

This tab use NGLVieweR (R package) to visualize where the significant peptides are located using the protein crystal structure. To start, you will need either a pdb file or a pdb code. Select how you want to upload the pdb structure and click calculate.

The screenshot shows a web interface titled "3D Structure". It has a blue header bar with a menu icon. Below the header, the text "Please select how to import your PDB file:" is followed by two radio buttons: "Using PDB file" (selected) and "Using PDB number". To the right, under "Select PDB file", there is a "Browse..." button and a "No file selected" button. Below these options is a "Calculate" button. Three orange arrows point from text boxes to the interface: one points to the "Using PDB file" radio button, another points to the "Browse..." button, and a third points to the "Calculate" button.

3D Structure

Please select how to import your PDB file:

- ☒ Using PDB file
- ☐ Using PDB number

Select PDB file

Browse... No file selected

Calculate

Select here if you want to use wither a pdb file or a PDB code.

Add your file or input the code.

Click calculate!

Once the calculate button is pressed, a cartoon representation of your protein will be displayed. The coloring scheme is the same as used in the global woodspot representation. Colored in gray are the non-significant peptides, in red peptides with increased flexibility (positive deltaD values (state 2-state ref)), in blue, peptides with increased protection in the HDX experiment (negative deltaD values (state 2-state ref)). Regions colored in yellow are the regions showing both increase in protection and increase in flexibility at different timepoints.

Below the crystal structure, there are basic commands to change the representation. The user can select either cartoon, ball+stick or surface representations and to turn the spin on/off.

Additionally, there is a box to add an amino acid offset. We understand that sometimes the crystal structure used might have either additional or reduced number of residues at the N-terminal. For those cases the user can add an offset to match the amino acid sequences from the HDX experiment and the crystal structure.

Two buttons are located below the structure controls. One to download a high-resolution PNG screenshot of the crystal structure and another one to download a Pymol script with the significant peptides.



## 3D Structure

Please select how to import your PDB file:

- ☐ Using PDB file  
☒ Using PDB number

Type PDB code here:

1hzb

Calculate



Click to download a high-resolution PNG screenshot.

Select Representation

cartoon

Spin

Amino acid offset

0

Structure controls

Save screenshot

Download pymol script

Click here to export the results into pymol.