

ENSnano 0.7.3 Quickstart Guide

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This quickstart guide sums up the main features of ENSnano graphical user interface (GUI).

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1 GUI overview

ENSnano GUI is decomposed into 5 parts:

1. **The top bar:** File managment, Views managment, Undo/Redo, Basic tool selection, Selection modes, Help
2. **The left panels** is split in 4 parts vertically:
 - **The 8 edition tabs**, from left to right: Grid tab, Strand/Helix tab, Camera display tab, Physics relaxation tab, Sequence tab, Parameters tabs, Bezier tab, Revolution surface tab.
 - **The camera panel:** standard view, incremental camera movements, screenshots (2D and 3D), export to STL, Saved camera positions
 - **The contextal panel:** provides information on the current selection
 - **The organizer tree:** a nested list to organize your design
3. **The 3D view:** a live editable 3D view of your design
4. **The 2D view:** a live editable 2D view of your design
5. **The statuc bar:** at the bottom of the 2D and 3D views, displays some relevant information when needed.

Most of the features are presented in details in the openly available article [Levy, Schabanel, DNA27, 2021].

2 The Top bar

From left to right:

- **File managment:**



New / Open an ensnano, cadnano or scadnano file / Reload / Save / Save as / Export to oxdna, PDB, or cadnano / Import a STL model

- **Views managment:**

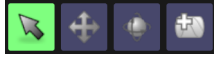


3D view only / Switch between Helix and Line helix representation / 2D view only / 2D and 3D view / Split or Unplit the 2D view / Switch the 2D view to stereographic / Exchange the two 2D split views / Translate the camera to fit the design in the 3D view / Make the camera horizontal

- **Undo / Redo:**



- **Basic tool selection:**



Select / Translate / Rotate / Add an helix to a grid

- **Selection mode:**



Nucleotide or crossover / Strand / Helix

- **Help:**



Display the help in the contextual panel / Link to online tutorial

3 The Left panel

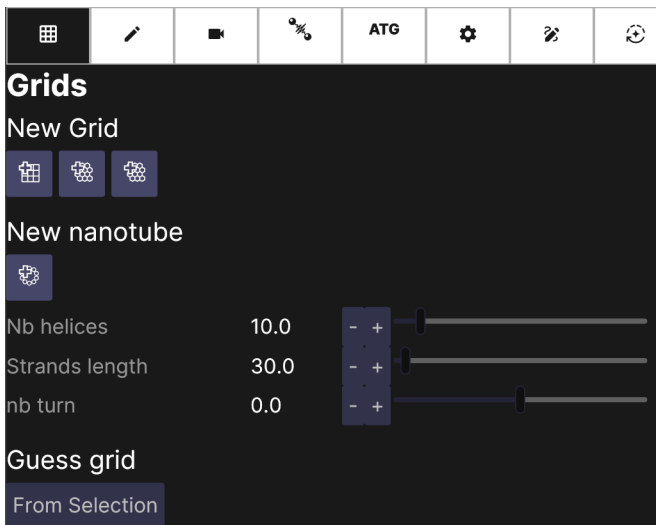
3.1 Tool tabs

There are 8 edition tabs:



From left to right:

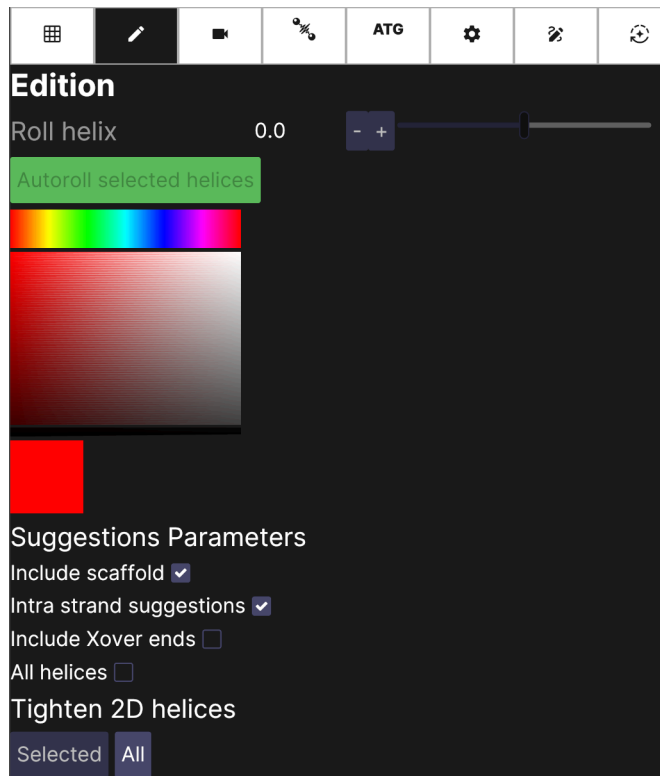
Grids tab



From top to bottom:

- Add a new Square / Honeycomb, Upright or Rotated
- Add a new nanotube with x helices, double strands of length y , making z turns
- **Guess grid:** Attach the currently selected helices to a guessed grid (useful when importing cadnano designs)

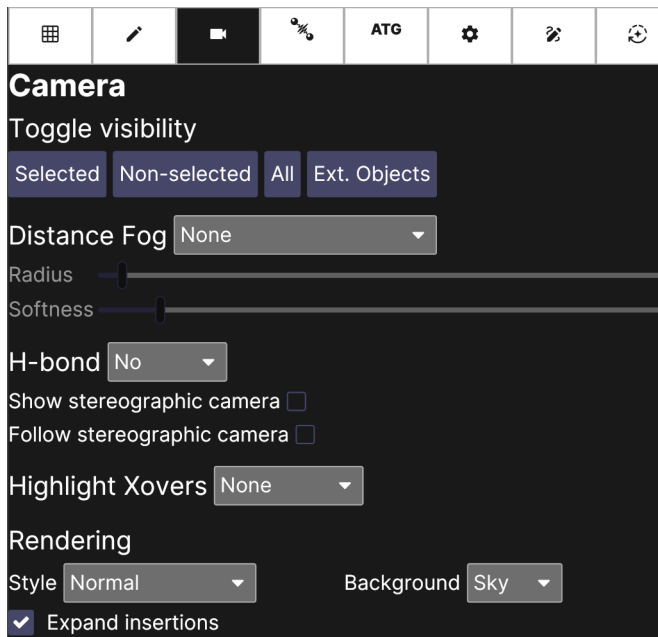
Edit tab



From top to bottom:

- Set the roll of the selected helices
- Autoroll the selected helices
- Set the color of the selected strands
- **crossover suggestion parameters:** choose which pairs of nucleotides should be considered
- **Tighten helices:** shorten the helices representation in the 2D view

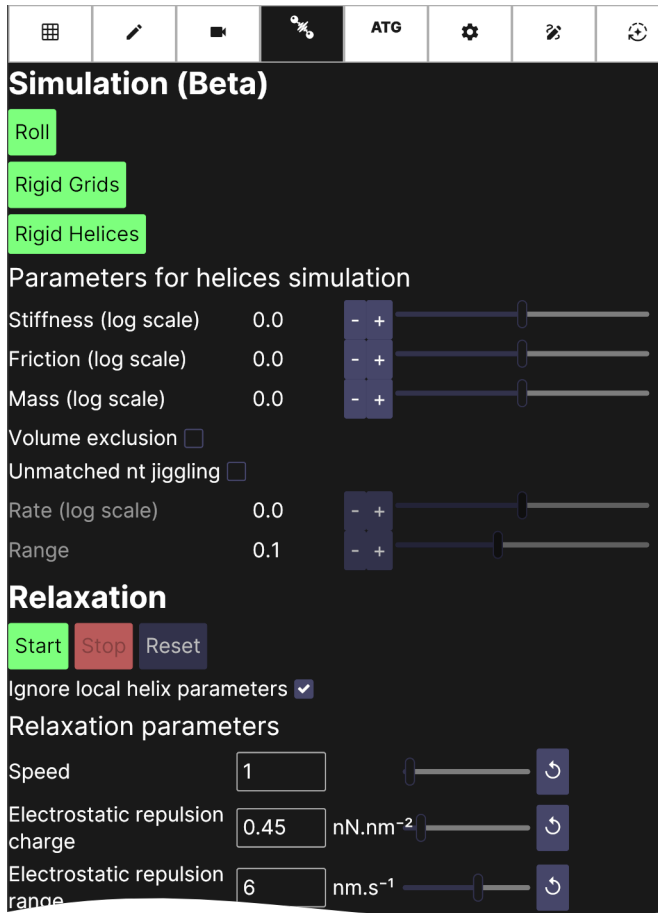
Camera tab



From top to bottom:

- Toggle the visibility of the current selection (helices, strands or crossovers), everything and external objects
- **Fog**: make invisible all objects that are too close or too far from the current pivot or the camera
- Show h-bonds
- **Stereographic view**: show the stereographic camera orientation in the 3D view; impose the 3D view camera to follow the stereographic camera
- **highlight crossover**: allows to mark crossovers in the 3D view
- **Rendering**: choose the rendering style and background
- Make insertions visible in the 3D view

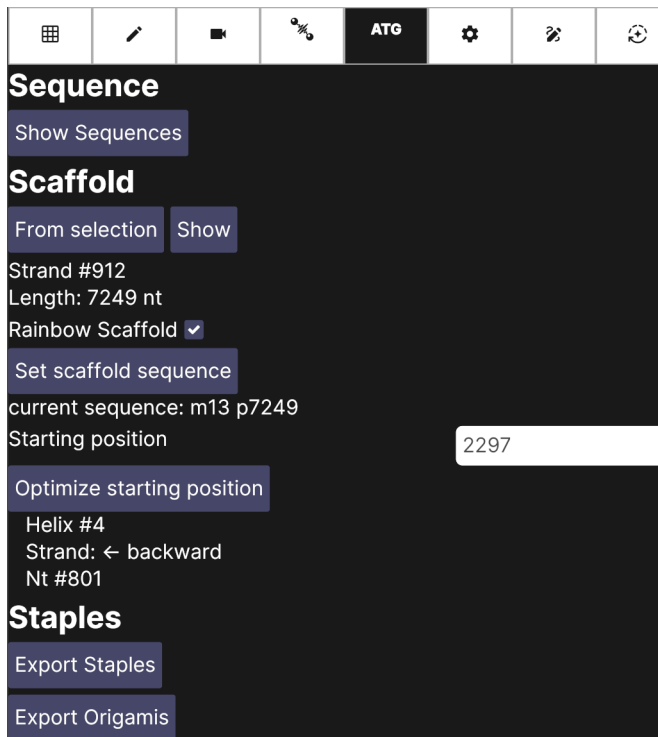
Relaxation tab



From top to bottom:

- **Roll:** Autoroll all the helices
- **Rigid grid:** Relax the design by making each grid a rigid body (experimental, only works for straight helices attached to a grid); mainly usefull when importing cadnano designs
- Relax the design by making each helix a rigid body (experimental, only works for straight helices); mainly usefull when importing cadnano designs
- Physics parameters for the two relaxations above
- **Relaxation (beta):** relax all the helices as non-intersecting beams
- Physics parameters for the relaxation above

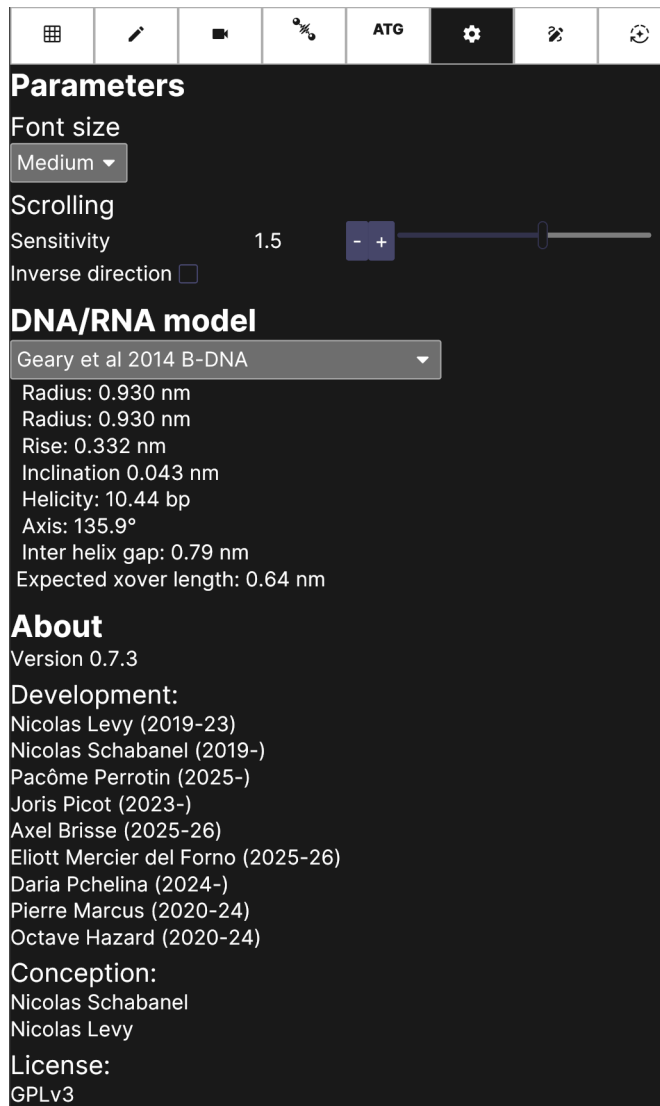
Sequence tab



From top to bottom

- Show/Hide the sequences in the 2D and 3D views
- **Scaffold:**
 - make the strand selected the scaffold
 - show the scaffold strand
 - display the scaffold in rainbow colors in the 3D view
 - choose the scaffold sequence and the location of its starting position in the scaffold strand
 - optimize the scaffold sequence starting position to minimize the staple strands possibly difficult to synthesis (minimize the numbers of $\{C, G\}^n$ for $n \geq 4$ and $\{A, T\}^m$ for $m \geq 7$)
- **Staples:**
 - export staples as a .xlsx file
 - export the design as a .origami json file listing the the scaffold domains spanned by each strand

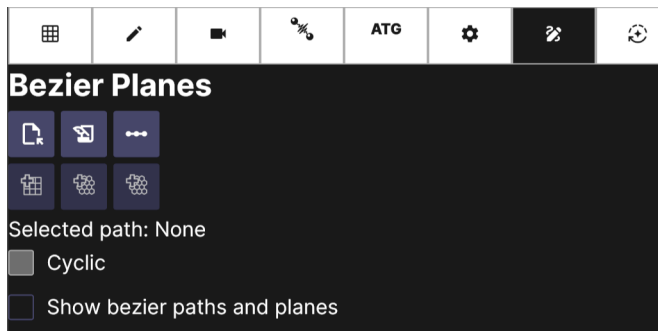
Parameters tab



From top to bottom:

- GUI font size
- Mouse scrolling sensitivity and direction
- Default DNA/RNA model: the default model is “Geary et al 2014 B-DNA”; RNA models are untested
- List of contributors
- License: GPLv3

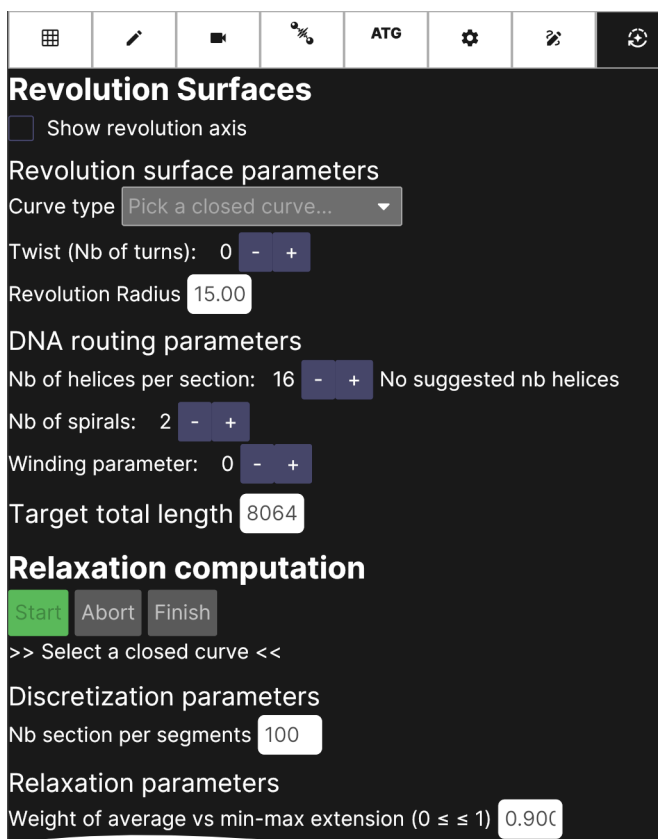
Bezier tab



From top to bottom:

- **Bezier planes:**
 - Import a bezier path in a pseudo svg format; Create a bezier plane; Switch to “Add bezier vertex” mode
 - Attach a Square / Honeycomb, upright or rotated, to the selected bezier path
- Make the selected bezier path cyclic
- Show/Hide bezier planes and paths

Revolution surface tab

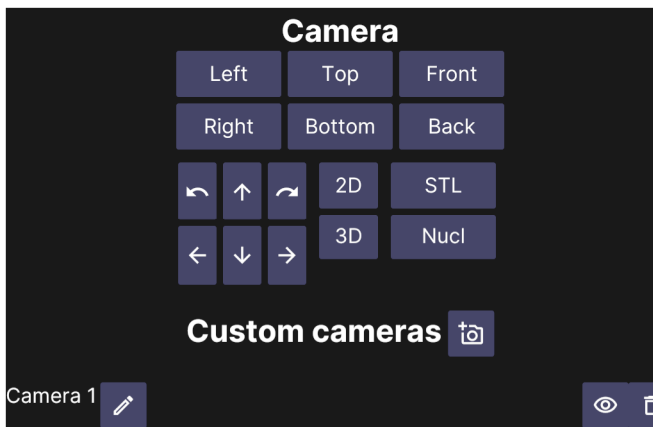


From top to bottom:

- Show/Hide revolution axis and plane
- **Revolution surface definition:**

- **Curve type:** choose and parametrize the closed curve defining the section of the revolution shape
- Define the twist of the revolution shape (number of turns of the section upon itself per revolution)
- set the revolution radius
- **DNA routing parameters:**
 - Choose the desired number of helices crossing per section, the number of spiraling helices and the winding parameter, see [Levy, Mills, DNA28, 2022; Finkel, Levy *et al*, FNANO21, 2024; Levy, Finkel *et al*, 2025, in revision]
- Total target total length of the spiraling helices
- **Relaxation computation:** Start / Abort / Force finish the relaxation of the spiraling helices according to the pattern defined above
- Physics parameters of the relaxation above

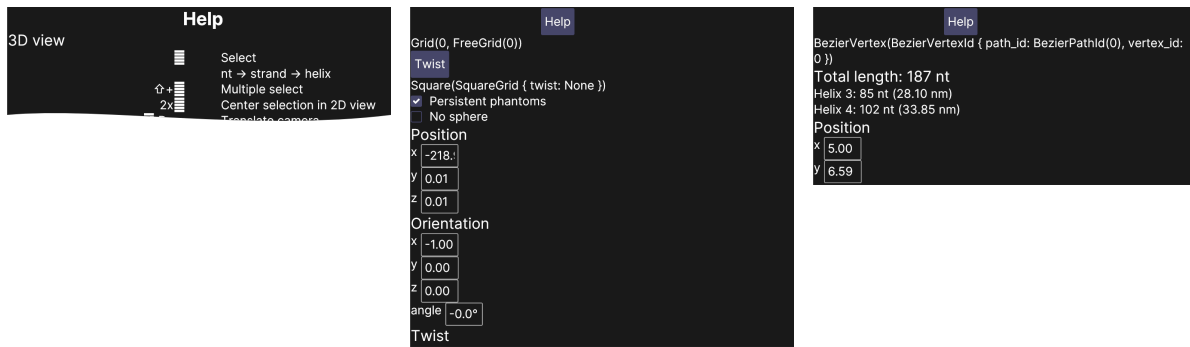
3.2 Camera panel



From top to bottom:

- Left / ... / Back buttons place the camera in the six standard directions, fitting the design in the frame
- The six arrows on the left rotates the camera frame around the pivot, if any, or the camera position otherwise
- The 2D/3D buttons take high resolution snapshots of the 2D and 3D views and automatically save them at the same location as the design file
- The STL button saves an STL model of the design at the same location as the file
- The Nucl button saves an ascii file at the design location containing the 3D coordinates of all nucleotides.
- The +camera button saves the camera location which is added in the list bellow and saves within the design file

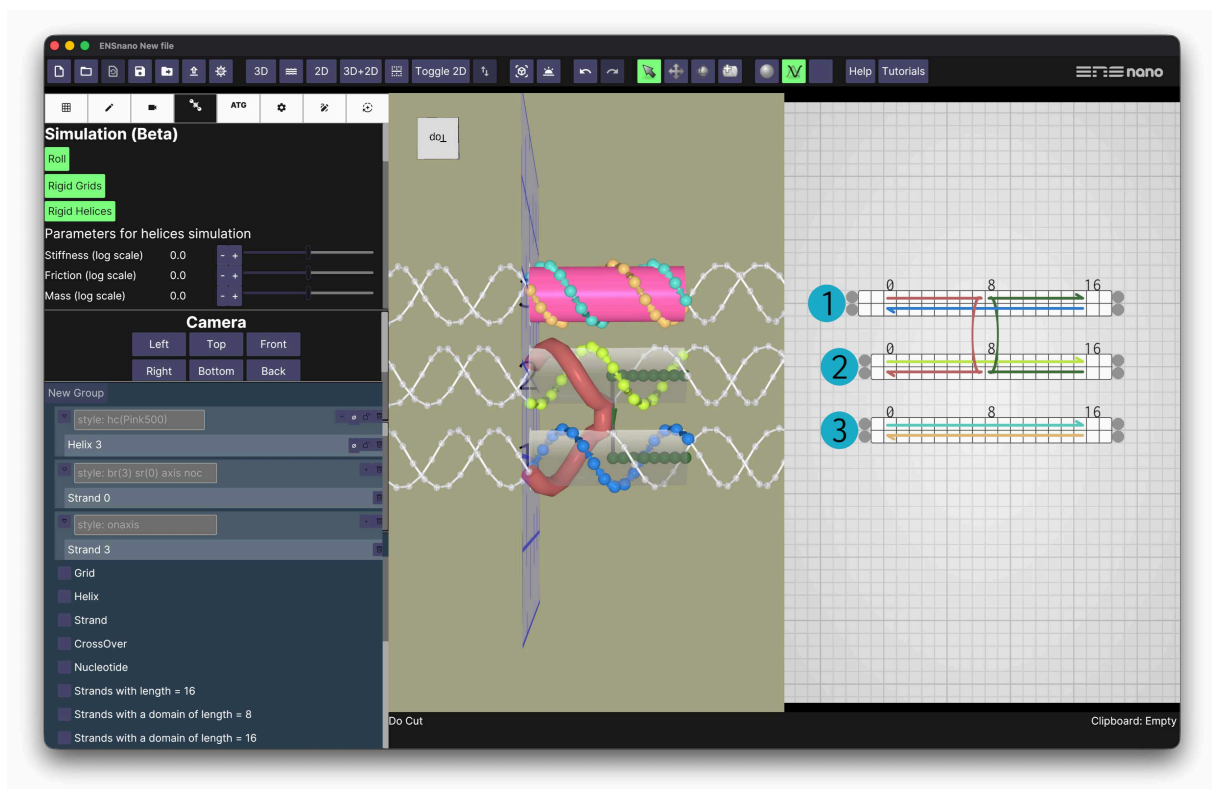
3.3 Contextual panel



The contextual panel displays by default an help notice. However when some object are selected, it displays some useful and possibly editable informations, such as:

- when a grid is selected: its position, orientation and angle; whether phantom helices are drawn or not
- when a bezier vertex is selected: its position inside its bezier plane; and the lengths of all the helices attached to its path

3.4 The organizer tree



The organizer tree allows to organize, change the appearance of, and check your design. It consists in automatically generated groups and custom groups.

- **Automatically generated groups:**
 - *Grid* contains all the grids for easy access; their visibility can easily be switch on/off there
 - *Helix* contains all the helices sorted by id
 - *Strand* contains all the strands sorted by id

- ▶ *Crossover* contains all the crossovers; it is very useful to click on this group to select all the crossovers and then click on “Toggle non-selected visibility” in the Camera tab to only see the crossover and check their pattern and lengths easily
- ▶ Then, the strands are grouped by length and also by subdomain lengths; very useful to check that all strands have adequate lengths
- **Custom groups** allow:
 - ▶ to tag strands within a group, indeed the groupname will be exported in the .xlsx file for readability.
 - ▶ to change the appearance of the helices, strands and crossovers in the 3D view. The groupname must start with `style:` (see image above). As shown in the image above, one can then write a series of keywords that will affect the 3D representation of the objects inside the group:
 - `rs / nors` to display the strands in rainbow color or not (default: `nors`)
 - `xc / noxc` to color the crossover by length or not (default: `xc`)
 - `sr( $r$ )` to set the nucleotide sphere radius to r in Å
 - `sc( $color$ )` to set the color of the nucleotides to $color$ where $color$ is the hexadecimal code AARRGGBB or a material color name (e.g., Blue500), see <https://materialui.co/colors/>
 - `br( $r$ )` to set the radius of the covalent bonds to r in Å
 - `bc( $color$ )` to set the color of the covalent bonds
 - `hr( $r$ )` to set the radius of the helix cylinder to r in Å
 - `hc( $color$  [,  $\alpha$ ])` to set the color of the helix cylinder; the optional floating number α in $[0, 1]$ sets the opacity
 - `wc / noc` to display the strand with cone-arrows or not (default: `wc`)
 - `cs( $color$  [,  $\alpha$  [,  $\beta$ ]])` for color shading the strands near a given color $color$ with optional opacity α and Hue range β : when pressing the shortcut key `k`, ALL the strands are recolored randomly and the strands in the group get a color variation of $color$
 - `onaxis / offaxis` to impose the strands to be positioned on the axis of the helix (*line-representation*) or at its natural helicoidal representation (default: `offaxis`)
 - `cv( $r_{min}, r_{max}$ )` `colordisplays` using a Purple-to-Blue gradient the *curvature radius* of the helix cylinder for radius within the range $r_{min} \cdots r_{max}$
 - `to( $\tau_{min}, \tau_{max}$ )` `colordisplays` using a Blue-to-Purple gradient the *torsion* of the helix cylinder for radius within the range $\tau_{min} \cdots \tau_{max}$
 - ▶ keywords are processed from top to bottom in the tree

4 The 2D and 3D views

The functioning of the 2D and 3D views is described in details in [Levy, Schabanel, DNA27, 2021]. We just recall the main functionalities. `ensnano` is best used with a **three-button mouse**.

A thumb rule is that in both views of `ensnano`:

- Left click is most of the time for *selecting and editing*
- Right click is most of the time for *rotating* camera (3D) or helices (2D)

- Middle click is for *moving* the camera / view
- Double left-click on an object in one view makes the other view focus on it as well.
- Middle click can be replaced by Alt/Opt + Left click in absence of a middle button.

4.1 The 3D view

- **Middle click** translates the camera
- **Right click:**
 - A right click on a selectable object (grid, nucleotides, bezier vertex,...) places the *pivot* (a yellow ball) there; right clicking elsewhere removes the pivot
 - Right dragging rotates the camera: around the pivot if any; or around the camera position otherwise. Note that the rotation maintains the horizon horizontal by default (press Alt/Option to rotate the camera freely)
 - Shift + right dragging rotates the frame of the camera
 - Alt/Option + right dragging rotates the camera freely
- **Left click:** Almost everything is editable in the 3D view with a left click
 - A single Left click selects an object
 - A left double click focuses the 2D view on the same object
 - Left dragging the extremity of a strand domain, moves it
 - **Long left press a nucleotide to create a crossover in the 3D view**
- **Crossover coloring:** in the 3D view the crossover are by default colored according to their length from light grey (good) to black (long) to provide an immediate feedback on the quality of the crossover. This can be turned off using the noxc keyword in the organizer tree.

4.2 The 2D view

- **Middle click** translates the 2D view
- **Right click:**
 - Right click in the middle of a domain of a strand and it will nick it
 - Right click at the extremity of a domain of strand and it will ligate to the neighboring domain if it is not bound by a crossover
 - Right click at the extremity of a domain of strand next to a crossover and it will double the crossover if possible.
 - Right drag on the helix id to rotate the helix representation
- **Left click:** Almost everything is editable in the 3D view with a left click
 - A single Left click selects an object (nucleotide, strand, crossover or helix depending on the selection mode selected in the top bar); Shift+ left click adds the clicked object to the current selection
 - Left dragging the extremity of a domain parallel to the helix moves the extremity
 - Left dragging a nucleotide of a domain perpendicularly to the helix will create a crossover
 - Left dragging an helix id moves the helix
 - A left double click focuses the 3D view on the clicked object

- Furthermore, when the 2D view is **split** in two parts, one can left drag nucleotides from one part to the other to create crossover between parts that are displayed apart in the 2D view
- **Copy/Paste is possible in the 2D view:**
 - It is possible to copy-paste strands of crossovers in the 2D view: just select some strands/crossover and press Ctrl/Cmd+C and then Ctrl/Cmd+V to paste and move the mouse to place the pasted object and left click to finish.
 - We refer to [Levy, Schabanel, DNA27, 2021] for the more sophisticated copy-past-and-repeat using Ctrl/Cmd+J which allows to paste several time by repeating and identical translation between the copies.

4.3 Crossover creation

To sum up, crossovers can be created either:

- By Long left pressing on a nucleotide in the 3D view
- Left dragging a nucleotide of a domain perpendicularly to the helix in the 2D view or to the other part of the 2D view when splitted

Here is an example:



5 Known issues

- **Sometimes key shortcuts do not work anymore:** just left-click on a **white text input box** in one the of tab (e.g. the starting point text input box in the Sequence tab) and then click outside of the text input box and it should work again. *This bug arises typically after having edited the organizer tree and will be fixed in the near future.*

- **Copy/Paste only works inside a given grid.** It is not yet possible to copy paste between different grids.
- **Some object cannot be moved in the GUI for now**, e.g. the STL model. However it is easy to edit the ensnano file (an easy-to-read and edit json file format) to modify the position and orientation of the object.

