molfig

A Typst package for rendering molecular structure files in static documents.

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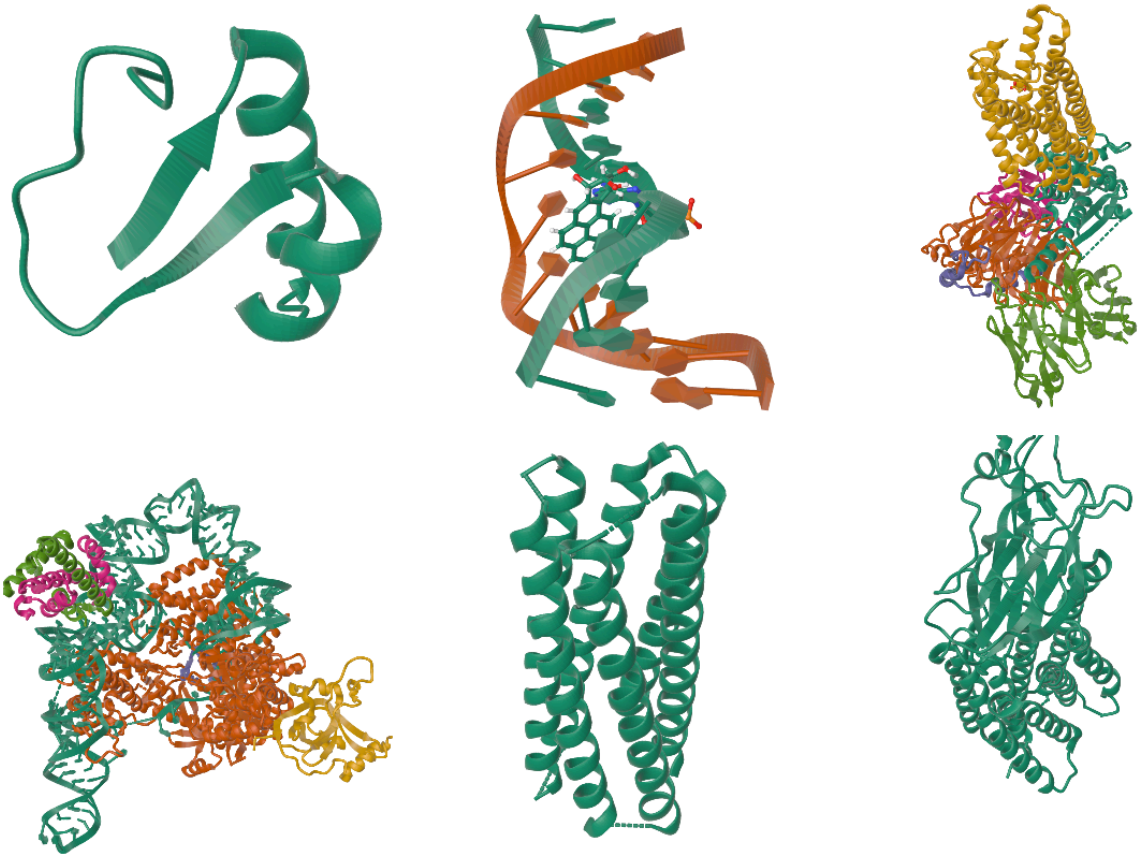
Molfig is a Typst package for rendering molecular structure files in static documents.

It accepts PDB, mmCIF, and BinaryCIF input, converts structures through a CPU-side Mol*-style Model/Structure/Unit layer, exports static OBJ/STL/PLY mesh bytes, and delegates final document rendering to `maquette`.



Quickstart

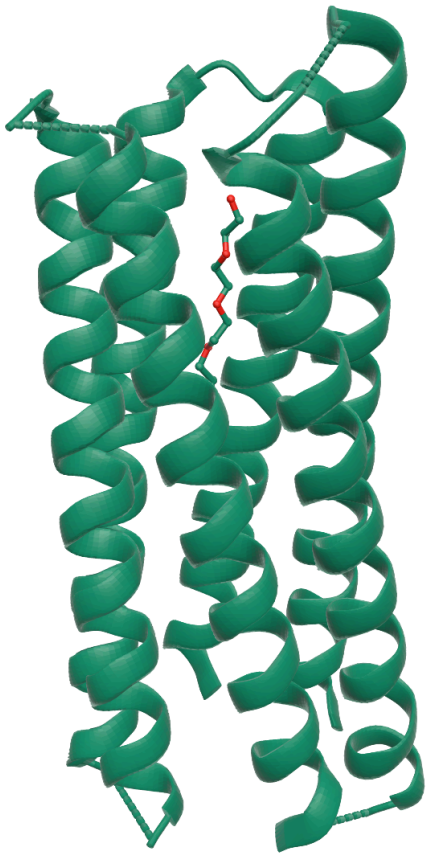
```
#import "@preview/molfig:0.1.3"
#set page(width: auto, height: auto, margin: 0mm)

// Uses structural data from RCSB PDB / wwPDB.
// PDB ID: 9R1O
// PDB DOI: https://doi.org/10.2210/pdb9R1O/pdb
// Deposition authors: Petrenas, R.; Ozga, K.; Chubb, J.J.; Woolfson, D.N.
// PDB archive data files are available under CC0 1.0.
#let pdb = read("9R1O.pdb", encoding: none)

#molfig.render(
  pdb,
  format: "pdb",
  representation: "molstar",
  assembly: "1",
  mesh-format: "obj",
```

```
  quality: "high",
  center: true,
  output-format: "svg",
  config: (
    azimuth: 35,
    elevation: 24,
    background: "",
  ),
)
```

The manual uses PDB entry 9R1O as its complete example. Put `9R1O.typ` and `9R1O.pdb` in the same directory, then compile the figure PDF:

```
typst compile 9R1O.typ
```

Rendered 9R1O Example



Structural data source: RCSB PDB / wwPDB, PDB ID `9R1O`, DOI `10.2210/pdb9R1O/pdb`. PDB archive data files are distributed under CC0 1.0.

Use `format: "mmcif"` or `format: "bcif"` for text mmCIF and BinaryCIF inputs. For reproducible documents, prefer explicit `format`, `representation`, `assembly`, `alt-loc`, `mesh-format`, and geometry quality options instead of relying on auto-detection.

Examples

The `package/examples` directory contains complete example sources, rendered PDFs, and their accompanying structural data files. The example data files are kept under `package/examples/data`, together with attribution metadata.

Features

- Inputs: PDB, text CIF/mmCIF, and BinaryCIF.
- Structure layer: Mol*-style Model/Structure/Unit concepts, assembly operators, altLoc handling, bond metadata, lookup3d/boundary summaries, secondary structure, coarse IHM spheres/gaussians, and semantic render-object metadata.
- Representations: `default` follows the Mol* Viewer preset, including pLDDT, QMEAN, and SB-NCBR partial-charge annotation themes before automatic size routing; `cartoon` is the Viewer Quick Styles Cartoon preset; `spacefill` is the Viewer illustrative Spacefill preset; and `polymer-cartoon` exposes the standalone Mol* Cartoon provider defaults. Ball-and-stick, ribbon, and backbone are also available.
- Assembly support: biological assemblies are represented as source model plus unit operators before static mesh export.
- Alternate locations: select a concrete altLoc, all altLocs, or the highest-occupancy conformer.
- Color themes: `color-theme` supports `chain-id`, `element-symbol`, `entity-id`, `operator-name`, `plddt-confidence`, `qmean-score`, and `sb-ncbr-partial-charges`. The optional `theme` dictionary mirrors Mol* Viewer overrides such as `globalName`, `carbonColor`, and `symmetryColor`; OBJ materials are forwarded to maquette.
- Outputs: OBJ, companion MTL, binary STL, and ASCII PLY.
- Rendering: `render` passes generated mesh bytes to maquette; `render-object` exposes the mesh, rendered content, and normalized metadata for advanced documents.

Public API

- `render(data, ..., config: (:), width: auto, height: auto)` converts and renders through maquette.
- `render-object(data, ...)` returns generated mesh bytes, rendered content, and metadata.
- `to-obj(data, ...)`, `to-mtl(data, ...)`, `to-stl(data, ...)`, and `to-ply(data, ...)` return export bytes.
- `info(data, ...)` returns molecular and mesh-planning metadata without rendering.
- `mesh-info(data, mesh-format: "obj", config: (:), ...)` delegates to maquette's mesh metadata helpers for the generated mesh.

Common options include `format`, `representation`, `color-theme`, `theme`, `assembly`, `alt-loc`, `block-index`, `block-header`, `quality`, `decimate`, `sphere-detail`, `linear-segments`, `radial-segments`, `radius-scale`, `atom-radius`, `bond-radius`, `ribbon-radius`, `ribbon-width`, `helix-profile`, `round-cap`, `sheet-arrow-factor`, `tubular-helices`, `infer-bonds`, and `center`.

The `data` argument accepts bytes from `read(..., encoding: none)`, inline string data for small examples, and Typst 0.15+ path values created with `path("...")`.

Choosing A Mesh Format

- Use OBJ for the closest static Mol* exporter parity and readable diffs.
- Use STL when a downstream tool specifically requires binary triangle data.
- Use PLY when package-owned face group metadata is useful in a compact text mesh.

OBJ output can be paired with `to-mtl`. During `render`, OBJ material colors are automatically converted to maquette's `materials` map; entries supplied through `config.materials` override generated colors. OBJ and PLY preserve Molfig group or operator metadata where the format can represent it. Binary STL follows Mol* static exporter behavior and keeps the two-byte facet attribute field at zero.

Documentation

The full Molfig manual is available at `package/docs/documentation.pdf`. It documents:

- installation and import conventions;
- input format handling and BinaryCIF block selection;
- every public command and return shape;
- mesh, representation, assembly, altLoc, and quality options;
- maquette passthrough configuration;
- metadata fields returned by `info` and `render-object`;
- licensing, third-party notices, and example data attribution;
- troubleshooting and development commands;
- the embedded 9R1O rendering and its data source.

The manual source is `package/docs/documentation.typ`, and it reads the package version from `package/typst.toml`.

Notes And Limits

Molfig emits static presentation meshes. `representation: "surface"` implements the * Viewer Quick Styles Molecular Surface preset on the CPU and exports the result as OBJ/STL/PLY. Gaussian volume and density/volume visuals remain outside the static export contract; the size-dependent ViewerAuto path uses a CPU Gaussian surface for Huge and Gigantic structures.

IHM coarse sphere and gaussian rows remain available as coarse model units and participate in the size-dependent ViewerAuto Gaussian-surface path.

License And Notices

Molfig project code is licensed under the MIT License. See `LICENSE`.

Molfig ports or adapts Mol* behavior and includes Mol*-derived reference data in the Rust/WASM implementation. Mol* is licensed under the MIT License, copyright (c) 2017 - now, Mol* contributors.

Bundled example structure files under `examples/data` are PDB archive data from RCSB PDB / wwPDB and are available under CC0 1.0. Per-file PDB IDs, DOIs, and recommended attributions are listed in `examples/data/README.md`.

See `NOTICE.md` and `THIRD_PARTY_NOTICES.md` for the full distribution notice.

Development

```
cd wasm-plugin
cargo fmt --check
cargo test
cargo build --release --target wasm32-unknown-unknown
cp target/wasm32-unknown-unknown/release/molfig.wasm ../package/molfig.wasm
cd ..
typst compile --root package package/docs/documentation.typ package/docs/documentation.pdf
```

The checked-in `package/molfig.wasm` should be regenerated after Rust changes that affect the Typst plugin. Regenerate `package/docs/documentation.pdf` after public API or documentation changes.