



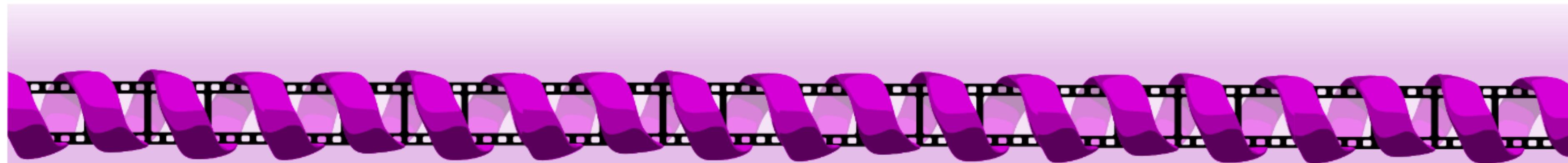
# Molecular movies made easy with

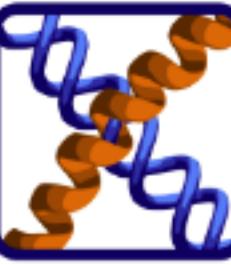
**MOLYWOOD**

BioExcel webinar  
22.10.2020

**Miłosz Wieczór**

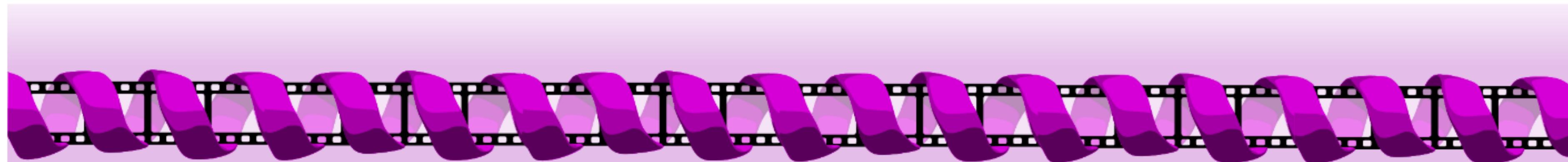
Molecular Modelling and Bioinformatics, IRB Barcelona  
Dept of Physical Chemistry, Gdansk University of Technology





# The background story

- Born out of a sense of common frustration
- Few tools available, mostly Python or Tcl libraries
- Either simplistic or complex: a big gap in between
- Simple syntax & extensive documentation
- Two guiding principles:
  1. make it 'plug-and-play'
  2. keep easy things easy, complex things doable



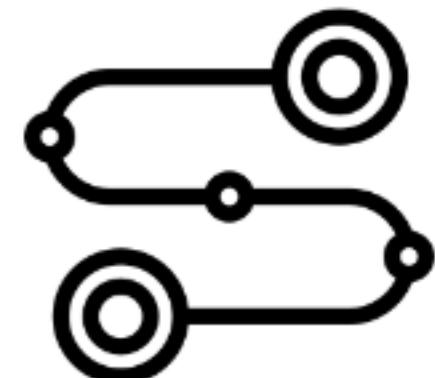
# The background story 2



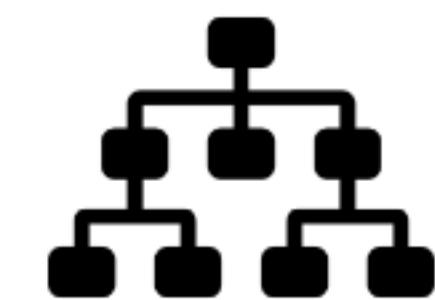
Users: computational biologists at all levels of expertise



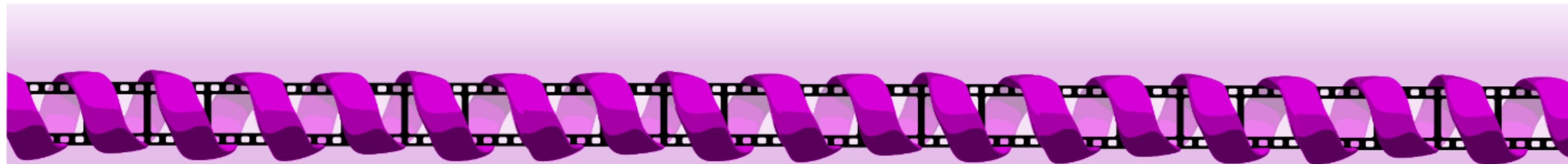
Goal: push for a broader recognition of movies as a tool for dissemination



Means: make movie design fun



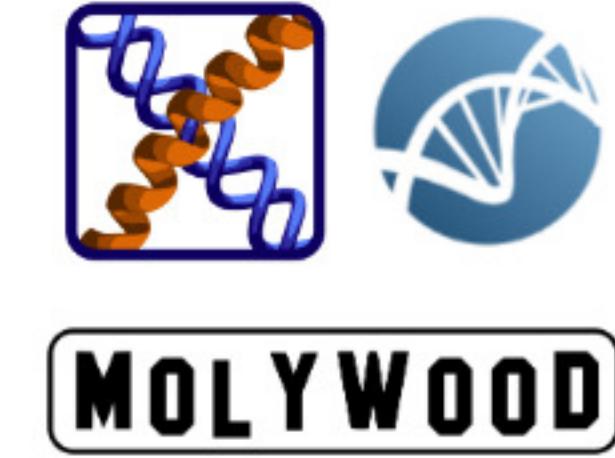
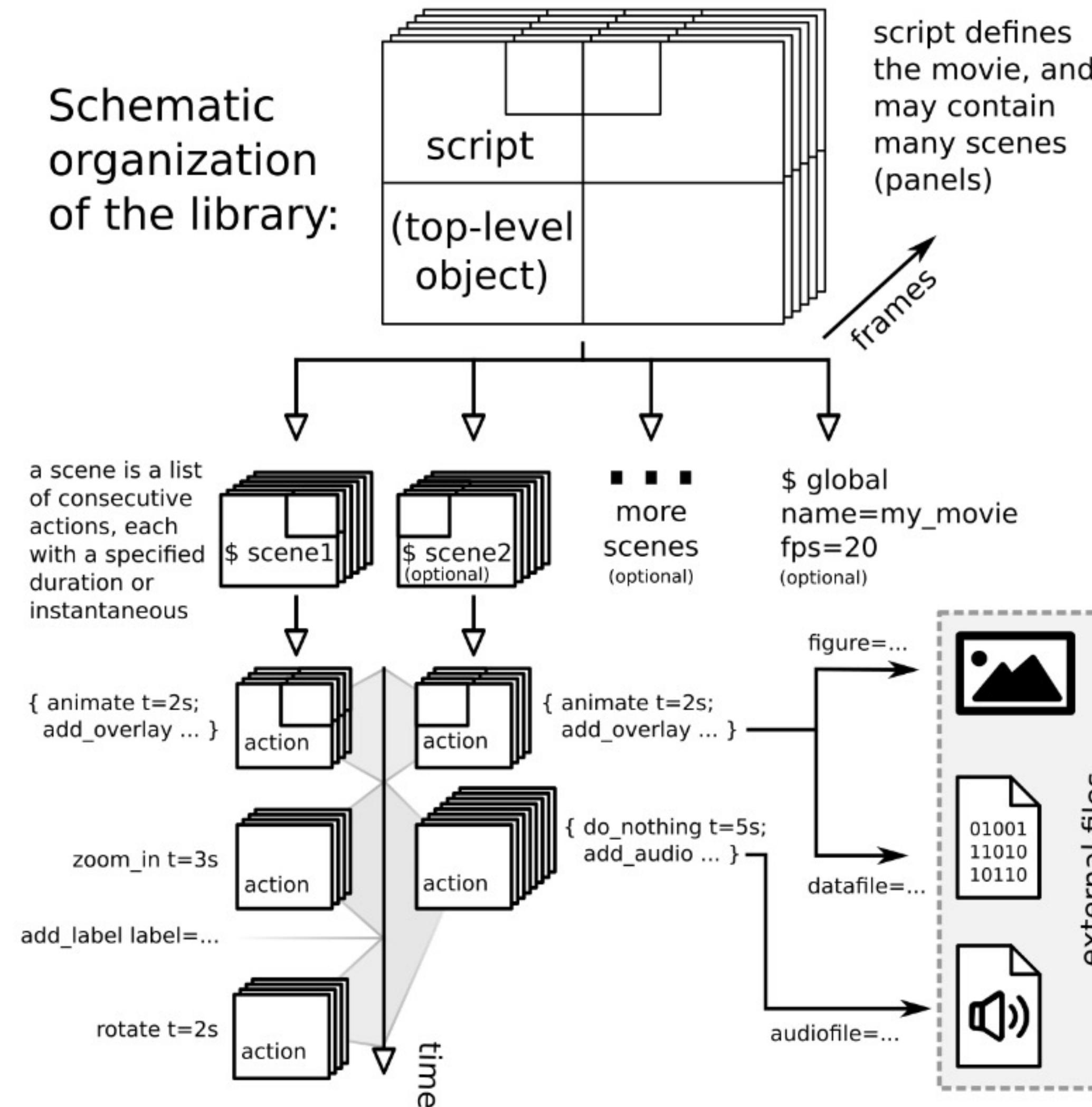
Structure: as modular and flexible as possible to foster creativity

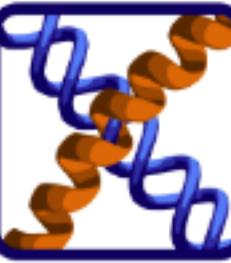




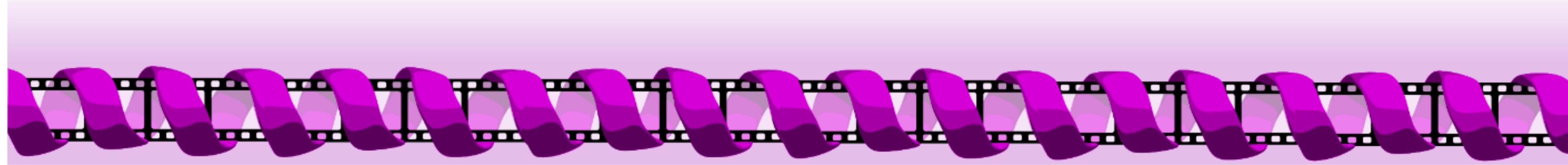
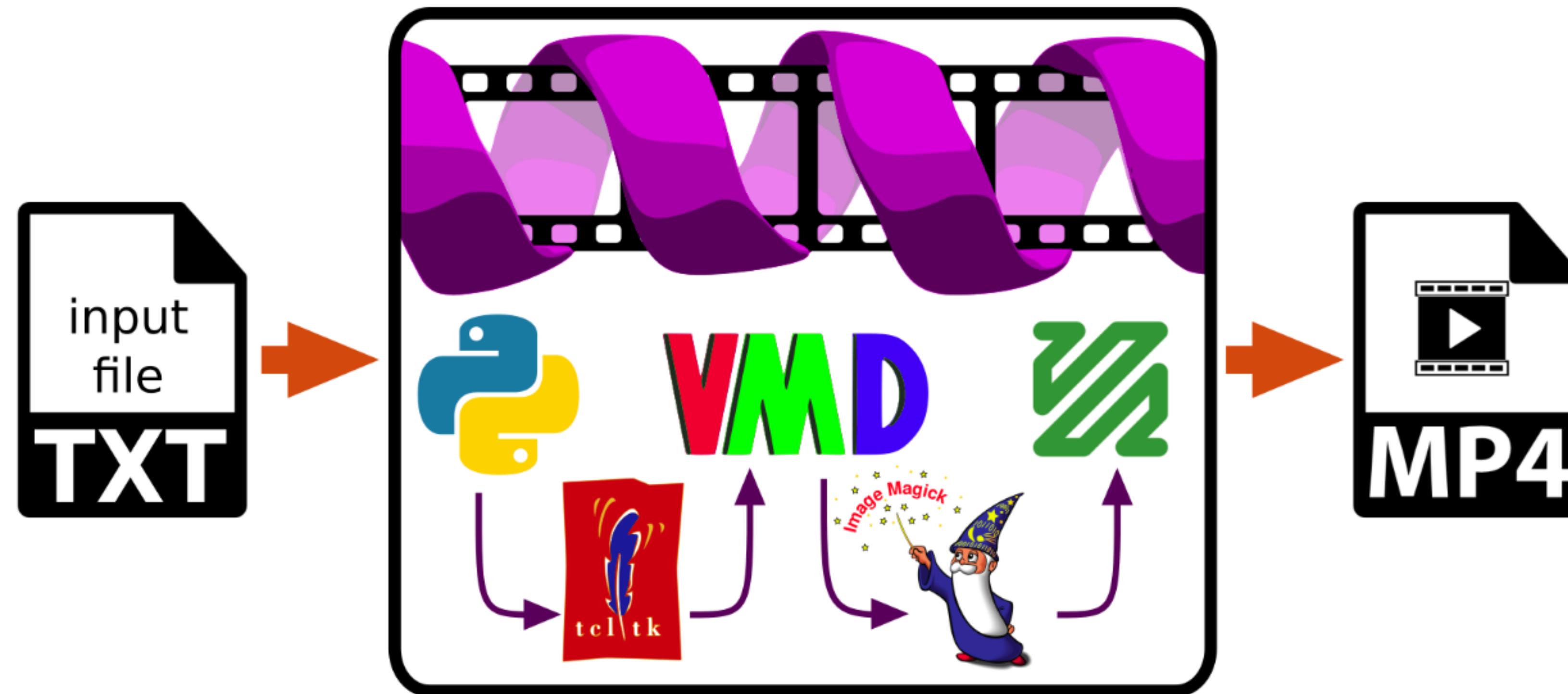
# Tool structure

Schematic organization  
of the library:



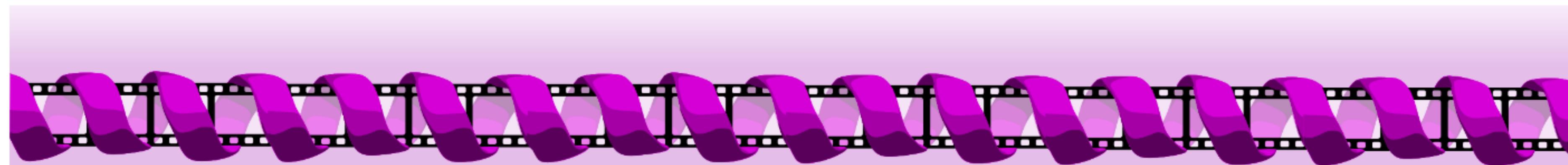
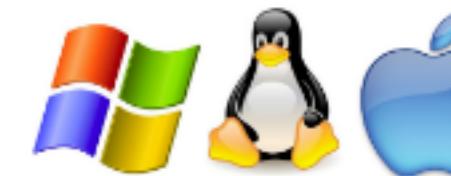


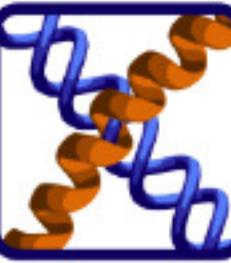
# What's under the hood



# Easy installation

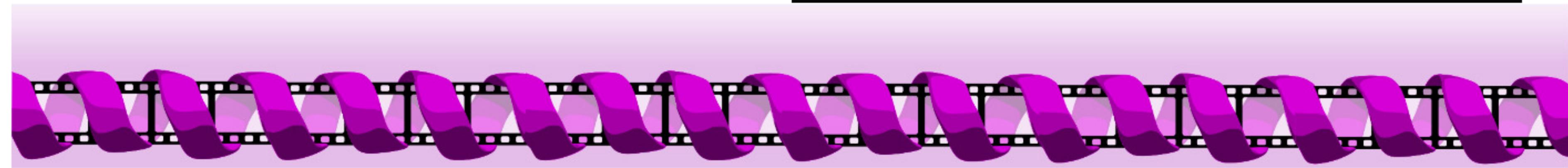
- Have ffmpeg, VMD and python/numpy? Just go for `pip install molywood`
- Safer version: through `CONDA` (see tutorials)
  1. modify existing venv
  2. create a new venv `molywood`
- Type `molywood-gen-env` to check and setup, and `molywood` to run
- Tested on Windows, Linux and Mac

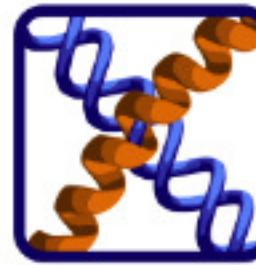




# A minimal example

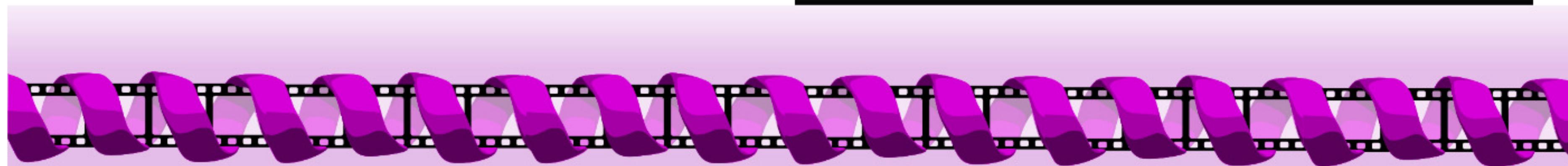
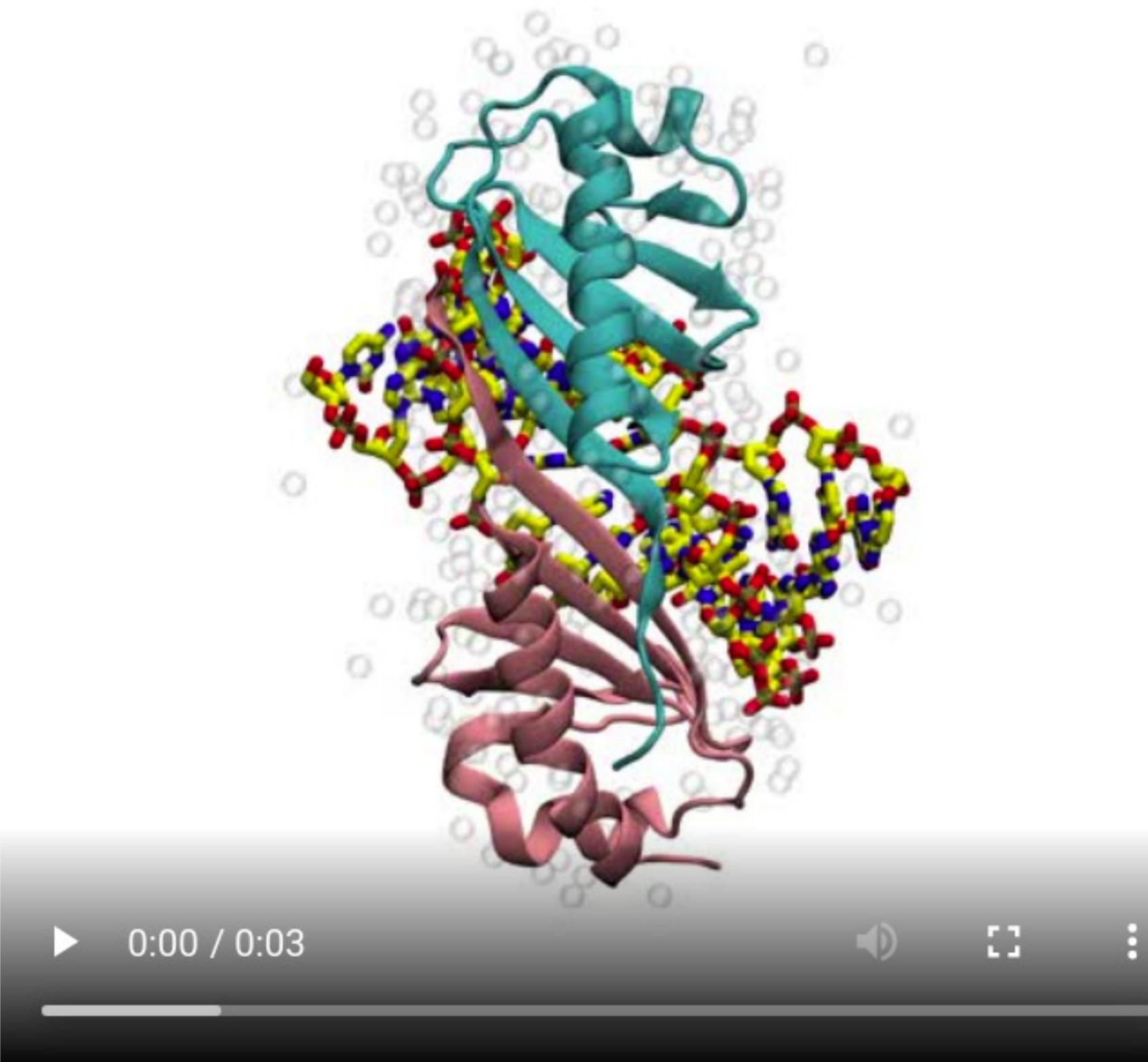
```
$ global name=movie1  
$ scene_tbp pdb_code=1cdw  
  
# scene_tbp  
zoom_in scale=1.4 t=2s  
rotate axis=y angle=360 t=2s
```





# Custom representations

```
$ global name=movie2  
$ scene_tbp visualization=cust.vmd  
  
# scene_tbp  
zoom_in scale=1.4 t=2s  
rotate axis=y angle=360 t=2s
```





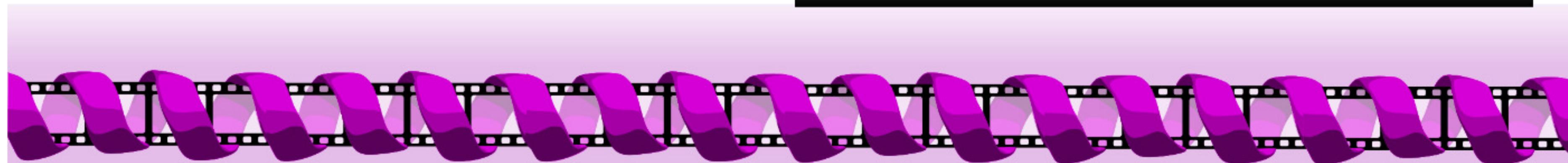
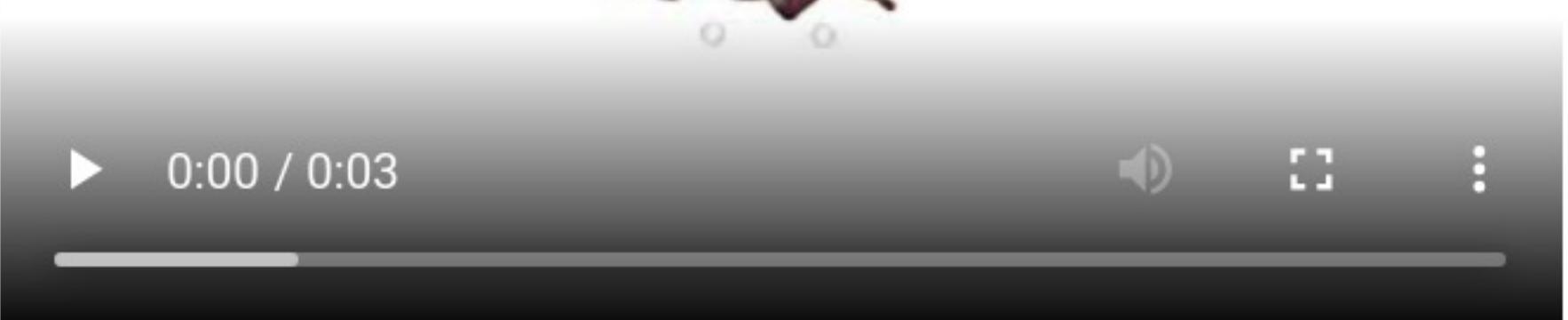
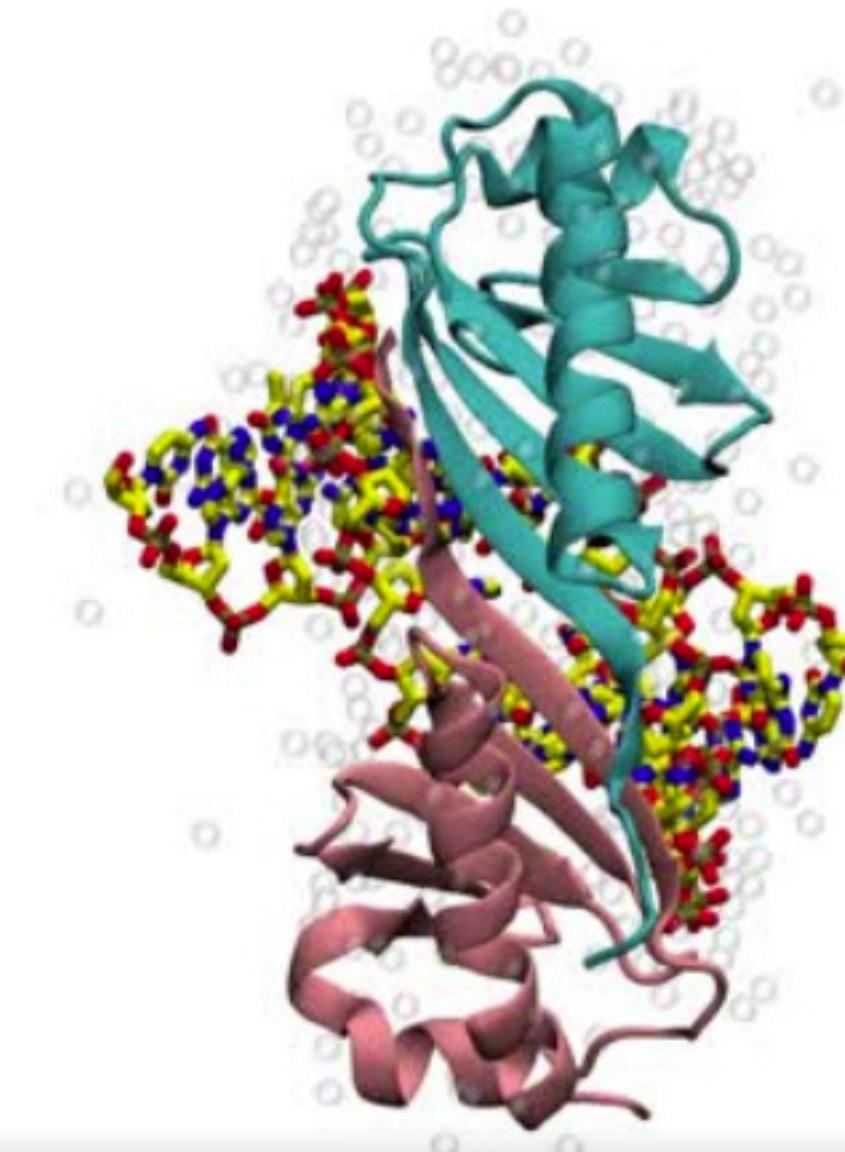
# ...or made from scratch

```
$ global name=movie3
$ scene_tbp pdb_code=1cdw

# scene_tbp
rotate axis=z angle=75
zoom_in scale=1.2
make_transparent material=opaque

highlight selection='nucleic and noh'
style=licorice color=type thickness=1.5 mode=u
material=diffuse
highlight selection='protein and resid < 247'
style=newcartoon color=10 mode=u material=diffuse
highlight selection='protein and resid > 247'
style=newcartoon color=9 mode=u material=diffuse
highlight selection=water style=vdw
thickness=0.5 mode=u alpha=0.1

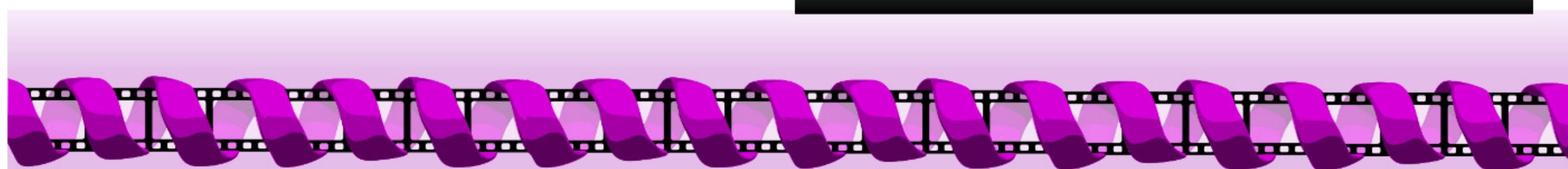
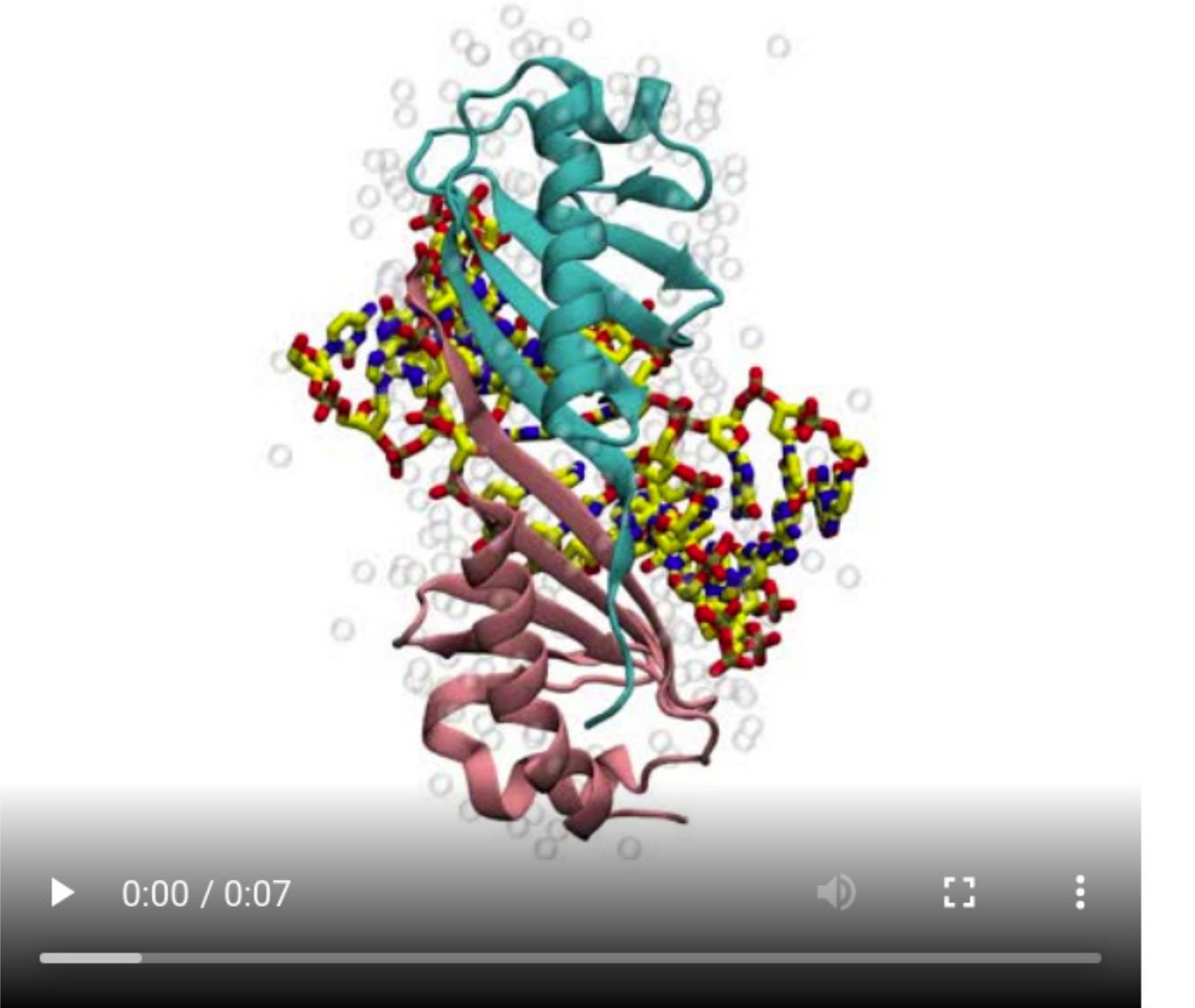
zoom_in scale=1.4 t=2s
rotate axis=y angle=360 t=2s
```

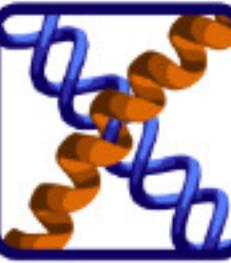


# Instantaneous or finite-time

```
$ global name=movie4
$ scene_tbp pdb_code=1cdw

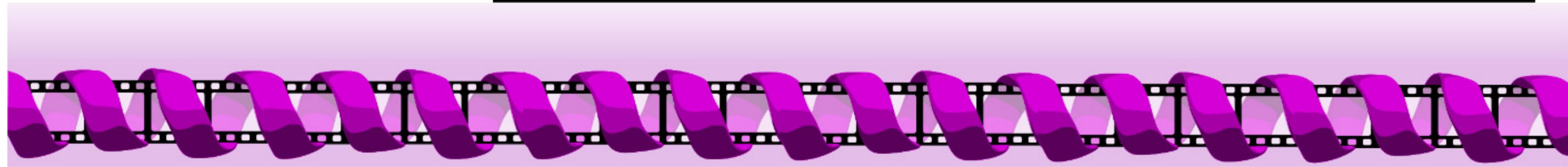
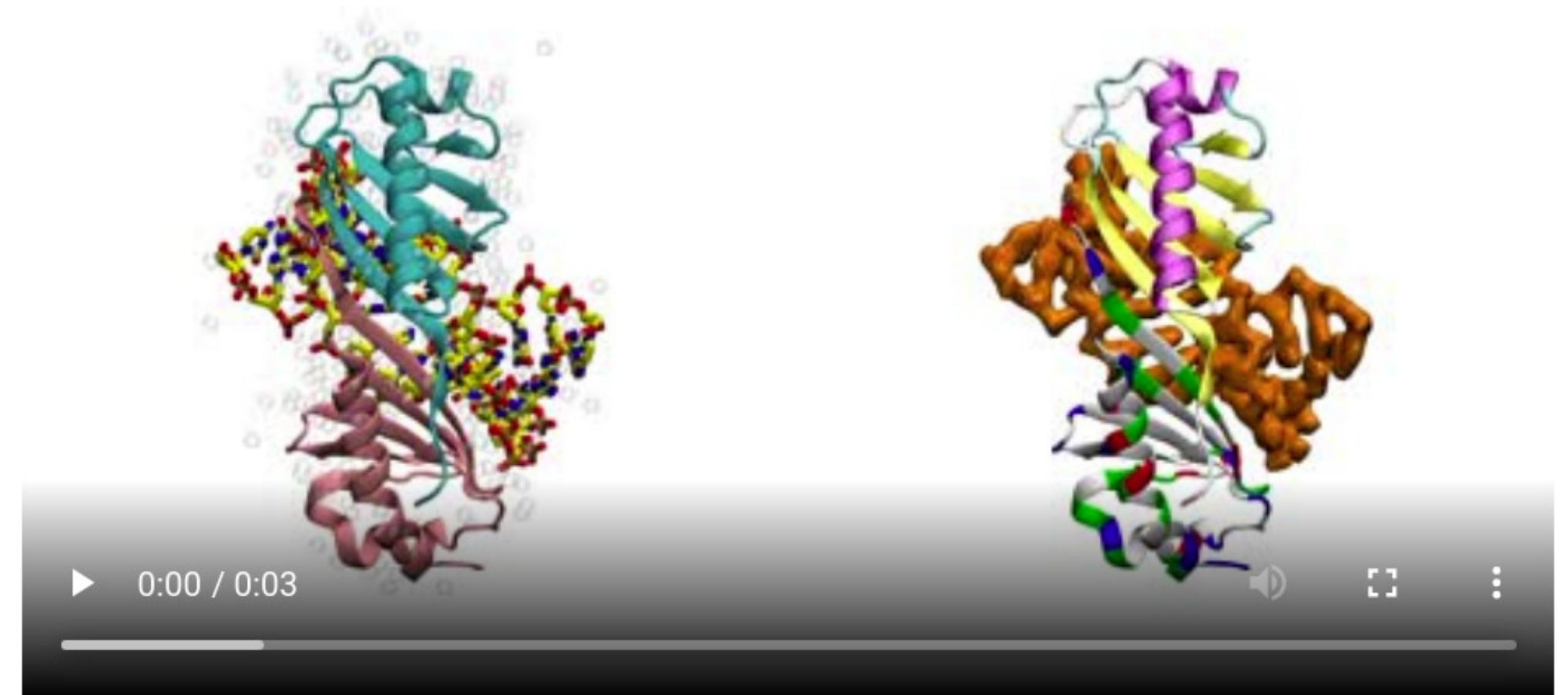
# scene_tbp
zoom_in scale=1.4 t=2s
rotate axis=y angle=15
zoom_out scale=1.4 t=2s
translate vector=0,0.2,0
rotate axis=y angle=120 t=2s
fit_trajectory selection=nucleic
axis=z
highlight selection='resname LYS'
style=vdw color=element mode=u
material=diffuse
rotate axis=y angle=-120 t=2s
```





# A grid of Scenes

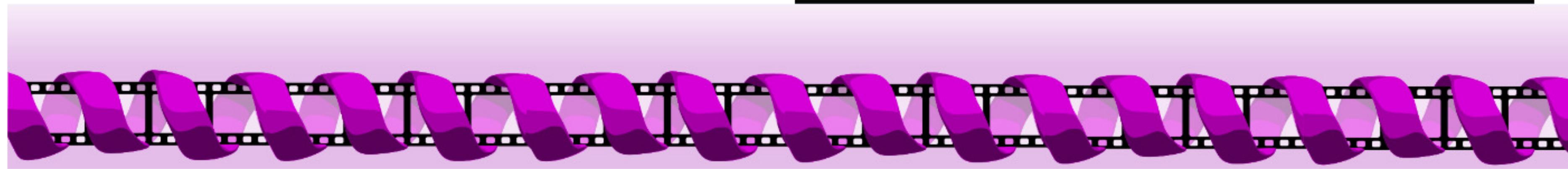
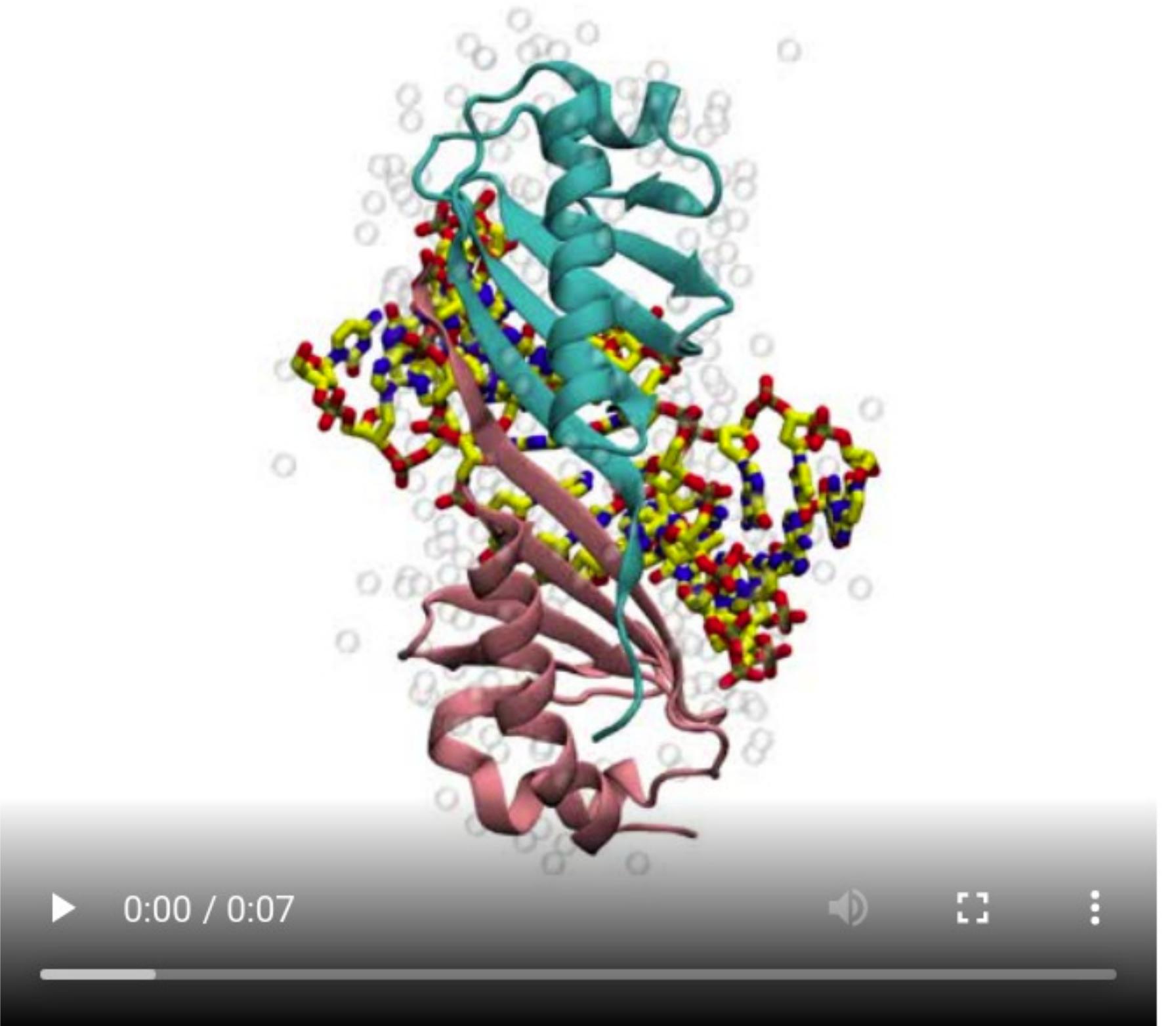
```
$ global name=movie5  
$ layout rows=1 columns=2  
$ sc1 visualization=custom1.vmd position=0,0  
$ sc2 visualization=custom2.vmd position=0,1  
  
# sc1,sc2  
zoom_in scale=1.4  
    t=2s  
rotate axis=y  
    angle=360 t=2s
```





# A sequence of Scenes

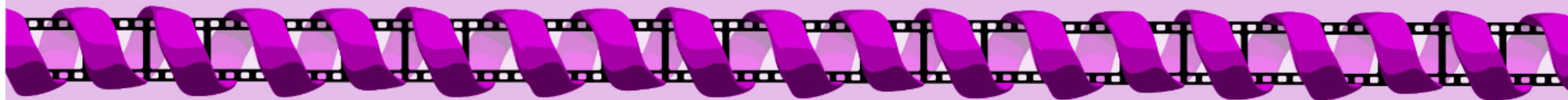
```
$ global name=movie6  
$ sc1 visualization=custom1.vmd  
$ sc2 visualization=custom2.vmd  
after=sc1  
  
# sc1,sc2  
zoom_in scale=1.4  
t=2s  
rotate axis=y  
angle=360 t=2s
```



# Overlays with text & images

```
$ global name=movie7
$ scene_tbp visualization=cu.vmd

# scene_tbp
zoom_in scale=1.4 t=2s
{add_overlay figure=logo.png
 origin=0,0.8 transparent_background=t
 relative_size=0.4;
rotate axis=y angle=-180 t=2s}
{add_overlay figure=logo.png
 origin=0,0.8 transparent_background=t
 relative_size=0.4;
do_nothing t=2s}
{add_overlay text=consensus:
 origin=0.02,0.93;
add_overlay text=TATAAAA
 origin=0.02,0.85;
rotate axis=y angle=180 t=2s}
```

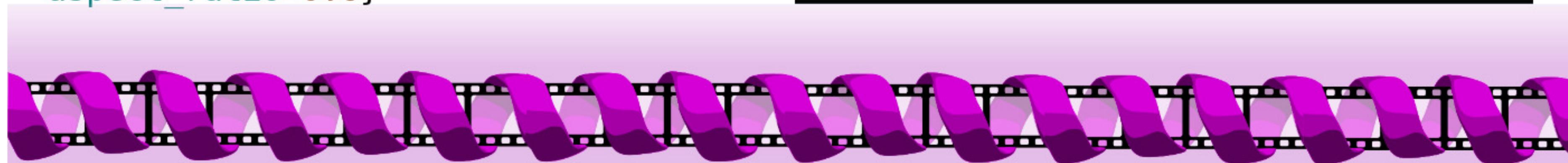


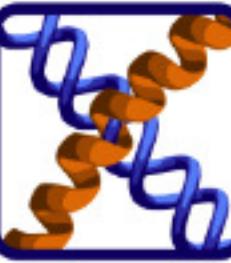
# Overlays with data

```
$ global name=movie8
$ scene_tbp visualization=cu.vmd

# scene_tbp
animate frames=150
fit_trajectory selection=protein
rotate axis=y angle=-90
rotate axis=y angle=90 t=2s

{animate frames=150:750 smooth=5 t=5s;
add_overlay datafile=data.txt
  origin=0,0.6 relative_size=0.4
  aspect_ratio=0.6}
do_nothing t=1s
{animate frames=750:150 smooth=5 t=5s;
add_overlay datafile=data2.txt
  origin=0,0.6 relative_size=0.4
  aspect_ratio=0.6}
```





# Scenes as overlays

```
$ global name=movie9
$ scene_tbp visualization=cu.vmd
$ scol visualization=cu.vmd

# scene_tbp,scol
animate frames=150
fit_trajectory selection=protein
rotate axis=y angle=-90

# scene_tbp
rotate axis=y angle=90 t=2s
{do_nothing t=1s;
add_overlay scene=scol transparent_background=t
  mode=u origin=0,0:0.65 relative_size=1:0.4}
animate frames=150:750 smooth=5 t=5s
do_nothing t=1s
animate frames=750:150 smooth=5 t=5s

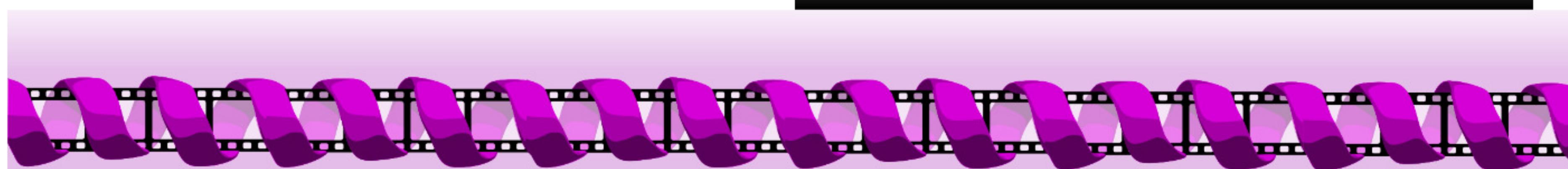
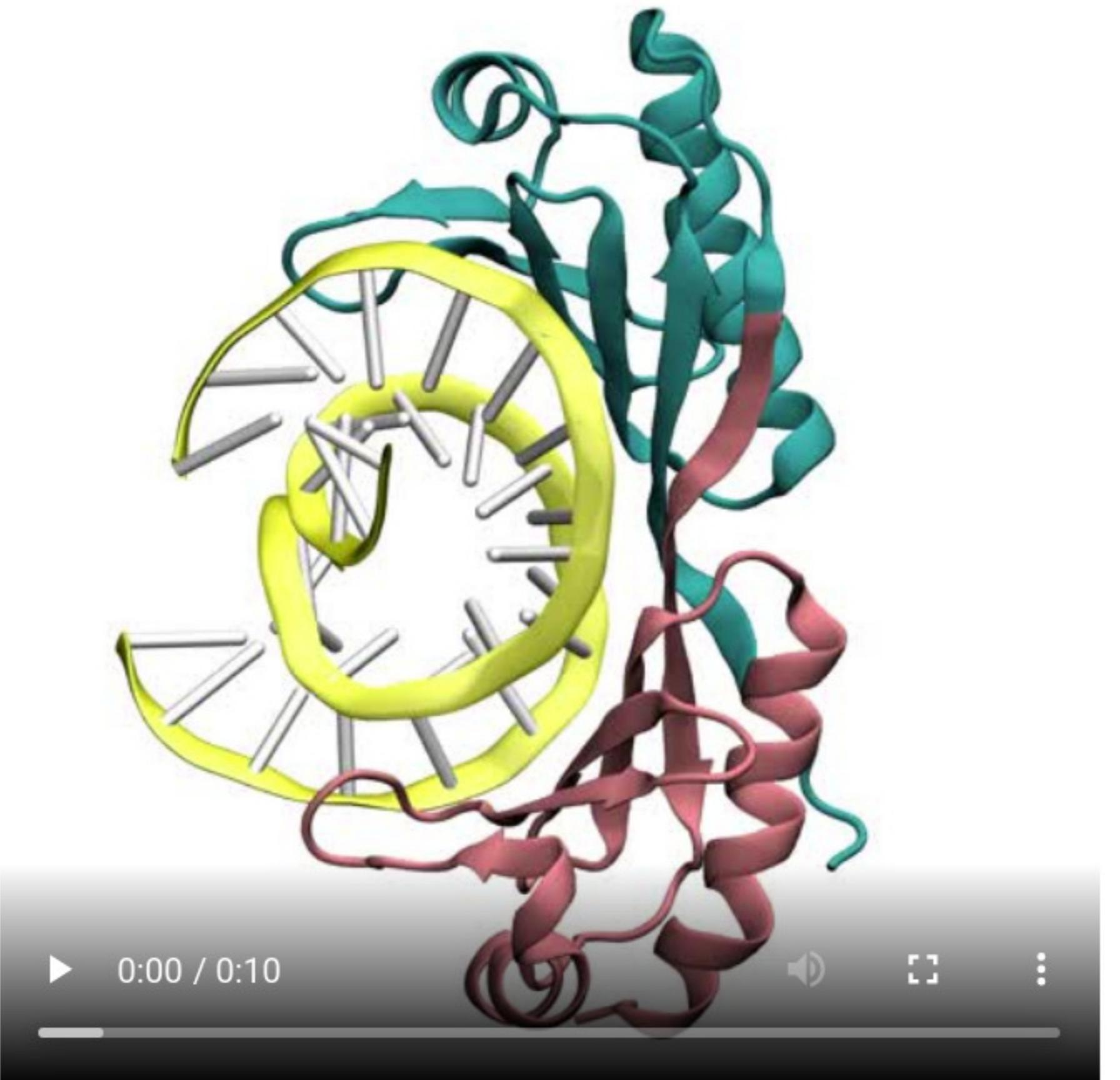
# scol
rotate axis=y angle=90
make_transparent material=Diffuse
do_nothing t=1s
animate frames=150:750 smooth=5 t=5s
do_nothing t=1s
animate frames=750:150 smooth=5 t=5s
```



# On-the-fly highlight edits

```
$ global name=movie10
$ scene_tbp visualization=cu.vmd

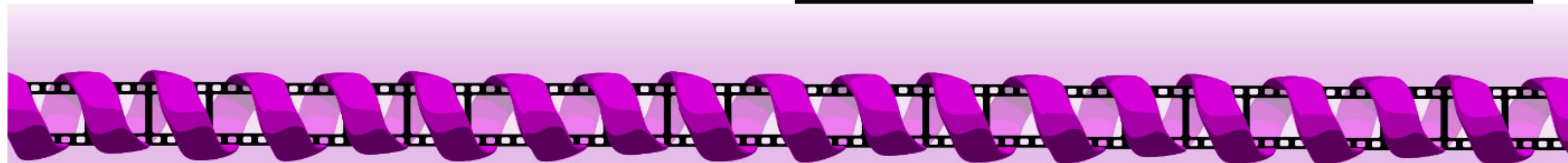
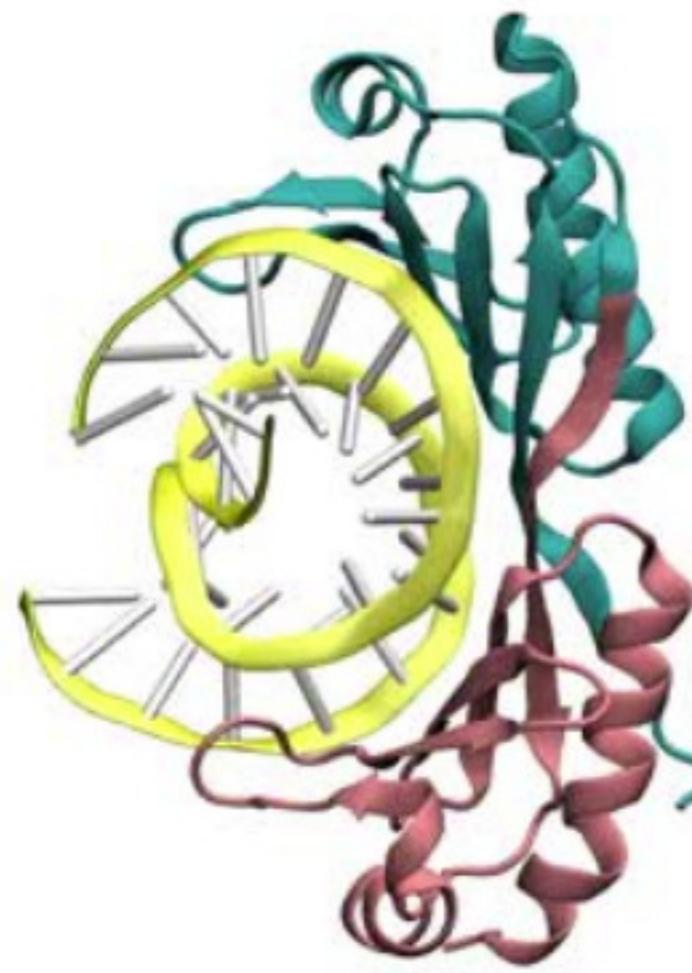
#scene_tbp
do_nothing t=1s
highlight selection='same residue as
(resname LYS ARG and within 5 of
nucleic)' style=licorice mode=u
color=type t=1s alias=sc fade_in=1.0
{rotate axis=y angle=360 t=3s
fraction=:0.5;
highlight alias=sc mode=n thickness=1:3}
{rotate axis=y angle=360 t=3s
fraction=0.5:;
highlight alias=sc mode=n thickness=3:1}
highlight alias=sc mode=d t=2s
do_nothing t=1s
```

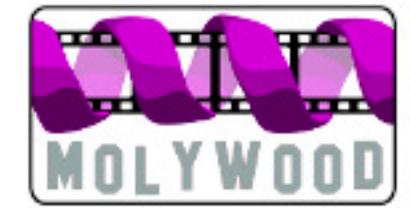


# Overlapping actions

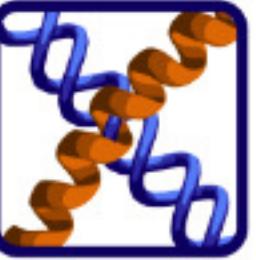
```
$ global name=movie11
$ scene_tbp visualization=cu.vmd

#scene_tbp
zoom_in scale=1.5 fraction=:0.5 t=2s
{rotate axis=y angle=360
 fraction=:0.5 t=2s;
zoom_in scale=1.5 fraction=0.5:}
{rotate axis=y angle=360
 fraction=0.5: t=2s;
translate vector=2.4,0,0
 fraction=0:0.5}
translate vector=-2.4,0,0
translate vector=2.4,0,0
fraction=0.5: t=2s
```





MOLYWOOD



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## Molywood Documentation

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### ¶ MOLYWOOD DOCUMENTATION

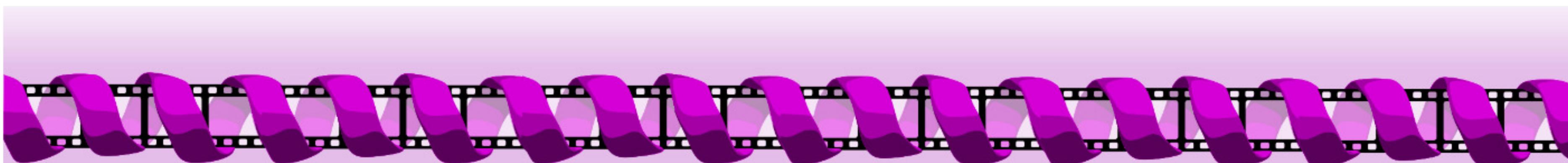
## Table of contents

- Input structure
  - Notes on input structure
- Global keywords
  - List of available global keywords and parameters
  - Notes on global keywords
    - Scene keywords
- Actions
  - List of available action keywords and parameters
    - Instantaneous actions
    - Instantaneous or finite-time actions
    - Finite-time actions
  - Notes on individual actions
    - Instantaneous actions
    - Instantaneous or finite-time actions
    - Finite-time actions

#### \* Known Issues

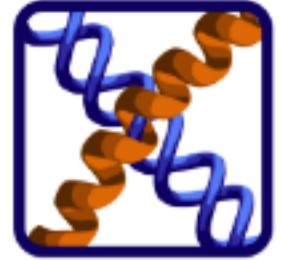
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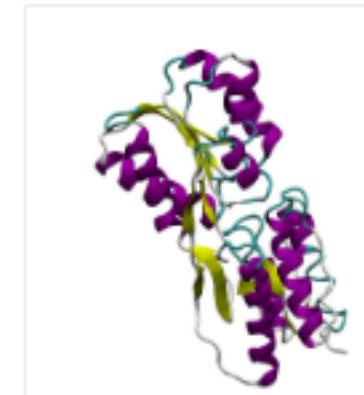


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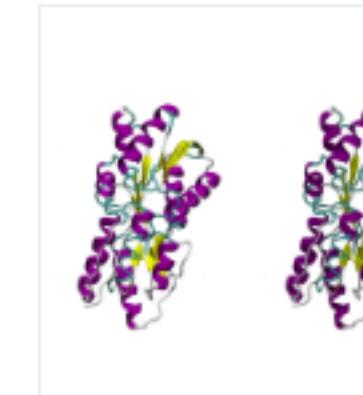
## Molywood samples

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### BASIC OPTIONS



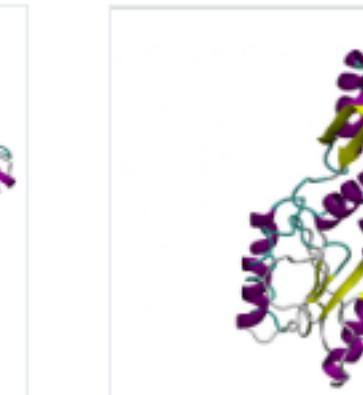
basic1



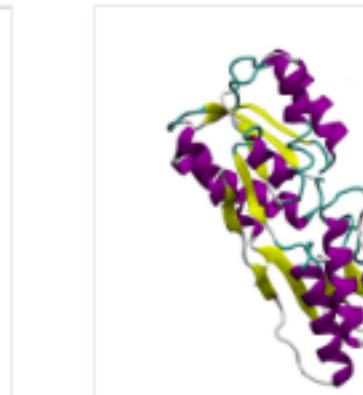
render1



render2



audio1



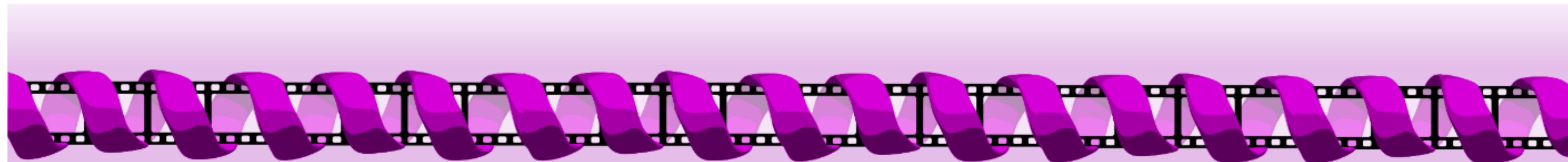
audio2



### CAMERA OPTIONS

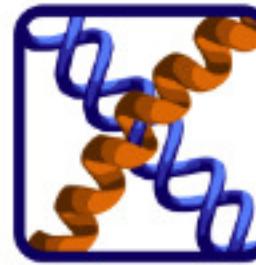
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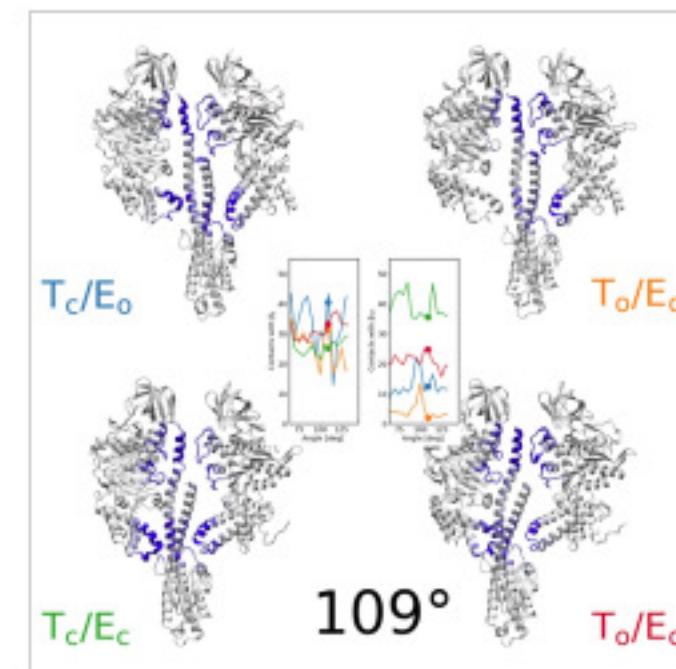


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## Molywood movies gallery

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### ■ $\gamma$ - $\beta^E$ AND $\gamma$ - $\beta^{TP}$ CONTACTS IN DIFFERENT F1-ATP SYNTHASE CONFORMATIONAL STATES



Rotation of the F1-ATP synthase  $\gamma$  subunit in all possible conformational states of  $\beta^{TP}$  (T, blue) and  $\beta^E$  (E, red). As the catalytic subunits assume an open or closed geometry, they maintain different number of contacts with the central  $\gamma$  subunit during the two shorter (25 and 30 degree) rotary substeps, moving from 65 to 120 degrees in the synthesis direction. The plots show  $\gamma$ - $\beta^E$  and  $\gamma$ - $\beta^{TP}$  contacts, and color-coding maps the contact frequency onto the structure of the enzyme.

● Open gallery example

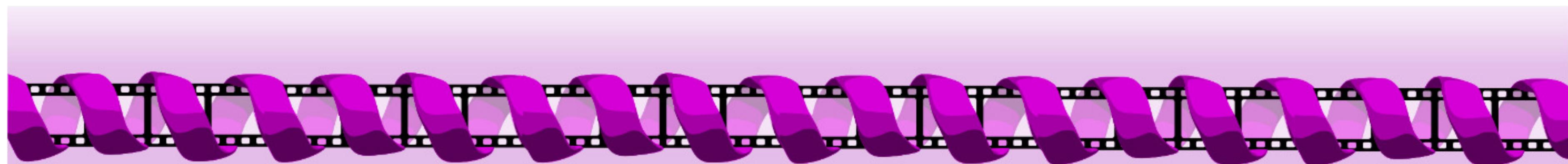
▷ Open code example

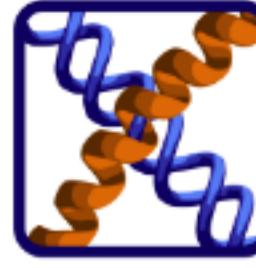
### ■ D-RIBOSE BINDING PROTEIN CONFORMATIONAL TRANSITION

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D-ribose binding protein conformational transition from a closed to an open conformation studied by means of an





# Movie design workflow:

Explore

Tweak

Adjust

`render=f draft=t  
t=1s`

`render=t draft=t  
fps=2`  
place overlays at  
low resolution

`render=t draft=t  
fps=5`  
adjust timing

Go HQ

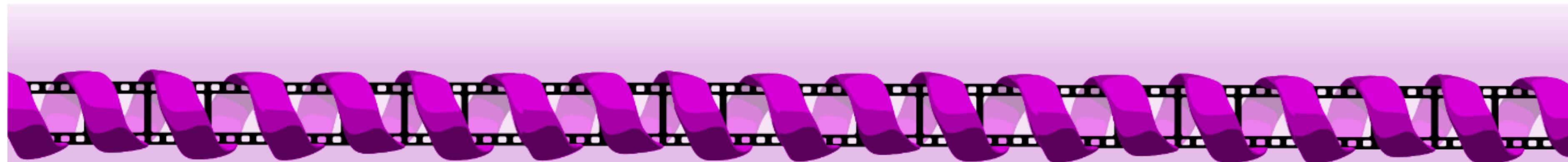
Full render

Test

`render=t draft=f  
fps=25  
ambient_occlusion=t`

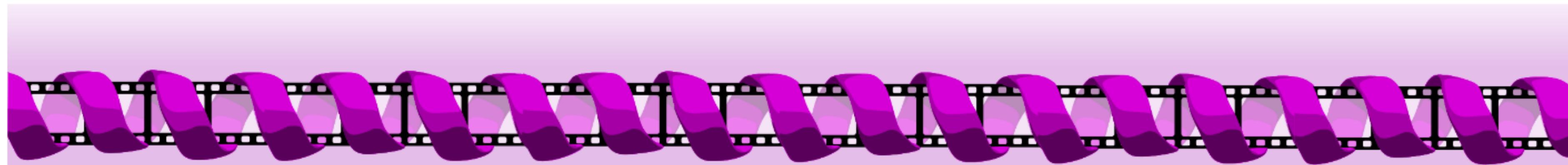
`render=t draft=f  
fps=25`  
wait a few minutes

`render=t draft=t  
fps=15`  
set final resolution



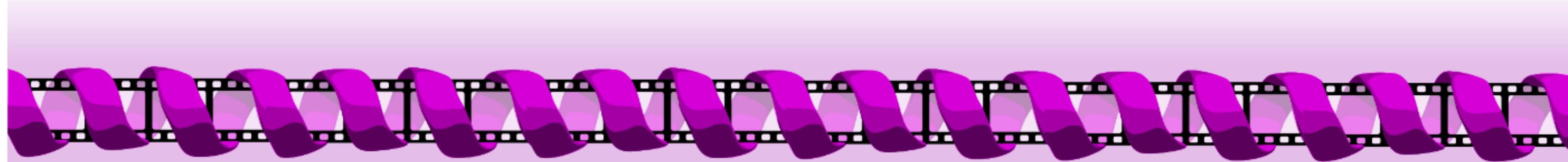
# Key features, summarized

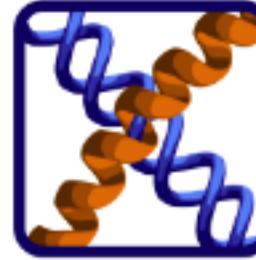
- From .txt to .mp4 with no extra requirements
- Ease of working with data, graphics, audio, movies
- Support for concurrent and/or asynchronous actions
- Flexibility in the treatment of scenes
- Highly customizable & dynamic representations
- Can be automated and run remotely
- Open and free



# Future developments

- Now entirely dependent on your feedback
- Add more actions?
- Enable editing of defaults?
- Support anything beyond VMD?
- GUI or TUI-only?
- Ongoing debugging
- Gallery open to your examples





# Thanks for your attention!

Now, go check out more at  
[mmb.irbbarcelona.org/molywood](http://mmb.irbbarcelona.org/molywood)

Bioinformatics, 2020, 1–2  
doi: 10.1093/bioinformatics/btaa584  
Advance Access Publication Date: 23 June 2020  
Applications Note



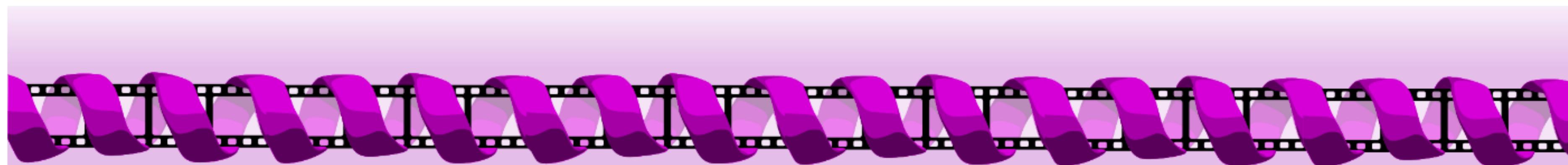
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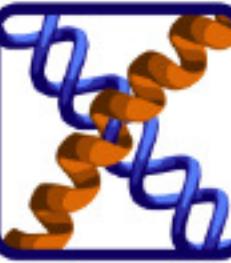
Structural bioinformatics

**Molywood: streamlining the design and rendering of  
molecular movies**

Miłosz Wieczór<sup>1,2,\*</sup>, Adam Hospital<sup>2</sup>, Genis Bayarri<sup>2</sup>, Jacek Czub<sup>1</sup>  
and Modesto Orozco<sup>2,3,\*</sup>

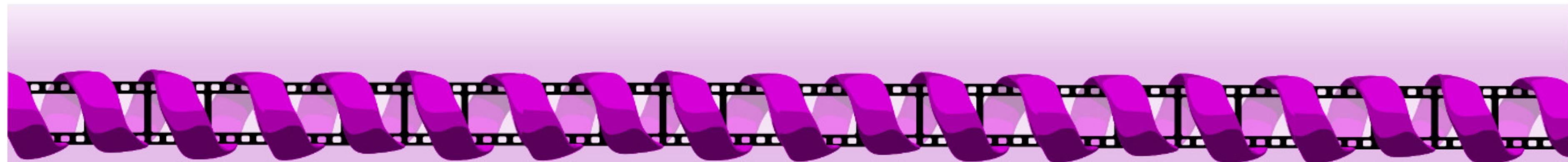
(& looking  
forward to  
questions)





# Audience Q&A session

- Please use the Questions function in GoToWebinar application
  - If you don't have audio, please mention that in the question.
- Any other questions or points to discuss after the live webinar? Join the discussions at <http://ask.bioexcel.eu>.





# Next autumn BioExcel webinar

*5 November at 15:00 CET*

Competency Mapper

Username  Password

Overview

Competency mapper is a web-based tool to support the creation and management of competency frameworks for professionals working in the biomolecular sciences [read more >](#)

**bioexcel**  
The BioExcel training programme is based on a competency profile. A competency is an observable ability of any professio... [»](#)

**CORBEL**  
We are using a competency-based approach to developing, delivering and monitoring the CORBEL training programme. CORBEL... [»](#)

**RITrain**  
This competency framework has been developed in partnership with Research Infrastructure leaders and is aimed to support... [»](#)

**ISCB**  
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Using competencies to guide training and professional development

*by Vera Master and Marta Lloret Llinares*

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