

Treinamento em Biologia Computacional - Módulo 2

Equipe de Dados Biológicos (EDB)

Grupo de Design de Proteínas (GDP)

Laboratório de Biologia Computacional (LBC)

Dia 2 (07/11/2025)



MINISTRY OF
SCIENCE TECHNOLOGY
AND INNOVATION



Módulo 2

Visualização molecular de biomoléculas no ChimeraX

Equipe de Dados Biológicos (EDB)

João V. S. Guerra

Grupo de Design de Proteínas (GDP)

Helder V. Ribeiro-Filho

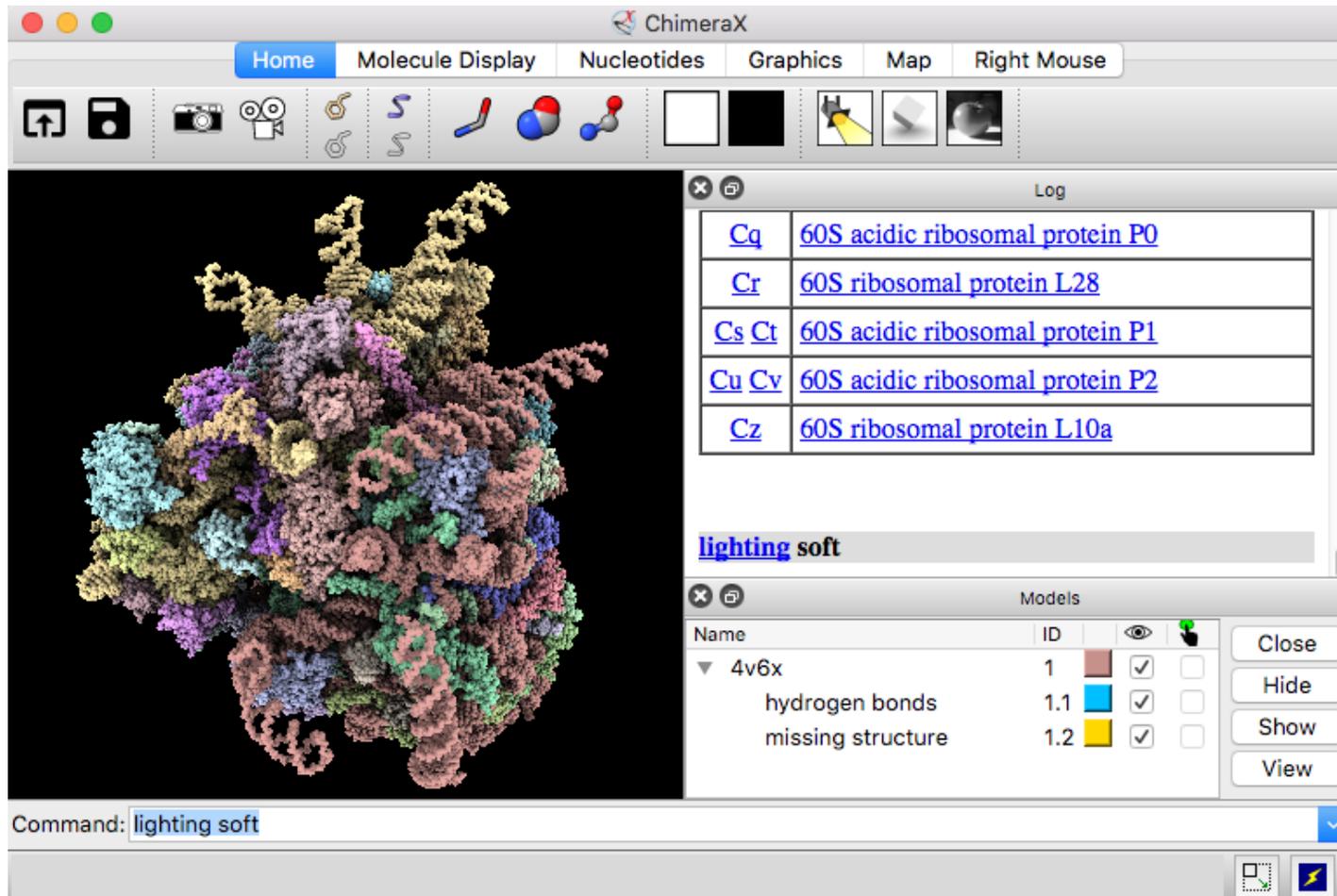
Dia 2 (07/11/2025)



MINISTRY OF
SCIENCE TECHNOLOGY
AND INNOVATION



- » O UCSF [ChimeraX](https://www.cgl.ucsf.edu/chimerax) é um software de código aberto de última geração para visualização, análise e manipulação de estruturas moleculares e dados relacionados.

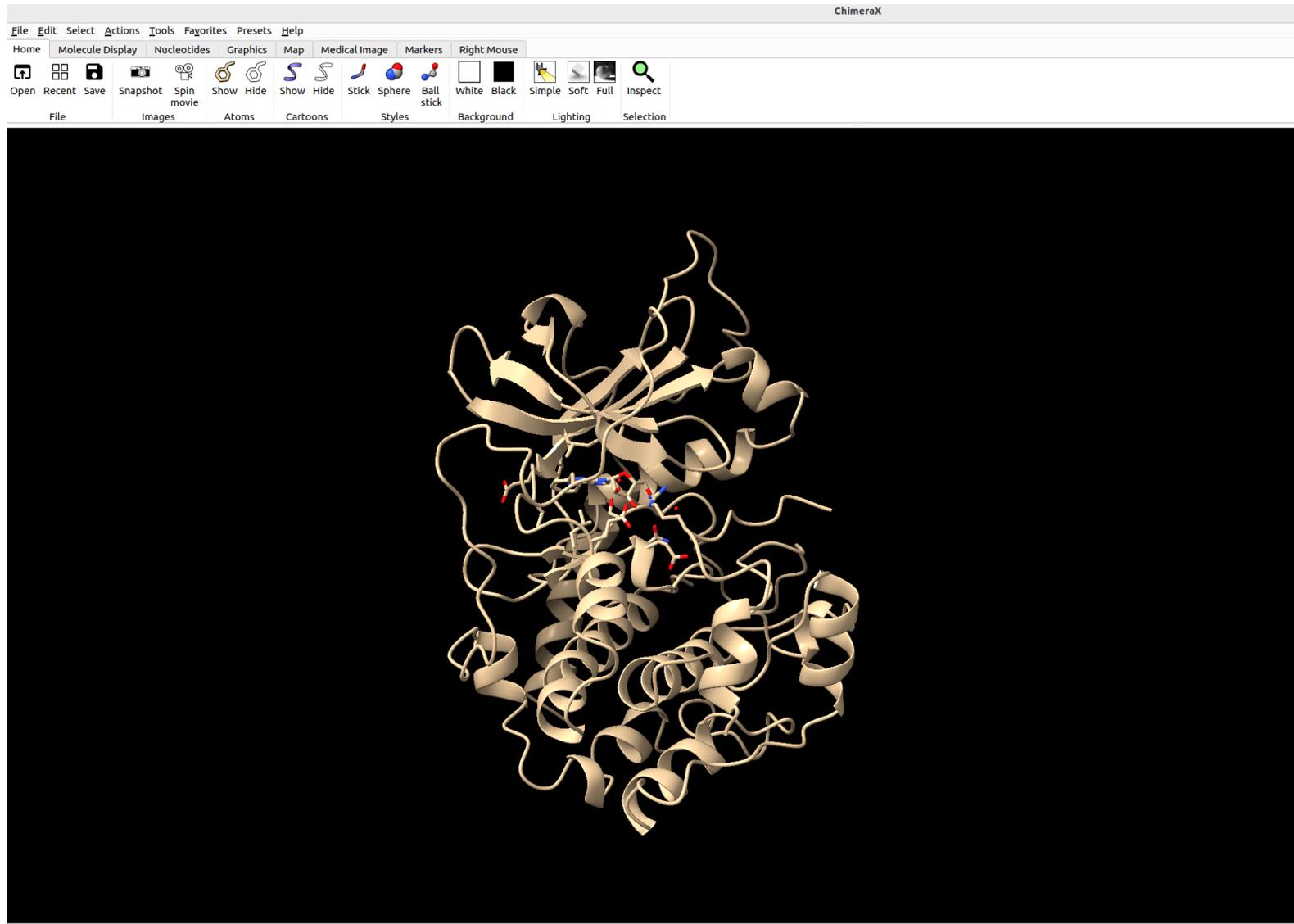


Principais funcionalidades:

- Visualização interativa de moléculas
- Suporte a múltiplos formatos (PDB, mmCIF, MRC etc.)
- Medições (distâncias, ângulos, contatos) e manipulação estrutural
- Análise de mapas de crio-EM e dados volumétricos
- Integração com bancos de dados (PDB, AlphaFold, UniProt)
- Geração de imagens e animações de alta qualidade
- Suporte a scripts em Python e plugins

Download: www.cgl.ucsf.edu/chimerax

A interface de visualização do ChimeraX



Show Sequence from Structure

Usage: `sequence chain chain-spec [viewer true | false]`

Log

Startup Messages	
note	available bundle cache has not been initialized yet

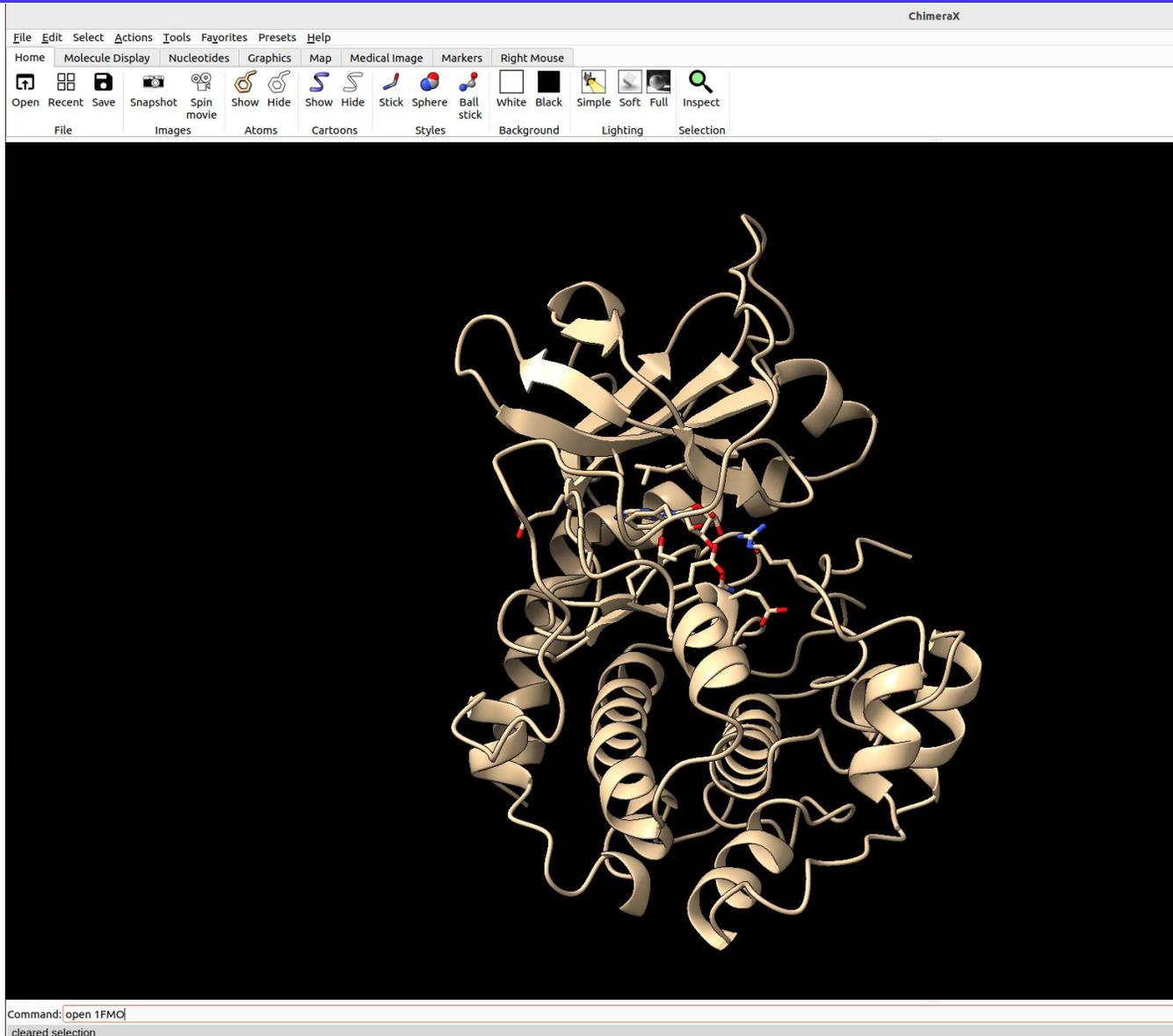
UCSF ChimeraX version: 1.9.dev202410230938 (2024-10-23)
© 2016-2024 Regents of the University of California. All rights reserved.
[How to cite UCSF ChimeraX](#)
open 1fmo format mmCIF fromDatabase pdb
1fmo title:
Crystal structure of A polyhistidine-tagged recombinant catalytic subunit of camp-dependent protein kinase complexed with the peptide inhibitor pki(5-24) and adenosine
[\[more info...\]](#)

Chain information for 1fmo #1		
Chain	Description	UniProt
E	CAMP-DEPENDENT PROTEIN KINASE	KAPCA_MOUSE 1-350
I	HEAT STABLE RABBIT SKELETAL MUSCLE INHIBITOR PROTEIN	IPKA_RABIT 5-24

Non-standard residues in 1fmo #1
[ADN – adenosine](#)

Models						
Name	ID			Skip		Close
1fmo	1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>		Hide Show View Info

Abrindo e salvando uma estrutura/seção no ChimeraX



ChimeraX

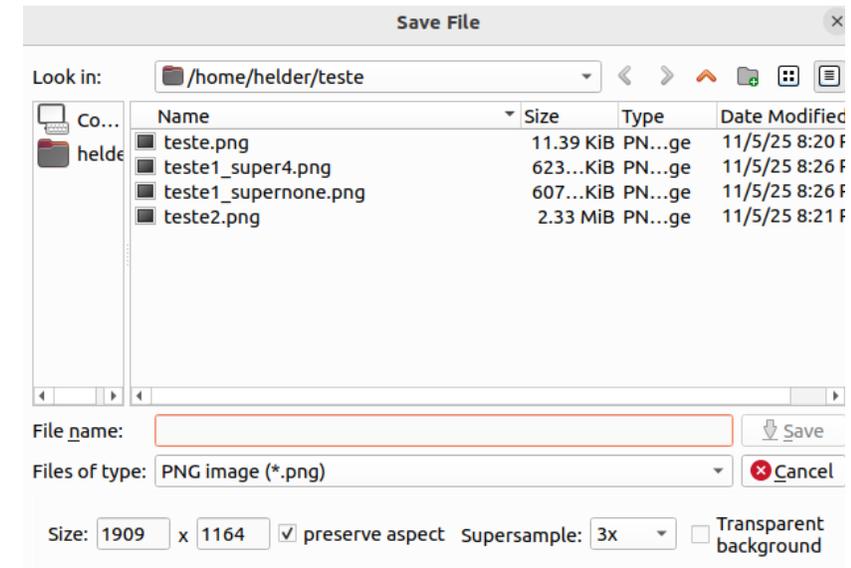
File Edit Select Actions Tools Favorites Presets Help

Home Molecule Display Nucleotides Graphics Map Medical Image Markers Right Mouse

Open Recent Save Snapshot Spin movie Show Hide Show Hide Stick Sphere Ball stick White Black Simple Soft Full Inspect

File Images Atoms Cartoons Styles Background Lighting Selection

Command: open 1FMO
cleared selection



Save File

Look in: /home/helder/teste

Name	Size	Type	Date Modified
teste.png	11.39 KiB	PN...ge	11/5/25 8:20 F
teste1_super4.png	623...KiB	PN...ge	11/5/25 8:26 F
teste1_supernone.png	607...KiB	PN...ge	11/5/25 8:26 F
teste2.png	2.33 MiB	PN...ge	11/5/25 8:21 F

File name:

Files of type: PNG image (*.png)

Size: 1909 x 1164 preserve aspect Supersample: 3x Transparent background



Hierarchical Specifiers

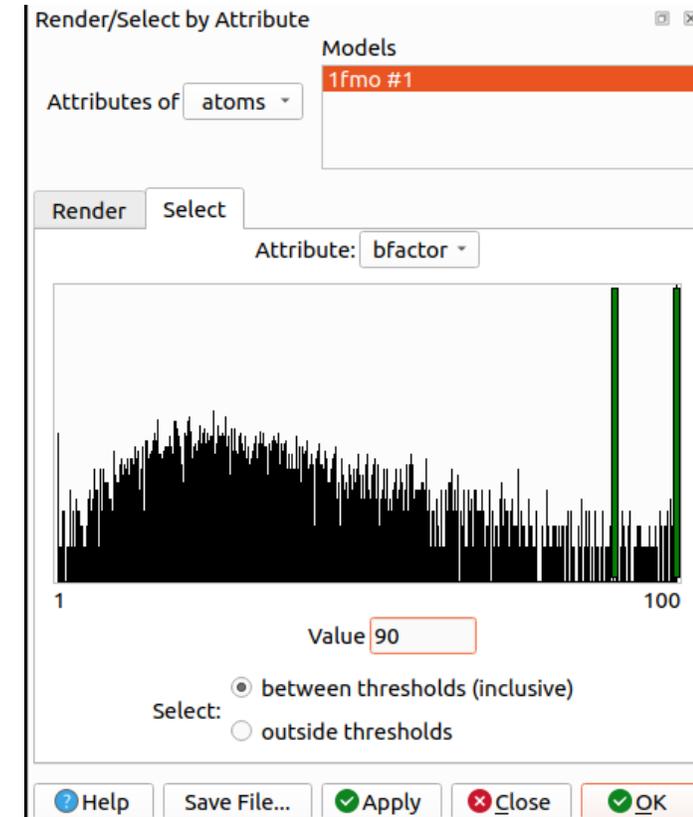
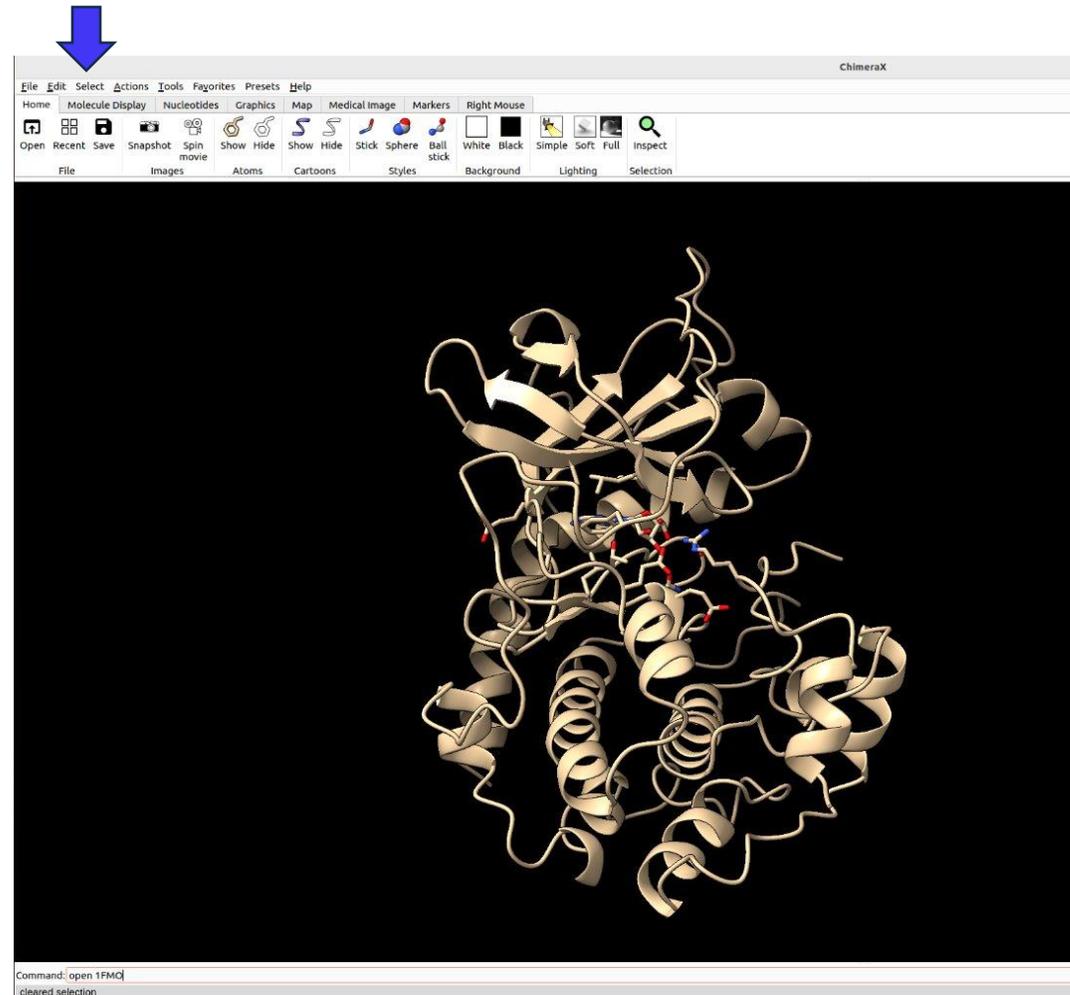
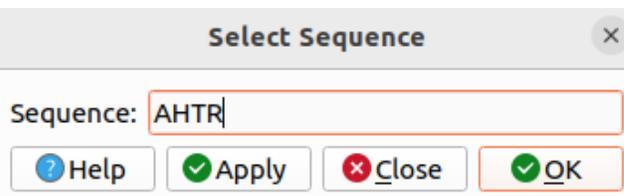
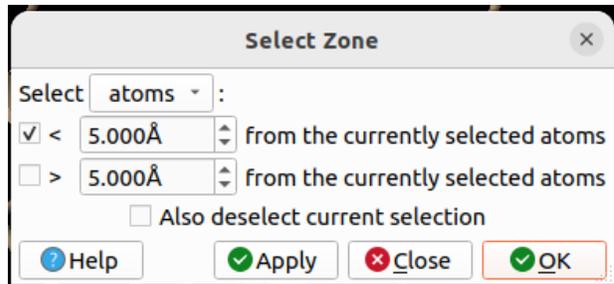
Symbol	Reference Level	Definition	Examples
#	model	model number assigned to the data in ChimeraX (hierarchical, with positive integers separated by dots: N, N.N, N.N.N, <i>etc.</i>)	#1 #1.3
/	chain	chain identifier (case-insensitive unless both upper- and lowercase chain IDs are present)	/A
:	residue	residue number <i>OR</i> residue name (case-insensitive)	:51 :glu
@	atom	atom name (case-insensitive)	@ca

<https://www.cgl.ucsf.edu/chimerax/docs/user/commands/atomspec.html#hierarchy>

Seleções no ChimeraX

Principais tipos de seleção:

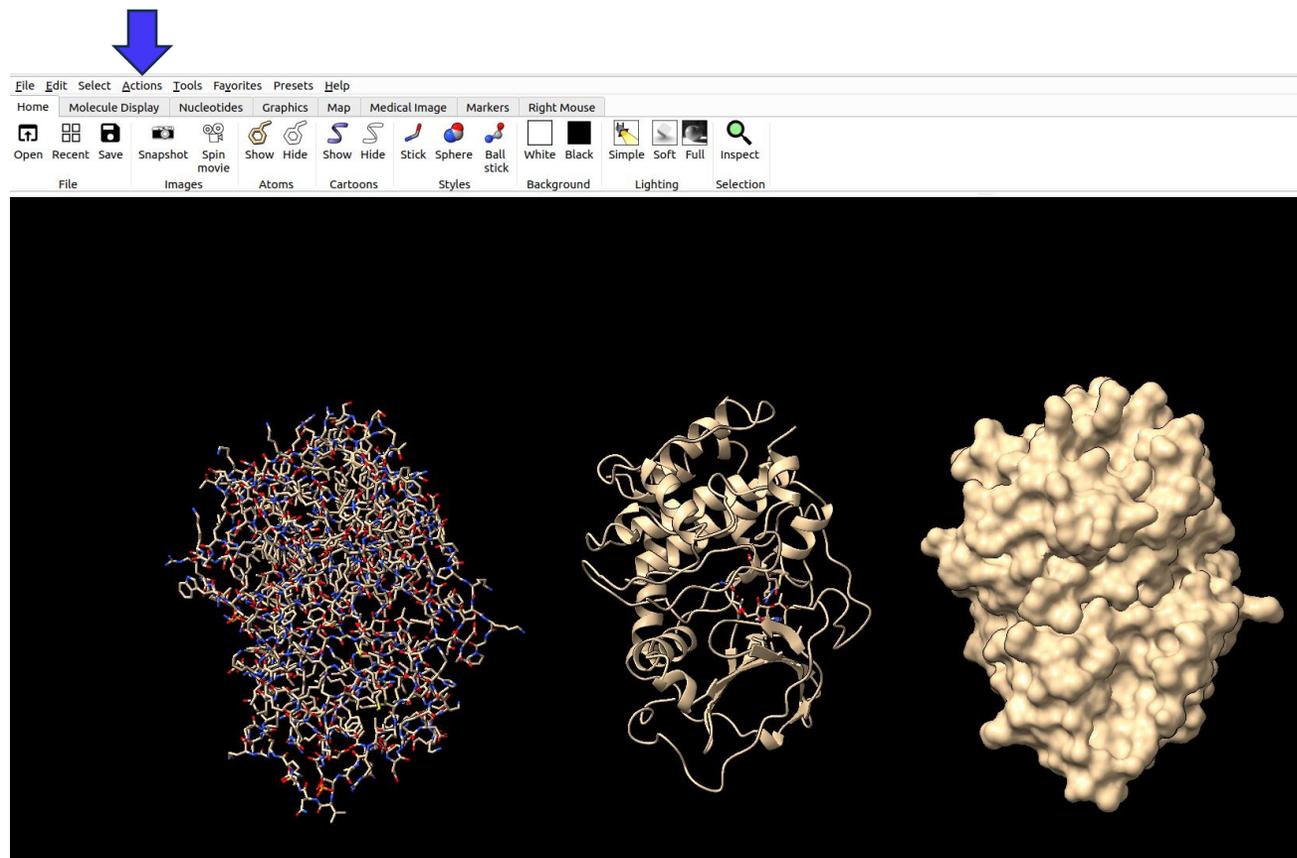
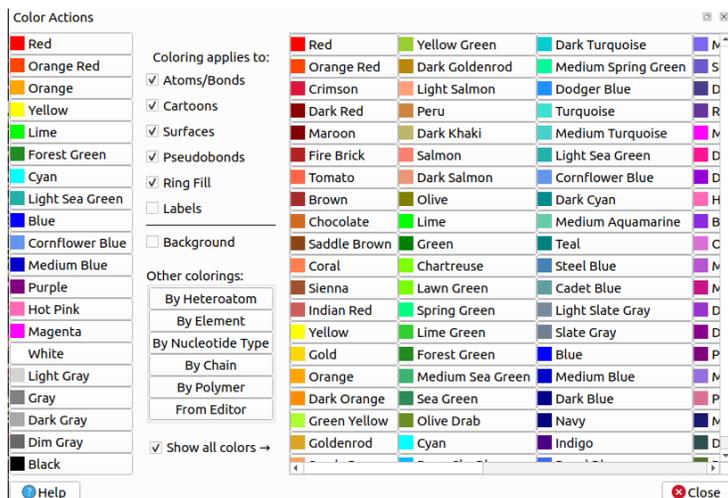
- Cadeia
- Resíduos
- Átomo
- Zona
- Sequência
- Atributo



Ações no ChimeraX

Principais tipos de ações:

- Alterar representações
- Funções *Delete*
- Cores e *labels*
- Funções *Focus* e *Pivot*



rainbow polymer palette Blues-5
color bychain

<https://www.cgl.ucsf.edu/chimerax/docs/user/commands/palettes.html>

Ferramentas do ChimeraX

Principais ferramentas:

- Gerais: side view
- Sequência: Visualizador e Alinhamento

CAMP-DEPENDENT PROTEIN KINASE (1fmo (#1) Chain E) [ID: 1/E]

```

chain E 1 GNAAA A K K G S E Q E S V K E F L A K A K E D F L K K W E T P S Q N T A Q L D Q F D R I K T L G T G S F G
chain E 56 R V M L V K H K E S G N H Y A M K I L D K Q K V V K L K Q I E H T L N E K R I L Q A V N F P F L V K L E F S F
chain E 111 K D N S N L Y M V M E Y V A G G E M F S H L R R I G R F S E P H A R F Y A A Q I V L T F E Y L H S L D L I Y R
chain E 166 D L K P E N L L I D Q Q G Y I Q V T D F G F A K R V K G R T W T L C G T P E Y L A P E I I L S K G Y N K A V D
chain E 221 W W A L G V L I Y E M A A G Y P P F A D Q P I Q I Y E K I V S G K V R F P S H F S S D L K D L L R N L L Q V
chain E 276 D L T K R F G N L K N G V N D I K N H K W F A T T D W I A I Y Q R K V E A P F I P K F K G P G D T S N F D D Y
chain E 331 E E E E I R V S I N E K C G K E F T E F
    
```

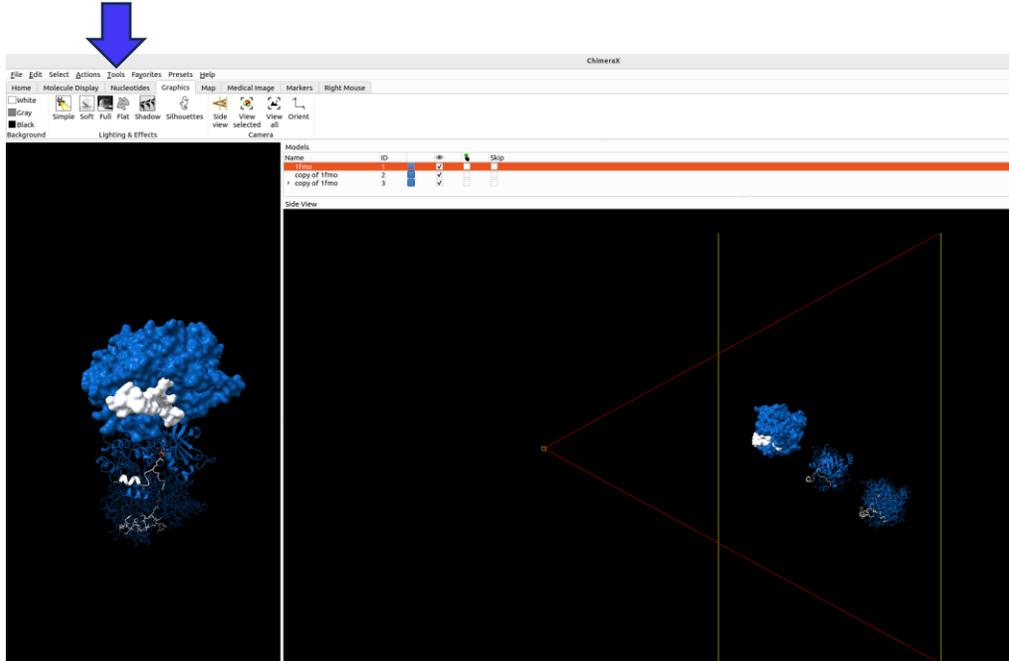
Clustal Omega Alignment [ID: 2]

```

Chain A ----- R A F W T E Q E G F E T W D G E T R K V K A H S Q T H R V D E G
Conservation
chain E ----- K G Y N K A V D W W A L G V L I Y E M A A G Y P P F
chain A T L R G Y Y N Q S E A G S H T V Q R M Y G C D V G S D W R F L ----- R G Y H Q Y

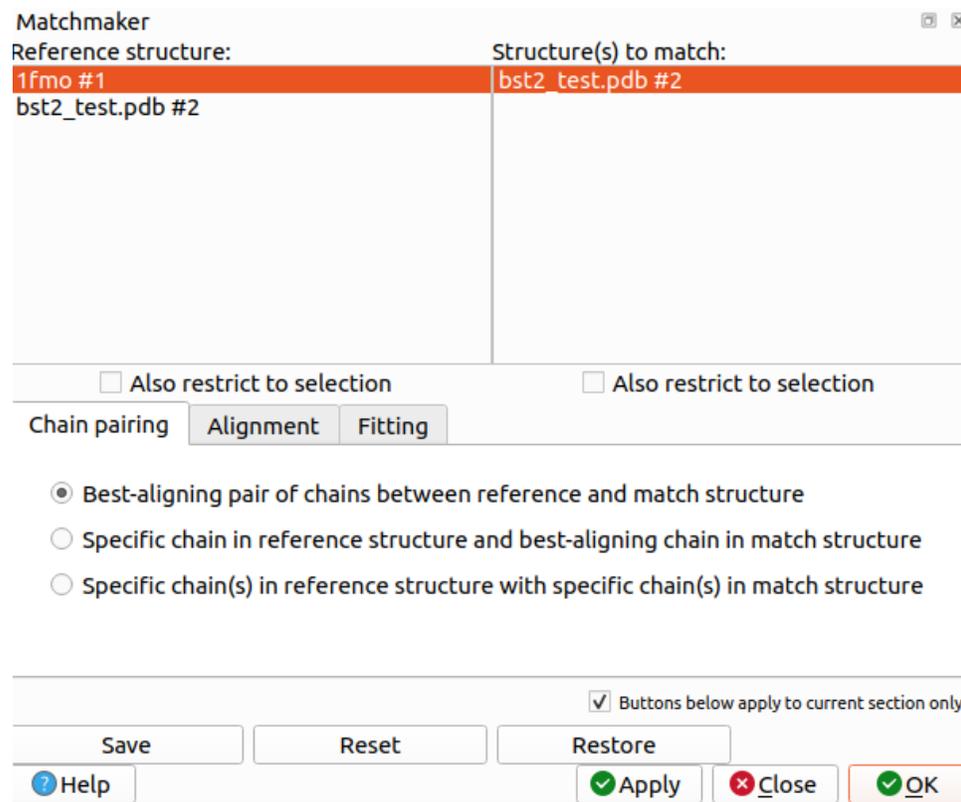
271          281          291          301          311
Conservation
chain E F A D Q P I Q I Y E K I V S G K V R F P S H F S S D L K D L L R N L L Q V D L T K R F G N
chain A A Y D G K D ----- Y I A L K E D L R S W T A A D M A -----
    
```

sequence align #1/A#2/A



Principais ferramentas:

- Análise de estrutura: distância, ângulos, ligações de hidrogênio e sobreposição (matchmaker)



Matchmaker

Reference structure: 1fmo #1
bst2_test.pdb #2

Structure(s) to match: bst2_test.pdb #2

Also restrict to selection Also restrict to selection

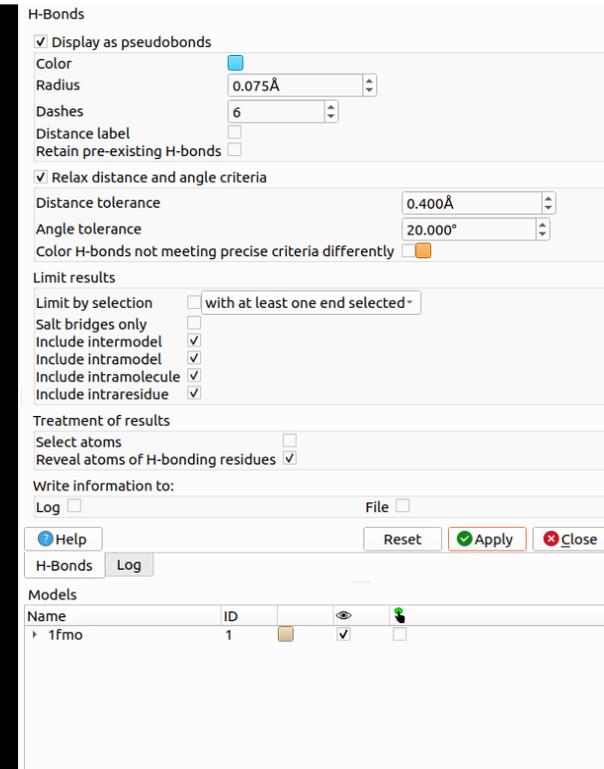
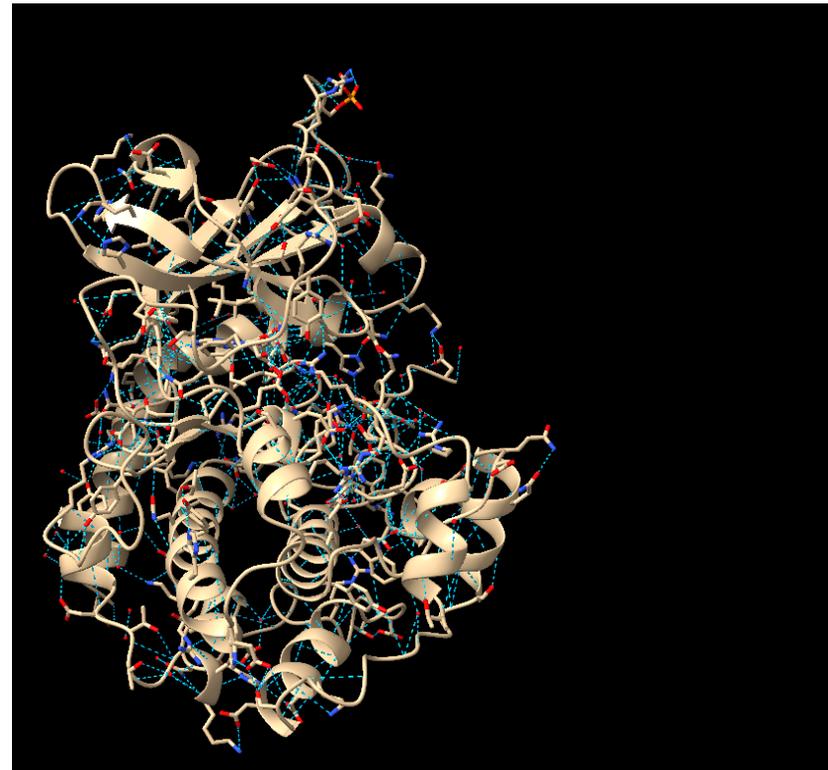
Chain pairing Alignment Fitting

- Best-aligning pair of chains between reference and match structure
- Specific chain in reference structure and best-aligning chain in match structure
- Specific chain(s) in reference structure with specific chain(s) in match structure

Buttons below apply to current section only

Save Reset Restore

Help Apply Close OK



H-Bonds

Display as pseudobonds

Color

Radius

Dashes

Distance label

Retain pre-existing H-bonds

Relax distance and angle criteria

Distance tolerance

Angle tolerance

Color H-bonds not meeting precise criteria differently

Limit results

Limit by selection with at least one end selected*

Salt bridges only

Include intermodel

Include intramodel

Include intramolecule

Include intraresidue

Treatment of results

Select atoms

Reveal atoms of H-bonding residues

Write information to:

Log File

Help Reset Apply Close

H-Bonds Log

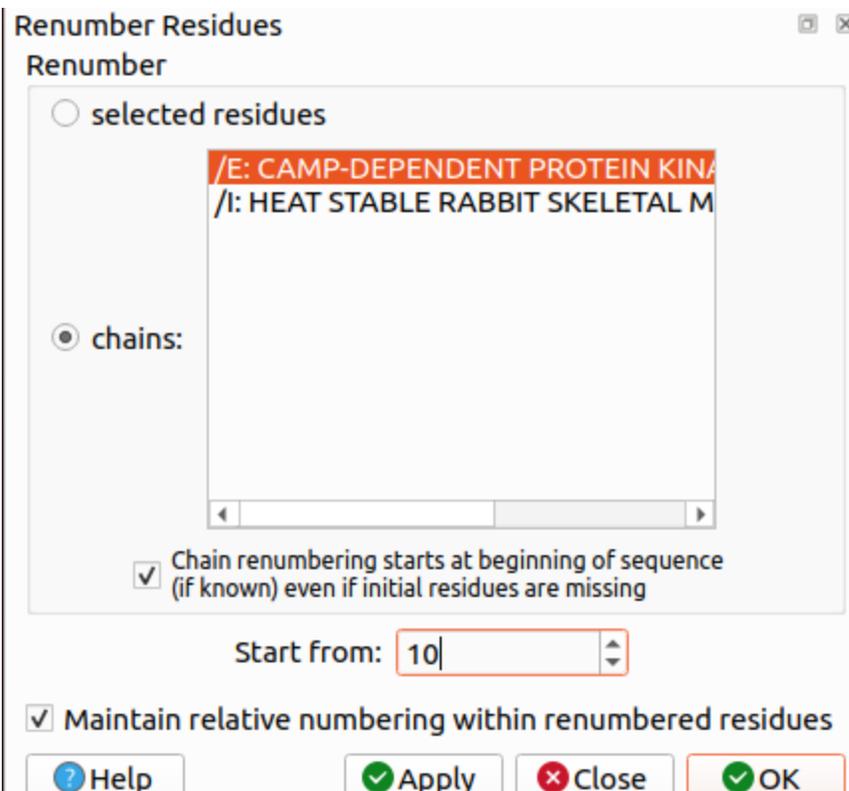
Models

Name	ID	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
1fmo	1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Ferramentas do ChimeraX

Principais ferramentas:

- Edição de estrutura: Rotâmeros, alterar chain ID e numeração de residues



Renumber Residues

Renumber

selected residues

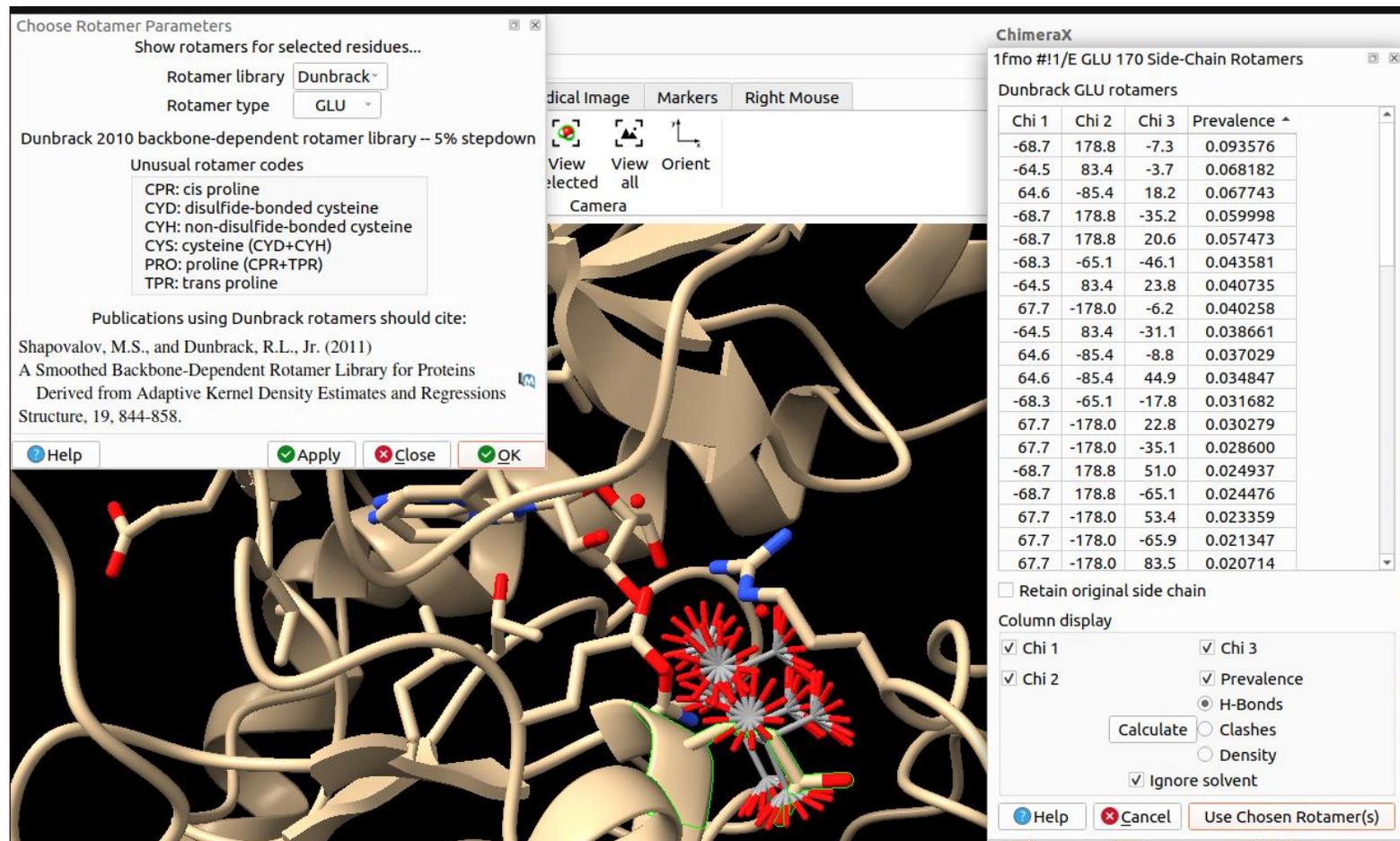
chains:

/E: CAMP-DEPENDENT PROTEIN KIN...
/I: HEAT STABLE RABBIT SKELETAL M...

Chain renumbering starts at beginning of sequence (if known) even if initial residues are missing

Start from: 10

Maintain relative numbering within renumbered residues



Choose Rotamer Parameters

Show rotamers for selected residues...

Rotamer library: Dunbrack
Rotamer type: GLU

Dunbrack 2010 backbone-dependent rotamer library -- 5% stepdown

Unusual rotamer codes

- CPR: cis proline
- CYD: disulfide-bonded cysteine
- CYH: non-disulfide-bonded cysteine
- CYS: cysteine (CYD+CYH)
- PRO: proline (CPR+TPR)
- TPR: trans proline

Publications using Dunbrack rotamers should cite:
Shapovalov, M.S., and Dunbrack, R.L., Jr. (2011)
A Smoothed Backbone-Dependent Rotamer Library for Proteins
Derived from Adaptive Kernel Density Estimates and Regressions
Structure, 19, 844-858.

1fmo #1/E GLU 170 Side-Chain Rotamers

Chi 1	Chi 2	Chi 3	Prevalence
-68.7	178.8	-7.3	0.093576
-64.5	83.4	-3.7	0.068182
64.6	-85.4	18.2	0.067743
-68.7	178.8	-35.2	0.059998
-68.7	178.8	20.6	0.057473
-68.3	-65.1	-46.1	0.043581
-64.5	83.4	23.8	0.040735
67.7	-178.0	-6.2	0.040258
-64.5	83.4	-31.1	0.038661
64.6	-85.4	-8.8	0.037029
64.6	-85.4	44.9	0.034847
-68.3	-65.1	-17.8	0.031682
67.7	-178.0	22.8	0.030279
67.7	-178.0	-35.1	0.028600
-68.7	178.8	51.0	0.024937
-68.7	178.8	-65.1	0.024476
67.7	-178.0	53.4	0.023359
67.7	-178.0	-65.9	0.021347
67.7	-178.0	83.5	0.020714

ChimeraX Toolshed - All Apps

https://cxtoolshed.rbvi.ucsf.edu/apps/all?platform=Linux&version=1.10



All Bundles

Categories

EM

Structure Analysis

Input/Output

User Interface

Structure Editing

atomic structure

MD

Fitting

external program

Protein Visualization

Model validation

crystallography

augmented reality

Sequence

Light microscopy

ligands

developer

Cytoscape

presets

NMR

more »

Get Started with the Toolshed »



AddH

Add hydrogens



AllMetal3D

Predicting metal and water binding sites in proteins



ArtiaX

Visualization and editing of cryo-ET particle lists.



Clipper

Adds support for crystallographic maps to



Cytoscape

This bundle provides an interface to Cytoscape's



DevelExtras

Work with non installed Bundles



DiffFit

Rapid Fitting of Molecular Structures to a Cryo-EM



EMalign

Fully automatic alignment of density maps



GenomeTools

Work with 3D genome models



HKCage

Depict icosahedral lattices for viruses



ISOLDE

Interactive Structure Optimization by Local Direct



LAMMPS

Import .data(.gz) and .dump(.gz) from LAMMPS



LeapMotion

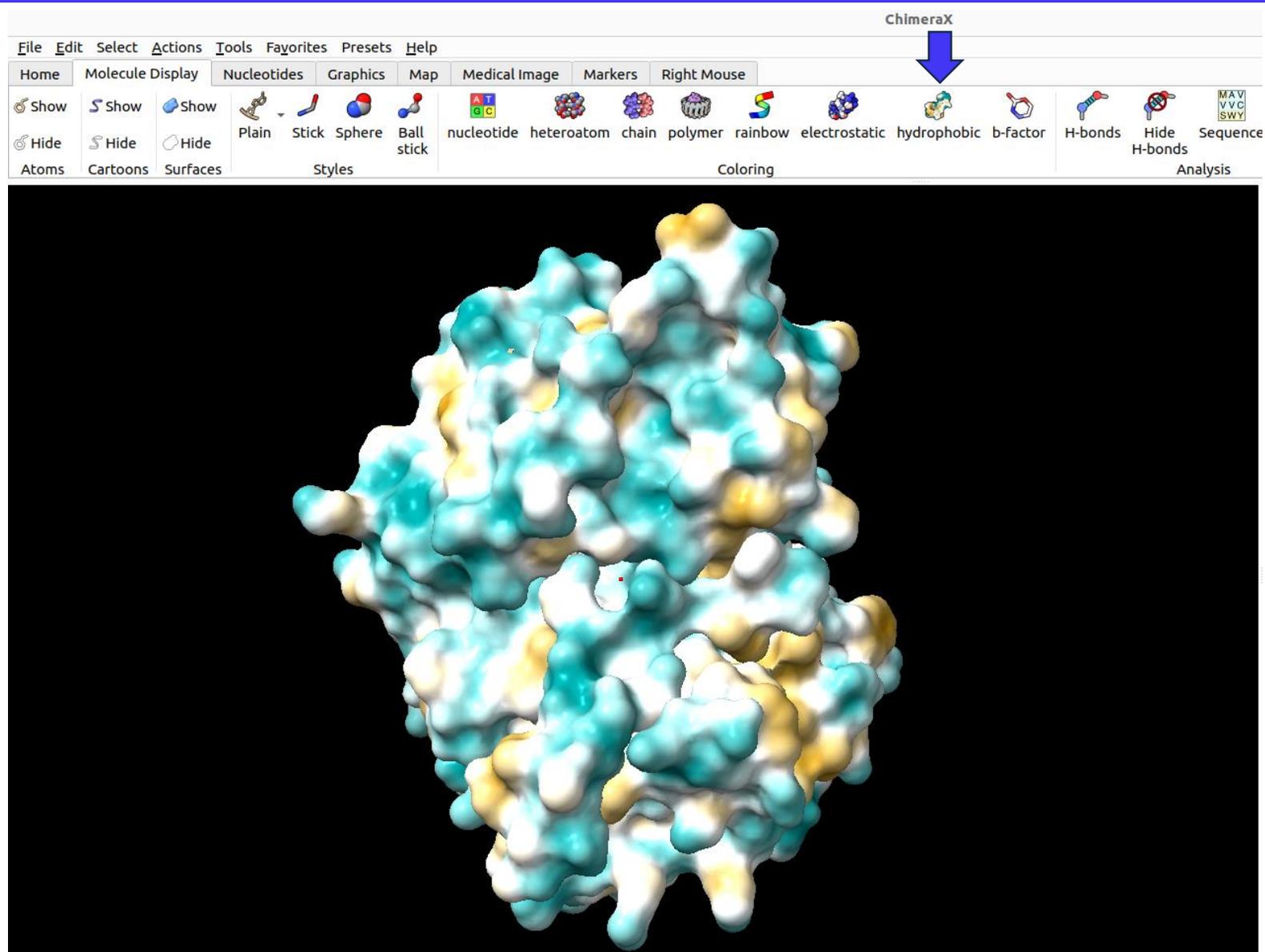
Leap Motion hand tracking



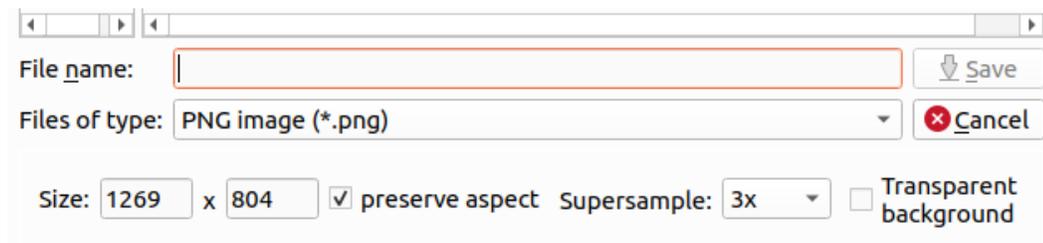
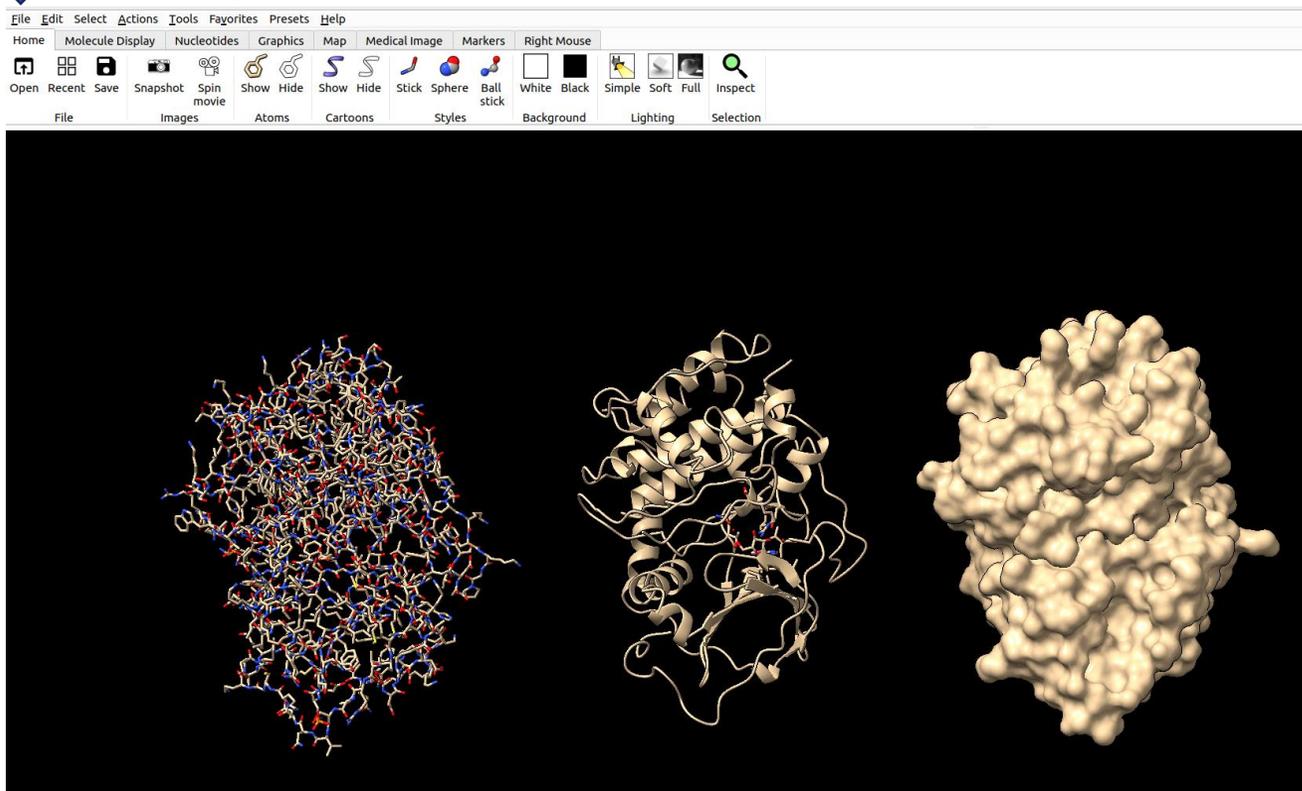
LigandRecognizer

Commands for recognizing ligands in cryoEM maps

Gerando representação de superfície colorida por hidrofobicidade



Salvando imagens no ChimeraX



Generating videos with ChimeraX

- [2dlabels](#) – add text, [symbols](#), and straight arrows to the display for presentation images and movies
 - [camera](#) – set mono or stereo viewing and related parameters
 - [clip](#) – control clipping planes
 - [cofr](#) – set center of rotation
 - [coordset](#) – play through frames of a [trajectory](#)
 - [crossfade](#) – interpolate between image frames
 - [fly](#) – smoothly traverse a series of named views
 - [morph](#) – morph (interpolate) between atomic structures; create a morph trajectory
 - [move](#) – translate
 - [movie](#) – record image frames and assemble them into a movie file
 - [mseries](#) – display an [ordered series of models](#)
 - [perframe](#) – specify operations to execute at every (or every Nth) display frame
 - [resfit](#) – show density fit of successive amino acid residues along a chain
 - [rock](#) – rock back and forth
 - [roll](#) – rotate continuously
 - [scenes](#) – save/restore named scenes
 - [stop](#) – halt ongoing motions
 - [torsion](#) – set or report torsion angles (rotate bonds)
 - [turn](#) – rotate
 - [view](#) – adjust the view to specified items; save/restore named views
 - [volume morph](#) – morph (interpolate) between two or more maps
 - [vr roomCamera](#) – in [virtual reality](#) (VR), set up a separate camera view fixed in the VR room coordinates
 - [vseries](#) – display, analyze, or process an [ordered series of maps](#)
 - [wait](#) – update the display and enforce ordered execution of commands in scripts
 - [window size](#) – set pixel width and height of the graphics window
 - [wobble](#) – perform a figure-eight rotation
 - [zoom](#) – change the apparent size of the view
- [record](#) – start recording frames
 - [encode](#) – stop any ongoing recording and encode the saved image frames into a movie file
 - [stop](#) – stop recording frames
 - [reset](#) – reset status to zero frames saved
 - [abort](#) – halt any encoding in progress and perform a **reset**
 - [crossfade](#) – interpolate from the preceding frame to the following frame
 - [duplicate](#) – expand the preceding frame into multiple frames
 - [ignore](#) – start/stop ignoring subsequent **movie** commands
 - [formats](#) – list the available movie file formats
 - [status](#) – report status (number of saved frames, *etc.*) in the [Log](#)

Obrigado!

Equipe de Dados Biológicos (EDB)

edb@lnbio.cnpem.br

+55 (19) 3512-1113

Grupo de Design de Proteínas (GDP)

+55 (19) 3512-2389

Laboratório de Biologia Computacional (LBC)

+55 (19) 3512-1255



Sign up to receive
newsletters
about **CNPEM**
and its units

cnpem.br



CNPem
Brazilian Center for Research
in Energy and Materials

MINISTRY OF
SCIENCE TECHNOLOGY
AND INNOVATION

