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Protein 3D representation

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Chimera

Chimera 1/3

Start Chimera

Open a 3D structure by PDB id:

Try 3PZD

This is human myosin X (chain A) in complex with a peptide (chain B)

Go to File > Fetch by ID > PDB

Type 3pzd in the window

Removing a structure

At the main menu go to
File > Close session

Then you can start again with the next structure
(otherwise structures are added)

Open again 3PZD

Viewing a structure

Click mouse left button and slide to rotate.

Click right button and slide to zoom in and out (or use your mouse wheel)

Pause pointer on a residue to see number and chain
This indicates amino acid, number and chain. (e.g. GLN1511.A)

Find residue 1723 in chain A.

Which type of amino acid is it?

What is the secondary structure conformation of this residue?

Open again 3PZD

Viewing a structure

These are fragments: the numbers correspond to the positions in the complete proteins.

Note the gaps, e.g. between positions 1963-1967 of chain A.

What do these gaps mean?

Note that there is a molecule represented, which is not a protein. That molecule is glycerol.

Selecting

Ctrl and click to select a single residue

Menu Select > Chain > to select a whole chain

Select chain B. What is the most abundant secondary structure for this chain?

Select > zone > (try a distance range < 5A)

If a residue or atom is selected: arrow up selects its secondary structure element, up again selects chain, up again selects all chains. Arrow down goes back.

Left/right arrows inverts selection.

Selecting by residue number

Select > Atom specifier >

This opens a little window where you can type ranges.

Examples:

:1510-1520.a

(Hint: Type Apply and not OK to keep the window open)

Selects residues 1510 to 1520 in chain A

:1425-1434.b

Selects residues 1425 to 1434 in chain B

Focusing

Select a residue (ctrl + click)

Actions > Focus

This will close the view on the selection

Get back to the original view by selecting the whole molecule (arrow up) and doing again:

Actions > Focus

Try this again with a selection of a protein fragment.
The view will focus on the selected fragment.

Set pivot

Select a residue

Actions > Set pivot

This will make the rotation center on the selection

Try these steps on the molecule of glycerol

You can see which residues are close to the molecule of glycerol:

Select > zone >

Then specify in the window that appears: select all atoms at <5.0 angstroms from the selection

How many residues are at less than 5.0 angstroms from the glycerol molecule?

Is there a cysteine among those? Which residue number?

To get back select all (arrow up) then
Actions > Focus

Measuring distances

Keep the focus on the molecule of glycerol. We can measure how far from it are the atoms of the side chains of the residues around it.

Tools > Structure analysis > distances

To define a distance select one atom in the glycerol with Ctrl+click and a second in a side chain of an amino acid in the protein with Shift+Ctrl+click. Then press the button "Create" in the small window.

What is the closest distance of an oxygen of the glycerol to the sulfur of cysteine 1706?

To get back select all (arrow up) then

Actions > Focus

Colouring a peptide chain

Select chain B

Select > chain > B

Actions > color > red

Changing representation

Default is ribbon

Try other things:

Actions > Atom/Bonds > Show

Actions > Atom/Bonds > sticks

You can hide the ribbon of the (selected) chain B.

Actions > Ribbon > hide

Represent the glycerol as spheres.

How can you use representation to check if the glycerol is exposed to the solvent or not? What is the result?

Chimera 2/3

Close session and load 3PQR

This is rhodopsin, a transmembrane protein
Let's find the hydrophobic part of the protein

Color residues by property

First select: Select > Residue > amino acid category
> hydrophobic

Then color:

Actions > colour > blue

Generate a surface

Select > chain > A

Actions > surface > show

Chimera 3/3

Close session and load 1GLU

This is the glucocorticoid receptor dimer bound to DNA
Let's find out if the interface of interaction with DNA
has positively charged amino acids

Color residues by property

First select: Select > Residue > Amino acid category >
positive

Then color: Actions > Color > blue
(Also color negative residues red)

Chimera 3/3

Generate a surface

(Script is a bit buggy when things are on the way – we remove the DNA first)

Select the DNA chains and then delete them:

Actions > Atoms/Bonds > Delete

(This cannot be undone!)

Now we do the surface:

Actions > Surface > Show

How to get back the DNA?

Fetch again 1GLU without closing the session
(the new molecule will be overlapped)