It may be useful to quickly identify how to use several commands.
4. Open Jmol and complete this workshop.
5. Use Jmol to open the structure file for glucagon, 1gcn.pdb
6. Learn to use the following commands in Jmol: zoom, rotate, view, spin on/off, atom size, bond size, measure bond length, measure bond angle, and measure dihedral angle. Refer to the "Using Jmol" guide as needed.
7. Describe the orientation of the X, Y, and Z axes for a front view of glucagon.
Hints: to visualize axes: Display > Axes
to obtain front view: View > Front

Description of front view	
Axis	Position of axis
Positive X	
Positive Y	
Positive Z	

8. Which axes (+X, -X, +Y, -Y, +Z, or -Z) comes out of the screen toward the viewer for each view?

View	Axis coming toward viewer
Front	
Top	
Bottom	
Right	
Left	
Back (use pop-up menu)	

9. Identify the N-terminal nitrogen in the structure of glucagon.

Hints: Nitrogens are blue.

N-terminal nitrogen is on an end of the backbone.

N-terminal nitrogen is bonded to an α -carbon.

What is the N-terminal amino acid?

Hints: The positions of hydrogens are not usually determined by X-ray diffraction.

Use the structures of amino acids in your textbook if needed.

Which end of which axis is closest to the N-terminus?

10. Identify the C-terminal carboxyl group in glucagon.

Hints: Oxygens are red.

C-terminal carboxyl group is on an end of the backbone.

C-terminal carbonyl carbon is bonded to an α -carbon.

What is the C-terminal amino acid?

Which end of which axis is closest to the C-terminus?

11. Identify the N-terminus of glucagon and determine the sequence of the first three N-terminal amino acids. Use the three-letter designation for each amino acid.

N-terminus: _____ - _____ - _____ -

12. Identify the C-terminus and determine the last three amino acids in glucagon. Be sure to report your answer in the N \rightarrow C-terminal direction.

- _____ - _____ - _____ :C-terminus

13. In this part you will learn to use the "Script Console" to manipulate the structure of glucagon. Shut off any measurements that remain on the figure (Pop-up menu > measurements > delete measurements). Reset the view to the front view (Home button on top menu). Open the "Script Console" window (Pop-up > Console).

In the console window enter the following commands. After typing each command touch enter (return).

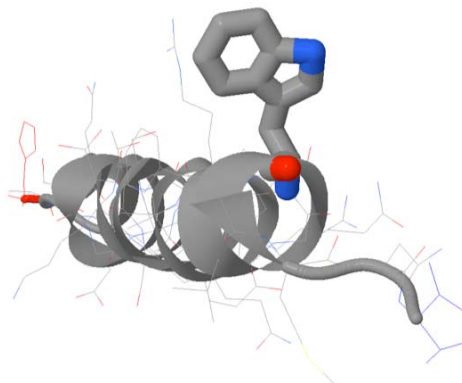
```
background white
spacefill off
wireframe
cartoon
rotate z -15
rotate y 90
rotate x 3
```

You should now be looking down the helical axis. We will now decide where the N-terminus is located in this view.

select 1
spacefill

Use the mouse to rotate the model to identify the N-terminus. Which amino acid is at the N-terminus? Hold the cursor over an atom in the N-terminal residue to see its identity.

color red
select 29
color blue
select
spacefill off
select 25
wireframe 0.5
zoom 200



Jmol

Use the mouse to rotate the model. Can you see a fuzzy caterpillar?
show sequence

The show sequence command indicates what is selected.

select
show sequence

Compare this result with what you reported in #11 and #12 above.

select acidic
spacefill

How many acidic residues are in glucagon?

Identify each of the acidic amino acids. Rotate with mouse as needed.

spacefill off
select basic
spacefill
color cpk

How many basic residues are in glucagon?

Identify each of the basic amino acids.

14. Use Microsoft Word to open the structure file for glucagon, 1gcn.pdb, and respond to the following:

How many amino acids are in glucagon?

Hint: Scroll down to the "SEQRES" (sequence) lines.

Paste the amino acid sequence of glucagon into the space below. It may be necessary to modify what you paste.

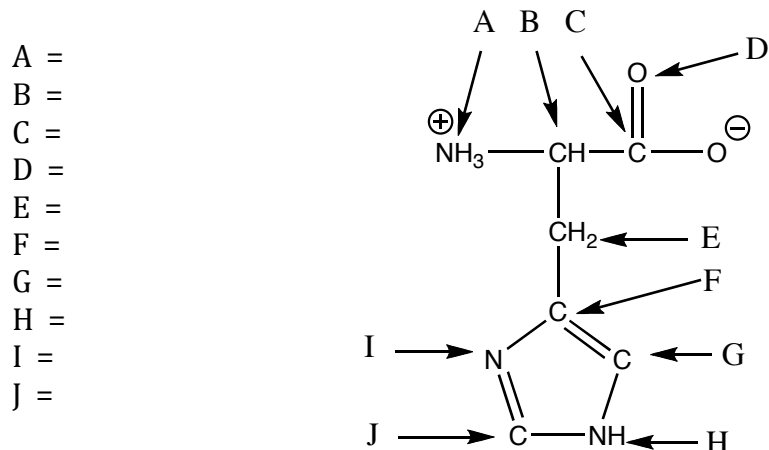
Check your answer for consistency with all previous questions.

The last pages of a protein database (pdb) file use one line for each atom whose position has been determined. Lines in a pdb file begin with a designation of the type of **record** on that line. Record designators include:

Record designator	Description
AUTHOR	lists authors
REMARK	various comments
SEQRES	primary structure
HELIX	region of helix structure
ATOM	identity and location of an individual atom

An ATOM record lists in order: a unique identifying number, a description of this atoms position within a particular amino acid, the identity of the amino acid, the identity of the chain in the overall structure, the sequence position for this amino acid, the X,Y, and Z coordinates, and other structure information.

For the structure of histidine, specify the label each atom (A - J in the figure) has as its designation in 1gcn to specify that particular atom.



15. From what organism was the glucagon described in 1gcn obtained?

16. Use Jmol to open the structure file for the lac repressor complex, 1lcd.pdb

17. Render the DNA as a violet cartoon:
Select DNA (Right mouse button > Select > Nucleic > All).
Render as cartoon (Right mouse button > Style > Scheme > Cartoon).
Make the cartoon violet (Right mouse button > Color > Structure > Cartoon > Violet).

18. Render the protein as space filling with the polar groups in red.
Select the protein (Right mouse button > Select > Protein > All).
Render as spacefill (Right mouse button > Style > Scheme > CPK spacefill).
Make the whole protein cyan (Right mouse button > Color > Atom > Cyan).
Make the polar residues red (Right mouse button > Select > Protein > Polar Residues),
then (Right mouse button > Color > Atom > Red).

19. Render the protein as a cartoon.
Select the protein (Right mouse button > Select > Protein > All).
Render as cartoon (Right mouse button > Style > Scheme > Cartoon).

20. Make the background white. Place the figure you have prepared using Jmol into this document in the space below. Scale the figure to fit on this page.

21. Which groove of the *lac* operon DNA has the most intimate contact with the Lac repressor?
22. Select the DNA (Select > Nucleic > DNA) and then change the color of the cartoon structure to CPK (Color > Structure > Cartoon > By Scheme > element cpk). When DNA is in cartoon style and CPK color, which end of the DNA is given a different color?
23. Hide the water molecules (Select > Hetero > All Water; Style > Scheme > CPK Spacefill; Style > Atoms > Off). List at least five of the polar residues in the Lac repressor that contact DNA when binding the *lac* operator. Indicate both the amino acid identity and the residue number. Hint, it may be helpful to select the polar residues of the protein and make them ball and stick with atoms at 50% of their van der Waals radii.
24. Place your name in the header of this document at the right margin. Save a copy of the completed worksheet in your "Molecular Modeling" folder.
25. Place a copy of your completed worksheet in the "Drop box" at the course D2L site.

Credits:

13 above is a modification from material developed by Jean-Yves Sgro, UW-Madison.

17, 18 and 19 above are from J. Gutow, UW-Oshkosh,

http://www.uwosh.edu/faculty_staff/gutow/Jmol_Web_Page_Maker/Export_to_web_tutorial.shtml

This worksheet was prepared by Warren Johnson, University of Wisconsin-Green Bay,

<http://www.uwgb.edu/johnsonw>. Permission is granted for use in education.