

## Exploring a protein structure using Chimera: Modeling missing loops

*Balaji Nagarajan, Ph.D.*

*Prof. Umesh R Desai's Lab*

*Institute for Structural Biology, Drug Discovery and Development, Virginia Commonwealth University, Richmond VA. \*Corresponding author:*

[bnagarajan@vcu.edu](mailto:bnagarajan@vcu.edu)

## Installing Chimera

1. Go to: <https://www.cgl.ucsf.edu/chimera/download.html>
2. Download Chimera according to your platform.
  - a. Windows: Download [chimera-1.12-win64.exe](#)
  - b. Mac: Download [chimera-1.11.2-mac64.dmg](#)
3. Follow default installation instructions and install Chimera with a desktop shortcut icon (please note the path of the installation (e.g. C:\Program Files\Chimera 1.12rc))
4. If you have problems installing, check:  
<http://www.cgl.ucsf.edu/chimera/docs/UsersGuide>

## Installing Modeller

1. First, you will need to request a KEY for installation. Go to:  
<https://salilab.org/modeller/registration.html>
  - a. Fill in your details – make sure to use your VCU email address.
  - b. Check your email for the license key.
2. Click on “Download and installation” on the left-hand side of the Modeller website. ([https://salilab.org/modeller/download\\_installation.html](https://salilab.org/modeller/download_installation.html).) Download the appropriate Modeller installation file and enter your license key when prompted.
  - a. Windows: Download modeller9.19-64bit.exe
  - b. Mac: Download modeller-9.19.dmg
3. Please note where you installed Modeller – this needs to be provided when performing Loop modeling. (e.g. C:\Program Files\Modeller9.19)

## Acknowledgement

1. Chimera (<https://www.cgl.ucsf.edu/chimera/>) UCSF Chimera--a visualization system for exploratory research and analysis. Pettersen EF, Goddard TD, Huang CC, Couch GS, Greenblatt DM, Meng EC, Ferrin TE. *J Comput Chem.* 2004 Oct;25(13):1605-12.  
<https://www.cgl.ucsf.edu/chimera/docs/credits.html>
2. Modeller (<https://salilab.org/modeller/contact.html>) A. Šali and T. L. Blundell. Comparative protein modelling by satisfaction of spatial restraints. *J. Mol. Biol.* 234, 779-815, 1993. 3) Prof. Umesh R Desai (PI). 4) Dr. Nehru Viji Sankaranarayanan (nvsankaranar@vcu.edu)