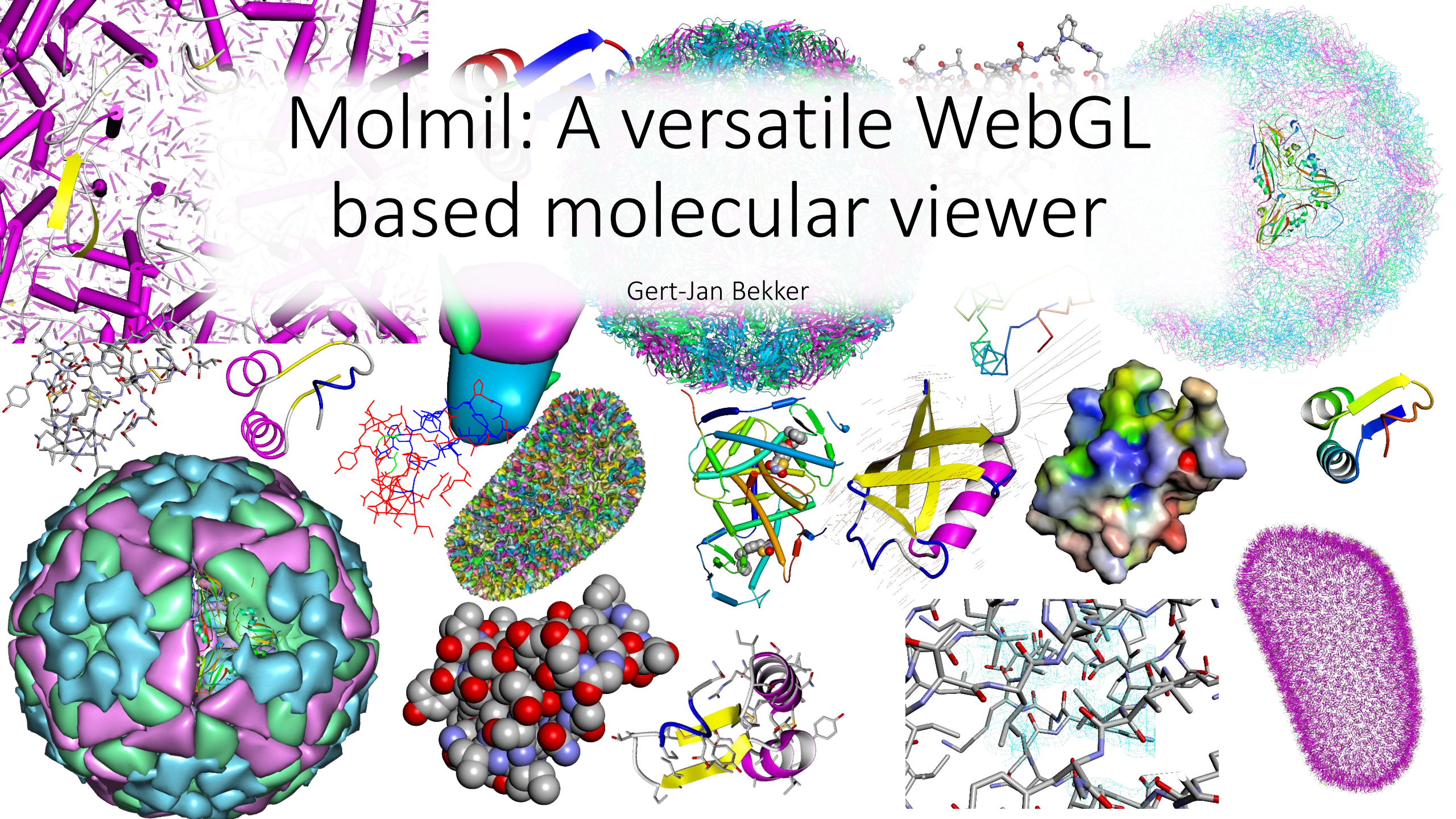
Molmil: A versatile WebGL based molecular viewer

Gert-Jan Bekker



Java on the web; the end of an age

- jV & Jmol applets were used on the web
- Oracle bought Sun (developer of Java) in 2009
- WebGL: prototypes in 2006 (Canvas 3D), WebGL Working Group (Khronos) in 2009, v1.0 specs released in 2011
- First draft implementation in Chrome in 2010, Firefox soon after, IE in 2013 and finally Safari in 2014
- 2015: Chrome drops Java support, Edge (IE12) never supported it; 2017: Firefox
- 2016: Oracle deprecates applets from JDK 9

Molmil: the start of a new one

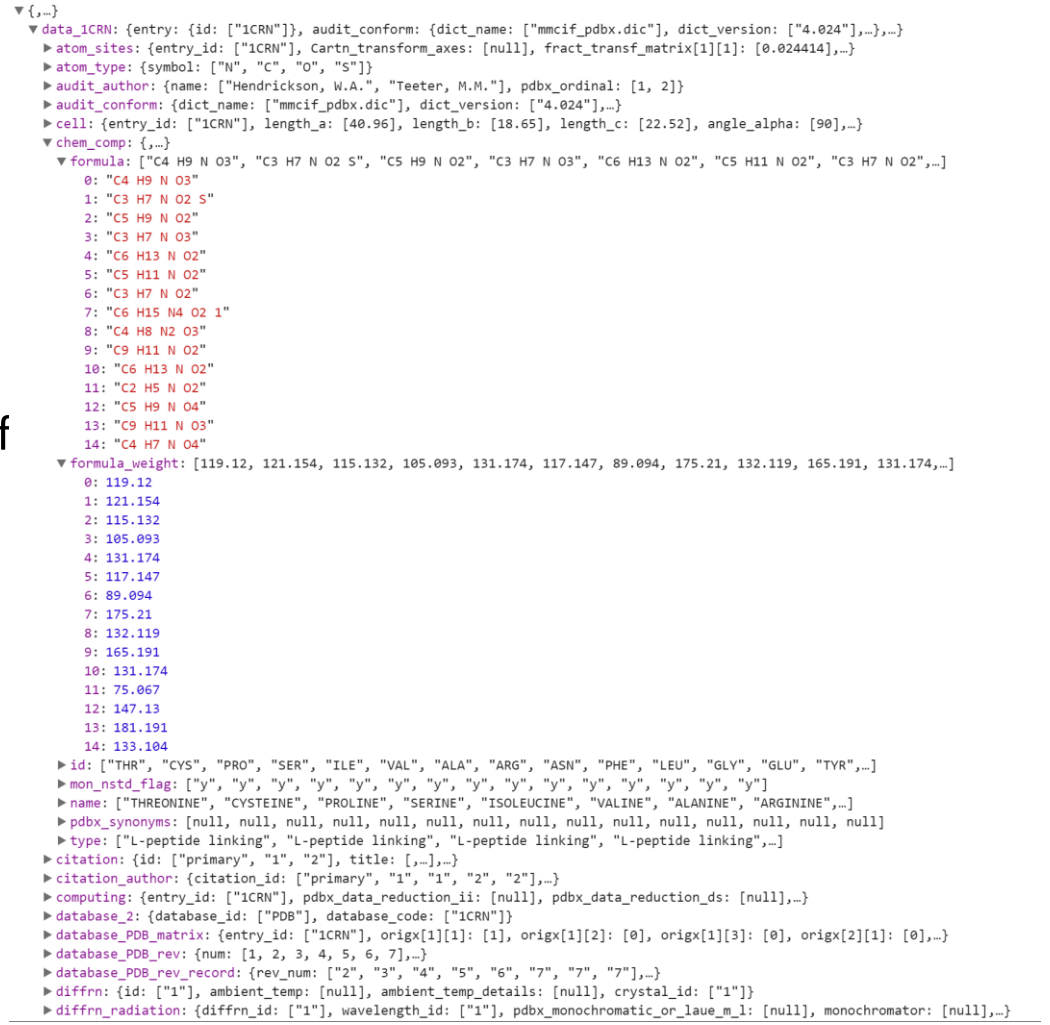
- Work on a molecular viewer for tablets started in 2012
- A new viewer for only tablets isn’t worthwhile; we wanted wide support
- WebGL was a new, but unproven technology with the potential for very wide support
- Beta version released in 2013; v0.9 in 2014, source (v1.0) published on GitHub in 2016 (along with J. Chem. Inf. paper)

Molmil Beta

- Released in 2013
- Part of PDBj website; not a standalone web app
- Only Mine PDB entry viewer
- Could only read PDBx/mmJSON format

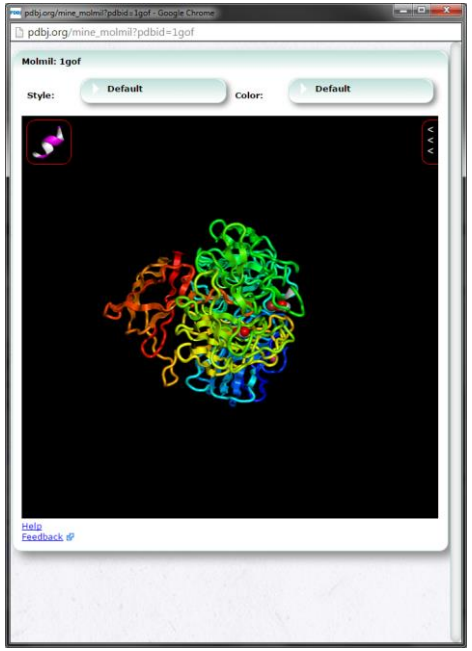
PDBx/mmJSON format

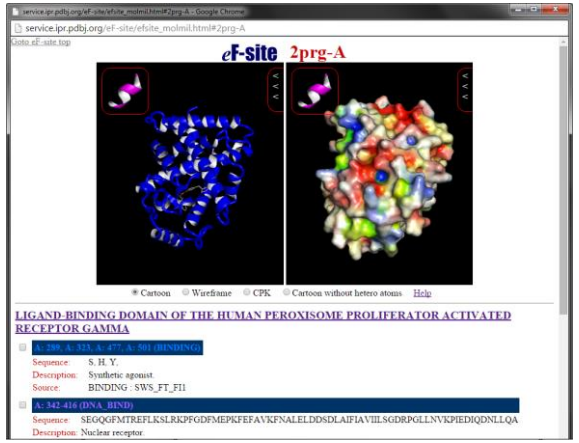
- Only a few programming languages have a PDBx/mmCIF parser
  - However many have a JSON parser (some have multiple)
- “Jsonified” version of PDBx/mmCIF format
  - Data structure of PDBx/mmJSON is very similar to that of PDBx/mmCIF
- Includes some optimizations for improved gzip compression
  - Gzipped ~40% smaller than PDBx/mmCIF
  - Simple typing (integer/float) is included in the format
- Metadata-only version used on PDBj website for displaying entries

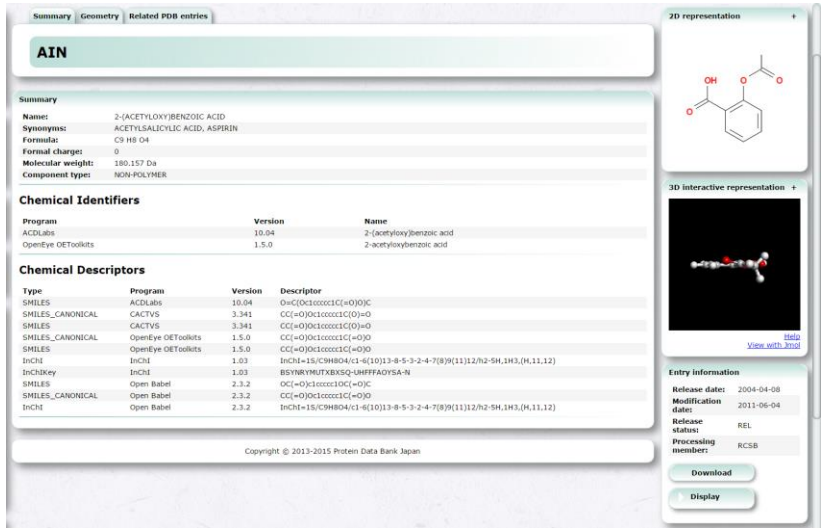


Molmil 0.9

- Revolutionary update
  - Standalone version (no longer requires the PDBj website to function)
  - Support for multiple file formats ➔ even USER specified files could be loaded
  - Molmil UI

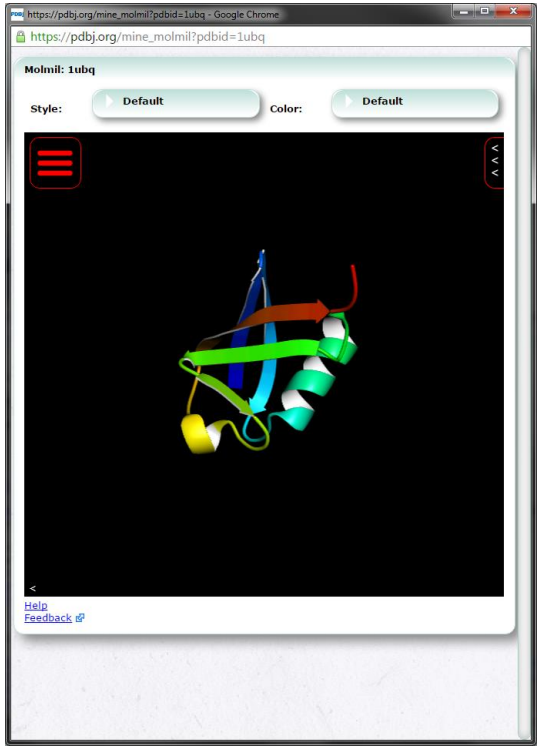


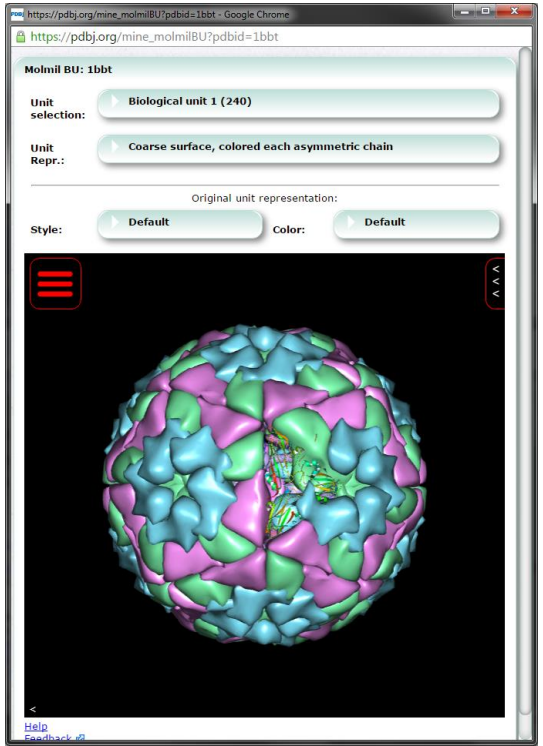


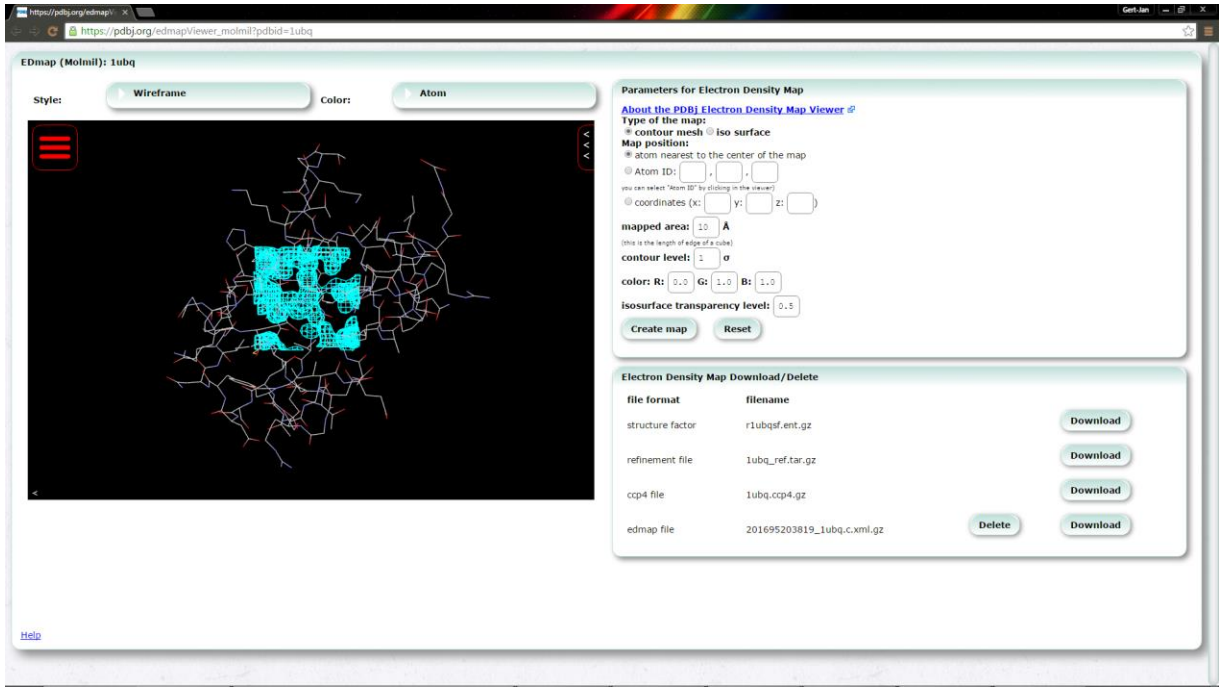


Molmil 1.0

- Evolutionary update
  - Many improvements and bugfixes
  - Support for additional PDBj services

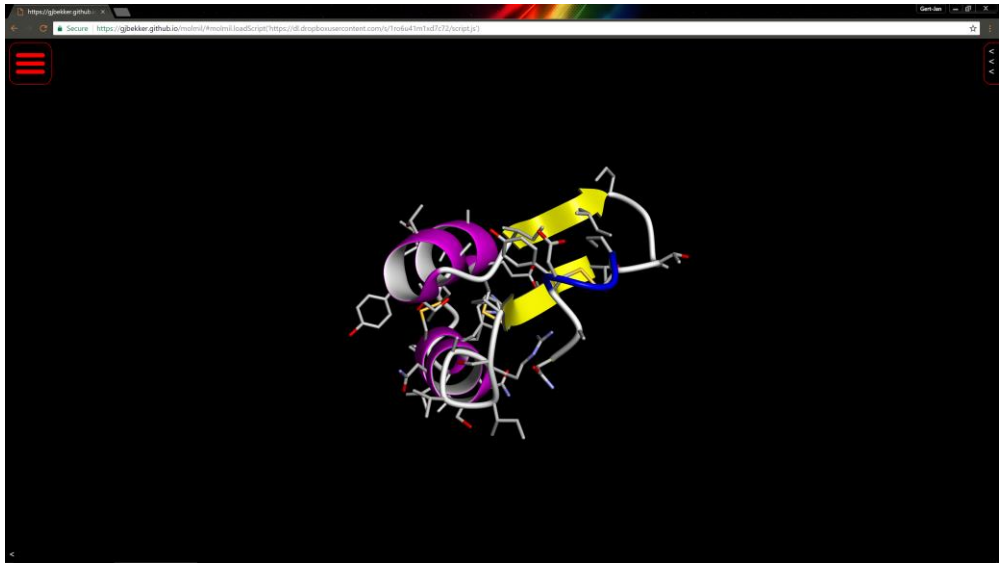






Beyond PDBj

- Rudimentary command line
  - Subset of Pymol commands
  - Molmil JavaScript API
  - Future: jV commands
  - Future: jmol commands
- Load Molmil script (e.g. from DropBox)
- Integrating Molmil & loading scripts/data from your local machine



https://github.com/gjbekker/molmil/wiki/Deploying-without-a-public-web-server

Local scripts & files

- Many programs with command lines support loading files by commands
- Molmil, which runs inside a web browser, is limited due to security issues
- You don’t want your browser to give any random website access to your files!
- Thus using Molmil in such a way is limited

Local scripting using Mozilla Firefox

- Mozilla Firefox allows running scripts locally, while having access to files in the same folder as where it was started from

- Files stored locally for easy reproducibility

- Perfect for making images for publication
  - Especially if you have to remake your images
  - Used extensively for my own paper:
    - Gert-Jan Bekker et al. *J. Chem. Theory Comput.*, **2017**, 13, 2389–2399

Load MD trajectories

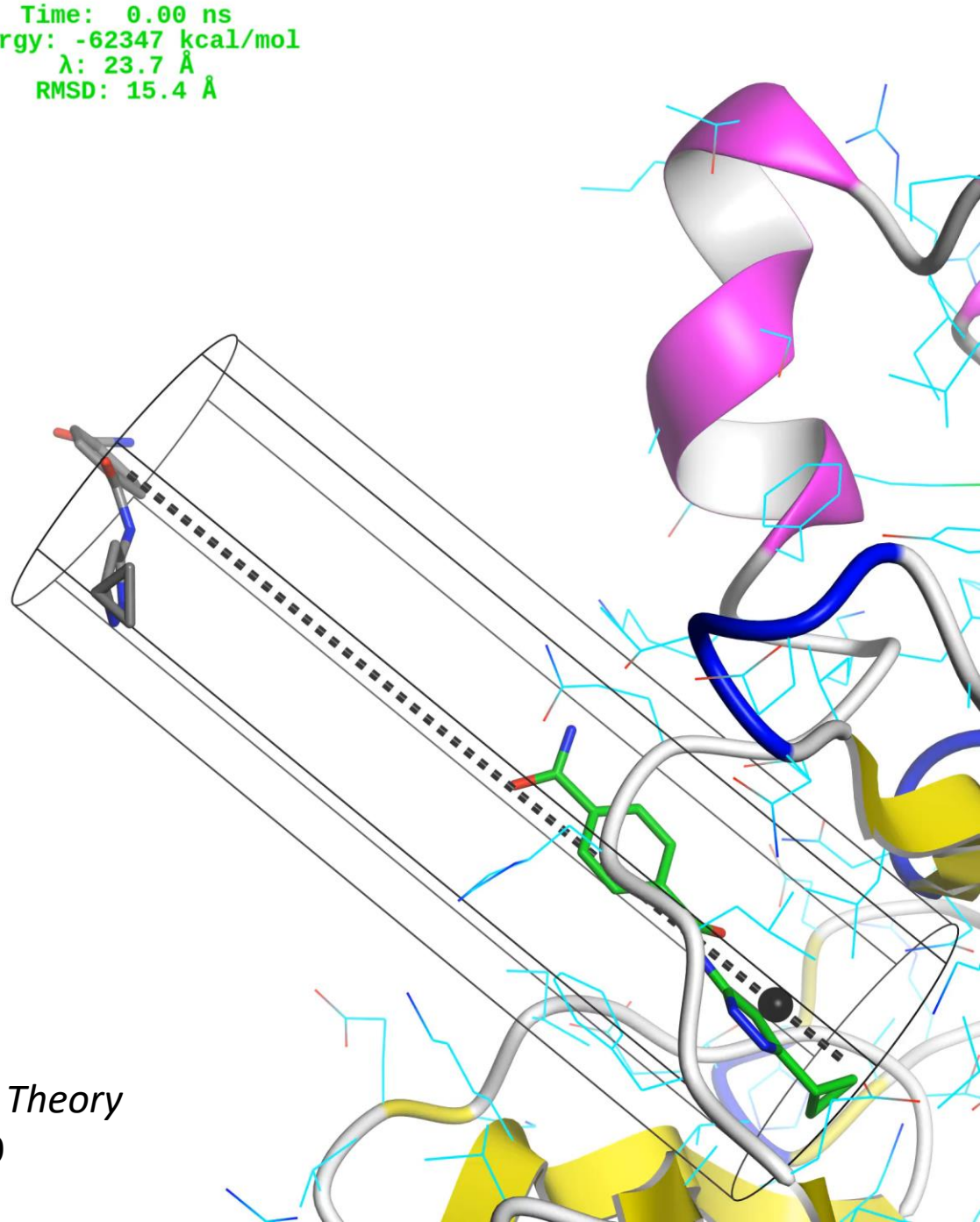
- Currently supported:
  - PDB models (not recommended)
  - Presto COD
  - Gromacs TRR
  - Gromacs XTC (compressed)

- Molmil can play MD trajectories using various representations

- Molmil can also be used to make MP4 movies

Movies

- Molmil can use the browser to generate PNG images
- Requires a “server-side” component to stitch the PNG images together to build a MP4 file
- This “server-side” component is just a script which runs on your local machine:
  - https://github.com/gjbekker/molmil/wiki/Load-MD-trajectory-files
- Combined with local scripting can produce very nice movies



Gert-Jan Bekker et al. *J. Chem. Theory Comput.*, **2017**, 13, 2389–2399

New features (currently in testing stage)

- New UI (menu)
- Show H-bonds function (if the structure includes hydrogens)
- Show nearby residues function

Future features

- Scripting: jV (rasmol-like) & jmol
- Superposition of structures (like Chimera’s MatchMaker)
- Improved rendering
  - VR/AR (first need a device for testing)
  - Improved graphics
  - More versatile render pipeline

Demos

- PDBj Services
- Basic usage of Molmil (standalone version)
- Custom local scripts examples

Questions, etc

- https://pdbj.org/contact
- https://github.com/gjbekker/molmil/issues
- gertjan.bekker@protein.osaka-u.ac.jp

Reference: Gert-Jan Bekker et al. *J. Cheminf.* **2016**, 8, 42