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)

LNBIO Brazilian Biosciences National Laboratory
CNPEM Brazilian Center for Research in Energy and Materials
MINISTRY OF SCIENCE TECHNOLOGY AND INNOVATION
BRAZILIAN GOVERNMENT BRASIL UNITING AND REBUILDING

Módulo 2

Visualização molecular de biomoléculas no ChimeraX

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Dia 2 (07/11/2025)

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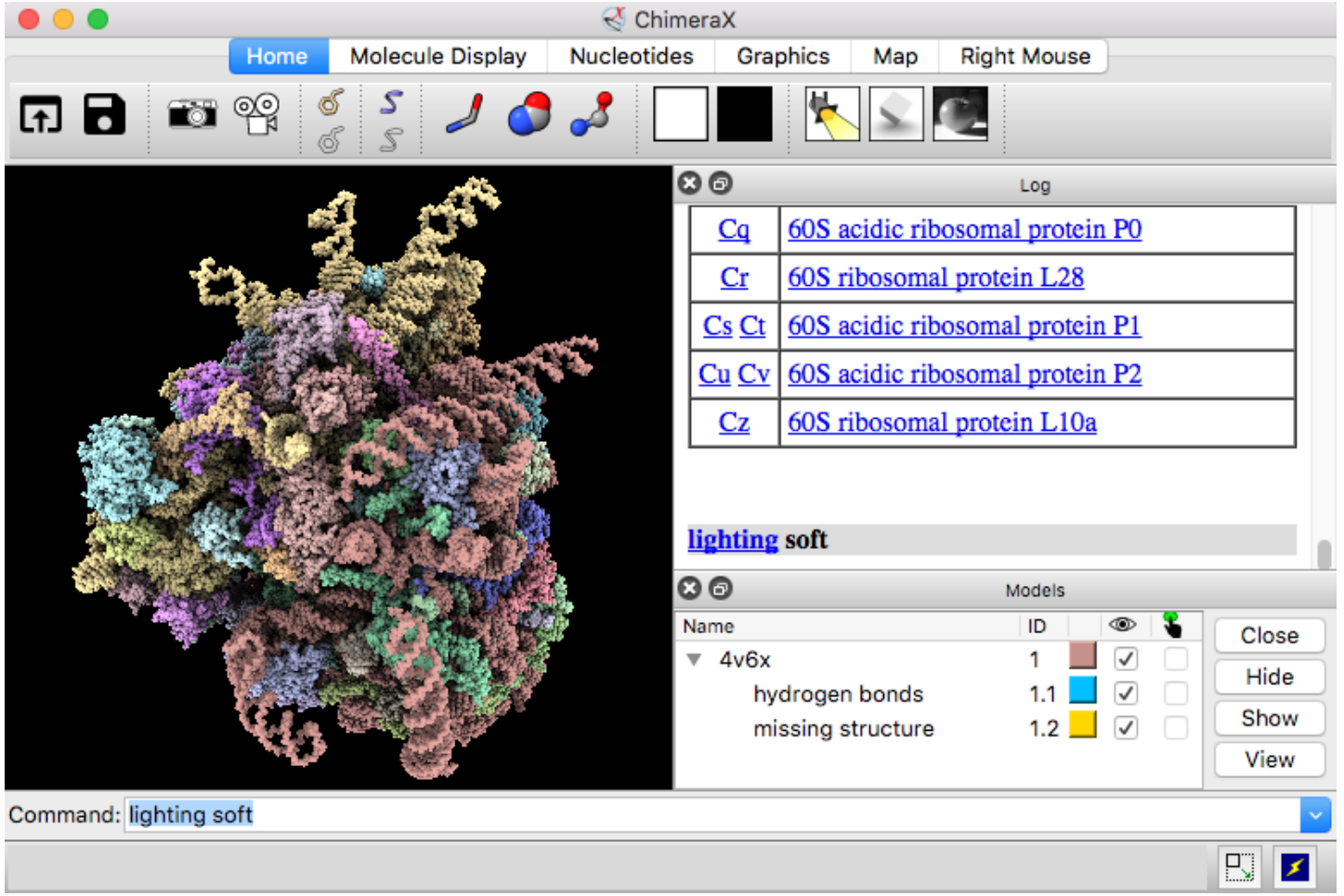
UCSF ChimeraX

» O UCSF ChimeraX é um software de código aberto de última geração para visualização, análise e manipulação de estruturas moleculares e dados relacionados.

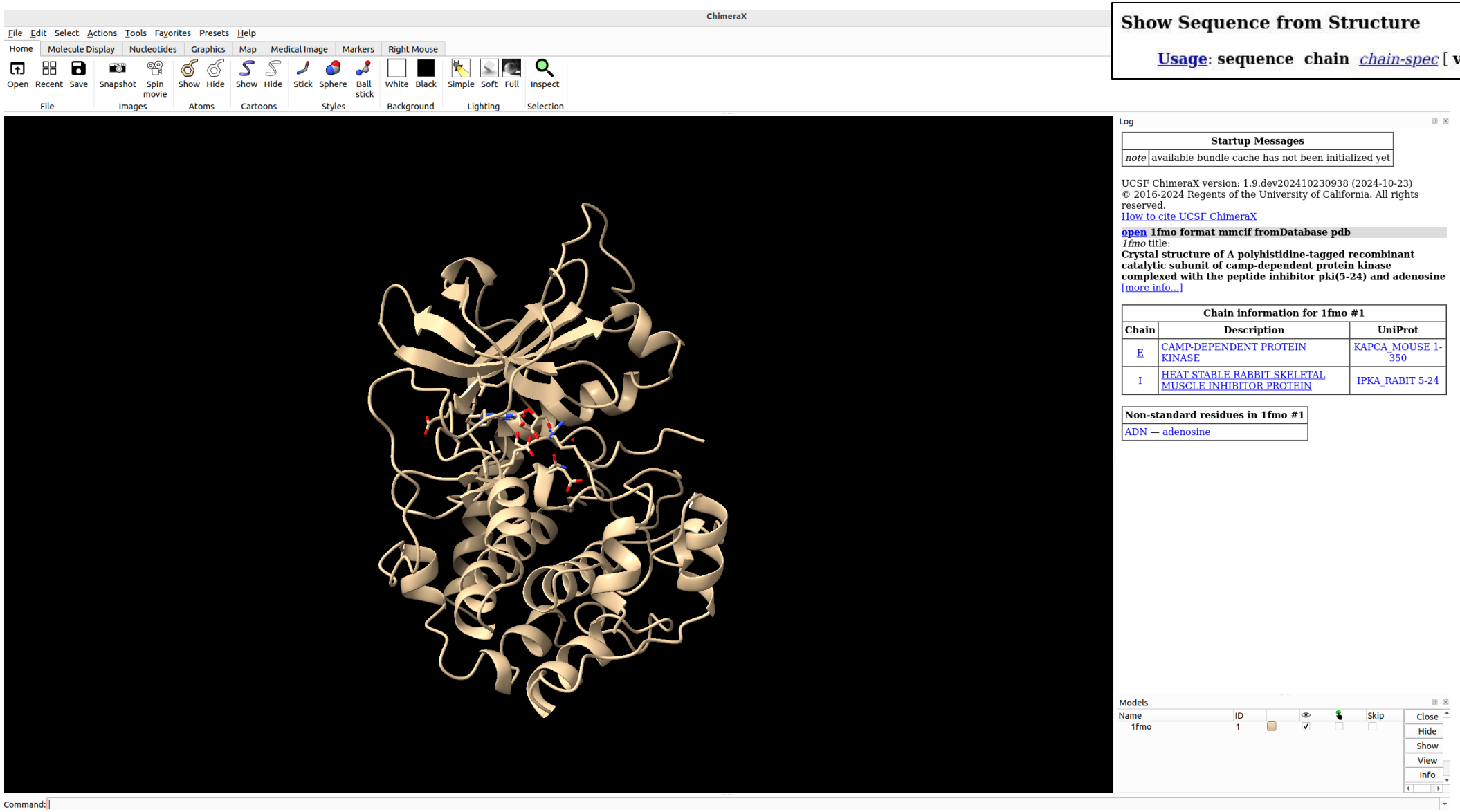


Principais funcionalidades:

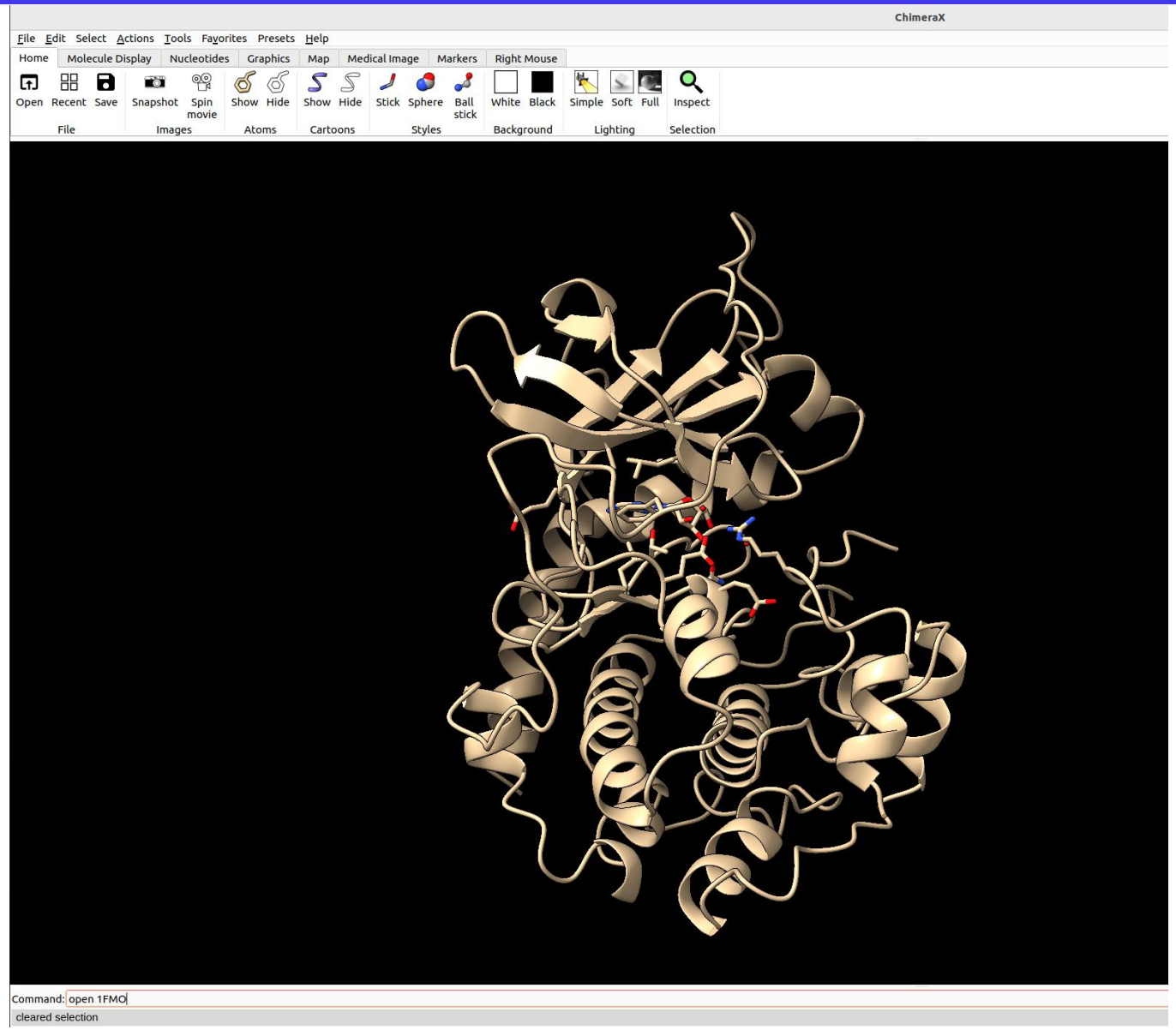
- Visualização interativa de moléculas
- Suporte a múltiplos formatos (PDB, mmCIF, MRC etc.)
- Medições (distâncias, ângulos, contatos) e manipulação estrutural
- Análise de mapas de crio-EM e dados volumétricos
- Integração com bancos de dados (PDB, AlphaFold, UniProt)
- Geração de imagens e animações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

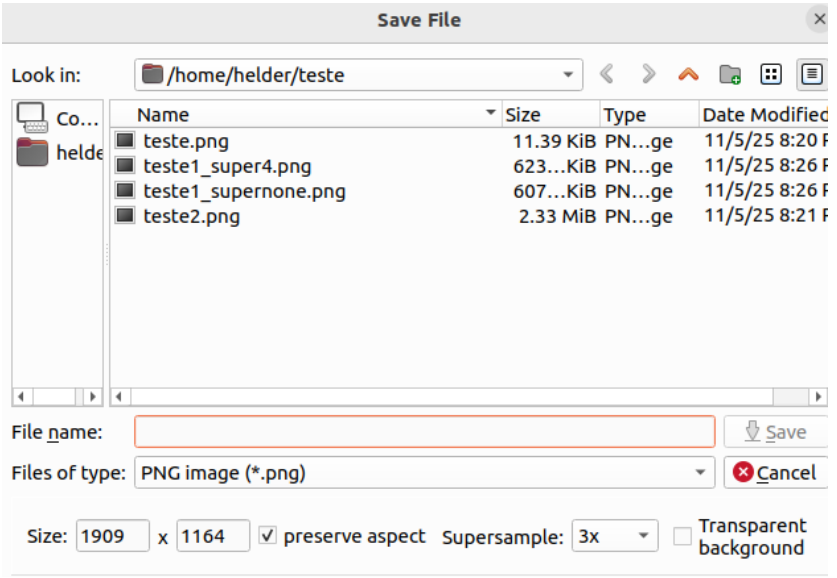
Download: www.cgl.ucsf.edu/chimerax

A interface de visualização do ChimeraX



Abrindo e salvando uma estrutura/seção no ChimeraX





Estrutura Hierárquica

Hierarchical Specifiers

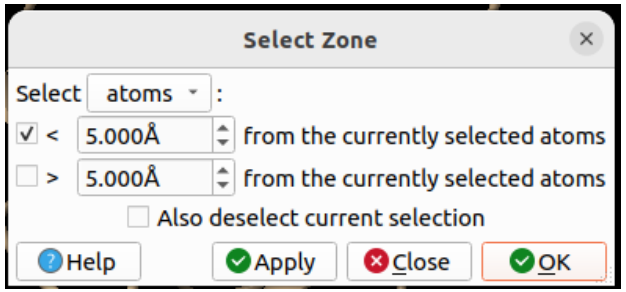
Symbol	Reference Level	Definition	Examples
#	model	model number assigned to the data in ChimeraX (hierarchical, with positive integers separated by dots: N, N.N, N.N.N, *etc.*)	**#1** **#1.3**
/	chain	chain identifier (case-insensitive unless both upper- and lowercase chain IDs are present)	**/A**
: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

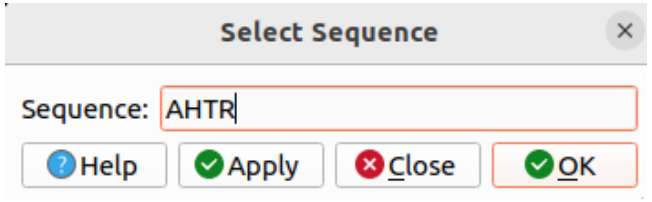
https://www.cgl.ucsf.edu/chimerax/docs/user/commands/atomspec.html#hierarchy

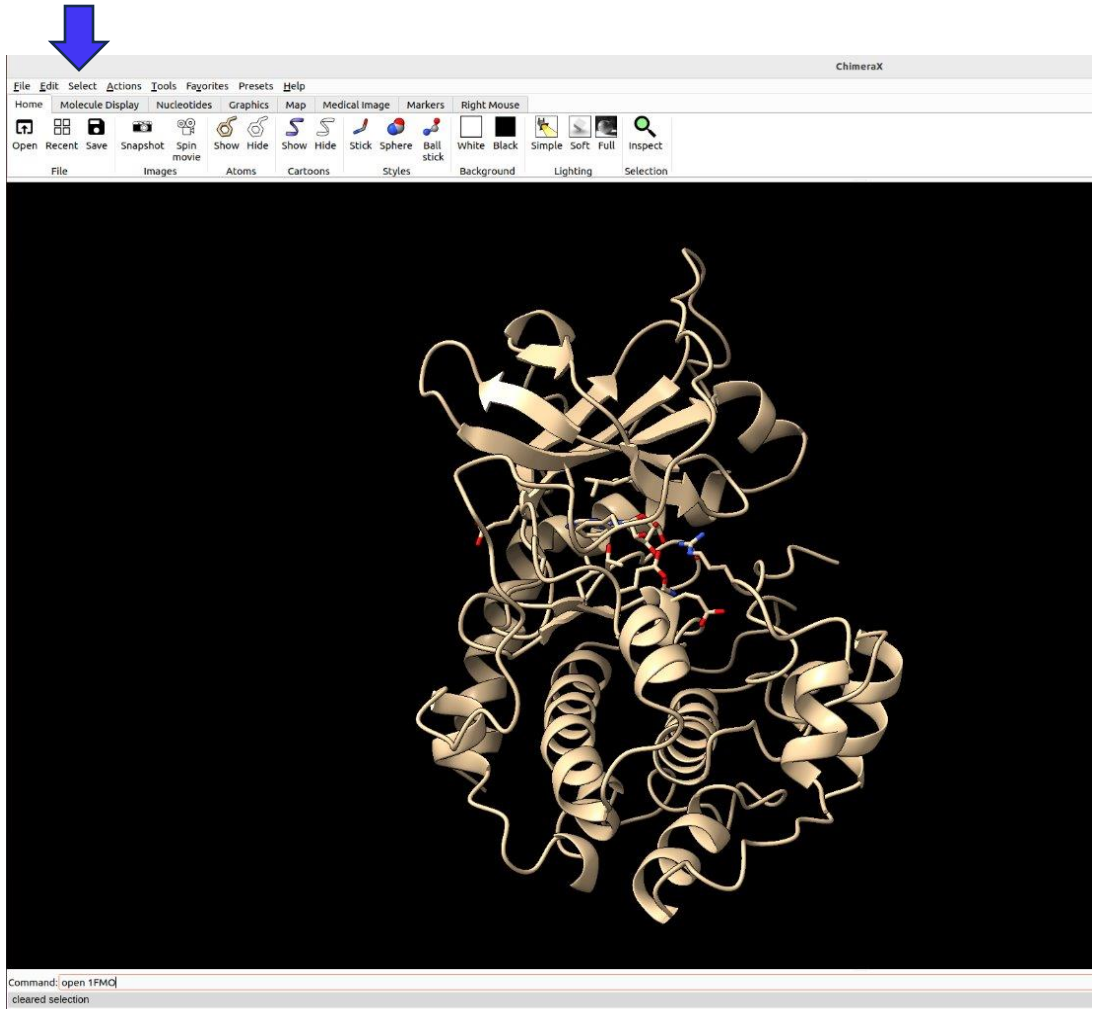
Seleções no ChimeraX

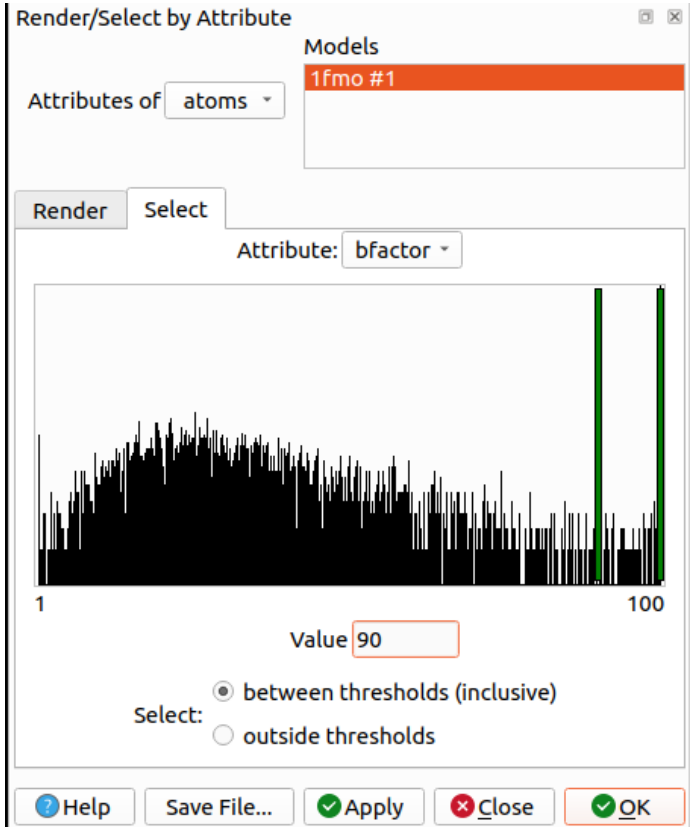
Principais tipos de seleção:

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





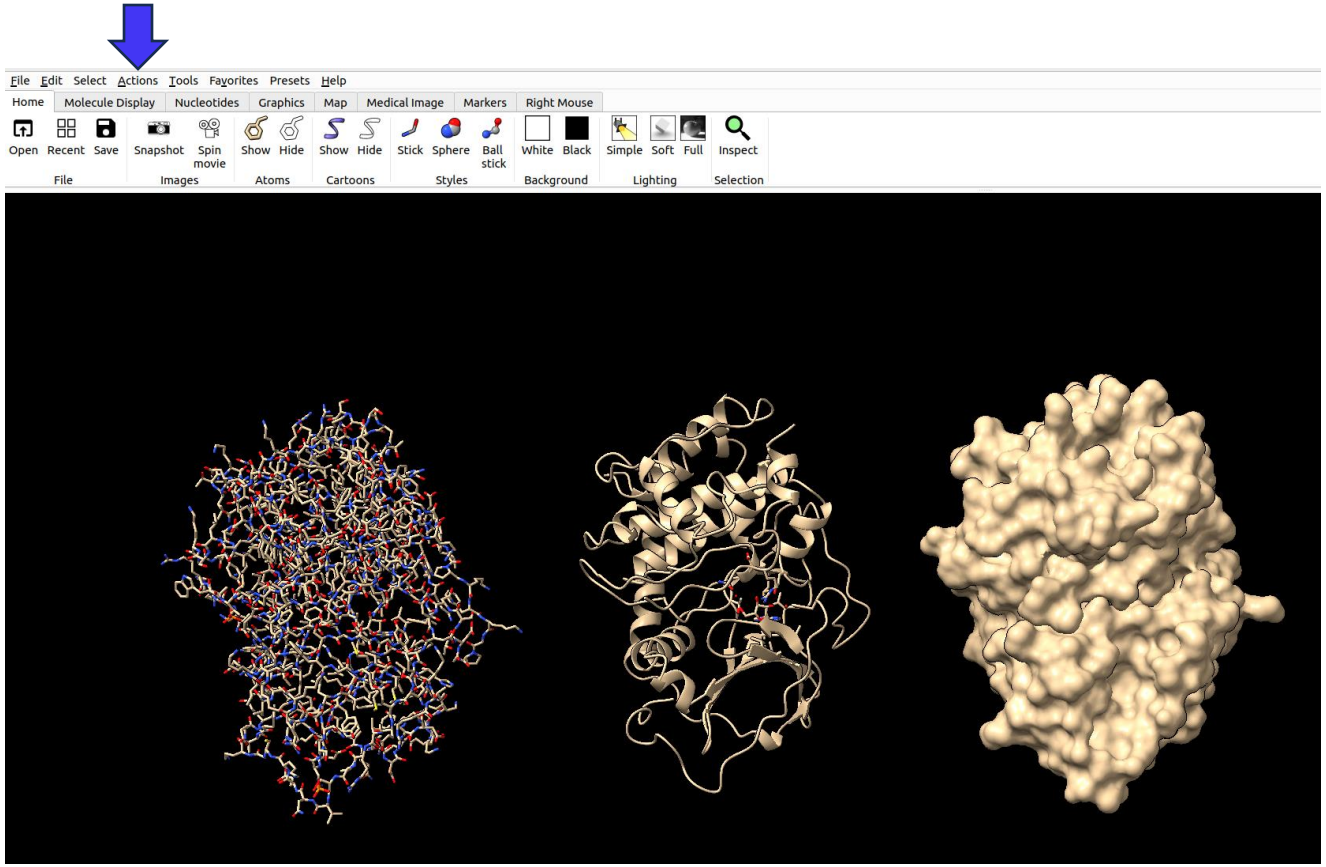


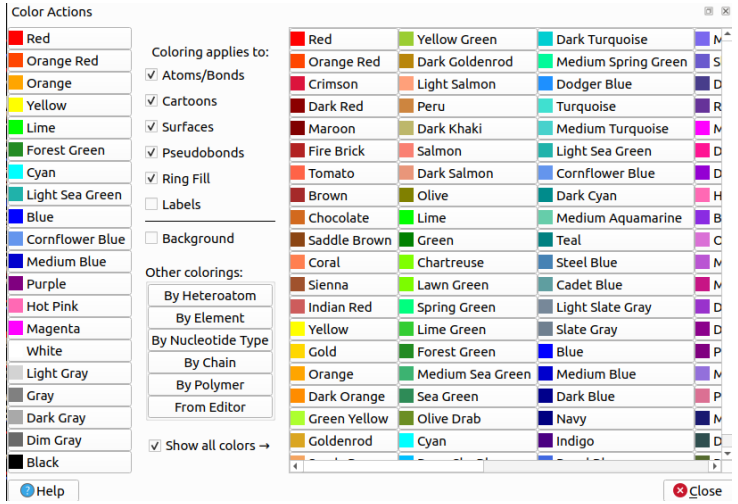


Ações no ChimeraX

Principais tipos de ações:

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





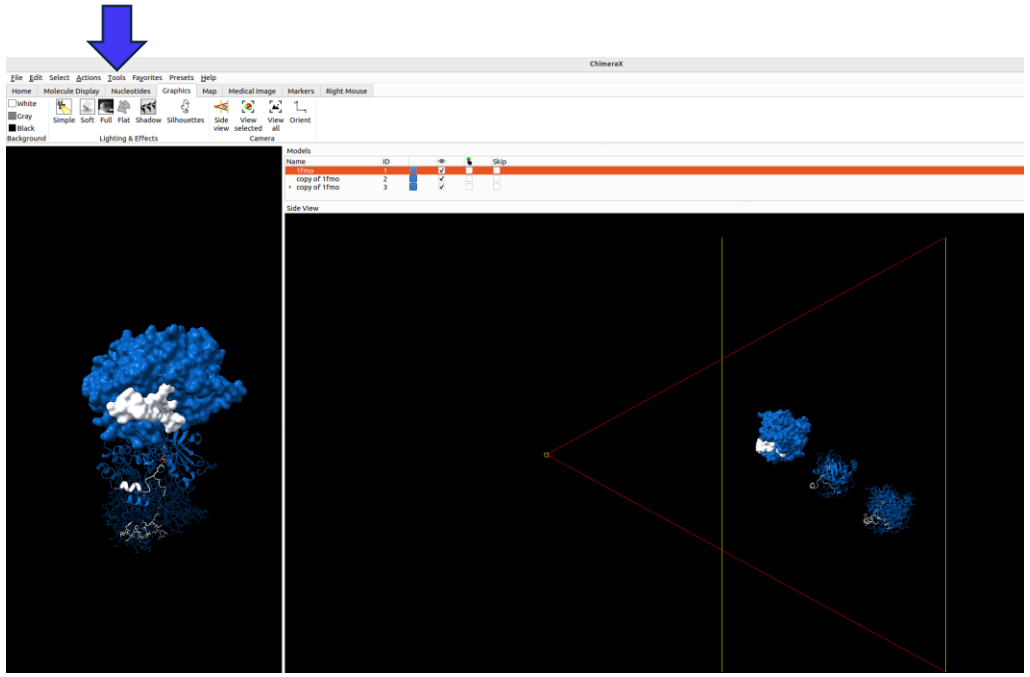
rainbow polymer palette Blues-5
color bychain

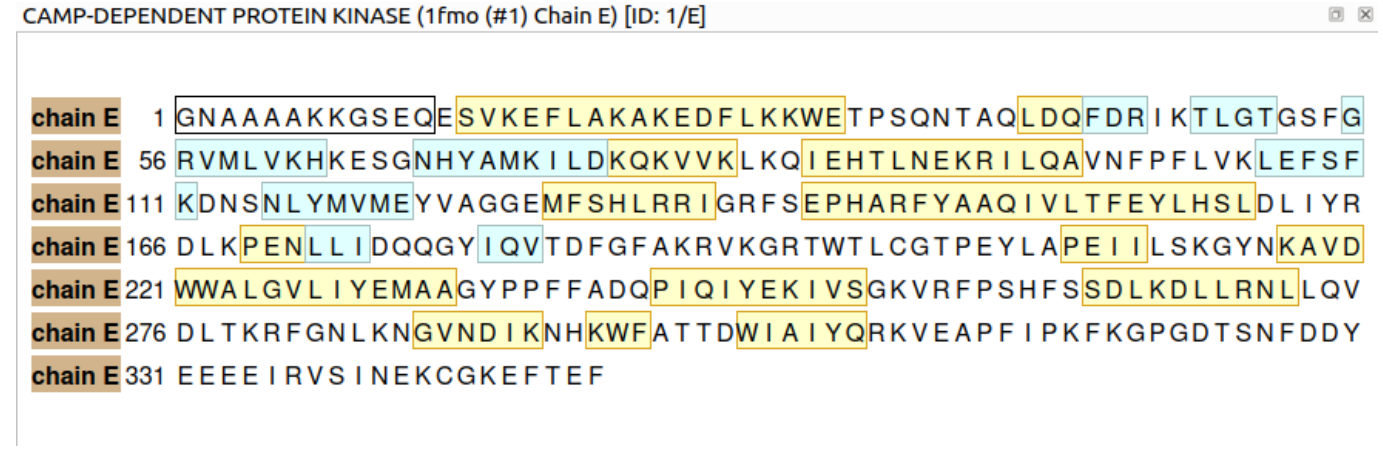
https://www.cgl.ucsf.edu/chimerax/docs/user/commands/palettes.html

Ferramentas do ChimeraX

Principais ferramentas:

- Gerais: side view
- Sequência: Visualizador e Alinhamento



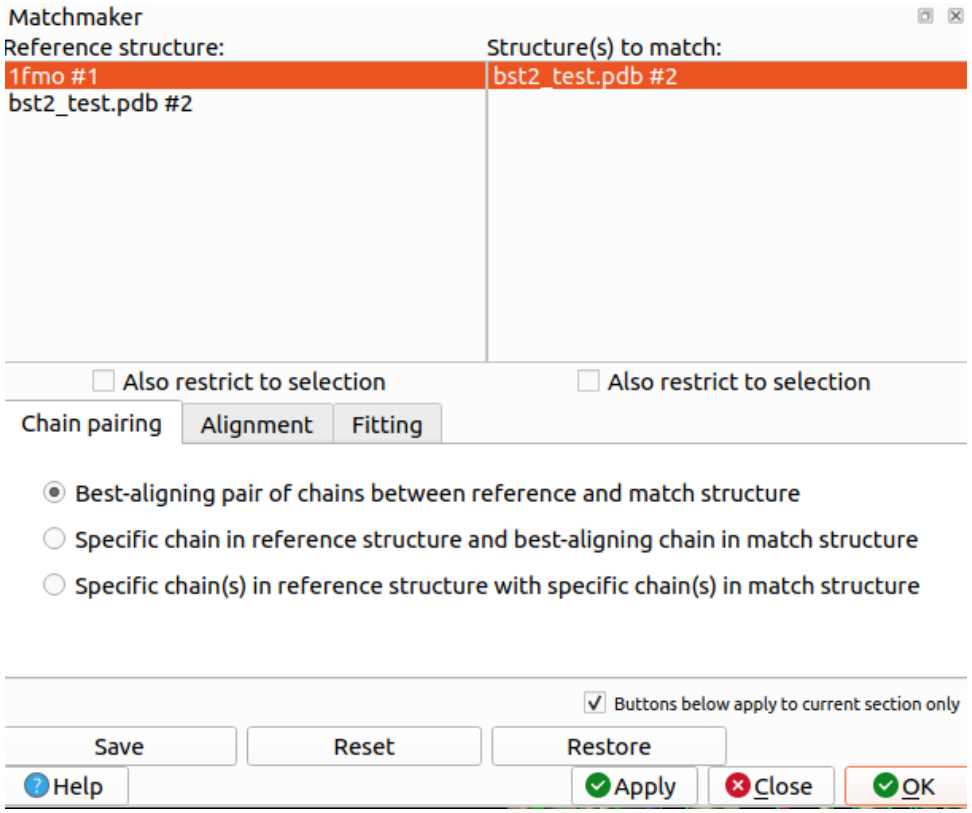


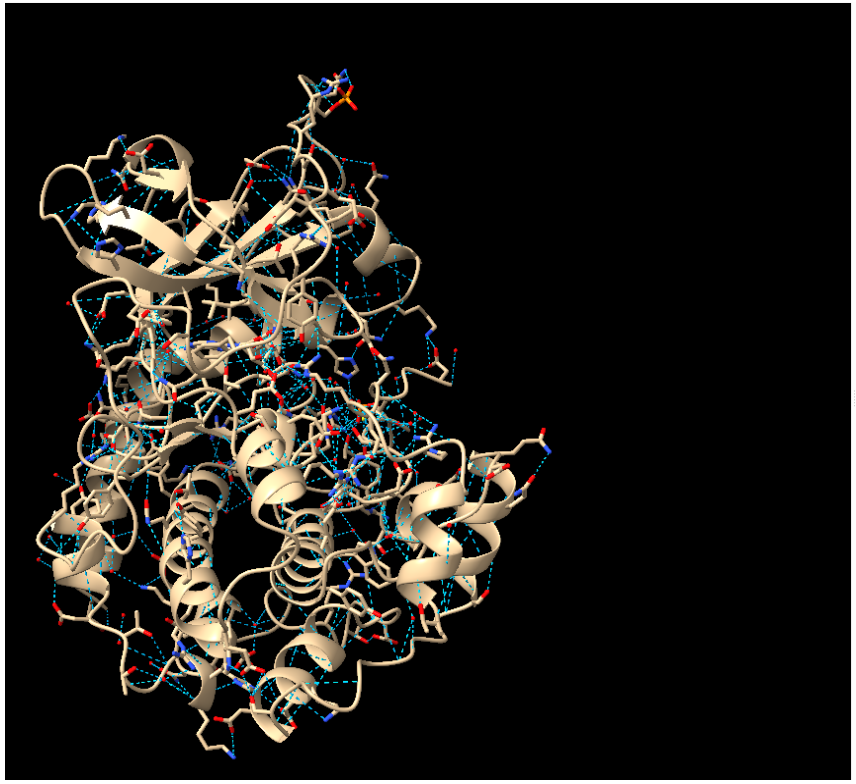
sequence align #1/A#2/A

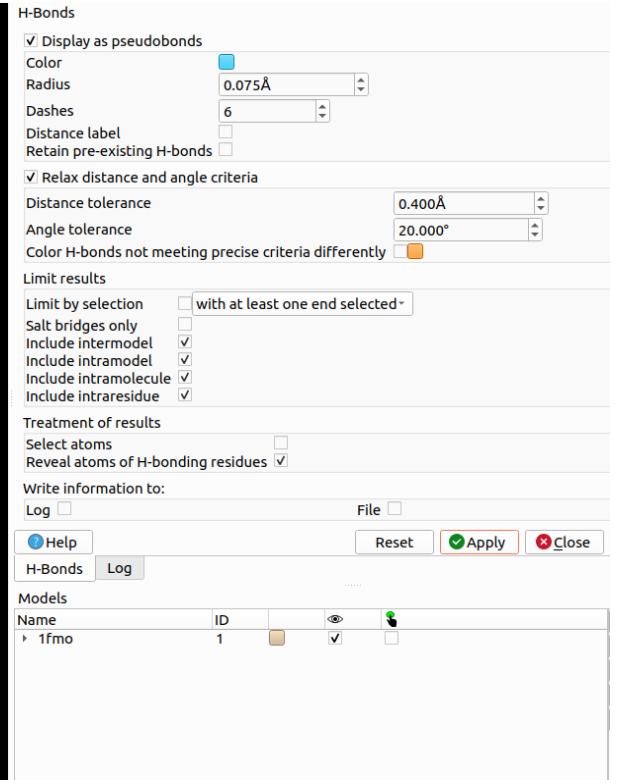
Ferramentas do ChimeraX

Principais ferramentas:

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



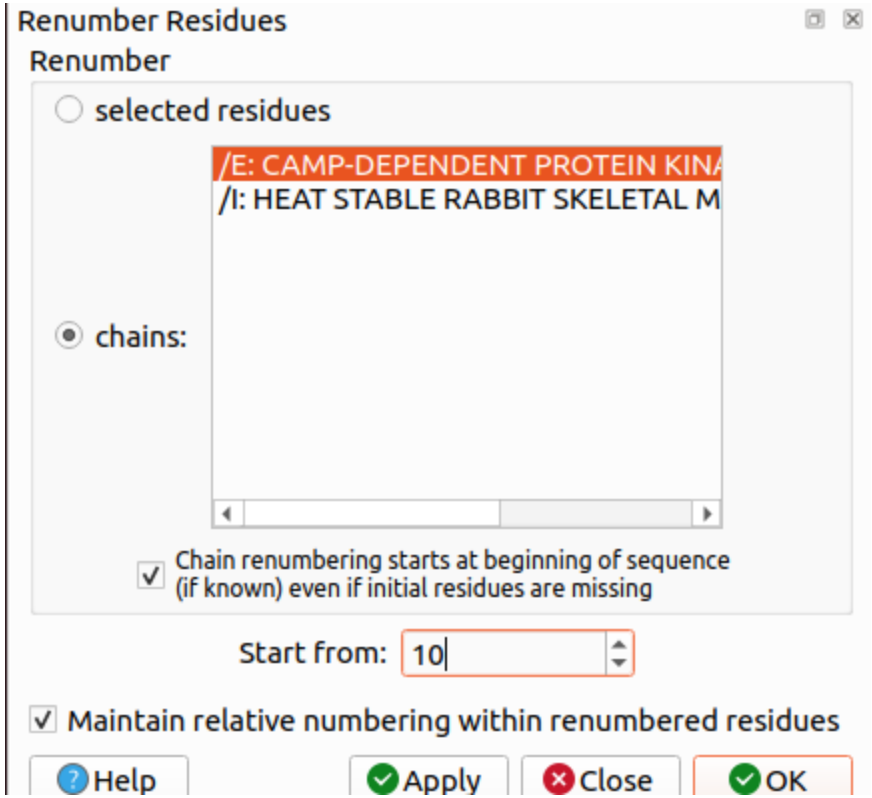


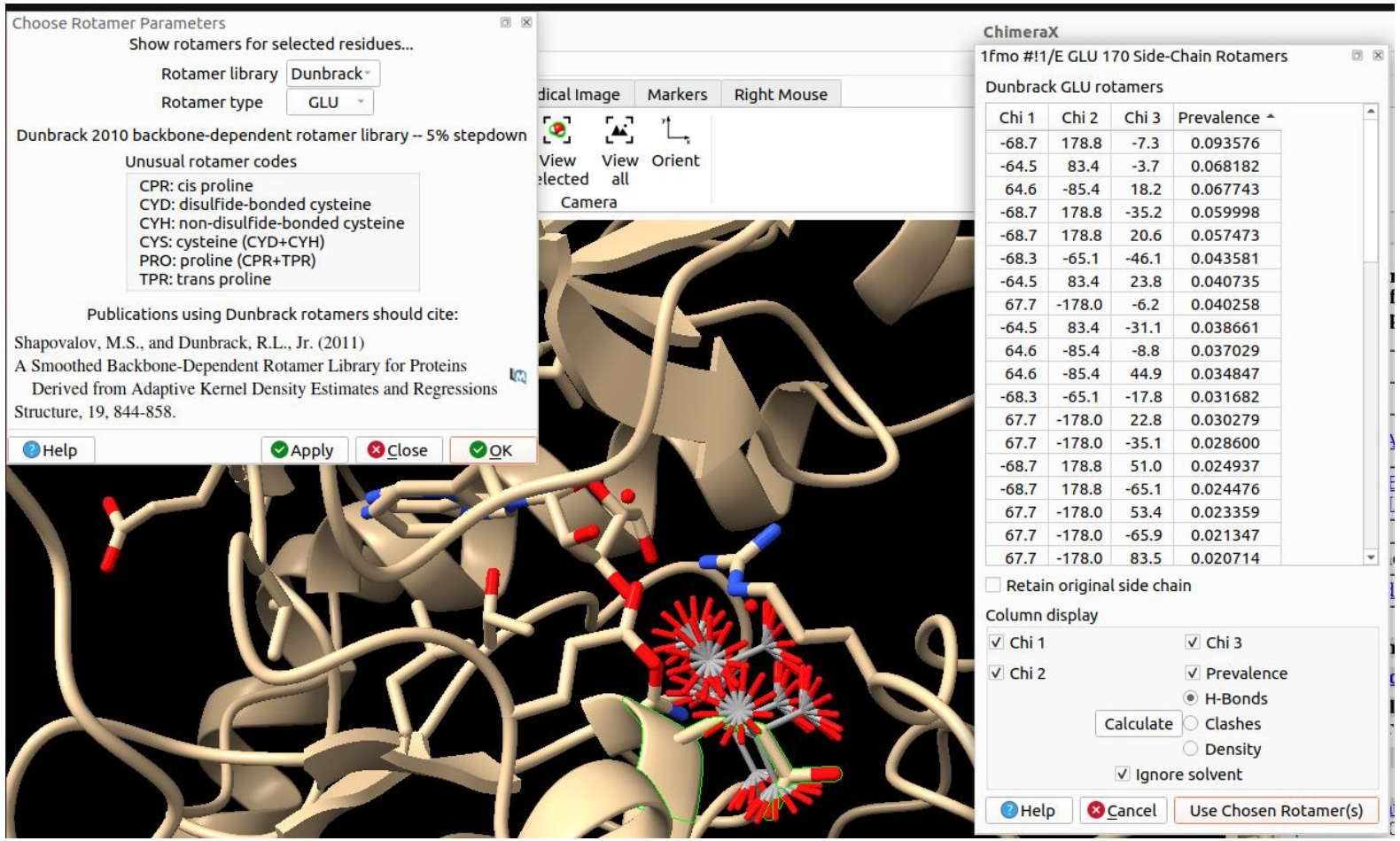


Ferramentas do ChimeraX

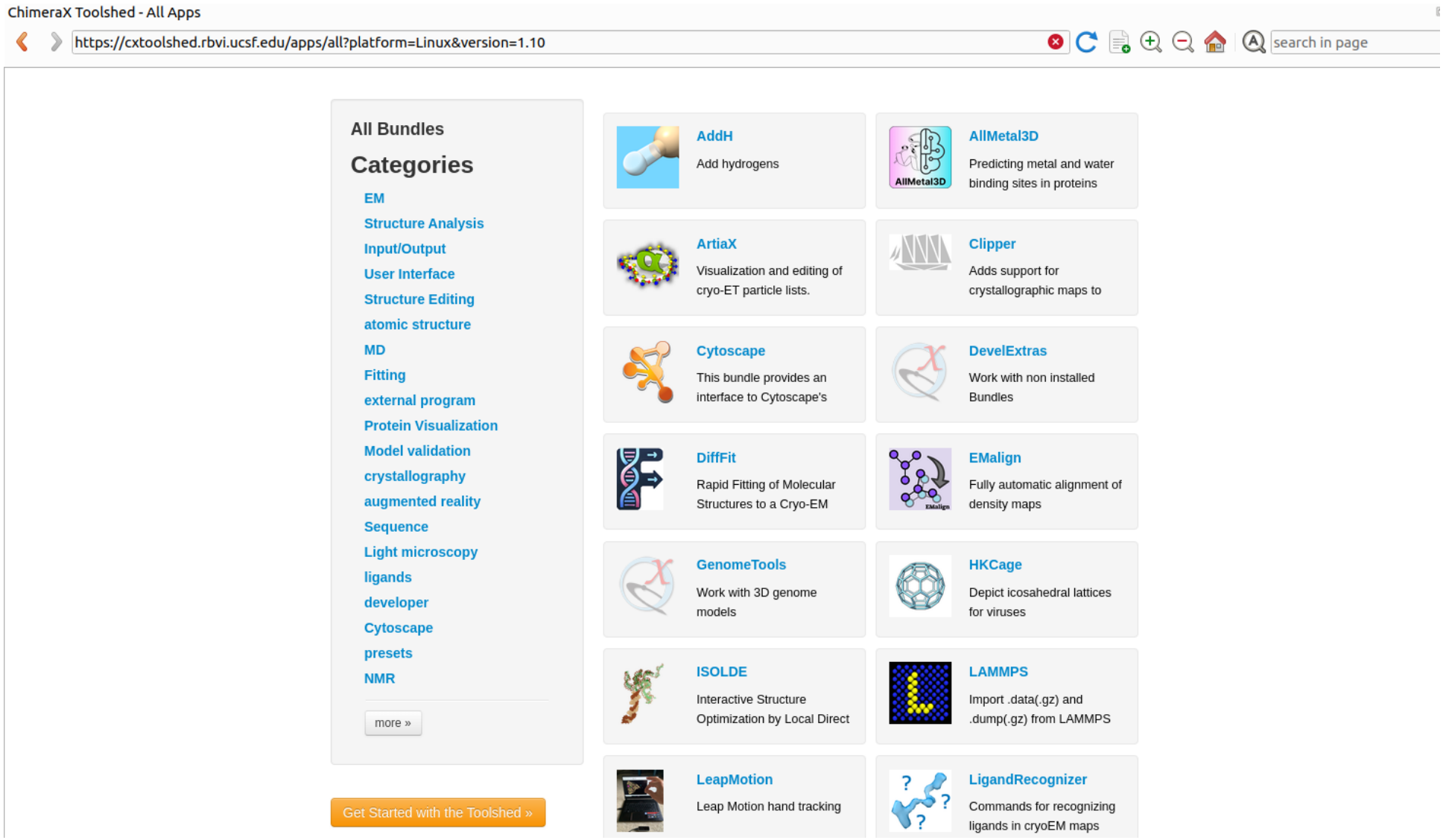
Principais ferramentas:

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

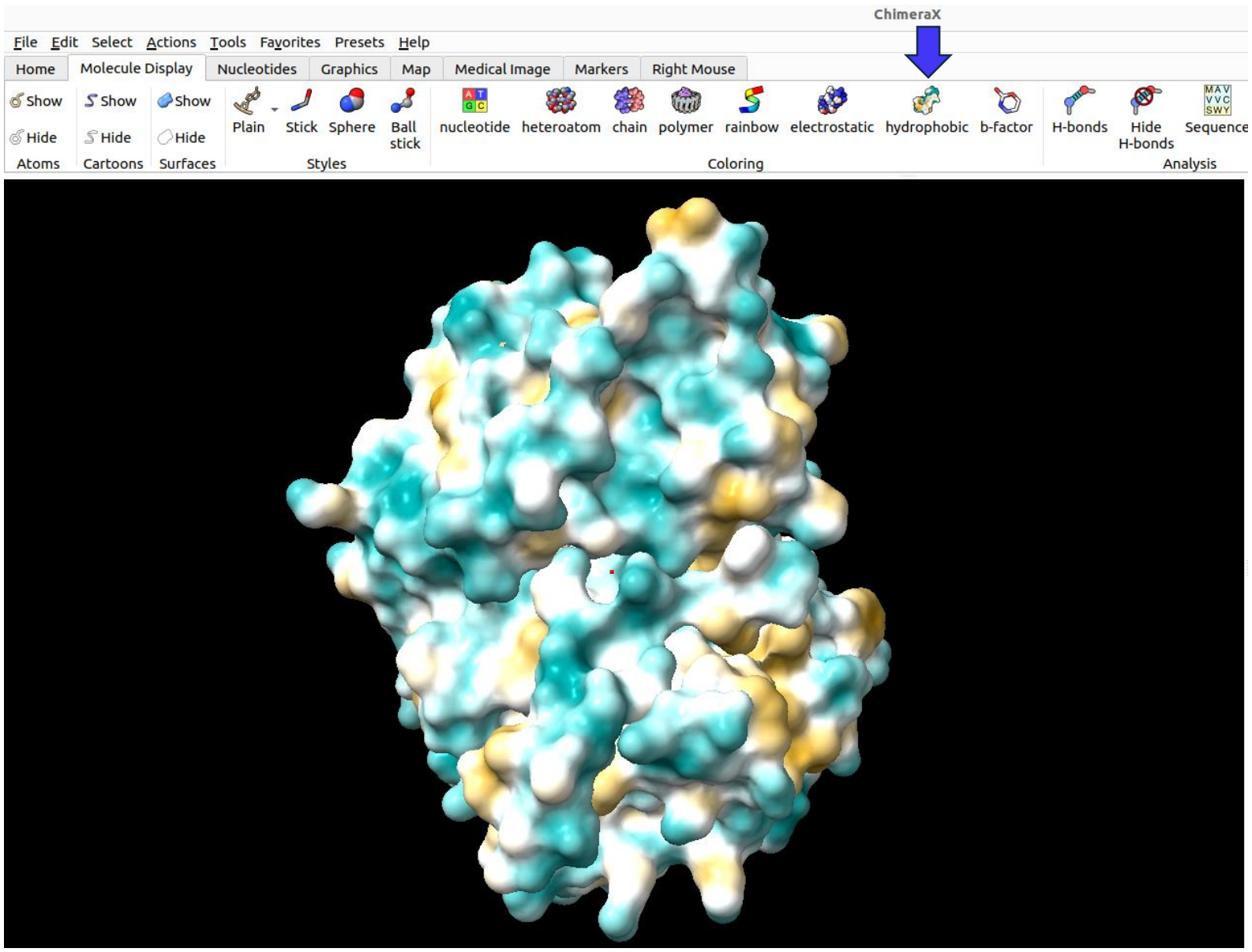




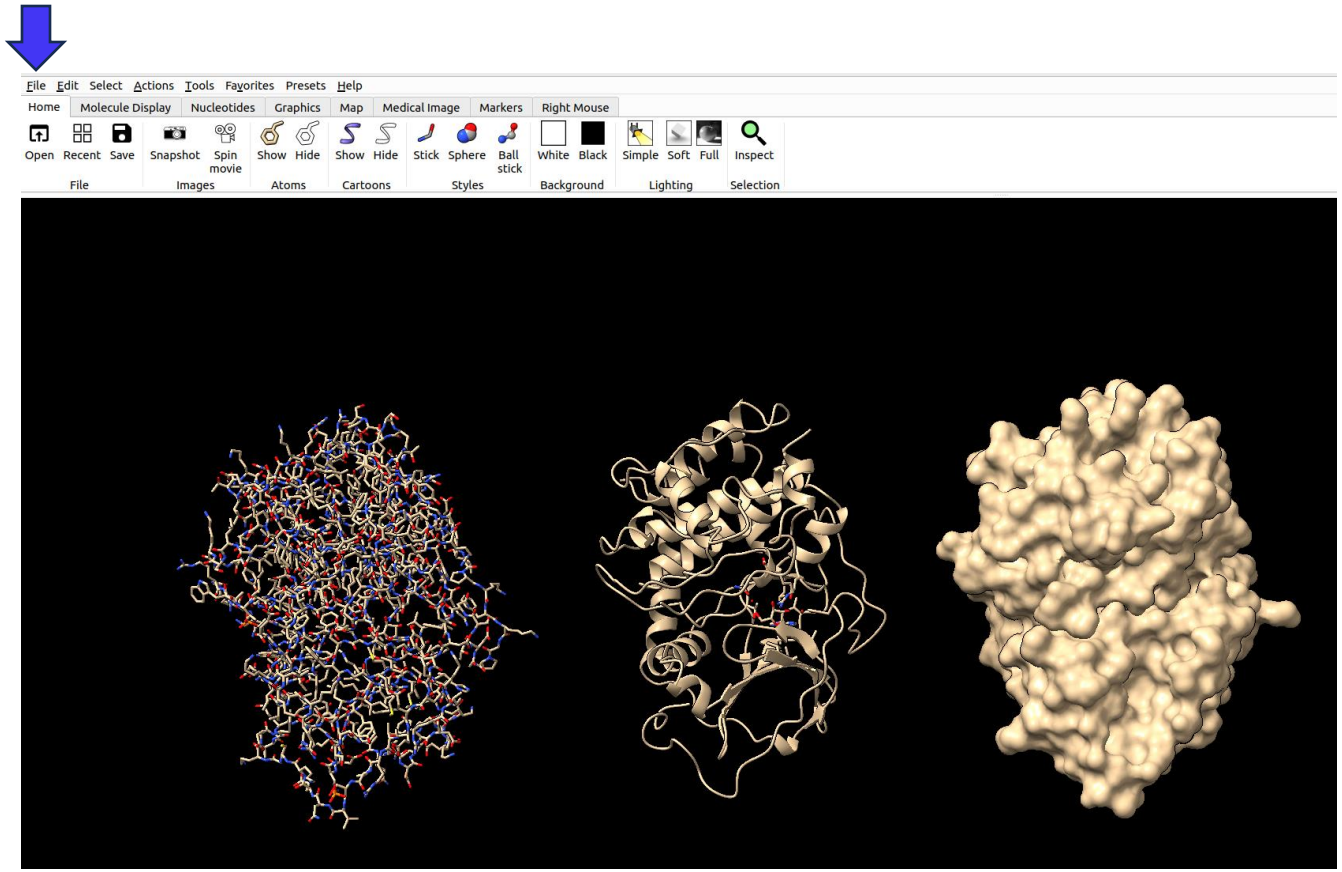
Mais ferramentas

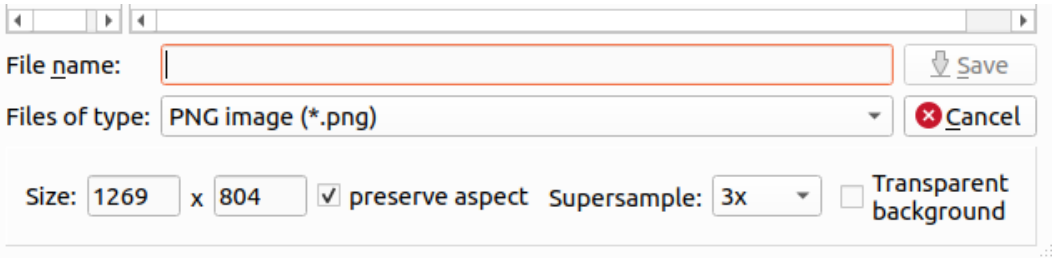


Gerando representação de superfície colorida por hidrofobicidade



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 N^{th}) 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
- **windowsize** – 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**

https://www.cgl.ucsf.edu/chimerax/docs/user/commands/movie.html

Obrigado!

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