FirstGlance.Jmol.Org

for BioMolViz.Org November 6, 2020

Eric Martz (Martz.MolviZ.Org) – This document: BioMolViz.MolviZ.Org

Main Goals:

- Ease of use (any macromolecular structure; >170,000 in the Protein Data Bank)
- Your 'first glance' is maximally informative
- Guidance for interpretation: explanations and examples
- Scrupulous attention to avoiding misinterpretations or failing to show important information.
- Free and open source

Example: 1IJW

- Google 'firstglance' (no space!)
- What do you see? Read the intro!
- FirstGlance is a user-interface wrapper for the separate project <u>Jmol.</u>
- Example of non-technical language and guidance: Reliability of this model (Rfree)
- Ligands and Non-Standard Residues: CBR, Isolate residue, View: Sticks (color key automatic), Click to identify.
- Reset & Make an animated slide (examples at tinyurl.com/movingmolecules)

How I Got Here:

- 1997 NSF-funded workshops: RasMol for college faculty
- One year later, clear that **command-language** *disempowered* nearly all participants.
- Protein Explorer 1998-2006: Great while it lasted ... Chime was its downfall.
- FirstGlance started 2005. Now 15 years of nearly continuous development.
- I am the primary architect and coder of FirstGlance (not of Jmol!).
- Many productive collaborations with Jaime Prilusky, Ángel Herráez, Joel Sussman, Bob Hanson, Frieda Reichsman and others.

Proteopedia.org & FirstGlance: A Synergy

- FirstGlance simplified because:
 - Canned representations and color schemes
 - Cannot customize the view, except it is easy to isolate or hide things.
- Proteopedia
 - Easiest way to make customized macromolecular scenes and share them.

Lesson Plans with Assessment – Each Participant:

- Chooses a different macromolecule.
- Answers a <u>list of questions</u> that relate structure to function with snapshots or animations from FirstGlance.
- Hands in answers in the form of slides for grading. (<u>Sample report</u>.)

Optional examples:

1F88

• Isolate one chain

6EF8

- Isolate one chain
- Contacts and non-covalent interactions with the 2nd heme from carboxy-end, HEC501.

Questions? Feedback? m0lviz@yahoo.com

I am happy to help you get started with FirstGlance in a one-to-one zoom session.