Universidad Nacional de San Agustín

Tópicos en Computación Gráfica

ArgosMol: A web tool for protein visualization

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Content

Overview

Definitions

Proteomics is the large-scale study of proteins [1]

Proteins are large, complex molecules that play many critical roles in the body. They do most of the work in cells. [1]

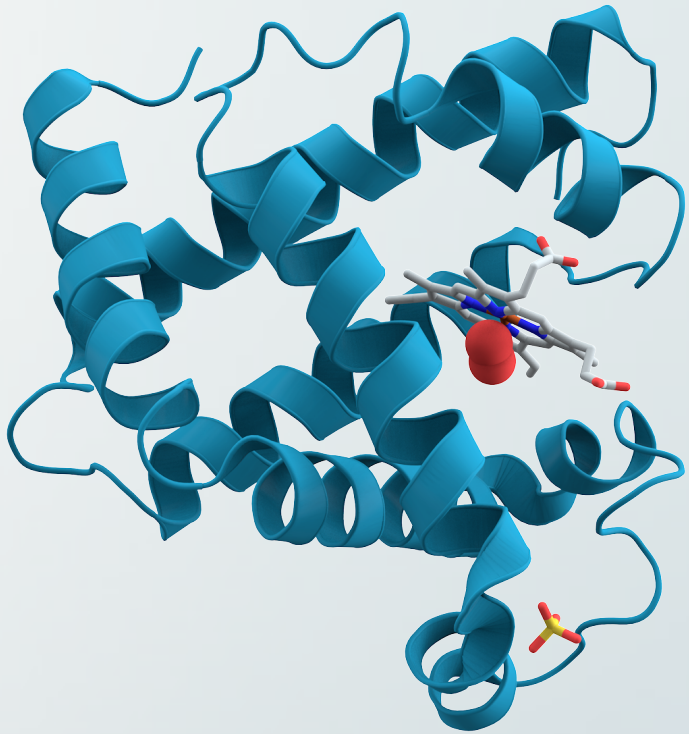

Figure: A representation of the 3D structure of the protein myoglobin. Source: PDB.

Protein structure

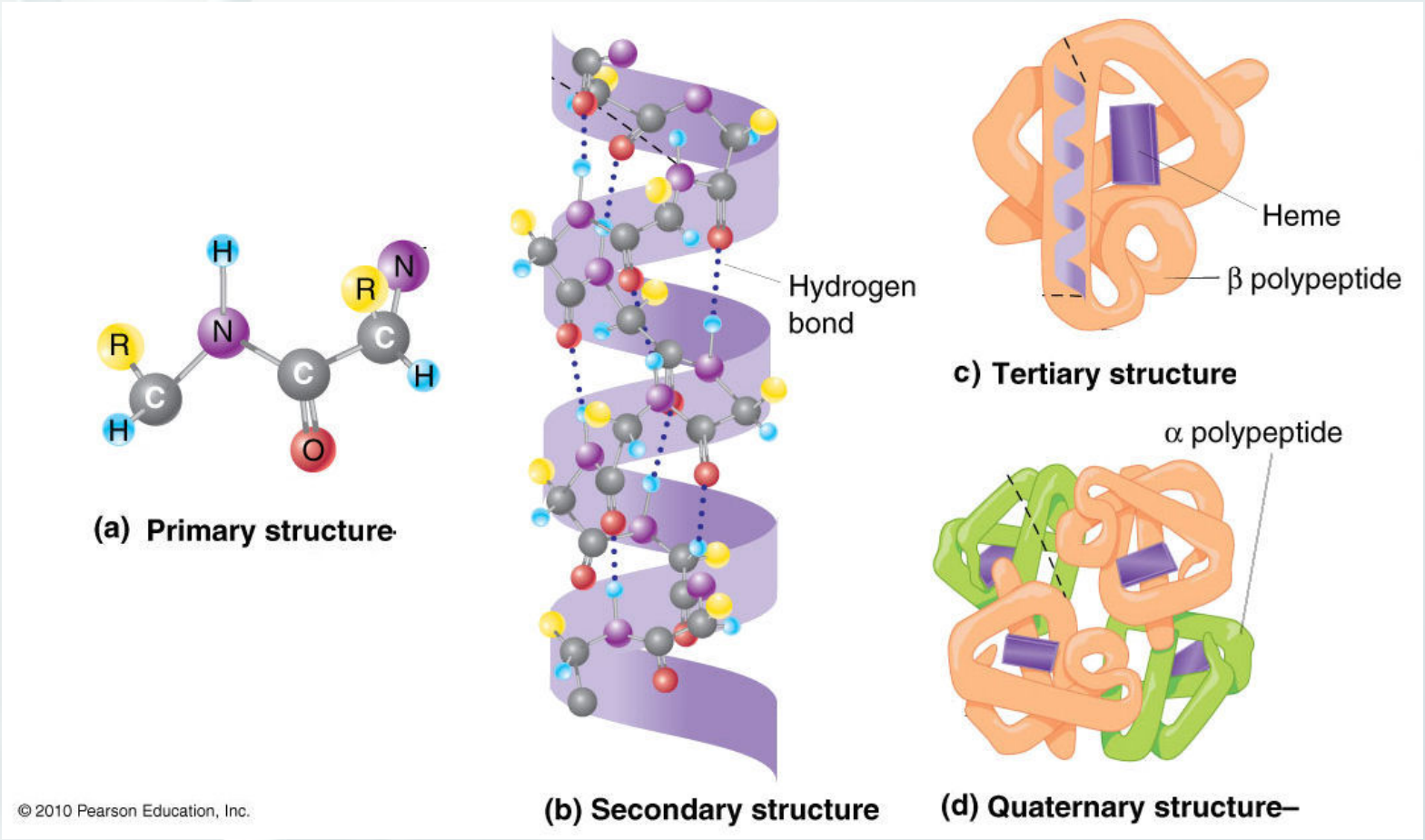

Figure: Types of protein structures. Source: [2].

Numbers

Protein structures are complex systems with several tens, hundreds and **thounsand** of residues (amino acids).

Only about **1%** of the total number of sequenced proteins has experimentally determined [3].

Overview

Motivation

Is one of the most used task in Bioinformatics [4, 5].

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Interactive visualization of large molecular structures can now be achieved via web-based 3D, It is not restricted to stand alone applications [7].

Overview

Problem

There is not a robust Web-based tool for protein visualization. The current applications are in development:

- They have bugs.
- They doesn't have all the functionality like stand-alone applications.
- They are not easy to use.

Related work
Jolecule

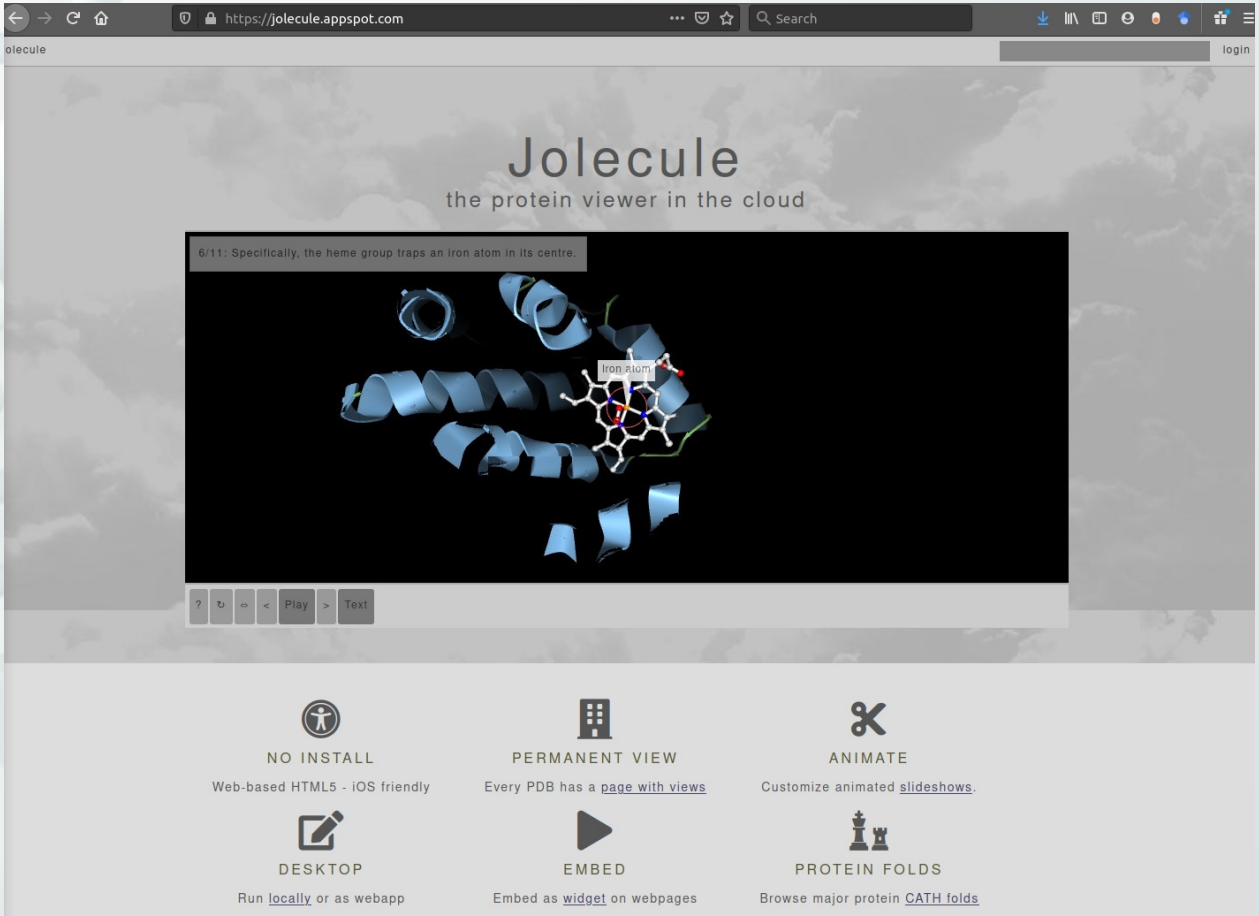

Figure: Web page of Jolecule.

Related work
NGL

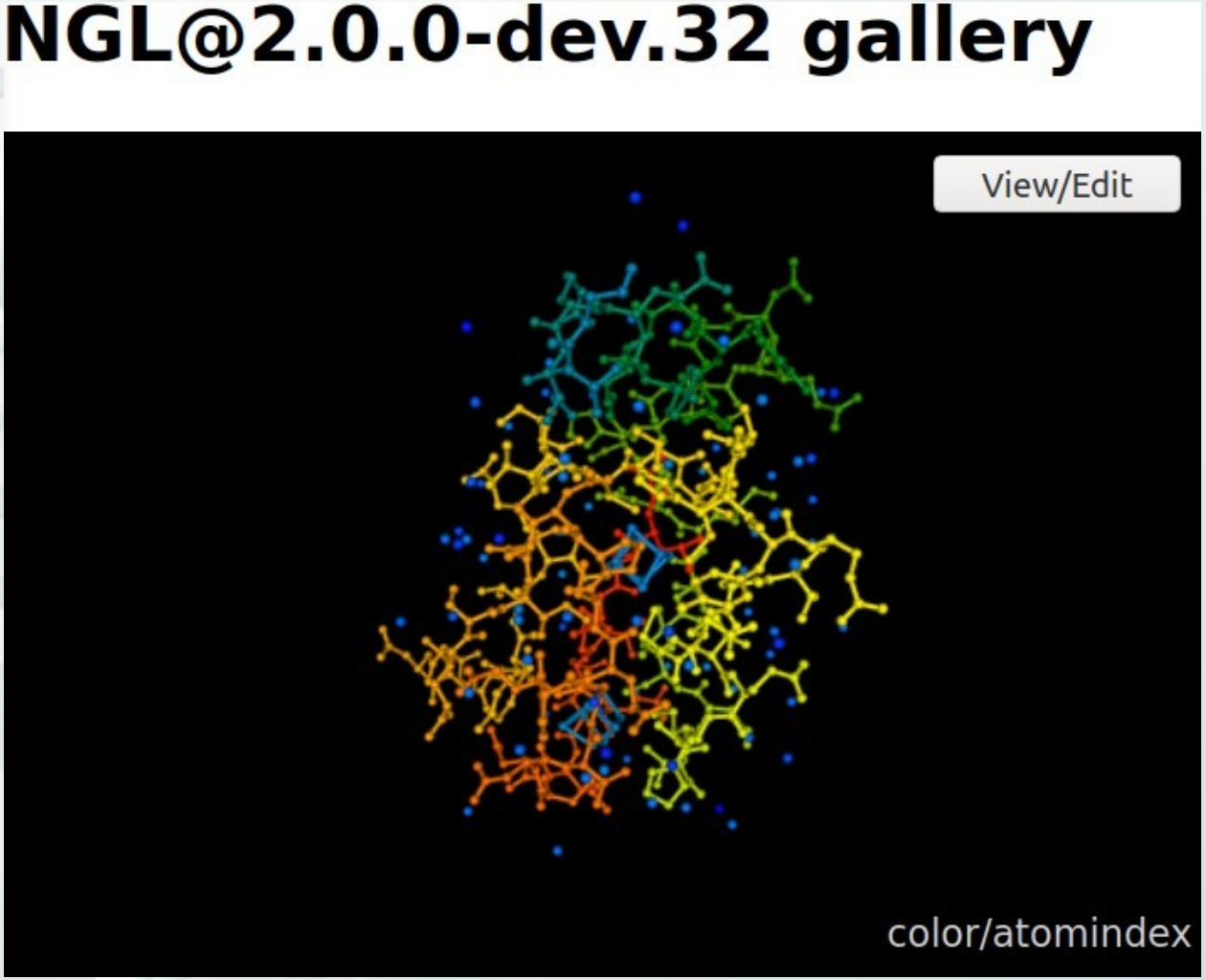

Figure: Web page of NGL [8].

Related work
EzMol

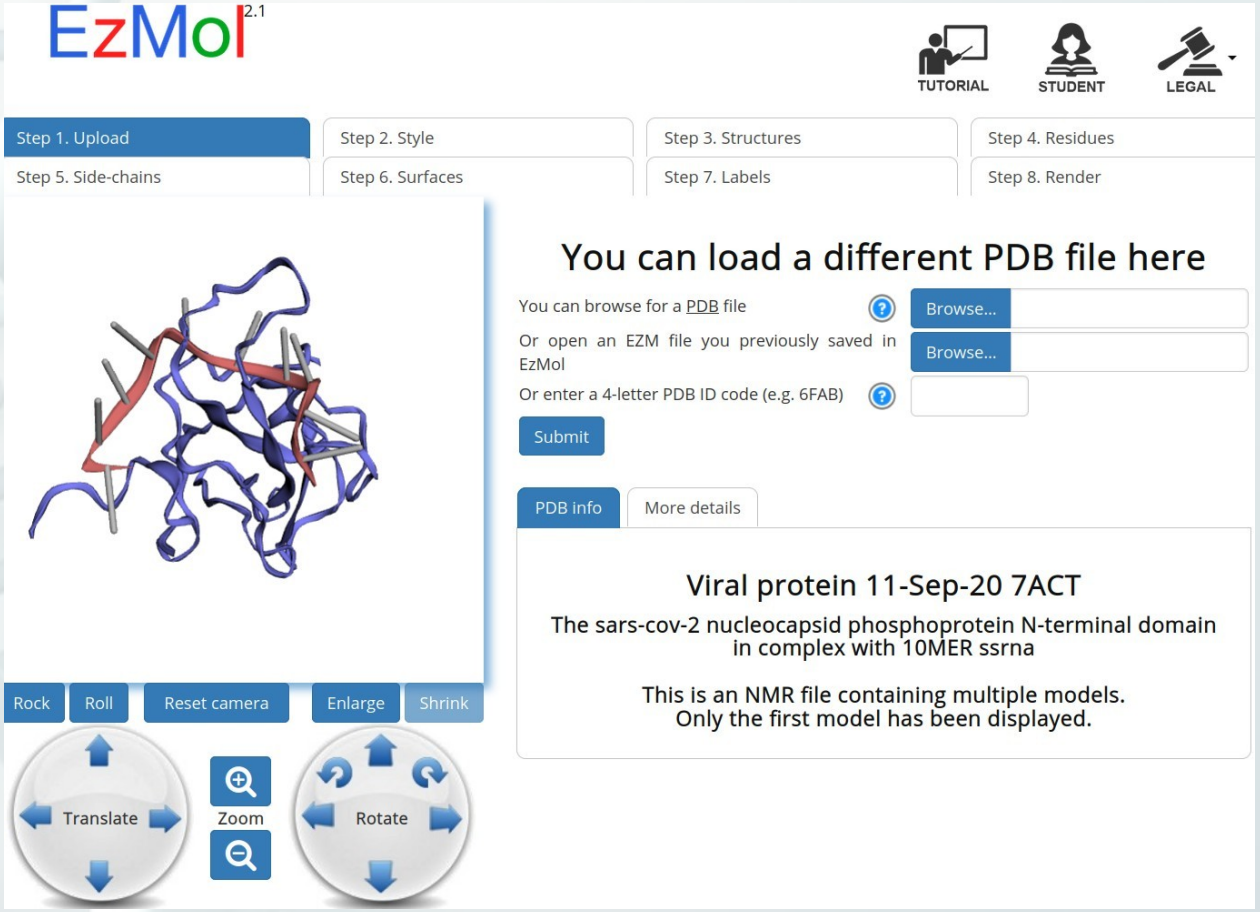

Figure: Web page of EzMol [6].

Related work
iCn3D

Figure: Web page of iCn3D [7].

Overview

- Introduction
  - Definitions
  - Motivation
  - Problem
- Related work
- Proposal
  - ArgosMol
- Conclusions

ArgosMol

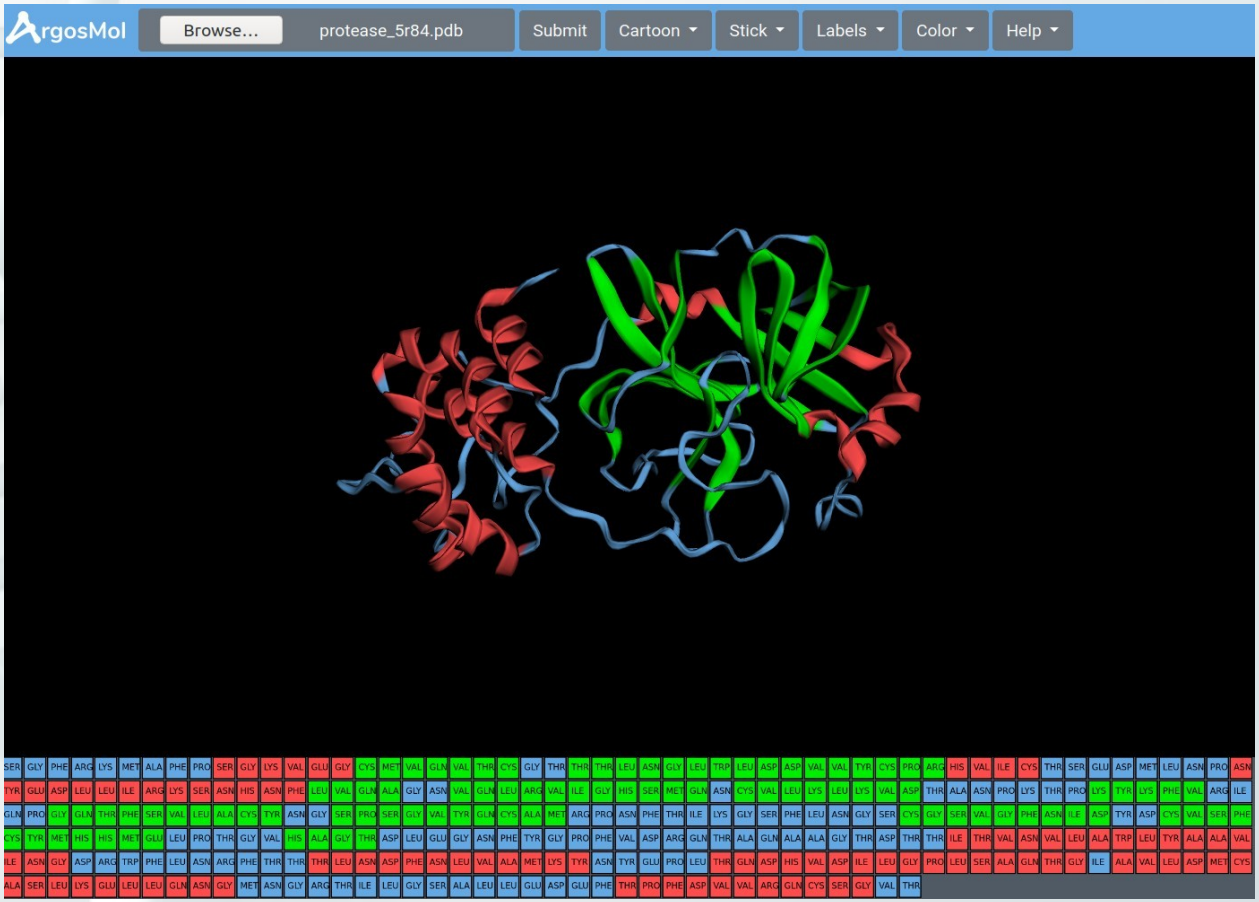

Figure: Web page of ArgosMol Enlace.

ArgosMol
Visualization

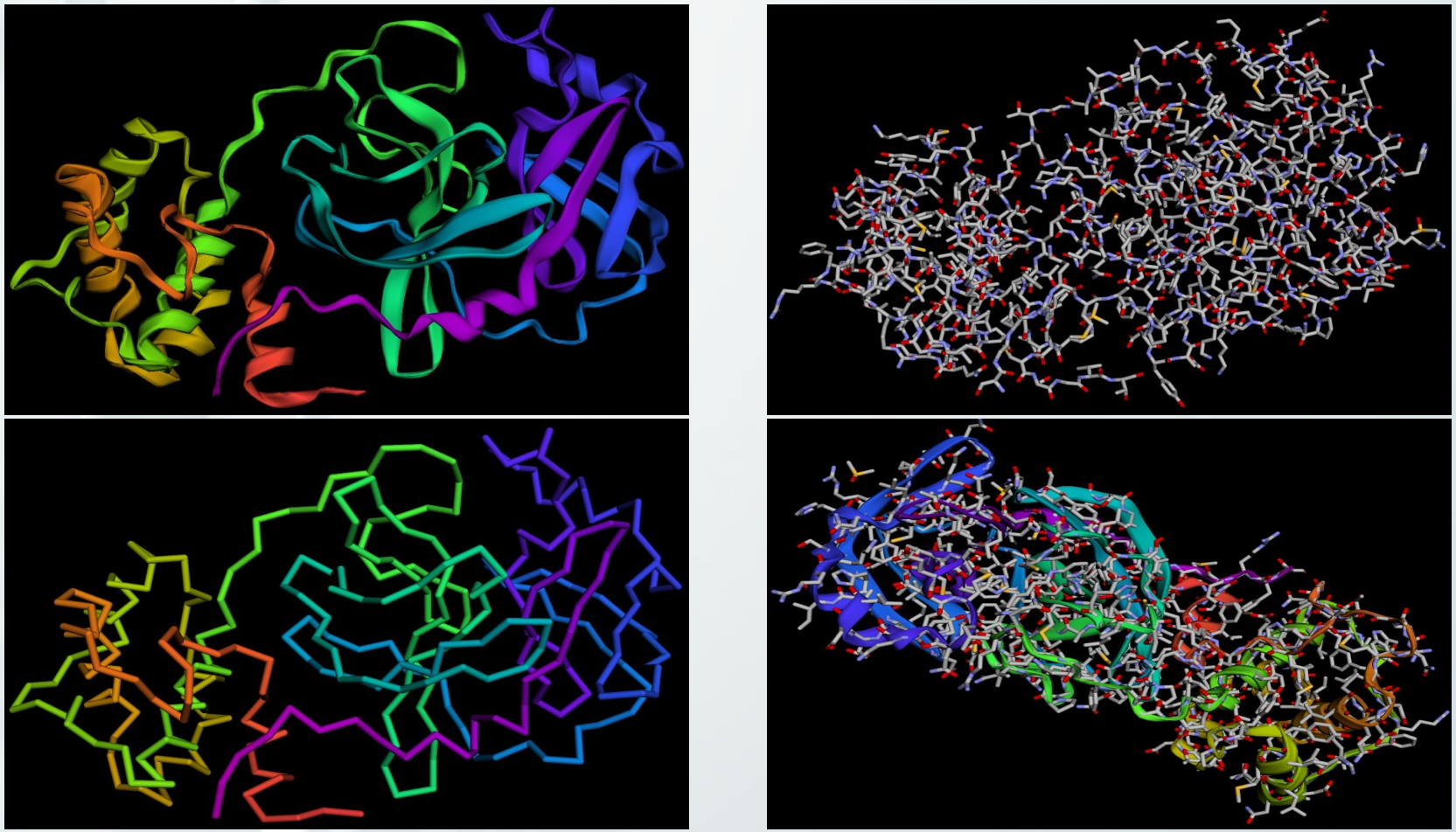

Figure: Visualization in ArgosMol.

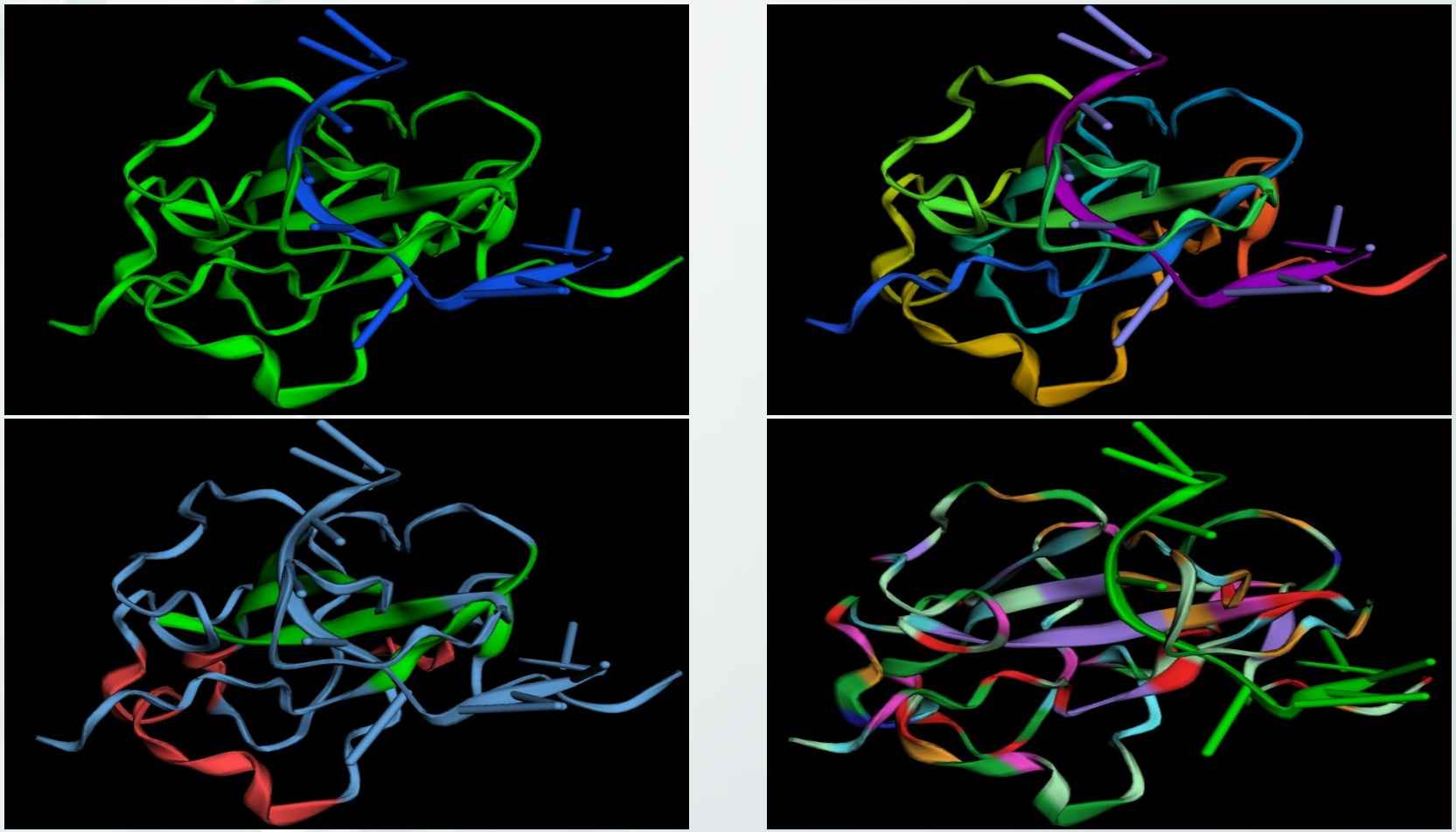

Figure: Colors in ArgosMol.

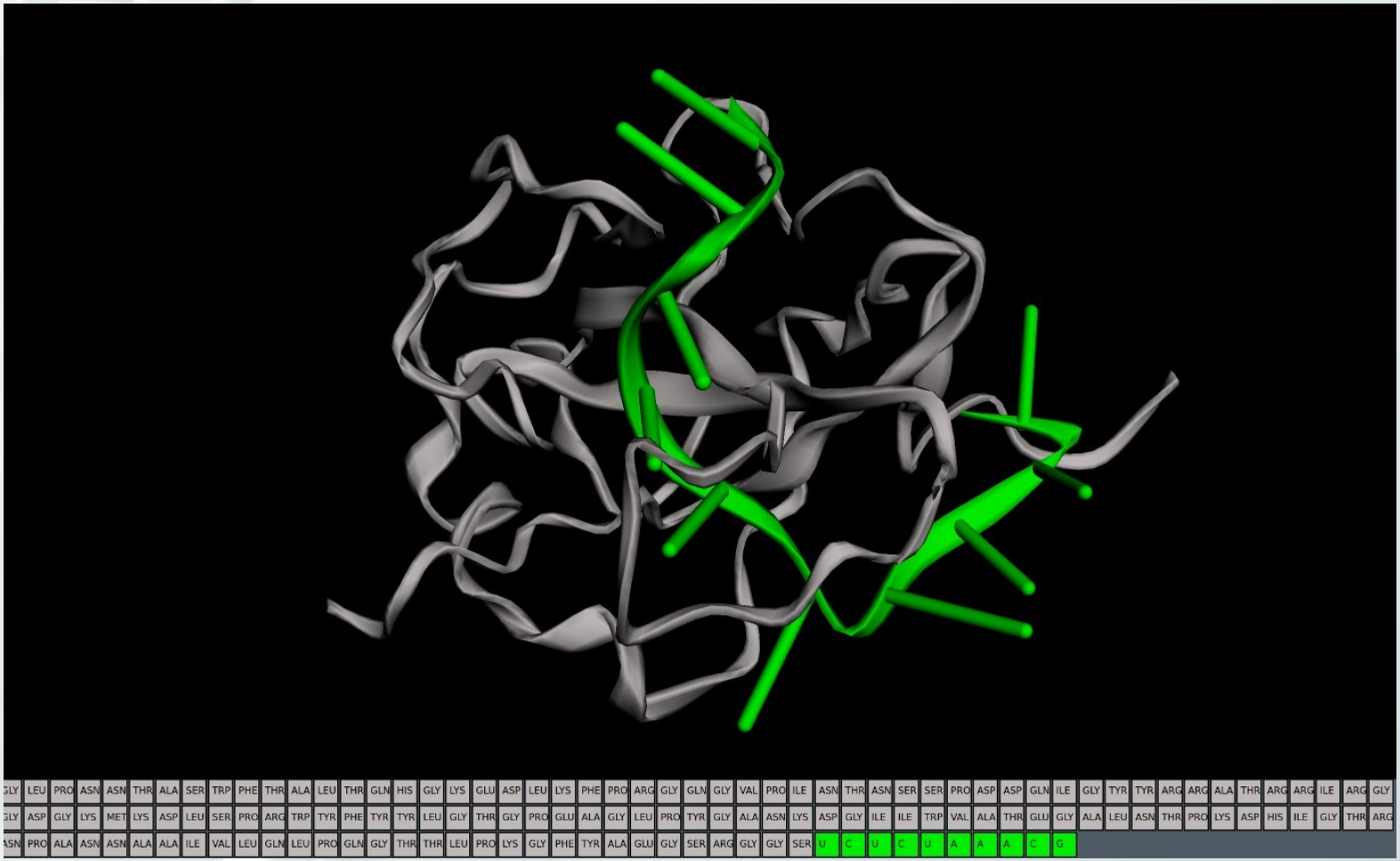

Figure: Relation between the model and the sequence in ArgosMol.

Conclusions

ArgosMol is an alternative to stand-alone applications that requiere instalation.

ArgosMol is part of a small number of Web-based tools for protein viosualization. Nevertheleses, ArgosMol improve the usability and the relation between the model and sequence.

In future version of ArgosMol, we will include protein structure prediction.

References I

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References II

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