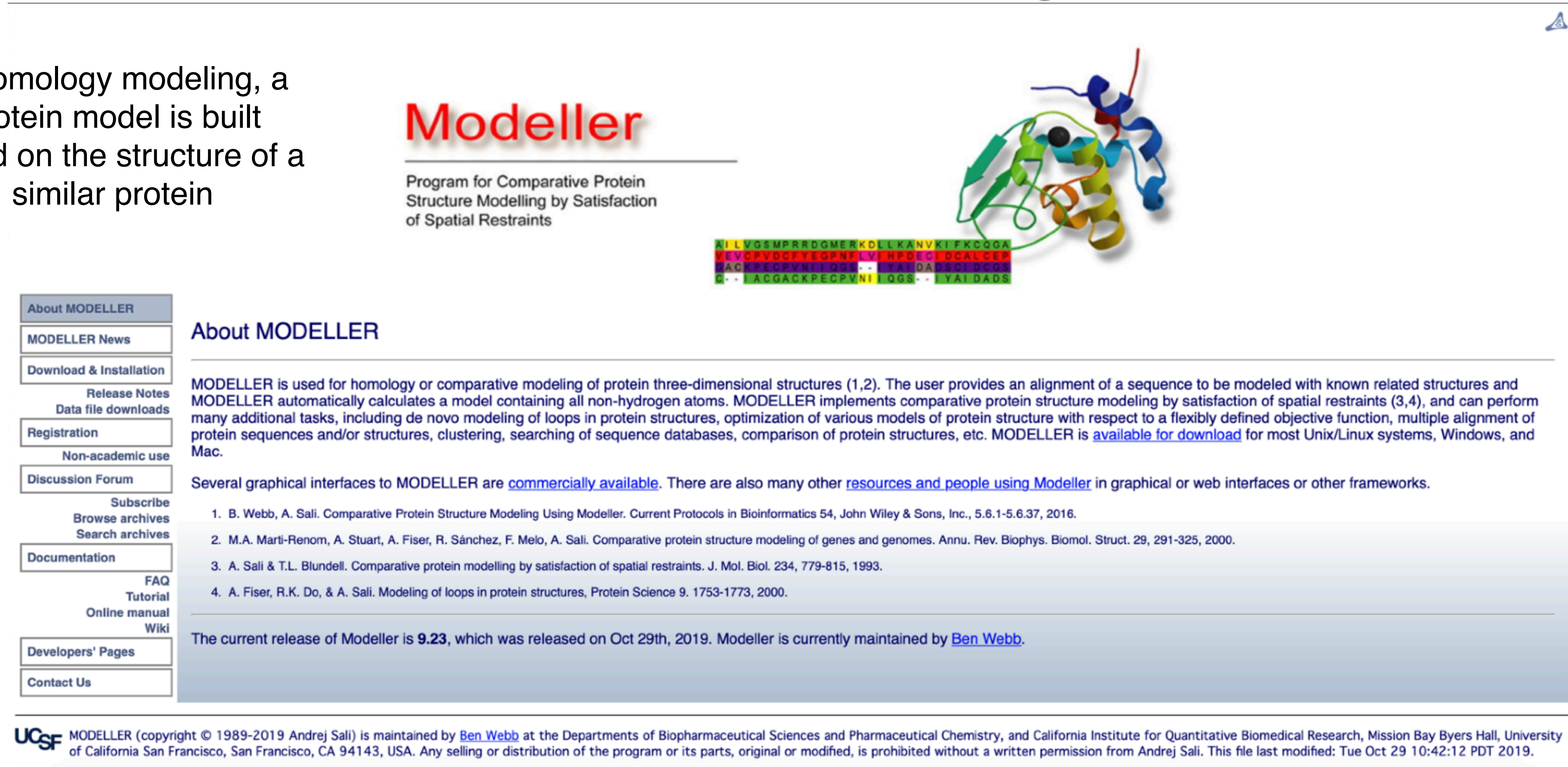


# Homology modeling further expands the range of accessible targets

In homology modeling, a protein model is built based on the structure of a similar protein



The screenshot shows the Modeller website interface. At the top, the word "Modeller" is written in a large, red, stylized font. Below it, the text "Program for Comparative Protein Structure Modelling by Satisfaction of Spatial Restraints" is displayed. To the right of the text is a 3D ribbon diagram of a protein structure, colored in green, yellow, and blue. Below the protein structure is a sequence alignment showing two sequences: "A I L V G S M P R R D G M E R K D L L K A N V K I F K C Q G A" and "Y E V C P N D C F Y E G P N F L V I H P D E C I D C A L C E P". The alignment is color-coded to show matches and mismatches. On the left side of the page, there is a vertical navigation menu with links: "About MODELLER", "MODELLER News", "Download & Installation", "Release Notes", "Data file downloads", "Registration", "Non-academic use", "Discussion Forum", "Subscribe", "Browse archives", "Search archives", "Documentation", "FAQ", "Tutorial", "Online manual", "Wiki", "Developers' Pages", and "Contact Us". The main content area is titled "About MODELLER" and contains a paragraph describing the program's capabilities. Below this paragraph is a list of four references. At the bottom of the page, there is a footer with the UCSF logo and a copyright notice.

**Modeller**  
Program for Comparative Protein Structure Modelling by Satisfaction of Spatial Restraints

**About MODELLER**

MODELLER is used for homology or comparative modeling of protein three-dimensional structures (1,2). The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms. MODELLER implements comparative protein structure modeling by satisfaction of spatial restraints (3,4), and can perform many additional tasks, including de novo modeling of loops in protein structures, optimization of various models of protein structure with respect to a flexibly defined objective function, multiple alignment of protein sequences and/or structures, clustering, searching of sequence databases, comparison of protein structures, etc. MODELLER is [available for download](#) for most Unix/Linux systems, Windows, and Mac.

Several graphical interfaces to MODELLER are [commercially available](#). There are also many other [resources and people using Modeller](#) in graphical or web interfaces or other frameworks.

1. B. Webb, A. Sali. Comparative Protein Structure Modeling Using Modeller. Current Protocols in Bioinformatics 54, John Wiley & Sons, Inc., 5.6.1-5.6.37, 2016.
2. M.A. Marti-Renom, A. Stuart, A. Fiser, R. Sánchez, F. Melo, A. Sali. Comparative protein structure modeling of genes and genomes. Annu. Rev. Biophys. Biomol. Struct. 29, 291-325, 2000.
3. A. Sali & T.L. Blundell. Comparative protein modelling by satisfaction of spatial restraints. J. Mol. Biol. 234, 779-815, 1993.
4. A. Fiser, R.K. Do, & A. Sali. Modeling of loops in protein structures, Protein Science 9. 1753-1773, 2000.

The current release of Modeller is **9.23**, which was released on Oct 29th, 2019. Modeller is currently maintained by [Ben Webb](#).

UCSF MODELLER (copyright © 1989-2019 Andrej Sali) is maintained by [Ben Webb](#) at the Departments of Biopharmaceutical Sciences and Pharmaceutical Chemistry, and California Institute for Quantitative Biomedical Research, Mission Bay Byers Hall, University of California San Francisco, San Francisco, CA 94143, USA. Any selling or distribution of the program or its parts, original or modified, is prohibited without a written permission from Andrej Sali. This file last modified: Tue Oct 29 10:42:12 PDT 2019.

**What is necessary/desirable about the physiological role of a SBDD target?**