2.0.4 questions

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Learning PyMOL video 4: Q1

0/1 point (ungraded)

All of the following questions relate to hemoglobin, PDB ID 2DN2.

Let's examine one of the inter-subunit salt bridges important in hemoglobin's allosteric mechanism. We'll select a specific residue in the protein and label its atoms.

First, find the C-terminal Arginine 141 in the "A" chain of hemoglobin. Recall the the "Display → Sequence On" and "orient" can be helpful here.

Apply labels to the **atoms** of Arginine 141.

What are the names of the terminal nitrogen atoms of the arginine side chain? Type the names here separated by a comma and a space.

Hint: you may need to zoom in to the arginine to see the names. You can do this in the action menu (select the arginine, then pick action → zoom).

NH1

Answer: NH1 and NH2 **or** NH1, NH2 **or** NH1 NH2 **or** NH2, NH1 **or** NH2 NH1 **or** NH2 and NH1

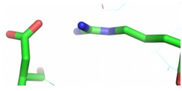
You can find these atoms by scrolling through the sequence display after you turn it on in the top window. OR, you could use the command line:

select CtermArg, chain A and resi 141

Where CtermArg is the name you are assigning to the selection and "chain A and resi 141" is used to select the specific amino acid.

Then zoom to the selection (A → zoom) and label the atoms (L → atom name)

NH1 and NH2 are the atom names given to the terminal amines of arginine.



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Answers are displayed within the problem

Learning PyMOL video 4: Q2

2/2 points (ungraded)

PyMOL can measure distances and angles in the molecular structures. The 'Wizard' menu provides a tool to easily make measurements by clicking on atom. A menu is in the bottom right selects between measurement types and includes distances and angles, with 'distance' as the default.

What is the distance between the "CB" and "CG" atoms in Arg141 of the A chain?

1.5 | **Answer:** 1.5

1.5

The Carbon–Carbon bond between CB and CG is 1.5 angstroms. You will need to be sufficiently zoomed in to the structure to see this to make the measurement!

Is this consistent with what you expect based on your knowledge of bond lengths?

- (•) Yes
- ( ) No

1.5 angstroms is the typical length for a carbon–carbon bond of this type.

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Answers are displayed within the problem

Learning PyMOL video 4: Q3

1/1 point (ungraded)

Select, orient, show as sticks only, and label only the atoms for Chain A Arg141 and Chain C Asp126 (Hint: type "help selections" for more info. You can use "residue identifier" to identify a residue by number like so : (resi #).

Booleans (and or) can be combined to refine selections.

Question: What is the distance between the amino groups of Chain A Arg141 (NH1 and NH2) and the oxygen groups (OD1 and OD2) of Chain C Asp126? Measure the distances from each amino nitrogen on the R-group to the oxygen atoms in the carboxyl functional group on the R-group of Asp126.

You should find four numbers, enter the shortest distance here. **Only enter the number one time!**

2.8 | **Answer:** 2.8

2.8

The closest atoms in this salt bridge are NH1 and OD2 which are 2.8 angstroms apart.

Here is an example of using the 'dist' command at the command line with boolean (AND) combination and wildcards (*) to measure four distances in a single step:

dist (chain A) AND (resi 141) AND (name NH*), (chain C) AND (resi 126) AND (name OD*)

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Answers are displayed within the problem

Learning PyMOL video 4: Q4

2/2 points (ungraded)

Next, let's measure some angles of this salt bridge.

Click the "Measurement Mode" toggle button in the Measurement Wizard and change it to "Angles" (it is in the viewer window and currently says "Distances").

Sequentially click on the first, second and third atoms in any given angle where the second atom is the vertex; (the command status will appear in the upper panel in case you are not sure if you clicked on an atom).

What is the angle between CB, CG and CD in Chain A Arg141?

109.6 | **Answer:** 109.6

109.6

The angle between CB, CG, and CD is 109.6.

Is this consistent with your knowledge of carbon chemistry?

- (•) Yes
- ( ) No

109.6 is typical of tetrahedral SP3 carbon geometry

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Answers are displayed within the problem

Learning PyMOL video 4: Q5

1/1 point (ungraded)

Hint - You can use the Display → Sequence ON, or use "select help" at the command line to get more info about the select command.

Once all Tyr residues are selected, change the representation to make the individual residues visible.

Hint: you don't need to manually select all the tyr residues from the sequence!

How many Tyr residues exist in the tetramer?

12 | **Answer:** 12

12

Here are 2 ways you could use to find the number of tyrosines in the structure:

1) With sequence displayed, use 'select (resn tyr)' at the command line to select all tyrosines. You can count these as selected, change the color to make them more visible in the sequence or use 'copy to object' to create a sequence showing 3 tyrosines in each chain for each of 4 chains in the model.

2) Selecting atoms will display the number of atoms in the external window. This provides a nice way to count residues - if you select for alpha carbons (CA) and Tyr residues, you can get a count in the external window.

select (resn tyr) and (name CA)

results in :

PyMOL>select (resn tyr) and (name CA)

Selector: selection "sele" defined with 12 atoms.

You can see here that 12 atoms are selected.

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Answers are displayed within the problem

Learning PyMOL video 4: Q6

0/2 points (ungraded)

How many acidic residues are in chain A?

Hint: to show certain classes of amino acids:
"select basic, (resn ARG+LYS+HIS)" or "select acidic, (resn ASP+GLU)"

464 | **Answer:** 12

464

How many basic residues are in chain B?

924 | **Answer:** 23

924

There are 12 acidic residues in Chain A and 23 basic residues in Chain B.

One way to figure this out is to select the C-alpha of each basic / acidic residue. For example:

select basic, chain B and (resn ARG+LYS+HIS) and (name CA)

Leads to a selection of 23 atoms, indicating 23 different basic residues.

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Answers are displayed within the problem