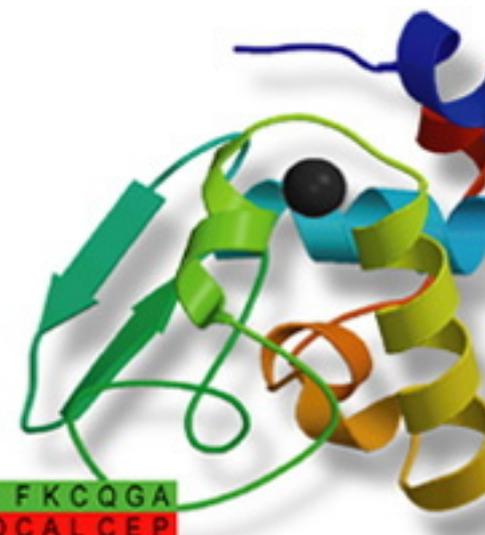




Modeller

Software for Comparative Protein
Structure Modelling by Satisfaction
of Local Restraints



```
AI LVGSMRRDGMERKDLLKANV KIFKCQGA
VEVCPVDCFYEGPNFLVIHPDECI DCALCEP
GACKPECPVNI IQGS - - YAI DADSCI DCGS
C - - I ACGACKPECPVNI IQGS - - YAI DADS
```

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Modeling with cryo-EM

This tutorial covers the use of MODELLER to build complete 3D models of an 'unknown' protein structure (i.e. not solved by X-ray crystallography) given three sources of experimental information:

- The amino acid sequence of the **unknown** protein structure.
- The PDB database of other, **known** protein structures.
- A cryo-EM map of the **unknown** protein structure.

In order to follow through this tutorial, the input files must first be downloaded. These files are available as a compressed archive in both [.tar.gz \(for Mac or Linux\)](#) and [zip \(for Windows\)](#) format (the same files are contained in each format archive). The archive contains a subdirectory for each step in the tutorial, and each step in turn contains a `results` subdirectory containing sample results from running the scripts.

The protein used in this example is a novel gene for lactate dehydrogenase that was identified from the genomic sequence of *Trichomonas vaginalis* (TvLDH). For some other sample studies with this system, please refer to the regular [MODELLER tutorial](#).

- [Step 1: Search for suitable templates](#)
- [Step 2: Select a template](#)
- [Step 3: Align sequence with structure\(s\)](#)
- [Step 4: Build comparative models](#)
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- [Step 6: Fit models into cryo-EM maps](#)
- [Step 7: Refine models with loop modeling](#)
- [Step 8: Flexible cryo-EM fitting with Flex-EM](#)

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