Universidad Nacional de San Agustín

Tópicos en Computación Gráfica

ArgosMol: A web tool for protein visualization

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2021

Content

Introduction
- Definitions
- Motivation
- Problem

Related work

Proposal
- ArgosMol

Conclusions

Overview

Introduction
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- Motivation
- Problem

Related work

Proposal
- ArgosMol

Conclusions

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]

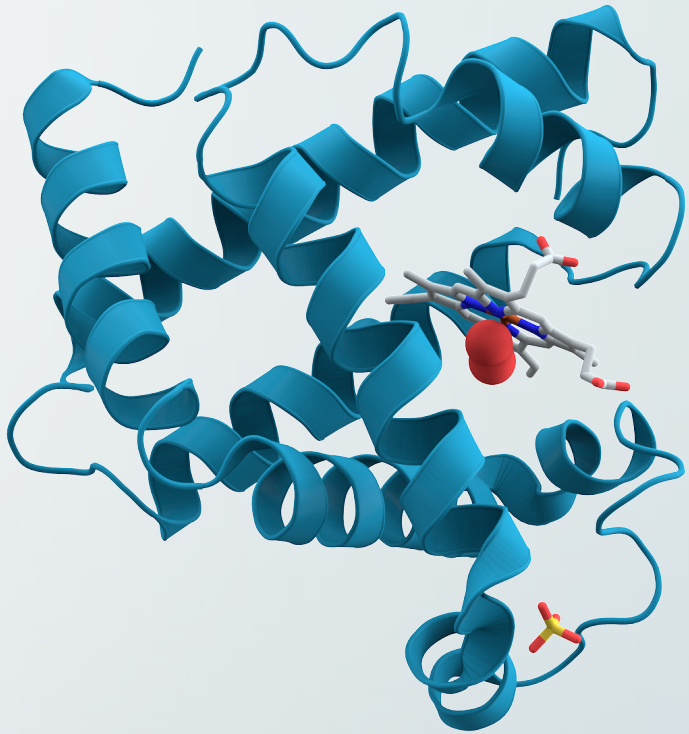

Figure: A representation of the 3D structure of the protein myoglobin. Source: PDB.

Protein structure

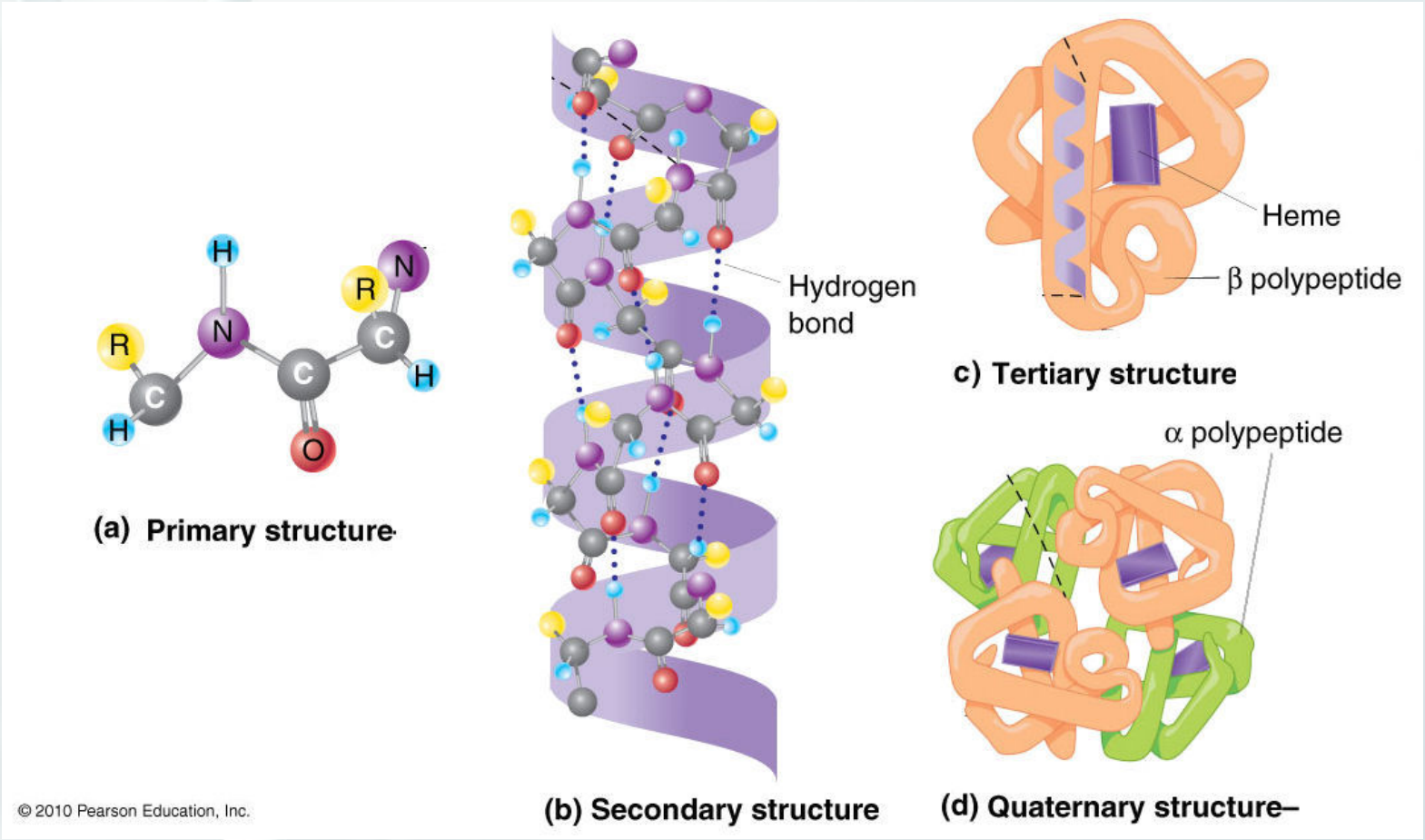

Figure: Types of protein structures. Source: [2].

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].

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Related work

Proposal
- ArgosMol

Conclusions

Motivation

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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].

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- Problem

Related work

Proposal
- ArgosMol

Conclusions

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

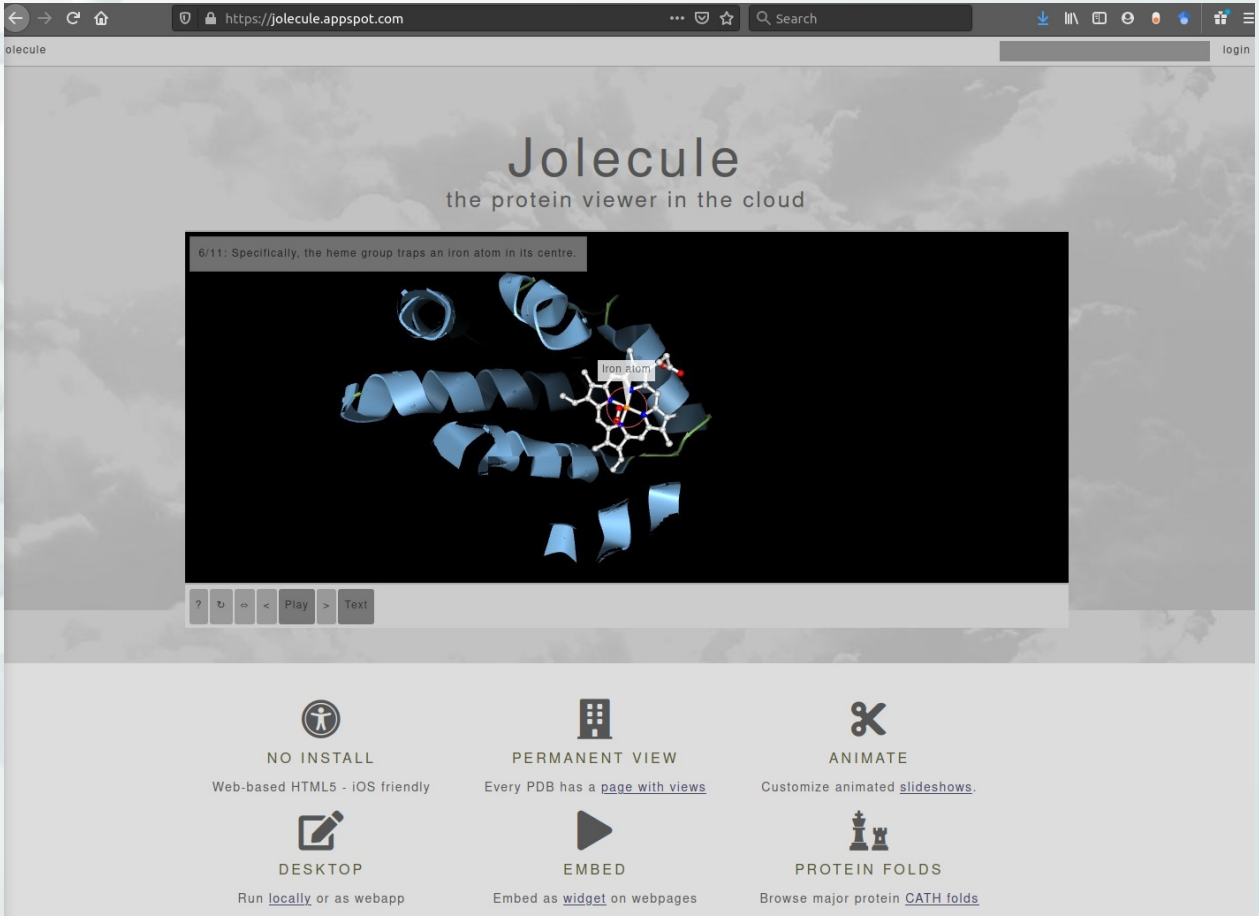

Figure: Web page of Jolecule.

Related work
NGL

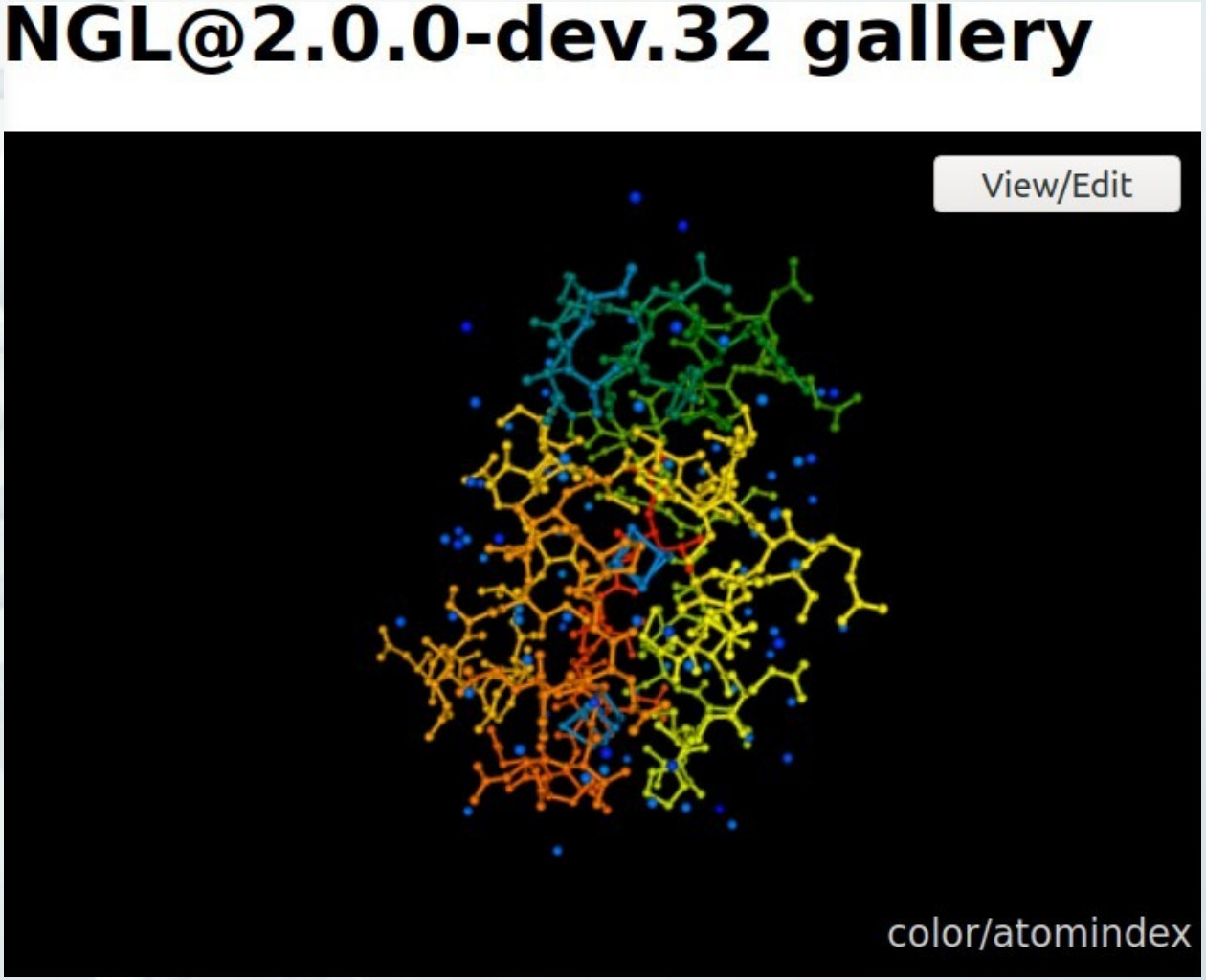

Figure: Web page of NGL [8].

Related work
EzMol

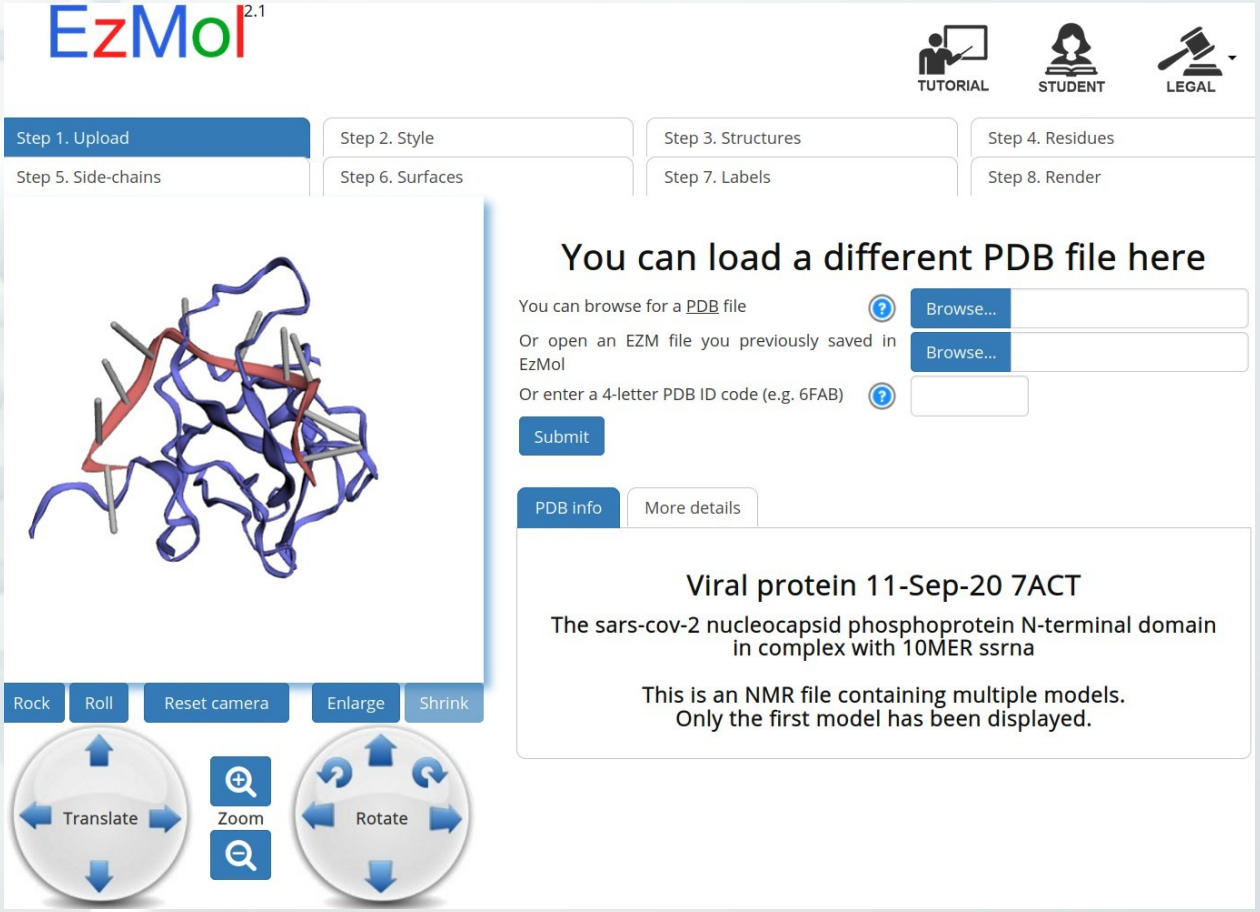

Figure: Web page of EzMol [6].

Related work
iCn3D

Figure: Web page of iCn3D [7].

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

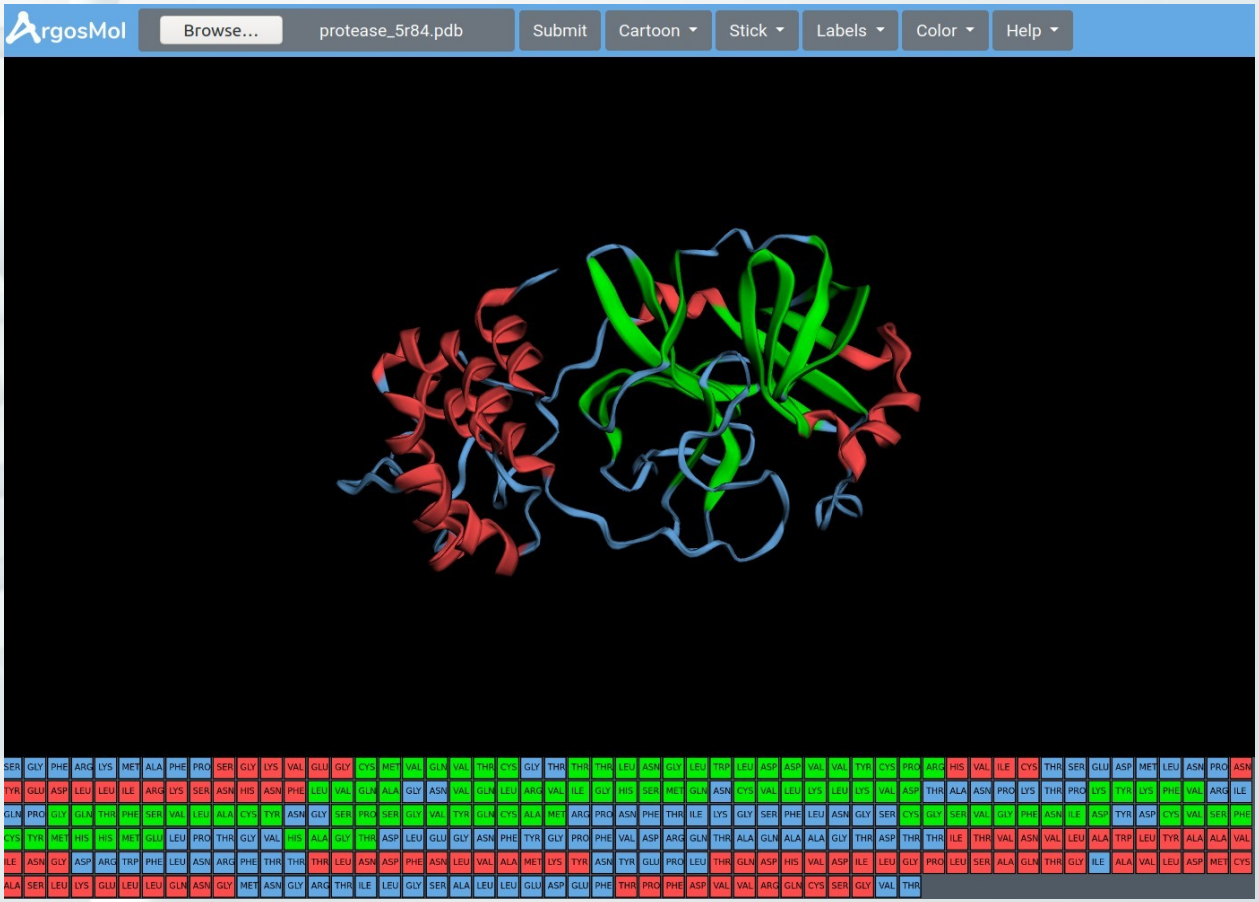

Figure: Web page of ArgosMol Enlace.

ArgosMol
Visualization

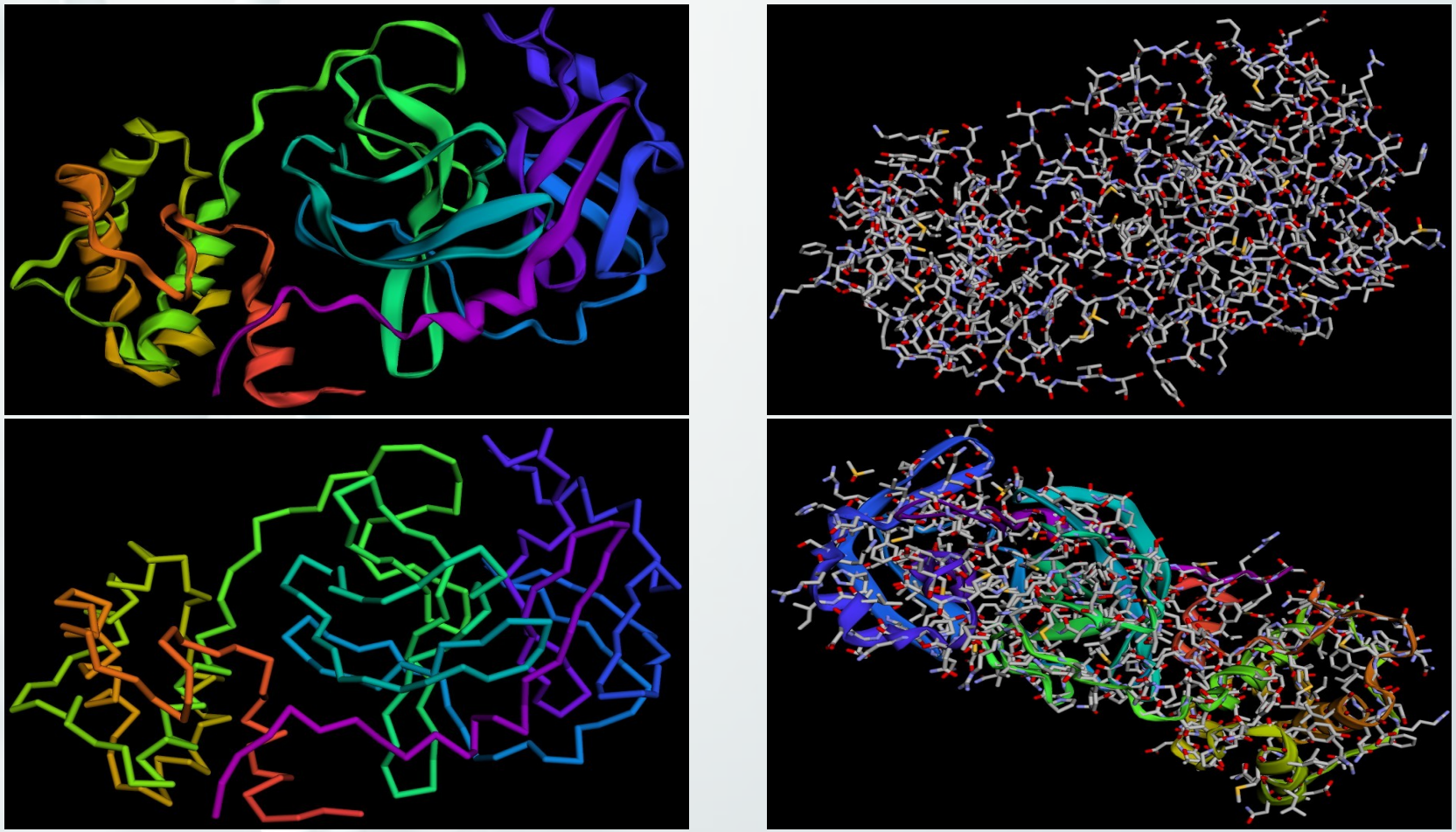

Figure: Visualization in ArgosMol.

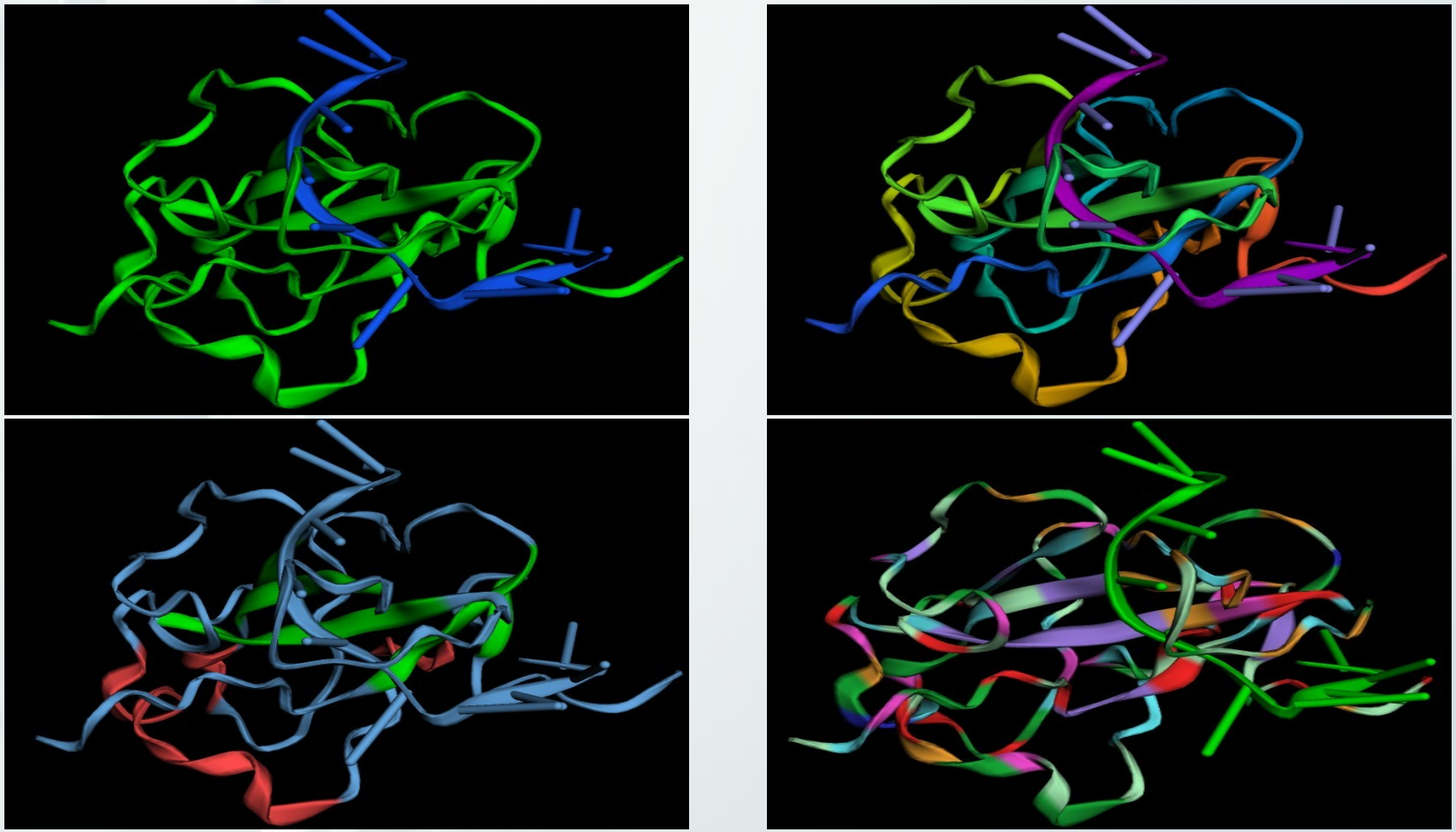

Figure: Colors in ArgosMol.

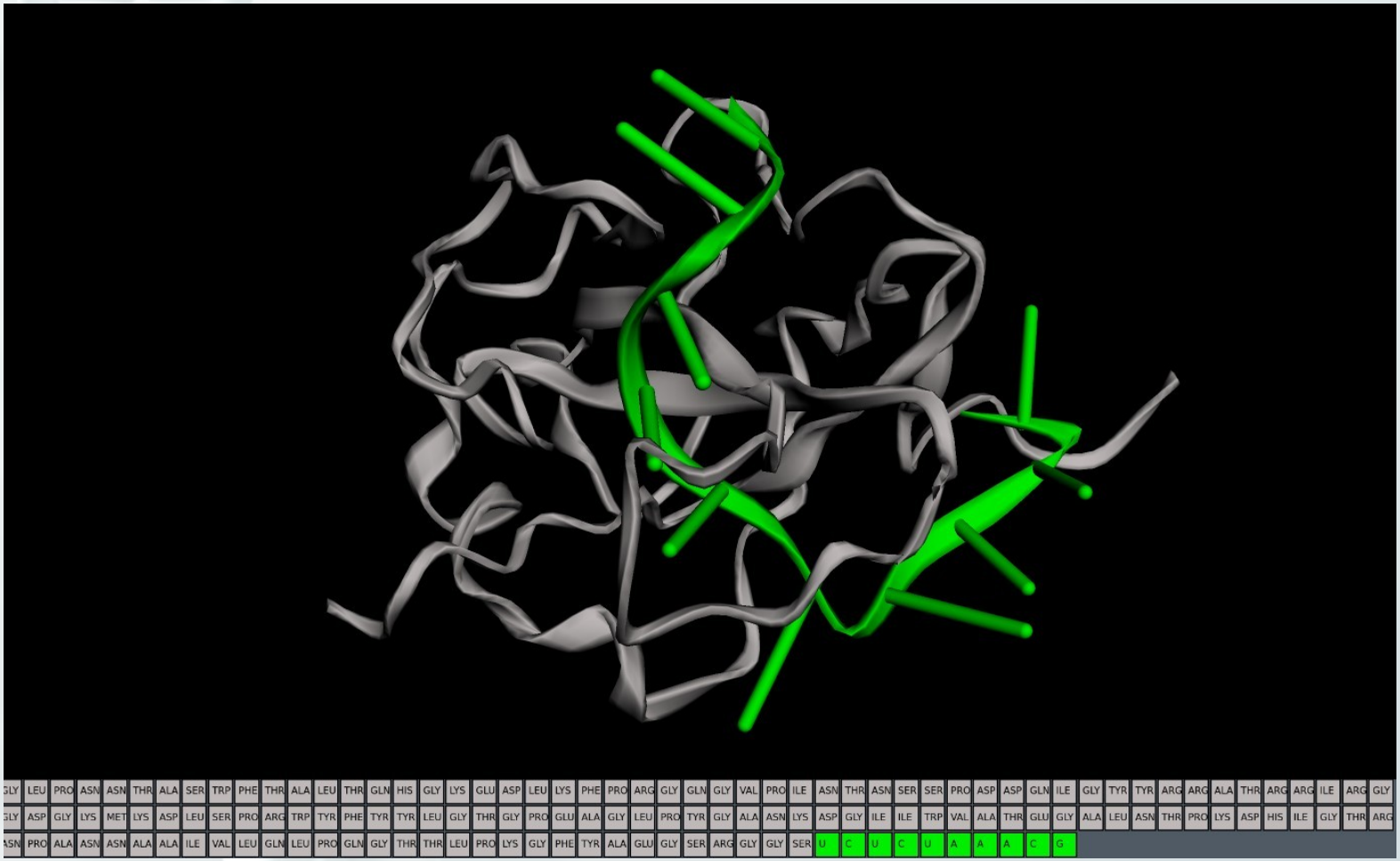

Figure: Relation between the model and the sequence in ArgosMol.

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

[1] N. L. Anderson and N. G. Anderson, “Proteome and proteomics: new technologies, new concepts, and new words,” *Electrophoresis*, vol. 19, no. 11, pp. 1853–1861, 1998.

[2] P. J. Russell and K. Gordey, *IGenetics*. Benjamin Cummings San Francisco, 2002, no. QH430 R87.

[3] H. Rangwala and G. Karypis, *Introduction to protein structure prediction: methods and algorithms*. John Wiley & Sons, 2011, vol. 18.

[4] S. I. O’donoghue, D. S. Goodsell, A. S. Frangakis, F. Jossinet, R. A. Laskowski, M. Nilges, H. R. Saibil, A. Schafferhans, R. C. Wade, E. Westhof *et al.*, “Visualization of macromolecular structures,” *Nature methods*, vol. 7, no. 3, pp. S42–S55, 2010.

[5] C. Mura, C. M. McCrimmon, J. Vertrees, and M. R. Sawaya, “An introduction to biomolecular graphics,” *PLoS Comput Biol*, vol. 6, no. 8, p. e1000918, 2010.

References II

[6] C. R. Reynolds, S. A. Islam, and M. J. Sternberg, “Ezmol: a web server wizard for the rapid visualization and image production of protein and nucleic acid structures,” *Journal of molecular biology*, vol. 430, no. 15, pp. 2244–2248, 2018.

[7] J. Wang, P. Youkharibache, D. Zhang, C. J. Lanczycki, R. C. Geer, T. Madej, L. Phan, M. Ward, S. Lu, G. H. Marchler *et al.*, “icn3d, a web-based 3d viewer for sharing 1d/2d/3d representations of biomolecular structures,” *Bioinformatics*, vol. 36, no. 1, pp. 131–135, 2020.

[8] A. S. Rose and P. W. Hildebrand, “Ngl viewer: a web application for molecular visualization,” *Nucleic acids research*, vol. 43, no. W1, pp. W576–W579, 2015.

[9] M. Shi, J. Gao, and M. Q. Zhang, “Web3dmol: interactive protein structure visualization based on webgl,” *Nucleic acids research*, vol. 45, no. W1, pp. W523–W527, 2017.