



University of Ljubljana  
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# P4EU ChimeraX workshop

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# Introduction

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- Overview of top menus
- How do we navigate the model pane
- command line
- Plugins
  - MD viewer is not standard anymore (yet):  
<https://cxtoolshed.rbvi.ucsf.edu/apps/moleculardynamicsviewer>

## **Links to more resources:**

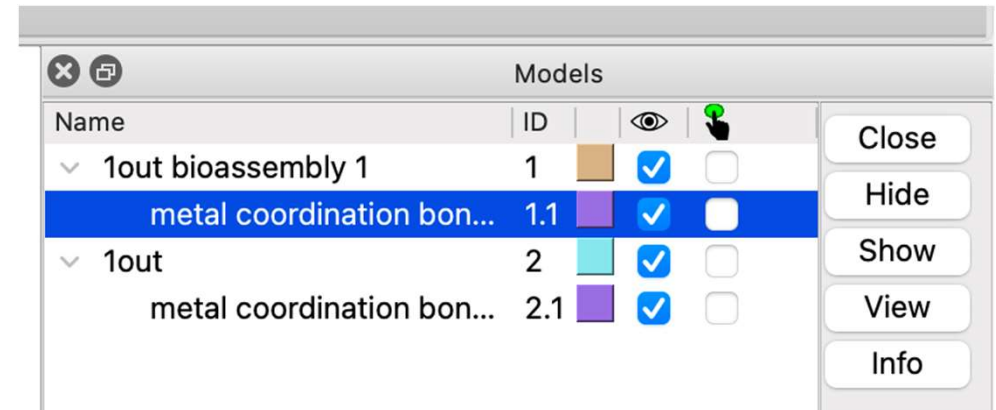
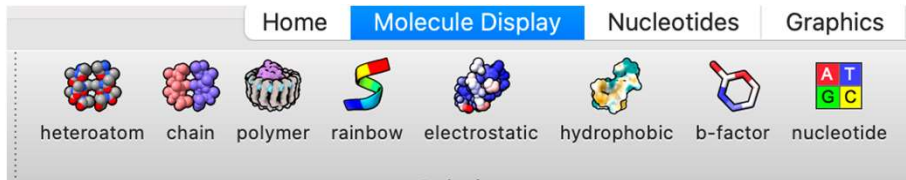
- Link to more tutorials: <https://www.cgl.ucsf.edu/chimerax/tutorials.html>
- Movie-making example: <https://kpwulab.com/2022/03/05/chimerax-make-movies/>

# Task 1.1: Structure of hemoglobin (1OUT)

1. Get the structure:

- open 1out
- open 1out fromDatabase rcsb\_bio

Do you notice the difference? Which is biologically relevant?



Concepts: model panel, coloring

## Task 1.2: Getting just a single subunit and observing the hem

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1. **Select>Chains> (select chain A)**
2. **Select>Invert**
3. **Action>Atoms/Bonds>Delete**
4. **Actions>Set pivot** (for easier manipulation)
5. **File>Save...** (saving session; there is no universal UNDO button!, saving PDBs if needed)

## Task 1.3: Colour the polypeptide chain and heme group differently

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1. **Select>Residues>Standard Amino Acids**

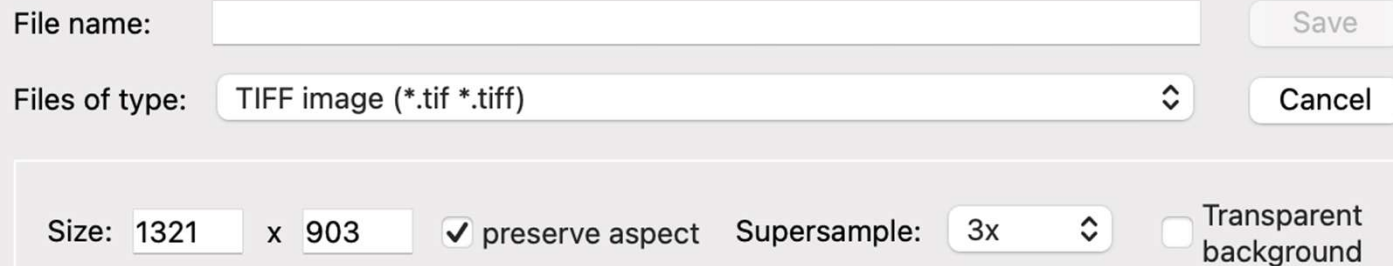
2. **Action>Color>(choose color)**

3. **Select>Residues>HEM**

4. **Action>Color>By Heteroatom**

5. **File>Save...**

by changing the format we can also save HIGH res pictures with transparent background



File name:  Save

Files of type: TIFF image (\*.tif \*.tiff)

Size:  x   preserve aspect    Supersample:   Transparent background

Task 1.4: Color by direction of the chain

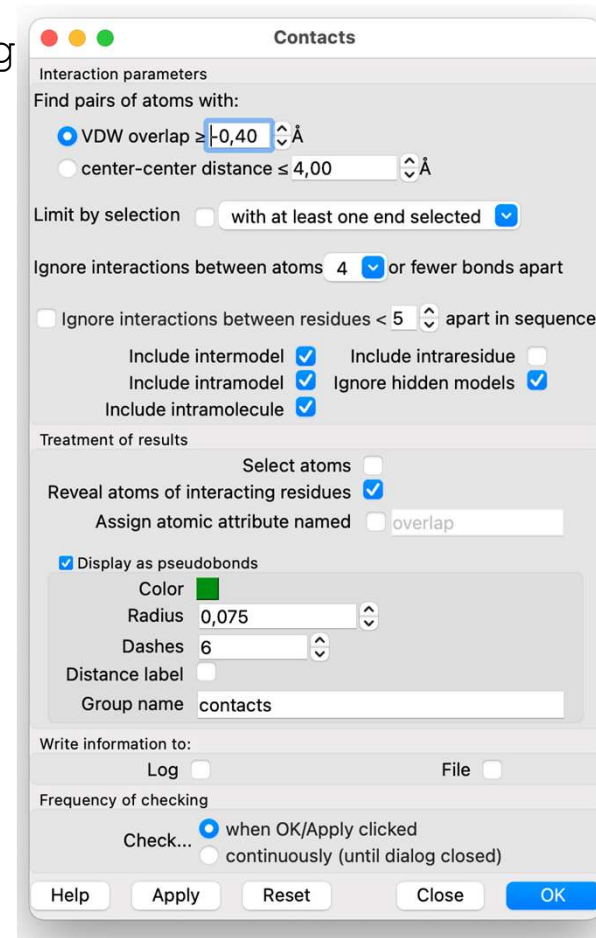
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Task 1.5: Display and color labels

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## Task 1.6: Observe interactions between hem and polypeptide chain

1. **Tools>Structure Analysis>Contacts** (mind the settings)
2. **Tools>Structure Analysis>H-Bonds** (mind the settings)
3. **Select>Zone...** or **Select>Broaden**
4. **Select>Define selector**
5. **Select polypeptide chain**
6. **Action>Surface>Show**
7. **color by hydrophobic (in menu)**



## Task 2: Analyze the cathepsin K complexes with chondroitin sulfate

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(PDB: 3C9E and 4N8W). What types of interactions are present between the molecules?

1. **Tools>Structure Analysis>Matchmaker**
2. **Editing model numbers in Models panel**
3. **Using contacts/H-bonds/surface**



# Task 3.1: Get active site of an enzyme

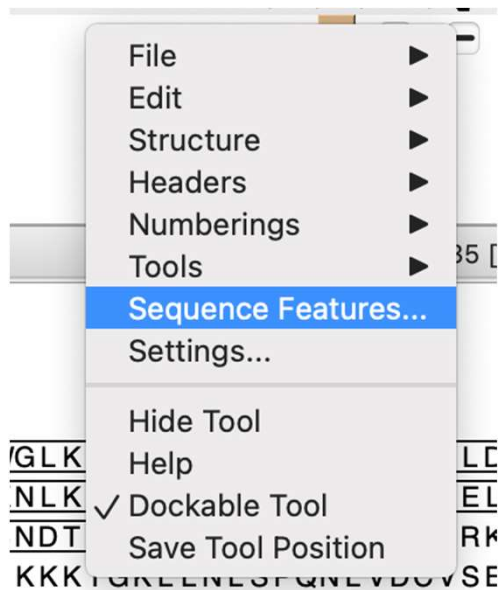
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(PDB: 1atk).

## 1. Get sequence connected to UniProt

Chain information for 1atk #1		
Chain	Description	UniProt
A	<a href="#">CATHEPSIN K</a>	<a href="#">CATK_HUMAN 1-215</a>

## 2. Check sequence properties in the sequence pane



## Task 3.2: Introduce mutation

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(PDB: 1atk).

Pycnodysostosis is an extremely rare hereditary skeletal disease. Thus far, only about 200 cases have been described, and it is estimated that currently 1-1.7 million people are affected. Several mutations in the cathepsin K gene have been identified as the cause of the disease. Explain what consequences these mutations have on the structure and consequently on the function of the enzyme. (In the exercises, we will focus only on the mutation that leads to the change of the amino acid residue Gly at position 146 to Arg - G146R)

### 1. Renumber residues correctly:

[https://www.uniprot.org/uniprotkb/P43235/entry#ptm\\_processing](https://www.uniprot.org/uniprotkb/P43235/entry#ptm_processing)

2. `sel :146` (is it a glycin?)

3. `renumber #1 start 115`

4. `sel :146`

5. **Tools>Structure Editing>Rotamers**

6. **And, ChimeraX does not have the energy minimization function anymore**  
(not?)