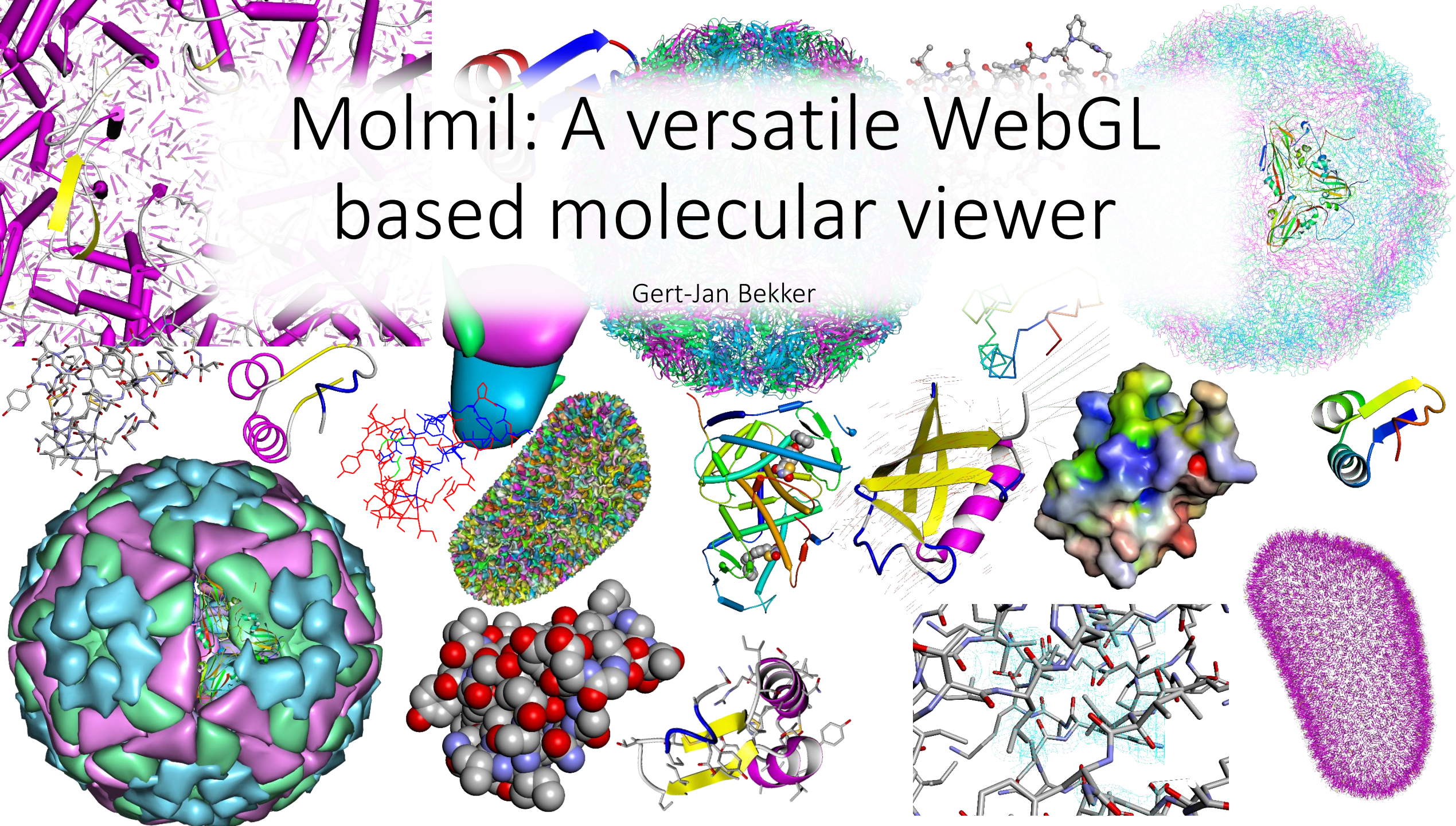


Molmil: A versatile WebGL based molecular viewer

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

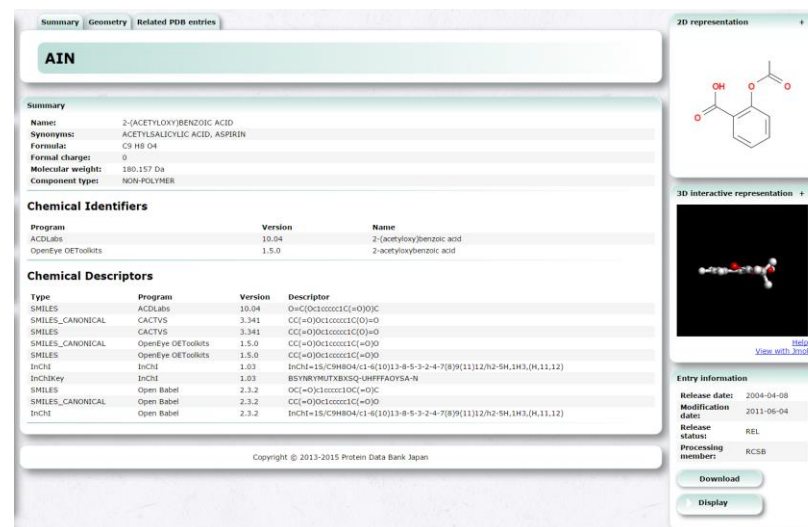
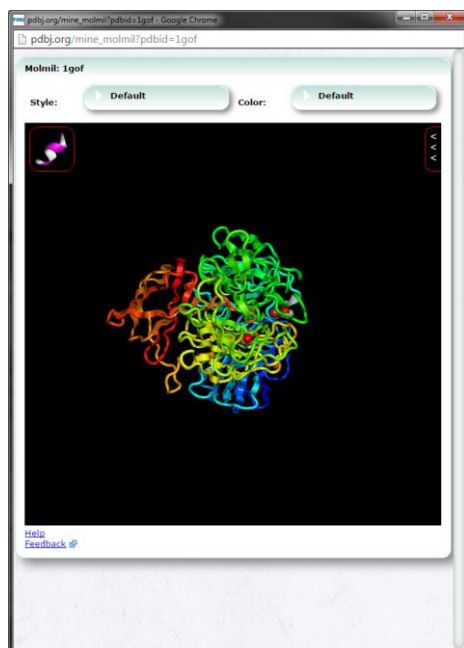
PDBx/mmJSON format

- 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

```
▼ {,--}
▼ data_1CRN: {entry: {id: ["1CRN"]}, audit_conform: {dict_name: ["mmcif_pdbx.dic"], dict_version: ["4.024"],...},...}
  ► atom_sites: {entry_id: ["1CRN"], Cartn_transform_axes: [null], fract_transf_matrix[1][1]: [0.024414],...}
  ► atom_type: {symbol: ["N", "C", "O", "S"]}
  ► audit_author: {name: ["Hendrickson, W.A.", "Teeter, M.M."], pdbx_ordinal: [1, 2]}
  ► audit_conform: {dict_name: ["mmcif_pdbx.dic"], dict_version: ["4.024"],...}
  ► cell: {entry_id: ["1CRN"], length_a: [40.96], length_b: [18.65], length_c: [22.52], angle_alpha: [90],...}
  ▼ chem_comp: {,--}
    ▼ formula: ["C4 H9 N O3", "C3 H7 N O2 S", "C5 H9 N O2", "C3 H7 N O3", "C6 H13 N O2", "C5 H11 N O2", "C3 H7 N O2",...]
      0: "C4 H9 N O3"
      1: "C3 H7 N O2 S"
      2: "C5 H9 N O2"
      3: "C3 H7 N O3"
      4: "C6 H13 N O2"
      5: "C5 H11 N O2"
      6: "C3 H7 N O2"
      7: "C6 H15 N4 O2 1"
      8: "C4 H8 N2 O3"
      9: "C9 H11 N O2"
      10: "C6 H13 N O2"
      11: "C2 H5 N O2"
      12: "C5 H9 N O4"
      13: "C9 H11 N O3"
      14: "C4 H7 N O4"
    ▼ formula_weight: [119.12, 121.154, 115.132, 105.093, 131.174, 117.147, 89.094, 175.21, 132.119, 165.191, 131.174,...]
      0: 119.12
      1: 121.154
      2: 115.132
      3: 105.093
      4: 131.174
      5: 117.147
      6: 89.094
      7: 175.21
      8: 132.119
      9: 165.191
      10: 131.174
      11: 75.067
      12: 147.13
      13: 181.191
      14: 133.104
    ► id: ["THR", "CYS", "PRO", "SER", "ILE", "VAL", "ALA", "ARG", "ASN", "PHE", "LEU", "GLY", "GLU", "TYR",...]
    ► mon_nstd_flag: ["y", "y", "y", "y", "y", "y", "y", "y", "y", "y", "y", "y", "y", "y", "y"]
    ► name: ["THREONINE", "CYSTEINE", "PROLINE", "SERINE", "ISOLEUCINE", "VALINE", "ALANINE", "ARGININE",...]
    ► pdbx_synonyms: [null, null, null, null, null, null, null, null, null, null, null, null, null, null, null]
    ► type: ["L-peptide linking", "L-peptide linking", "L-peptide linking", "L-peptide linking",...]
  ► citation: {id: ["primary", "1", "2"], title: {,--},...}
  ► citation_author: {citation_id: ["primary", "1", "1", "2", "2"],...}
  ► computing: {entry_id: ["1CRN"], pdbx_data_reduction_ii: [null], pdbx_data_reduction_ds: [null],...}
  ► database_2: {database_id: ["PDB"], database_code: ["1CRN"]}
  ► database_PDB_matrix: {entry_id: ["1CRN"], origx[1][1]: [1], origx[1][2]: [0], origx[1][3]: [0], origx[2][1]: [0],...}
  ► database_PDB_rev: {num: [1, 2, 3, 4, 5, 6, 7],...}
  ► database_PDB_rev_record: {rev_num: ["2", "3", "4", "5", "6", "7", "7"],...}
  ► diffrn: {id: ["1"], ambient_temp: [null], ambient_temp_details: [null], crystal_id: ["1"]}
  ► diffrn_radiation: {diffrn_id: ["1"], wavelength_id: ["1"], pdbx_monochromatic_or_laue_m_1: [null], monochromator: [null],...}
```

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



The screenshot shows the Molmil 2prg-A web interface. The URL is service.lpr.pdbj.org/ef-site/efsite_molmil.html#2prg-A. The interface includes a 'Style' dropdown set to 'Default' and a 'Color' dropdown set to 'Default'. The main display area shows a 2D representation of a chemical structure, colored by residue type. Below the structure, there is a section titled 'LIGAND-BINDING DOMAIN OF THE HUMAN PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA' with a sequence viewer showing the sequence: `Sequence: S H Y`, `Description: Synthetic agonist`, `Source: BINDING - SWS_FT_F11`, `A: 342-416 (DVA_HUNH)`, `Sequence: SEQQGFMTRFLKSLRKPQDFMEPLFEFAVKFNALELDSDLAIFAVIILSGDRPGLLNVPEDIQNLQA`, and `Description: Nuclear receptor`.

Program	Version	Name
ACDLabs	10.04	2-(acetyloxy)benzoic acid
OpenEye OEToolkits	1.5.0	2-acetyloxybenzoic acid

Type	Program	Version	Descriptor
SMILES	ACDLabs	10.04	O=C(C(=O)O)C(=O)O
SMILES_CANONICAL	CACTVS	3.341	CC(=O)OC(=O)C(=O)O
SMILES	CACTVS	3.341	CC(=O)OC(=O)C(=O)O
SMILES_CANONICAL	OpenEye OEToolkits	1.5.0	CC(=O)OC(=O)C(=O)O
SMILES	OpenEye OEToolkits	1.5.0	CC(=O)OC(=O)C(=O)O
InChI	InChI	1.03	InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8/9(11)12/h2-5H,1H3,(H,11,12)
InChIKey	InChI	1.03	BSYRVRWUTXBSQ-UHFFFAOYSA-N
SMILES	Open Babel	2.3.2	CC(=O)OC(=O)C(=O)O
SMILES_CANONICAL	Open Babel	2.3.2	CC(=O)OC(=O)C(=O)O
InChI	Open Babel	2.3.2	InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8/9(11)12/h2-5H,1H3,(H,11,12)

Entry information

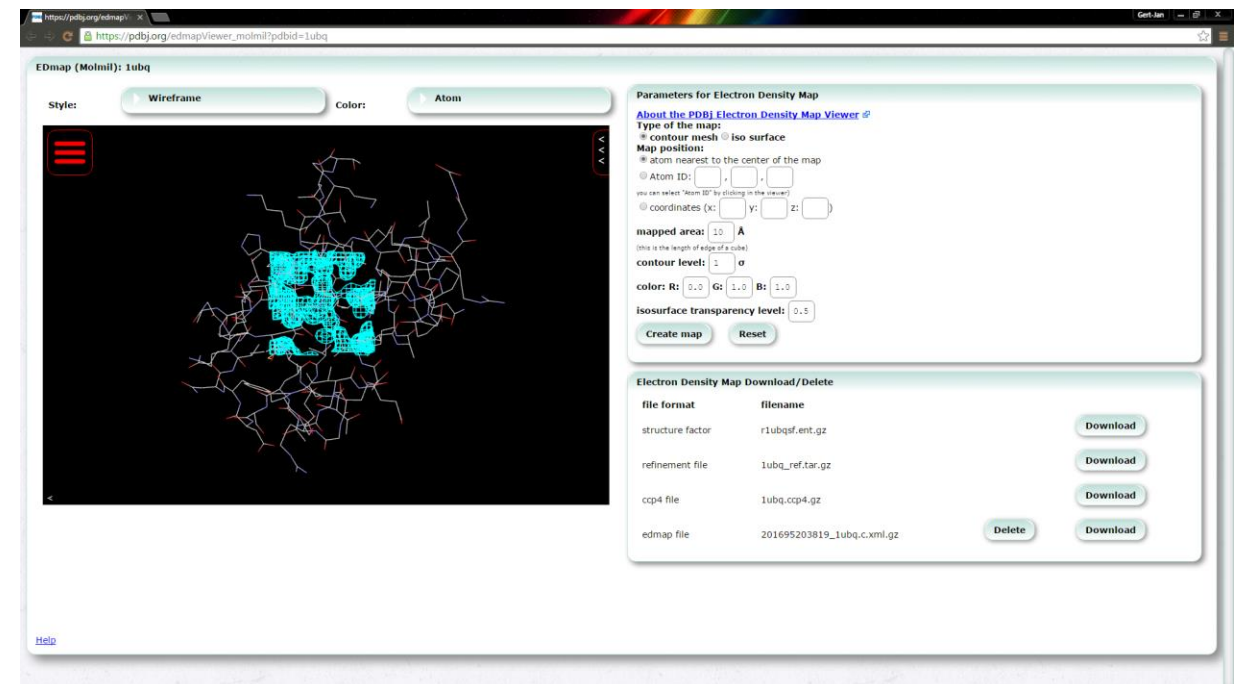
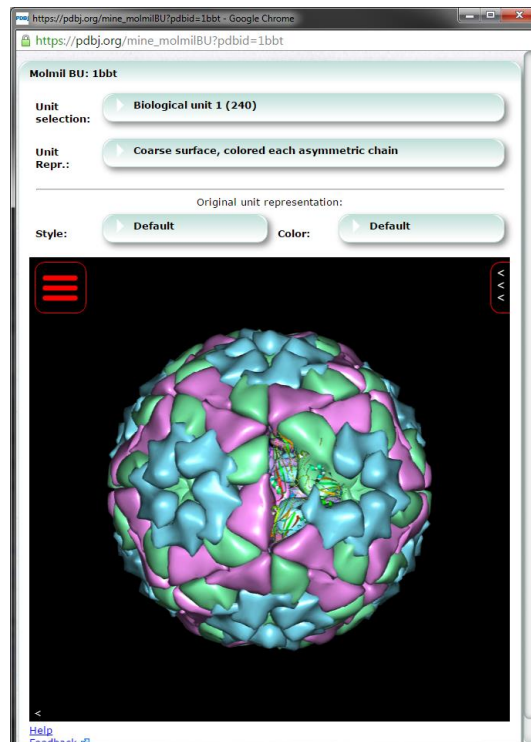
Release date:	2004-04-08
Modification date:	2013-06-04
Release status:	REL
Processing member:	RCSB

Download

Display

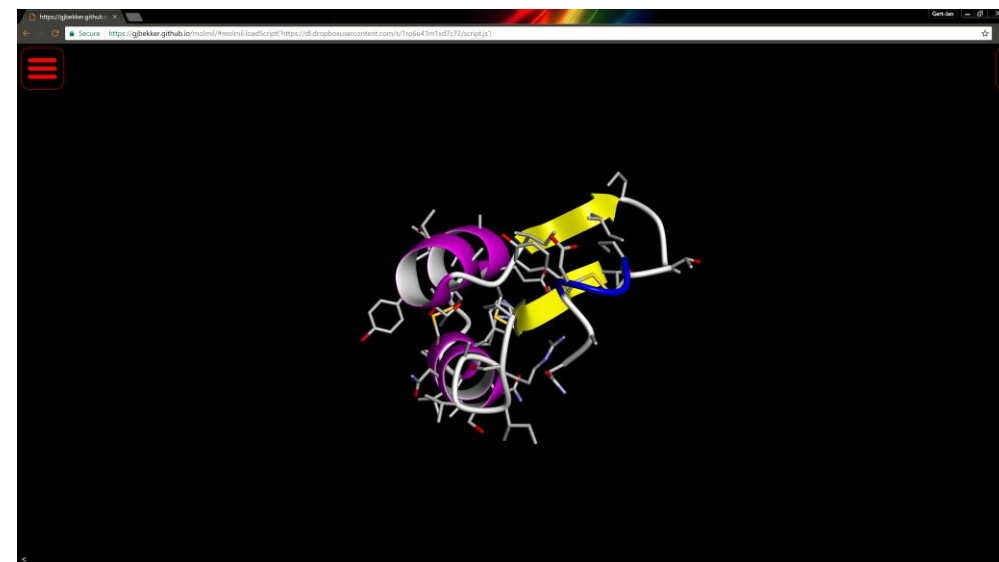
Molmil 1.0

- 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

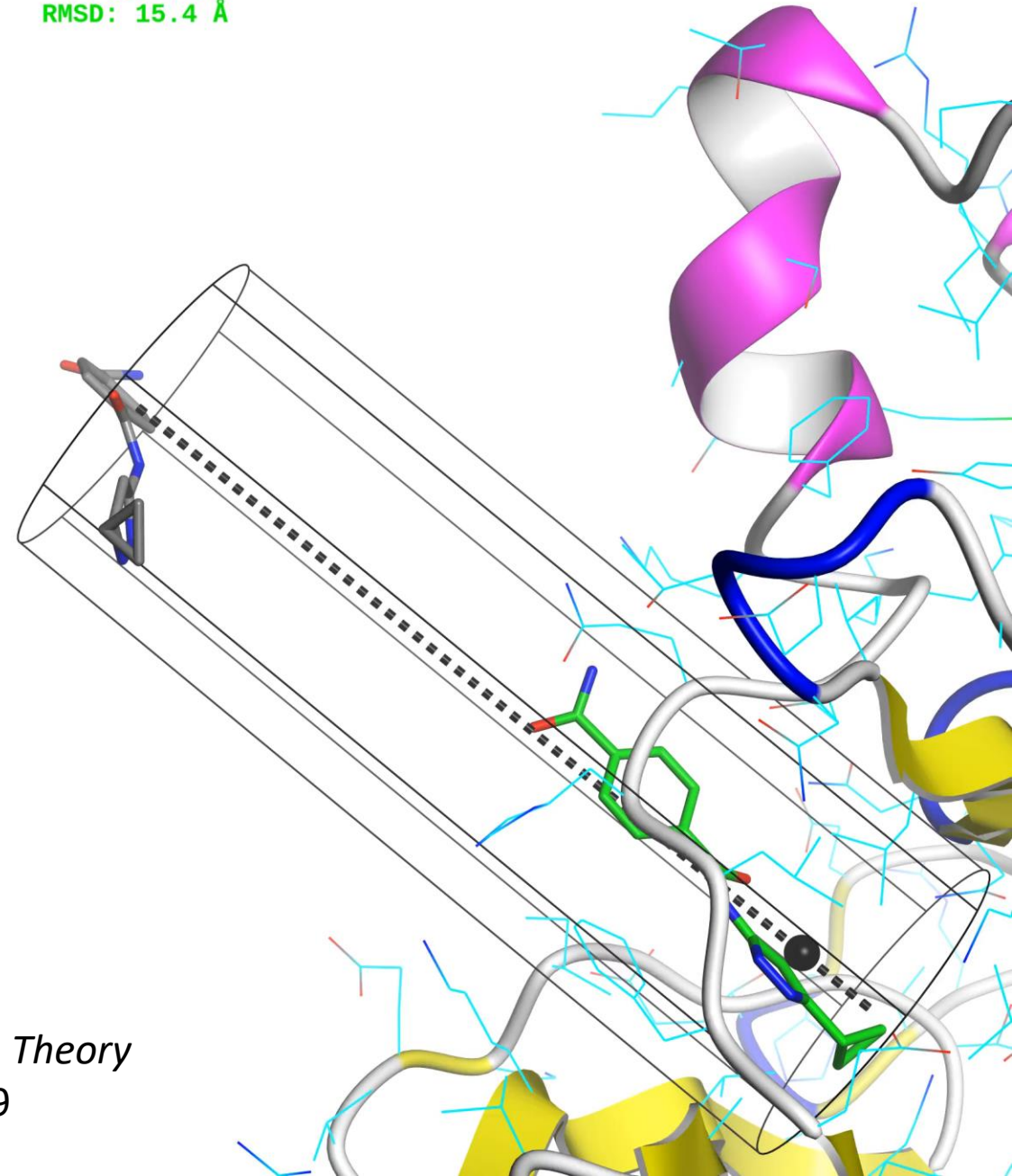
- Currently supported:
 - PDB models (not recommended)
 - Presto COD
 - Gromacs TRR
 - Gromacs XTC (compressed)
- Molmil can play MD trajectories using various representations
- Molmil can also be used to make MP4 movies

Time: 0.00 ns
Energy: -62347 kcal/mol
 λ : 23.7 Å
RMSD: 15.4 Å

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