# 3dRS$_{d}ocumentation Documentation$

***Release 1.1.1***

**3dRS Project**

**Aug 31, 2023**

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CHAPTER

ONE

# CONTENTS

## 1.1 3dRS documentation

### 1.1.1 Brief description

Documentation for the web application **3-dimensional structure Representation Sharing (3dRS)**. This application has been built with the aim of **sharing visualizations of 3D biological structures** through the web. In these visualizations, users will be able to draw several representations with different selections of the structure(s) previously **uploaded to the application**.

Our **philosophy for this project** is to make it accessible to everybody, so there is no private area and once a project is shared **everybody with the link can access it** with no restrictions.

For the sake of simplicity and to **improve the user experience** of the users, **this application has no *Save* button**. Each change performed over the stage or the panels will be **automatically saved** to the database, so anytime a user can close the browser and then come back to keep working on the edition at the same point it was.

**3dRS** has been built on top of **NGL Viewer** (a collection of tools for web-based molecular graphics that uses **WebGL** to display molecules like proteins and DNA/RNA with a variety of representations). **MDsrv** (a Molecular Dynamics streaming web server) has been used as well for **representing the trajectories**.

### 1.1.2 Publication

**3dRS, a Web-Based Tool to Share Interactive Representations of 3D Biomolecular Structures and Molecular Dynamics Trajectories** Genís Bayarri, Adam Hospital and Modesto Orozco . *Front. Mol. Biosci.*, 13 August 2021, doi: 10.3389/fmolb.2021.726232.

### 1.1.3 Demo

Below there is an embedded project of our gallery:

### 1.1.4 Version

v1.1.1

### 1.1.5 Documentation & help

All the documentation is accessible through Read the Docs.

### 1.1.6 Acknowledgements

This project has been developed on top of NGL Viewer and MDsrv:

- NGL viewer: web-based molecular graphics for large complexes
- NGL Viewer: a web application for molecular visualization
- MDsrv: viewing and sharing molecular dynamics simulations on the web

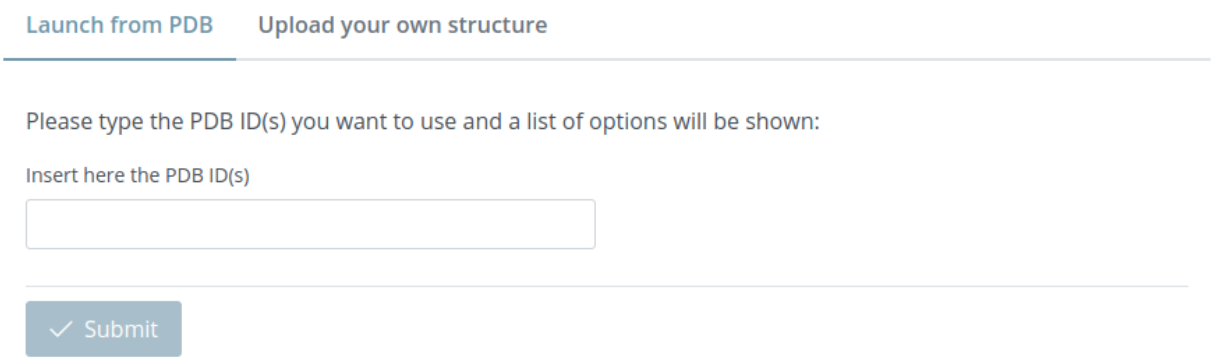
### 1.1.7 Copyright & licensing



## 1.2 Launch project

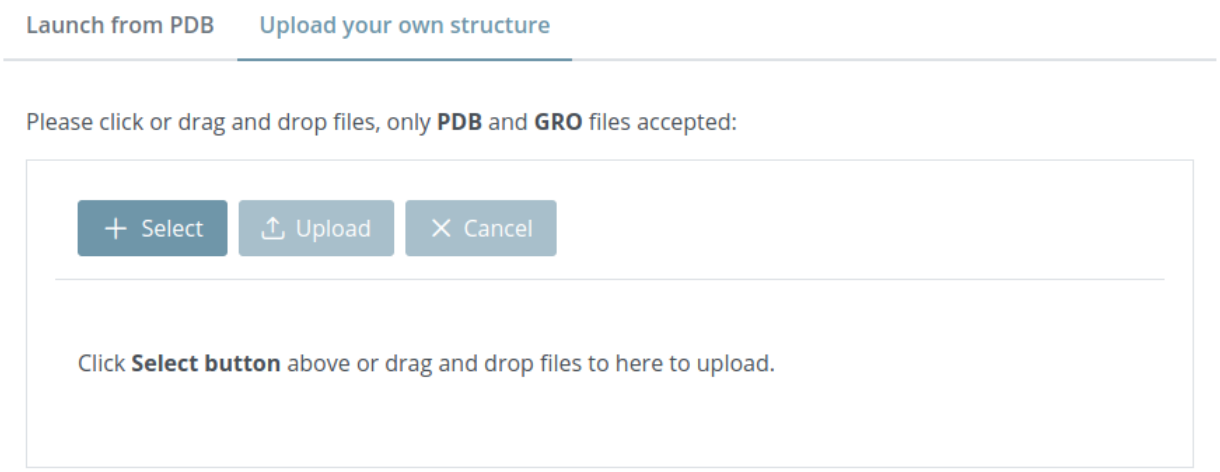
Go to the **Launch** page of the website for starting a new project. In this page there are two tabs: **Launch from PDB** and **Upload your own structure**.

### 1.2.1 Launch from PDB



In this tab, users simply must insert one or more PDB code(s) from the **Protein Data Bank** and, once selected, click the **Submit button**. The application will automatically download the structure(s) from the **Protein Data Bank** and then the application will redirect to the new project.

### 1.2.2 Upload your own structure




Custom structures can be uploaded from this tab just **clicking** the **Select button** or **dragging** them on the area below the submenu. Once the selection of files is ready, just clicking the **Upload** button the files will be processed by the application and then it will redirect to the new project.

Note that these custom structures **will be stored in our database** for the sake of sharing the representation later.

In the current version, only **PDB** and **GRO** formats are accepted and the maximum file size is **50MB**.

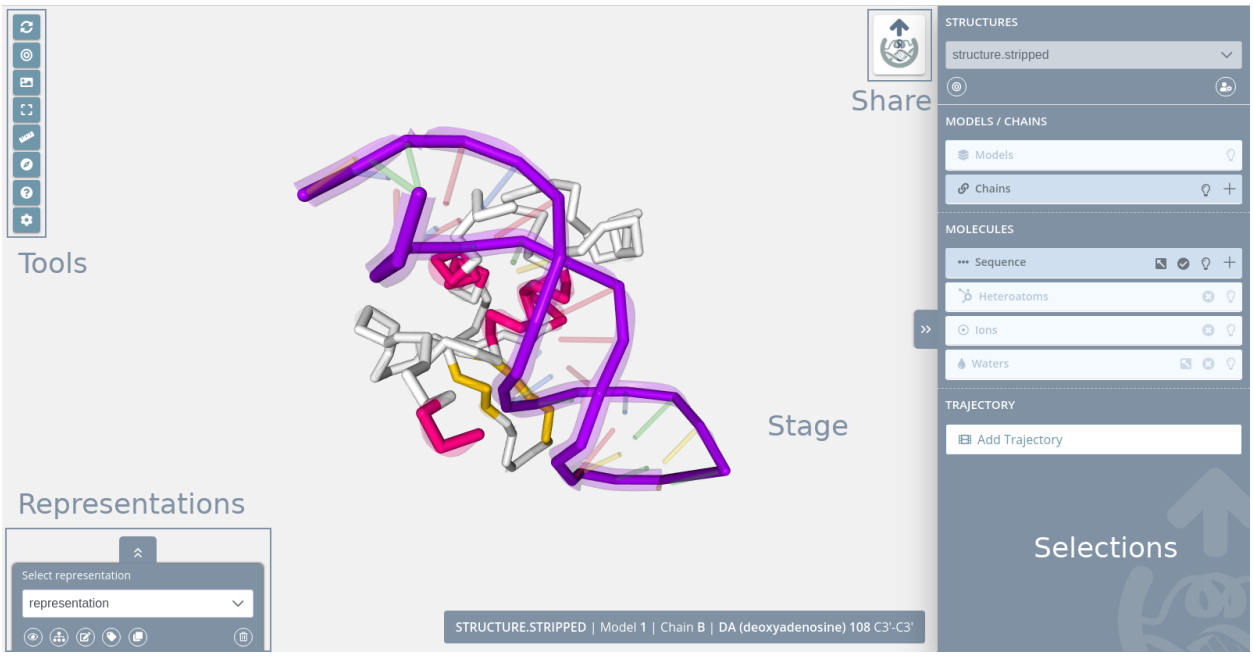
## 1.3 Edit representation

Once the structure or structures are uploaded, users will be redirected to the **Edit representation page**. This page loads the structure(s) and shows a notification warning that the project will expire unless it's shared. That means that users have **until the date shown** in the notification for editing and sharing a project. In case of not sharing it after this period of time, all the files and data related to the project will be **removed** from our database.

In the current version, the expiration time is **20 days**.

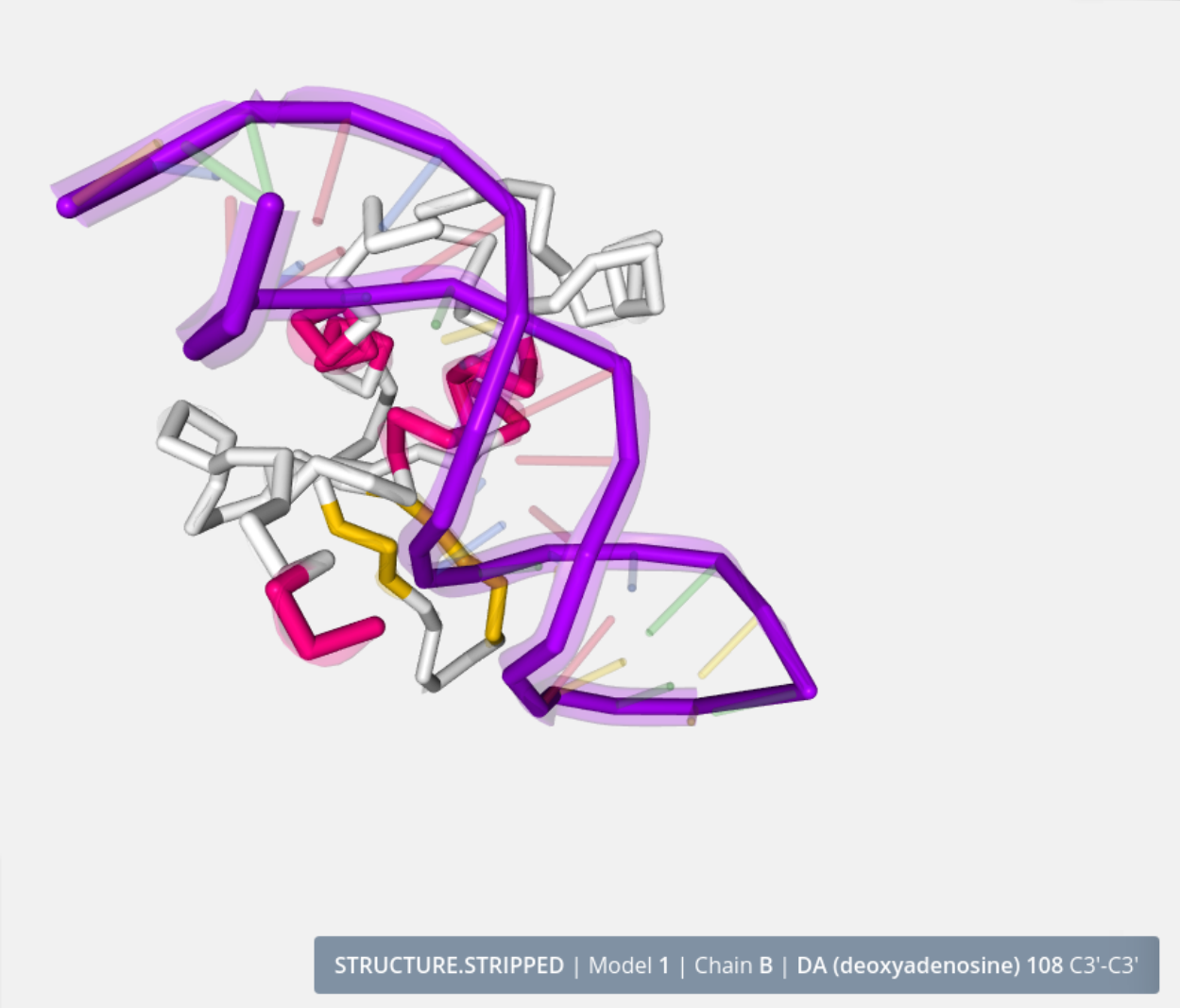
Following the philosophy of the project, this **Edit representation page** is open, but protected so that only user(s) with this URL address can access it.

This **Edit representation page** is the core of the application and we can split it into five parts:




- *Stage*
- *Tools*
- *Representations*
- *Selections*
- *Share*

### 1.3.1 Stage




The **stage** covers the entire screen and the rest of the parts are on top of it. In the stage the **structure is loaded** and users can interact with it in several ways. At this point it's important to remember that **this application has no Save button**. Each change performed over the stage or panel will be **automatically saved** to the database, so anytime a user can close the browser and then come back to keep working on the edition at the same point it was.

#### Zoom / Drag

Actions of **zoom in** and **zoom out** can be done with the **scroll mouse or the trackpad** of a notebook:

- Clicking **out of the structure** (that means in the "empty" part of the stage) with the **left button** and **dragging will rotate the view**.
- Clicking **out of the structure** (that means in the "empty" part of the stage) with the **right button** and **dragging will translate the view**.
- Double clicking **out of the structure** (that means in the "empty" part of the stage) with the **left button** will center the view.

#### Mouse actions

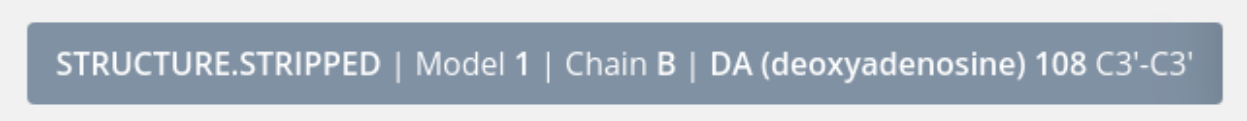
#### Mouse over actions

Passing the mouse over the molecules of the structure will **highlight** them and show **their information** in the **legend** on the bottom right of the stage.

#### Mouse click actions

- Clicking with the mouse **left button** on a molecule will **select it for the current representation**. Note that the **representations are explained in the Representations section**. Only a **new representation** accepts **new molecules**. In the **default representation** no molecules can be **selected** and this feature is disabled.
- Clicking with the mouse **left button** on a molecule **while pressing the Ctrl key** will make a zoom in at a molecule.
- Clicking **consecutively on two atoms** with the mouse **right button** will draw and calculate the distance in **ångströms** between these two atoms. In the **default representation** no distances can be **created** and this feature is disabled.
- Clicking **consecutively on three atoms** with the mouse **right button while pressing the Ctrl key** will draw and calculate the angle in **degrees** between these three atoms. In the **default representation** no angles can be **created** and this feature is disabled.

#### Legend

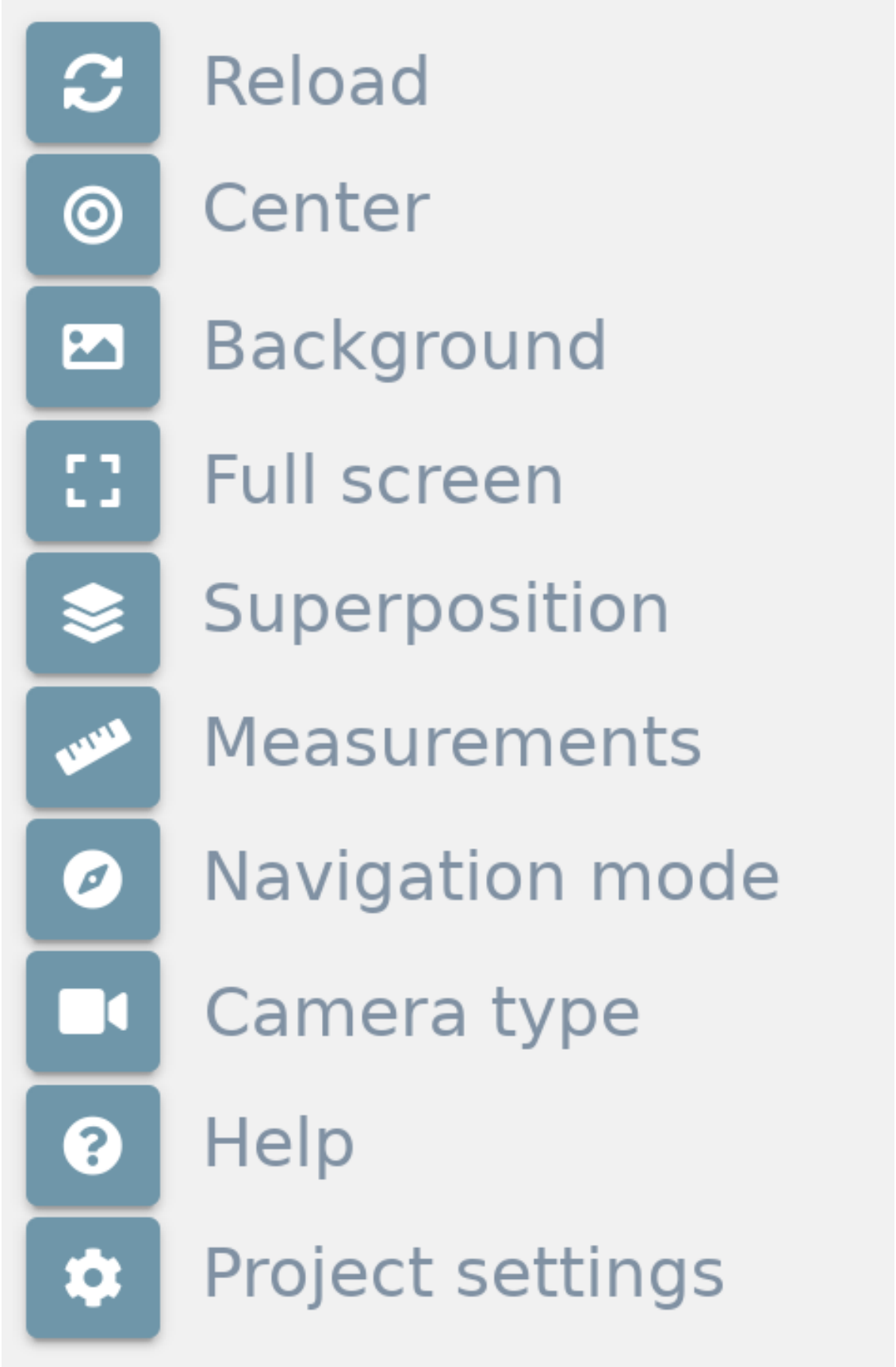



As explained in the previous section, passing the mouse over the molecules of the structure will **highlight** them and show **their information** in the **legend** on the bottom right of the stage. This legend shows information about the molecule in the next format:

> **Structure file name** | Model **number** | Chain **ID** | **Residue name (Residue long name) Residue number**
> Atom name (or Bond)

### 1.3.2 Tools

The tools menu is at the top left of the **stage** and allows users to make some actions over it:


Reload
Center
Background
Full screen
Superposition
Measurements
Navigation mode
Camera type
Help
Project settings

- *Reload*
- *Center*
- *Background*
- *Full Screen*
- *Superposition*
- *Measurements*
- *Navigation mode*
- *Camera type*
- *Help*
- *Project settings*

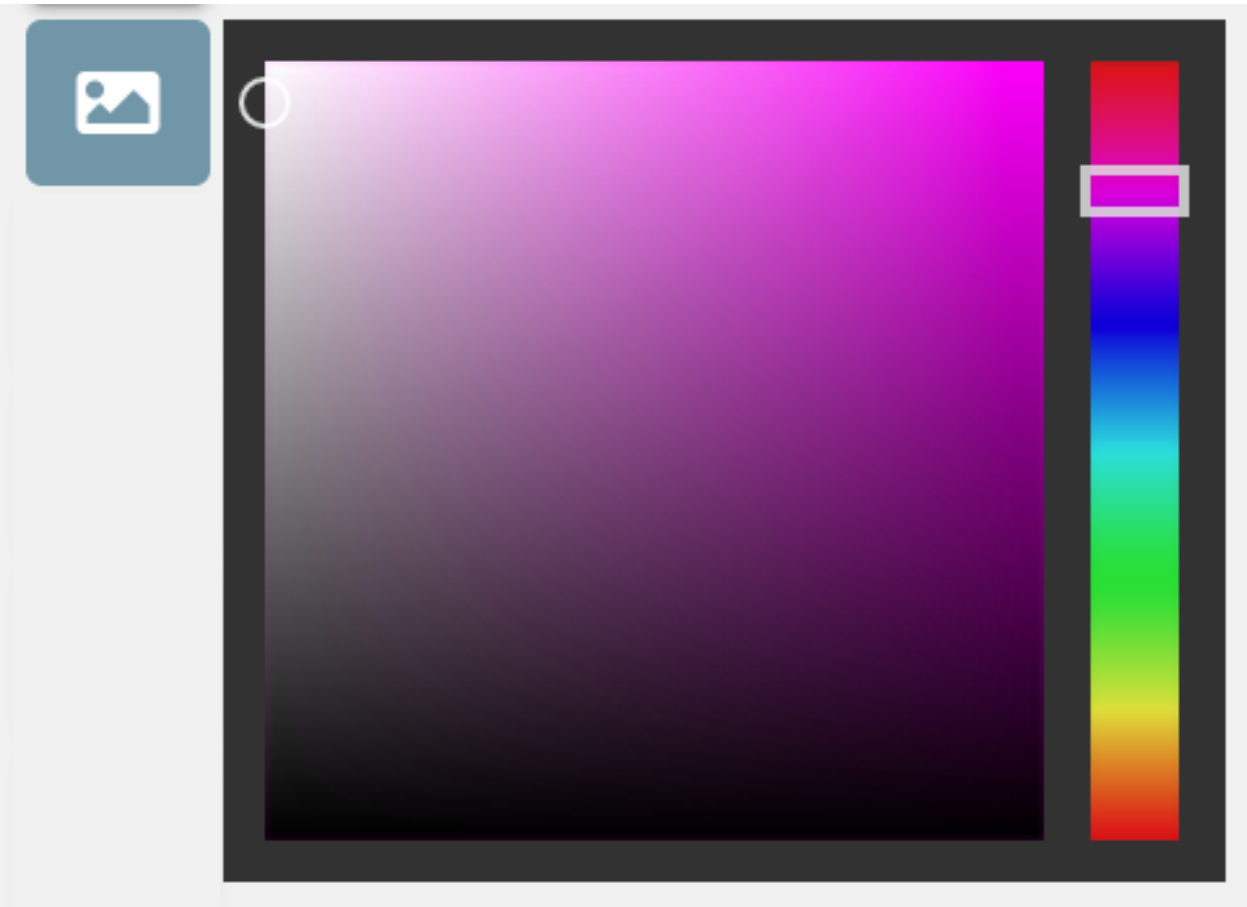
### Reload

Clicking this button **restores the view to the initial position** on the **stage**.

### Center

Clicking this button **centers** the structure(s) position on the **stage**.

### Background



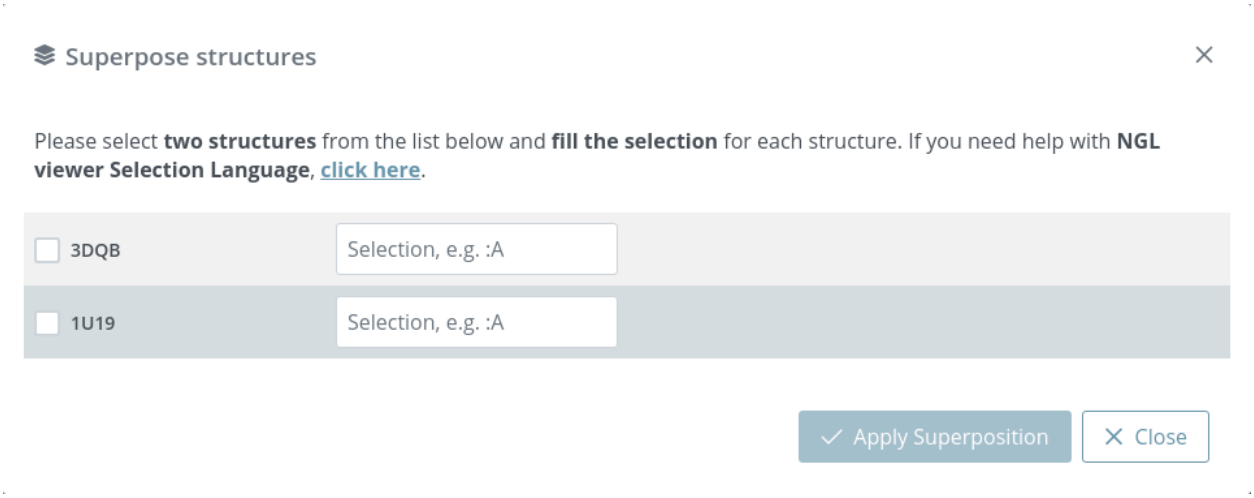
Clicking this button opens a **color picker** that allows users to change the **background color** of the **stage**.

### Full screen

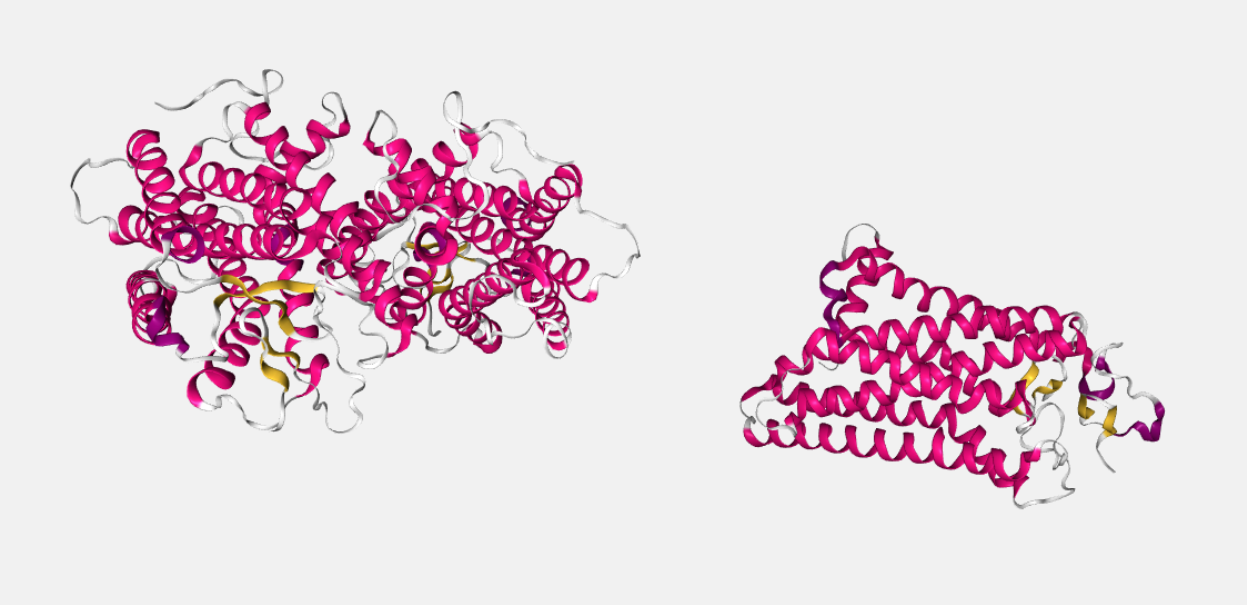
Clicking this button opens the **fullscreen mode**. For **exiting** full screen mode, just **click the button again** or press the **Esc key**.

### Superposition

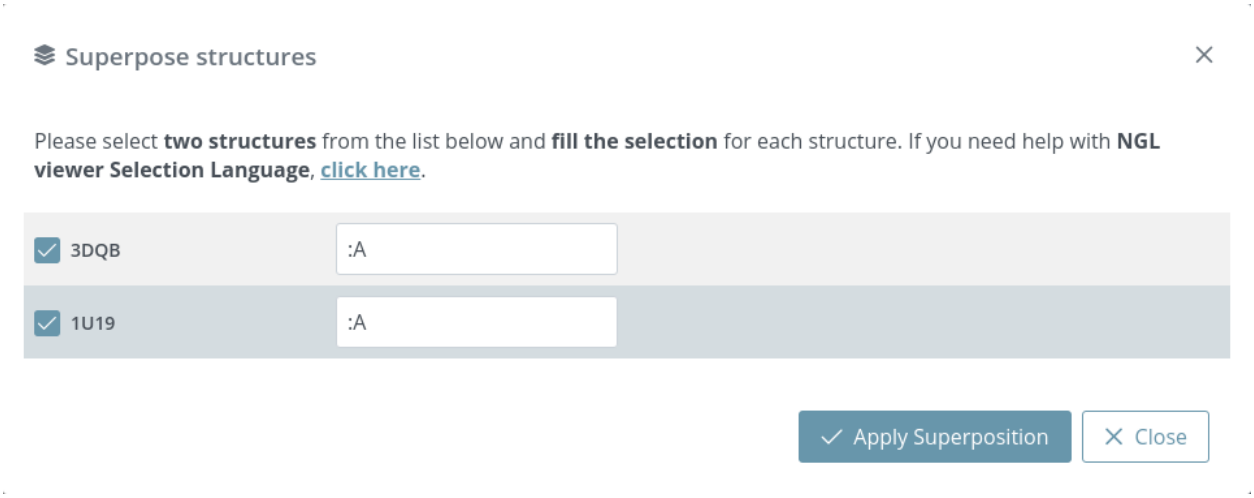
3dRS allows to **superpose** multiple structures **in pairs**. Clicking the Superposition button **opens a new modal dialog** with a list of **all the structures** present in the project:




As an example, **3DBQ** and **1U19** are shown before superposition:



Users must select **two structures** and specify in NGL viewer Selection Language the **superposition area** of each structure. If Selection field is empty, **all the structure** will be taken as a superposition area.



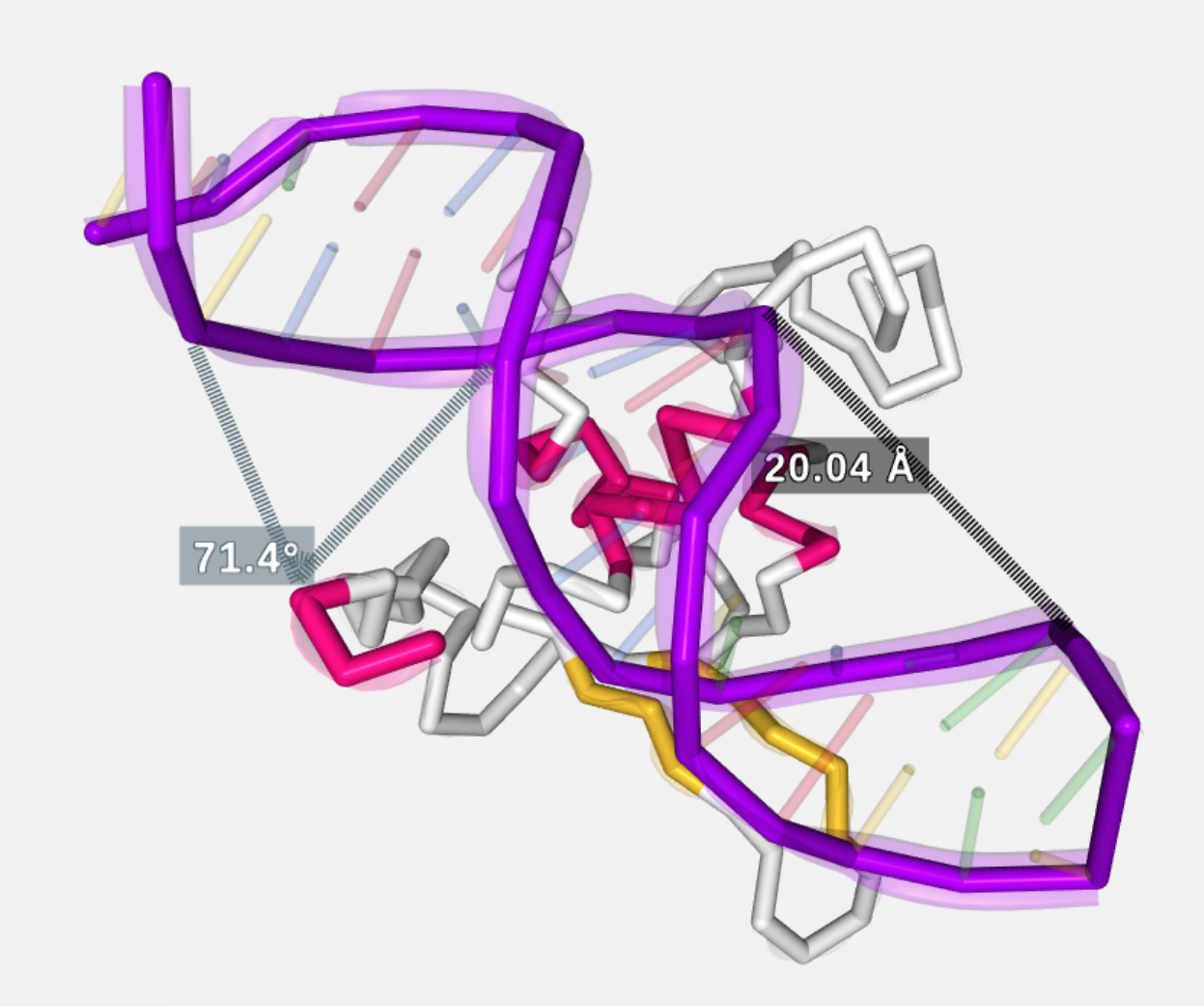

After **selecting** and **clicking** the **Apply superposition button**, both structures will be superposed (in the given example, they have been superposed on the A chain):

Note that this button **only appears in case more than one structure** has been uploaded.

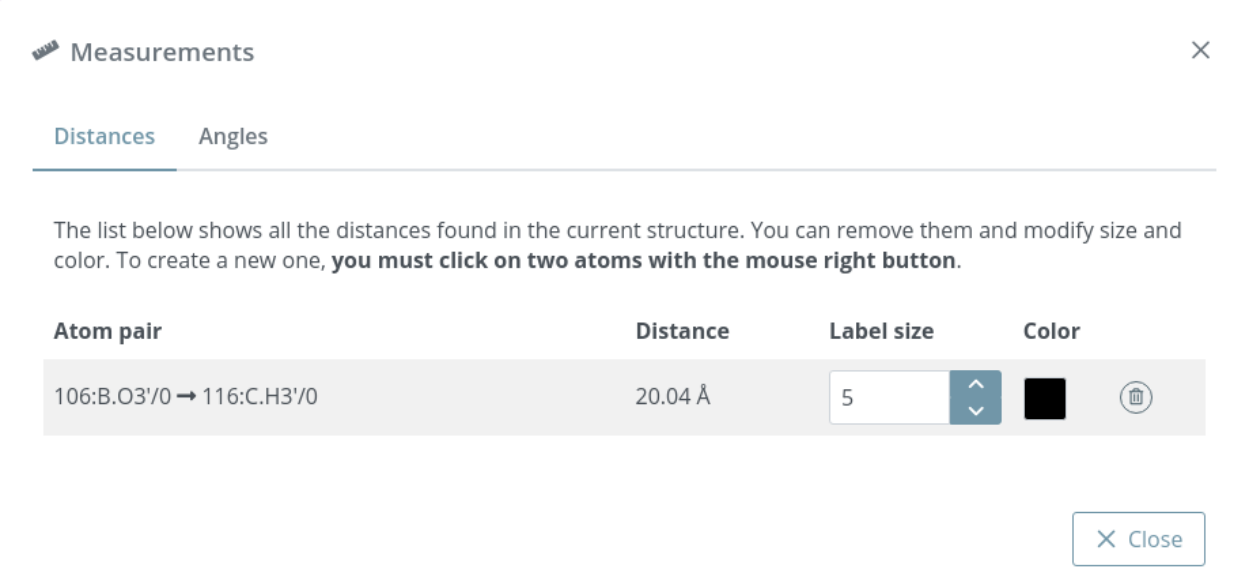
### Measurements

Clicking this button **opens a modal dialog** to edit the **distances and angles** created by users in the stage. For remembering how to draw them, please go back to the ***Mouse click actions section***.

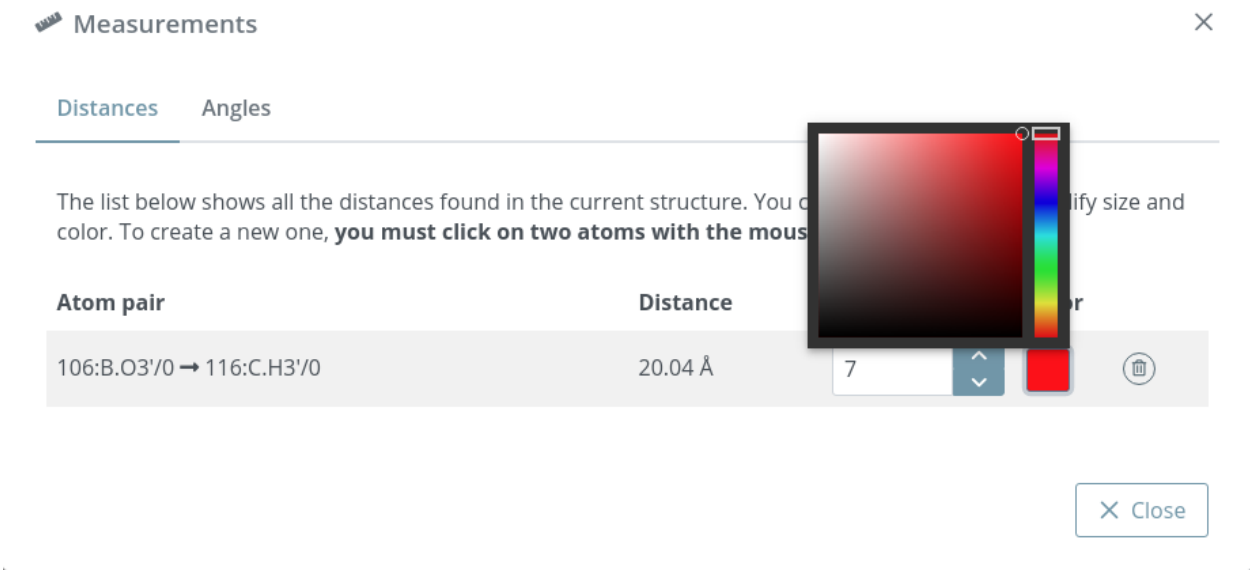
**Measurements** with size and color **by default**:




**Distances** before editing size and color:

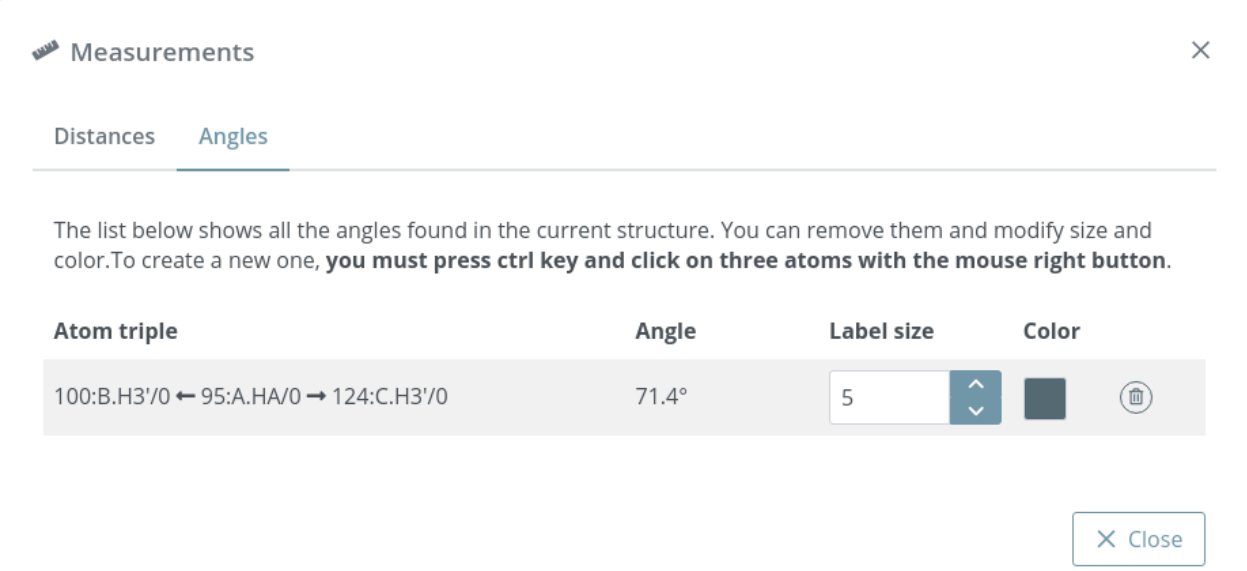



**Distances** after editing size and color:

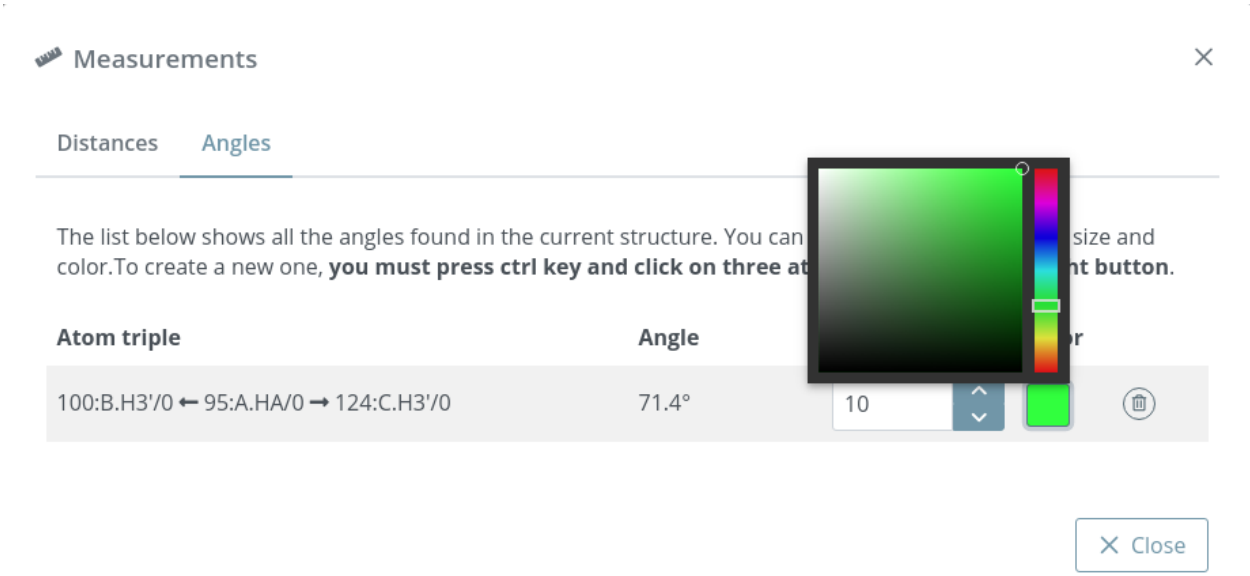



If **only a distance** is needed (**without label**), please set **0 as Label size**.

**Angles** before editing size and color:

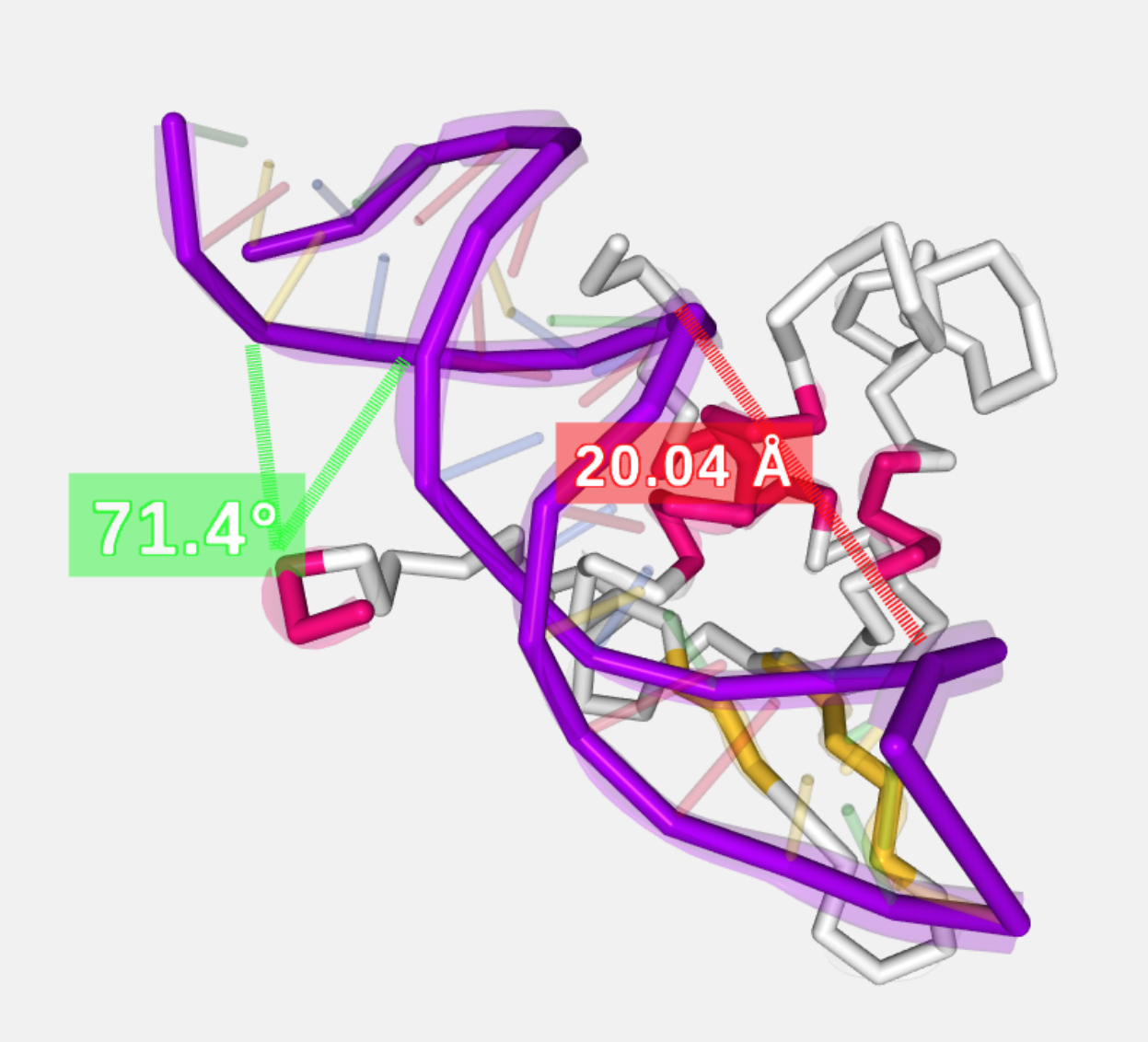



**Angles** after editing size and color:




If **only the lines** are needed (**without label**), please set **0 as Label size**.

**Measurements** after **size and color edition**:




In the current version, distances between different structures dont work.

### Navigation mode

Sometimes it's difficult to move the stage without **accidentally selecting** a residue from it. For the sake of avoiding these problems, a **Navigation mode button** is provided. Clicking it **disables** the **selection** of molecules and the creation of **distances** and **angles**.

Once the button is clicked, it turns out its background to white and the compass icon starts **spinning**:

During the navigation mode, the mouse pointer changes its aspect to a grabbing hand:

The **Navigation mode** will be enabled until users **click the button again**.

### Camera type

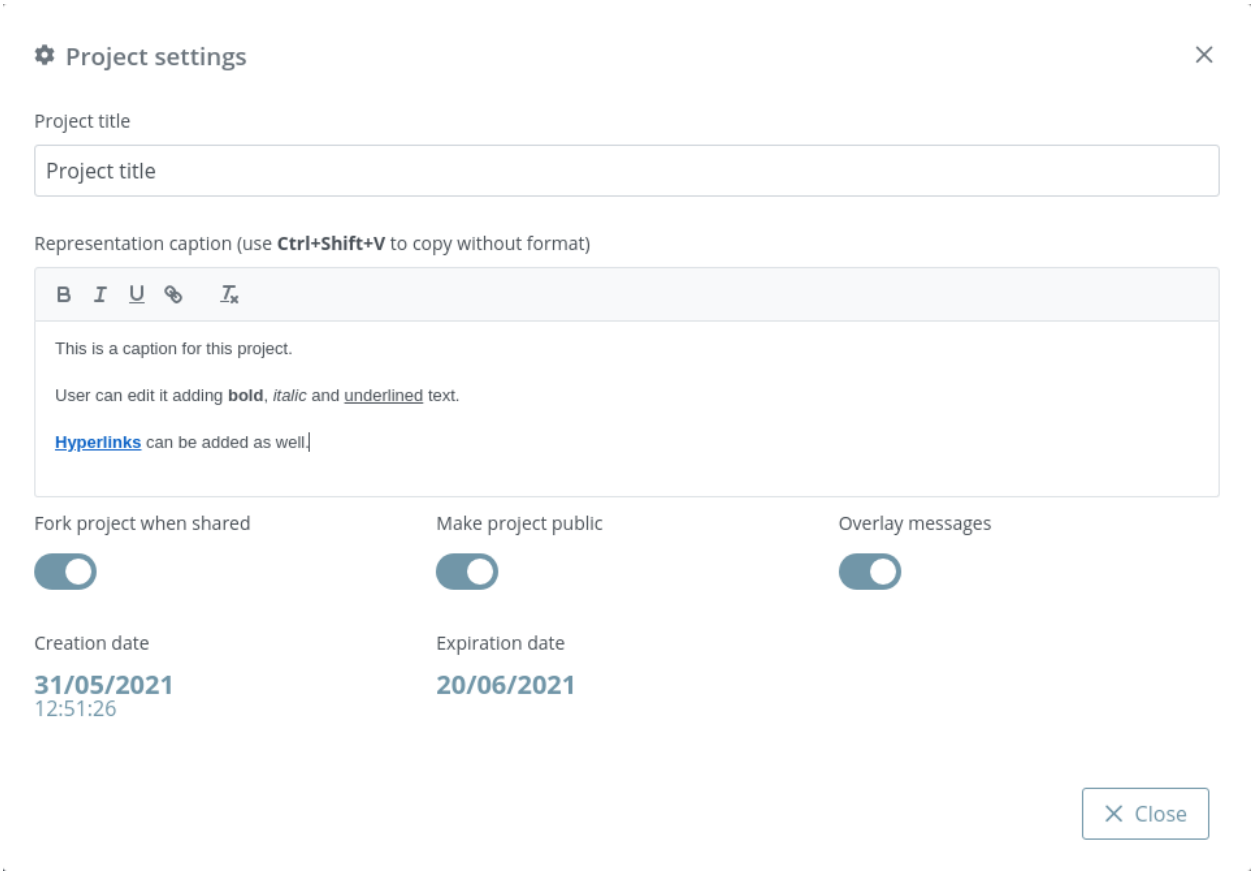
Switches camera type between **orthographic** and **perspective**.

### Help

Link to this same Read the Docs.

### Project settings

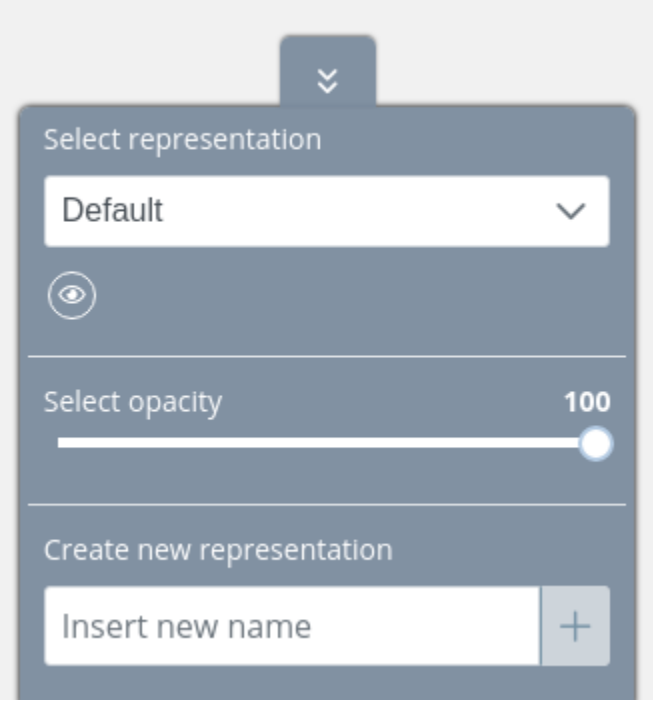
Clicking this button **opens a modal dialog** to edit the **project settings**:



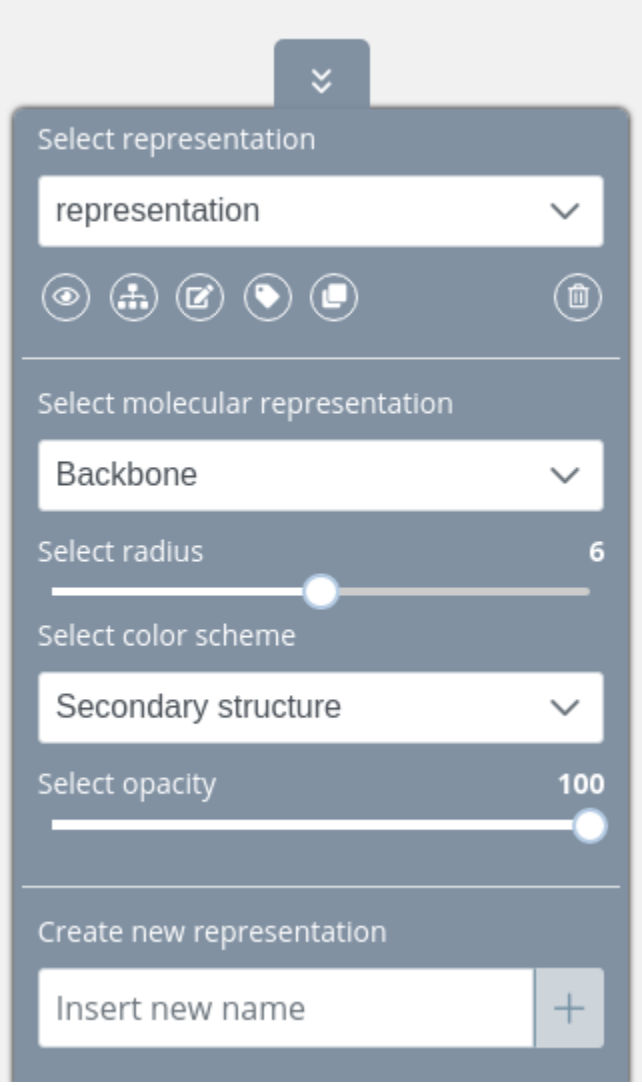

- **Project title:** title of the project. If this field is empty, neither title nor caption will be shown in the project once shared
- **Representation caption:** representative information of the project such as description, author(s), links and so on. Beware of copying **formatted text**, it can give problems. It's strongly reccomended to paste text without formatting (via **Ctrl+Shift+V** or **Tx** button).
- **Fork project when shared:** if enabled, the project will be able to be forked once shared. That means that anyone can make an editable copy of the project.
- **Make project public:** if enabled, the project will be shown in the home page list along with the rest of latest public projects.
- **Overlay messages:** there are notification messages for almost each action in the application. With this button they can be enabled / disabled. Note that although this option is enabled, the expiration notification will still appear as well as some error messages and the navigation mode prompt.
- **Creation date:** date of creation of the project.
- **Expiration date:** date of expiration of the project. This date will disappear once the project is shared for the first time, since then the project will be persistent.

### 1.3.3 Representations

The **Representations** panel is at the bottom left of the stage and is used for changing the properties of the representation. Initially, there is a **Default** representation that only allows to change the opacity and hide or show it:



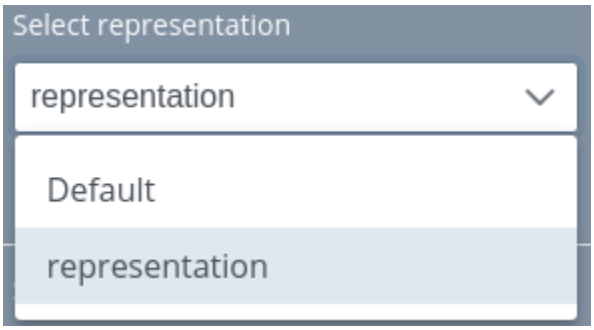

Once users create a new representation, there are **all the properties** available:




### Representation actions

Below there is a description of **all the actions** that can be performed in this panel.

### Select representation



In this dropdown menu, users can switch **between all the representations** of the project.

### Edit representations

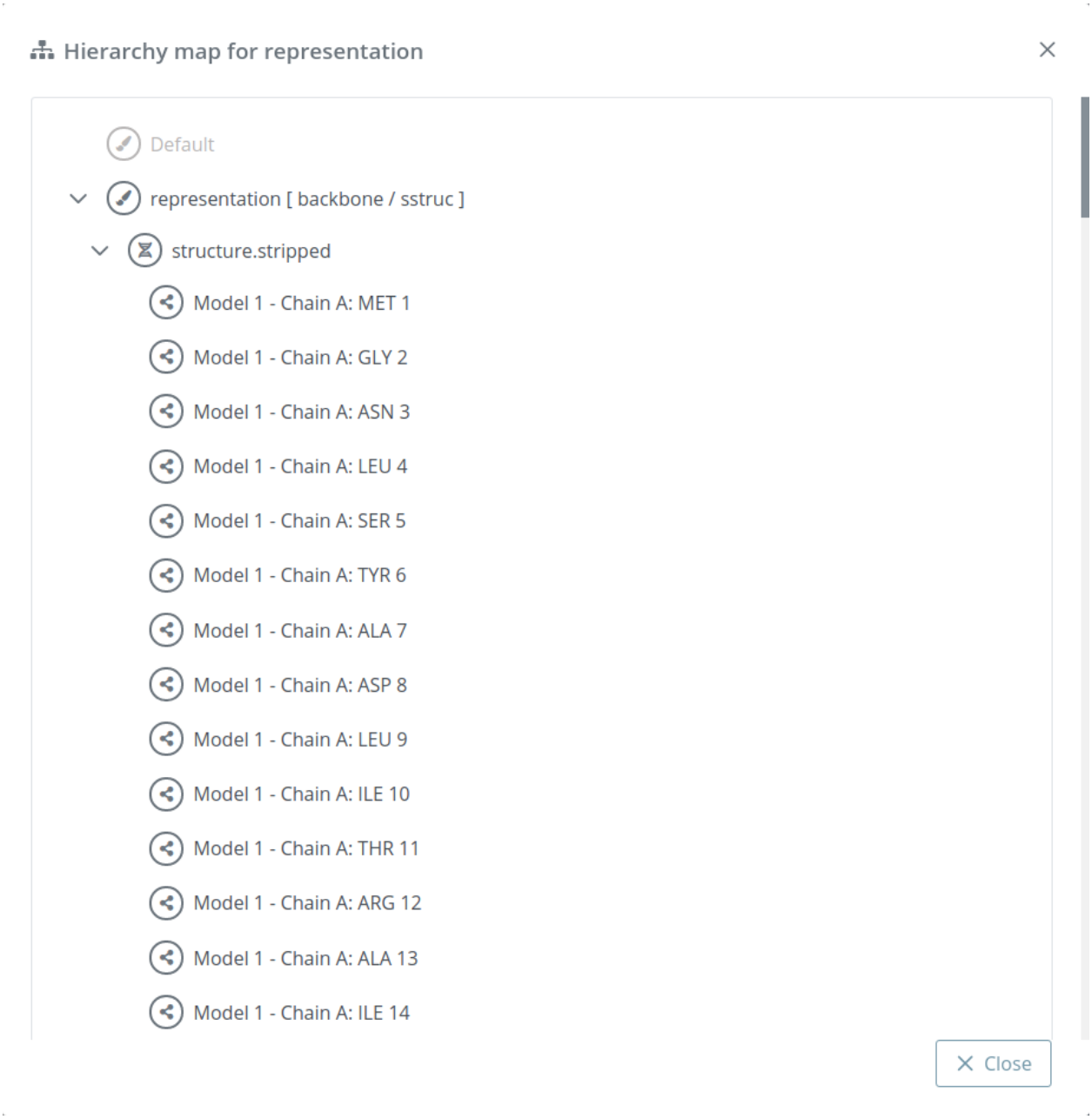
Below the select dropdown menu there is a tiny menu for making **some actions** over the **representations**.

### Hide / show

**Hides** or **show** the **current representation** selected on the dropdown above.

### Hierarchy map

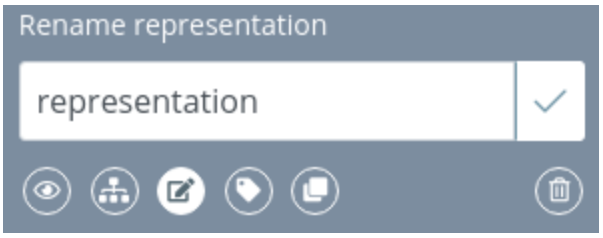
Shows a **modal dialog** with all the molecules selected in **each representation**:




In the default representation this feature is disabled.

### Edit representation name

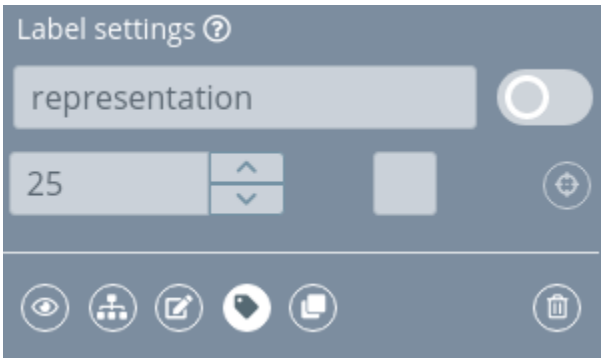
Allows to **rename** the **current representation**:




In the default representation this feature is disabled.

### Edit label

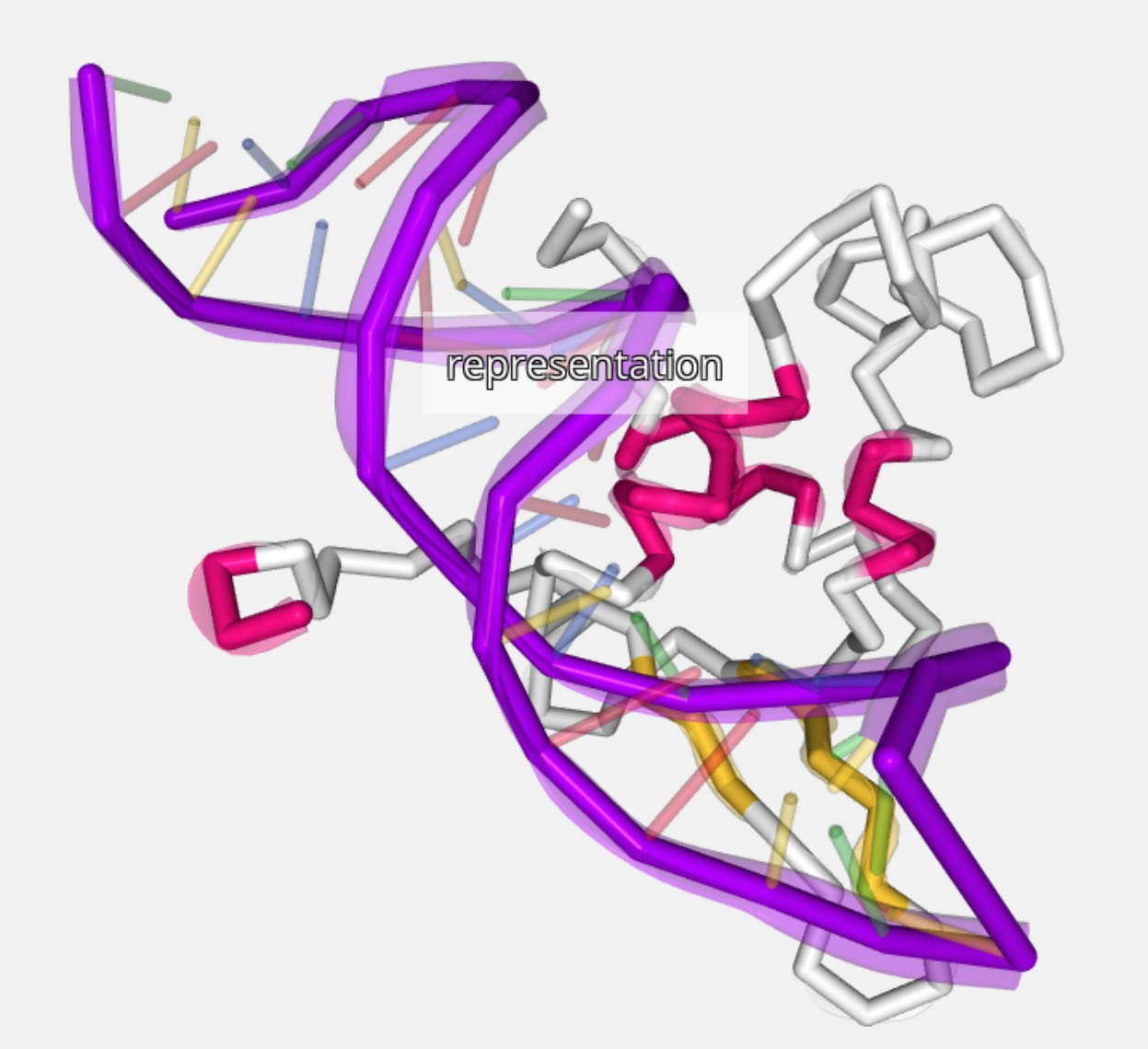
Clicking this button opens the **label edition area**:



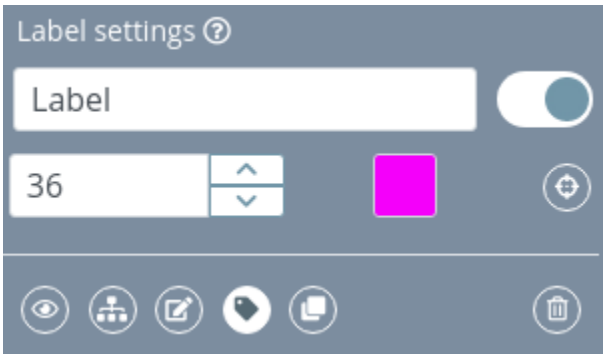

**By default**, all the actions are **disabled** until the label is **enabled** clicking the switch button.

Once the label is enabled, it will appear in the **stage** with generic size and color and centered in the current selection. Note that the **default position** varies depending on the structure and the atoms selected. Sometimes the label can be out of the selection or in a **non-representative position**. In order to fix that, a **place label button** is provided (explained below).

**Generic label** aspect:




In the **label edition area**, users can modify the label **name**, the label **size**, the label **background color** and the label **position**:



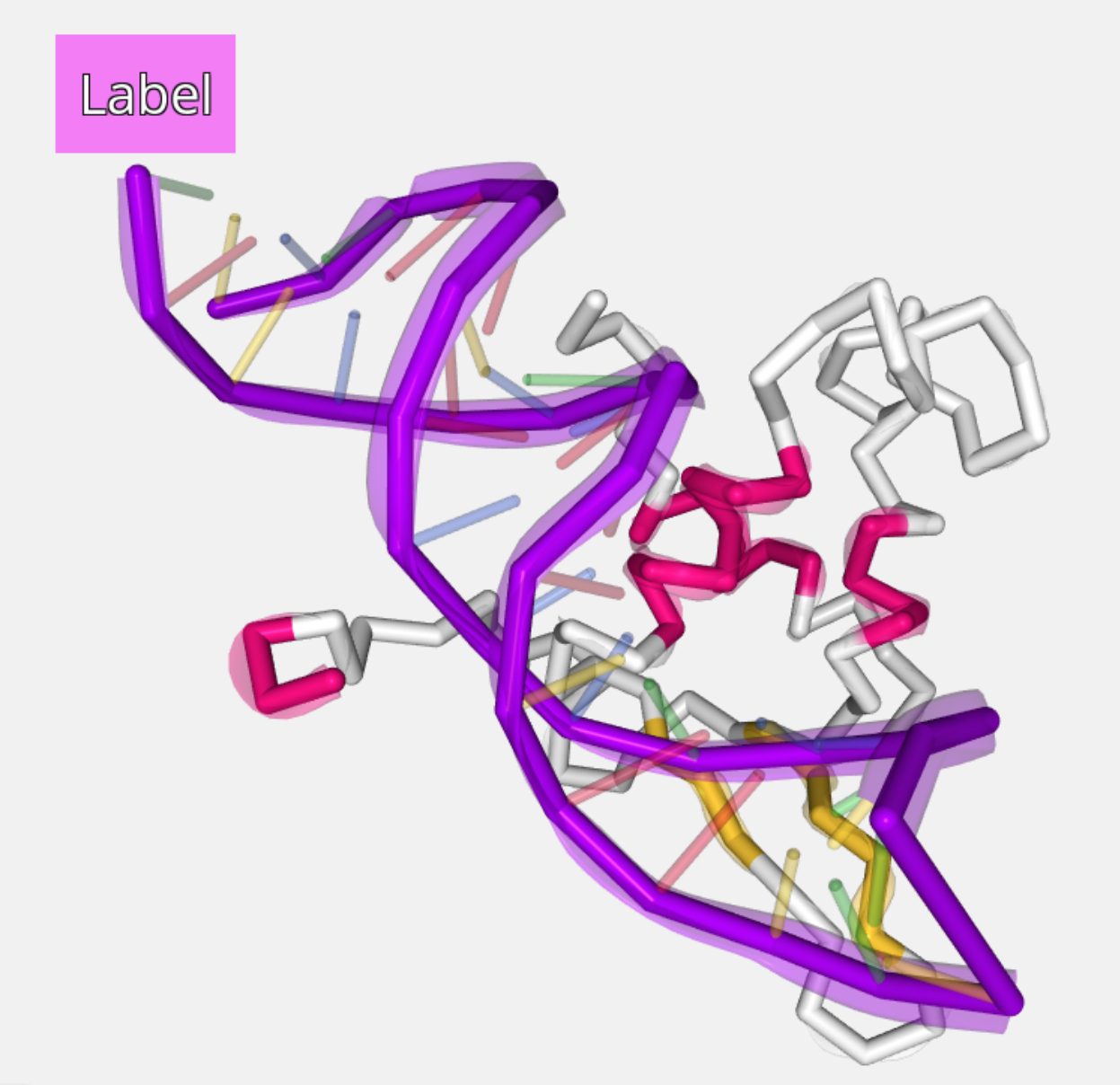

To **modify the label position**, the place label button must be clicked:

Once the button is clicked, it turns out its background to white and the crosshair icon starts **spinning**:

During this label position mode is active, the mouse pointer changes its aspect to a **crosshair**:

Note that during this mode, the **selection** of molecules and the creation of **distances** and **angles** are disabled. Picking a molecule only will translate the label to its position.

**Edited label** aspect:




In the default representation this feature is disabled.

### Clone representation

Clicking this button will **duplicate the current representation** with the same features and selection.

In the default representation this feature is disabled.

### Remove

**Removes** the **current representation and all the selections** linked to it. This button must be clicked **twice** in order to ensure that it has not been clicked by mistake.

In the default representation this feature is disabled.

### Representation properties

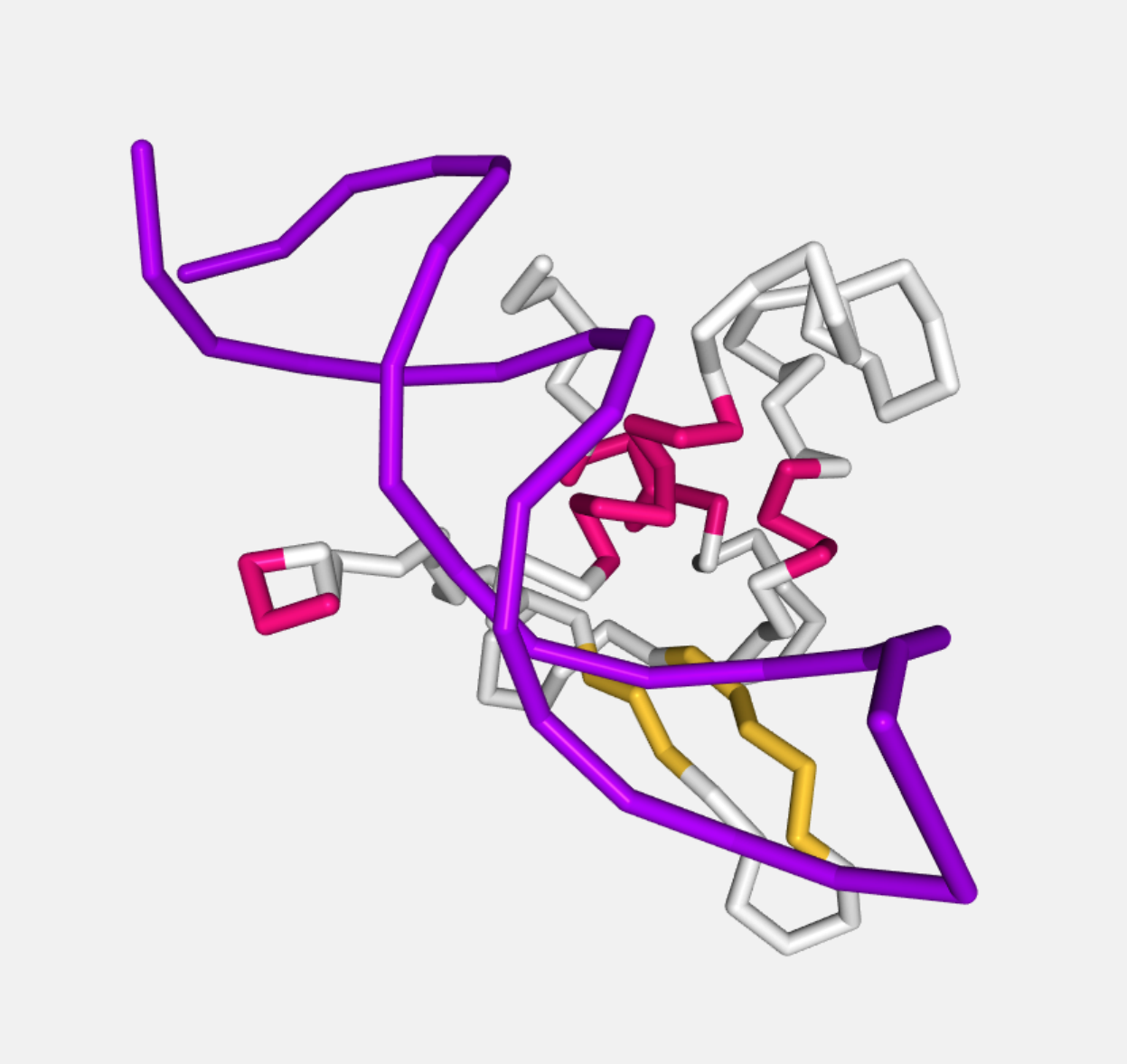
There are several properties that can be modified for each representation.

### Molecular representation


Each loaded **structure** can be displayed using a variety of **molecular representations**:

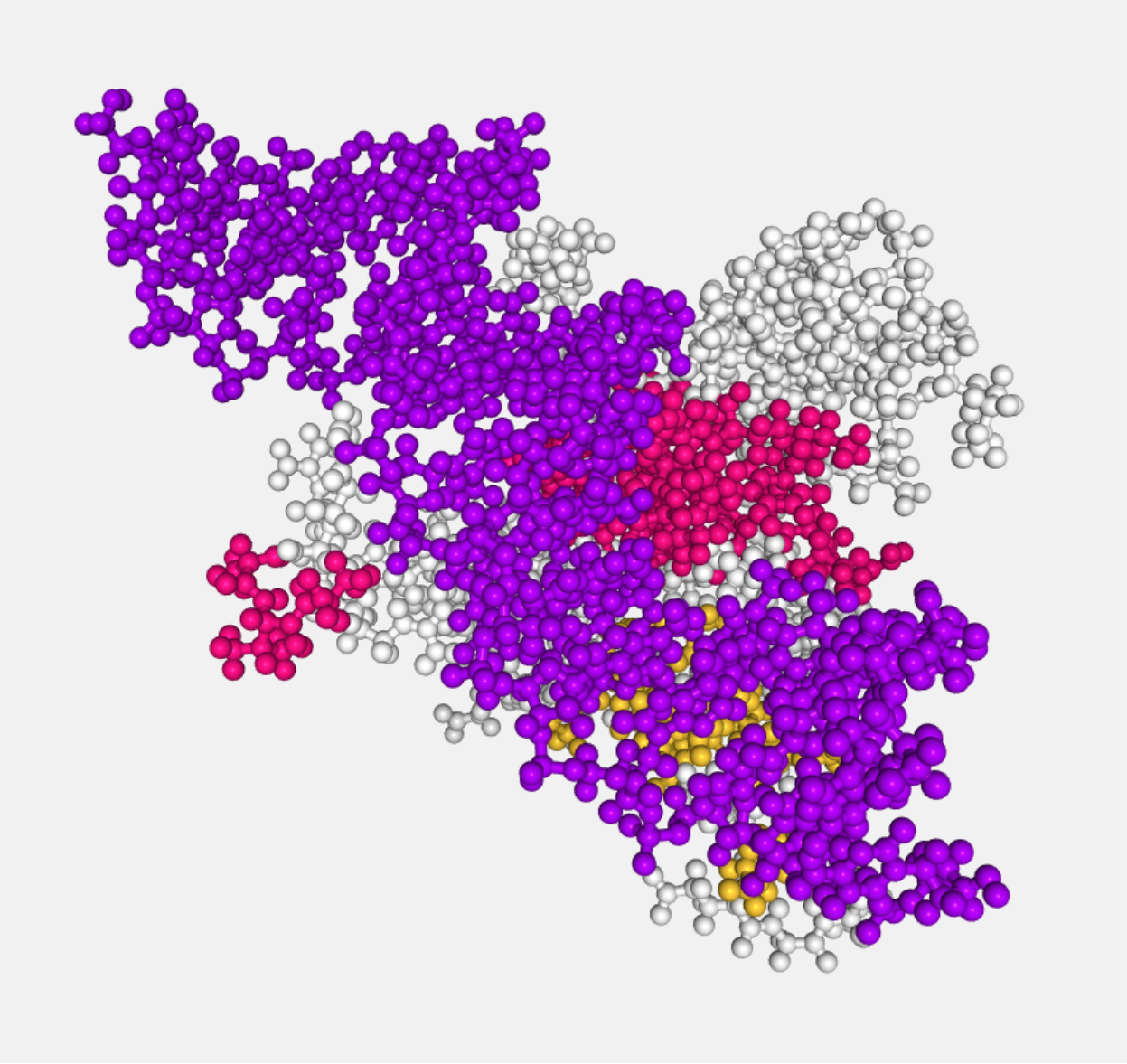
### Backbone

Cylinders connect successive residues of unbroken chains by their main backbone atoms, which are **.CA** atoms in case of proteins and **C4'/C3'** atoms for RNA/DNA, respectively. The main backbone atoms are displayed as spheres.



### Ball and stick

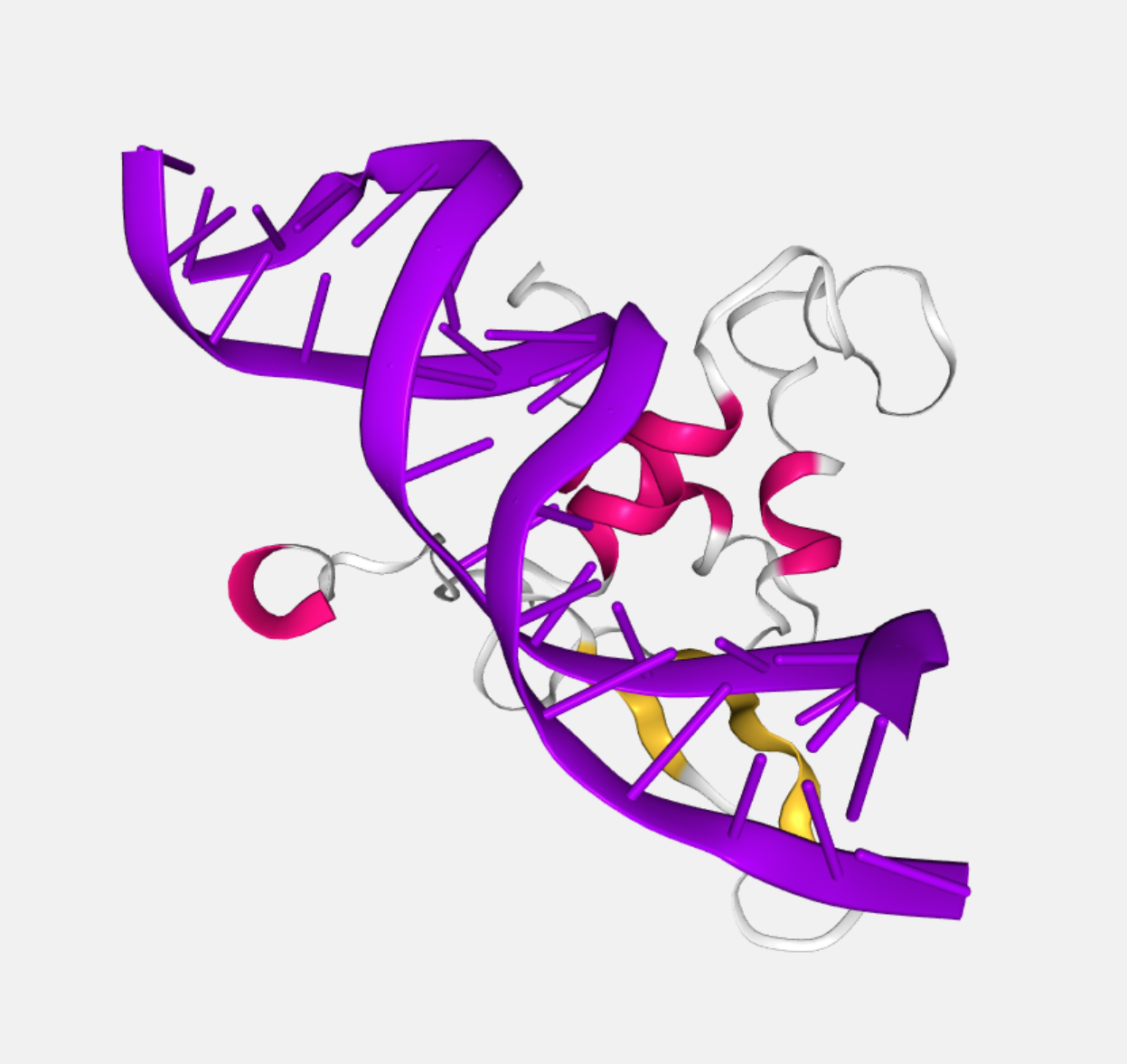
Atoms are displayed as spheres (balls) and bonds as cylinders (sticks).



### Cartoon

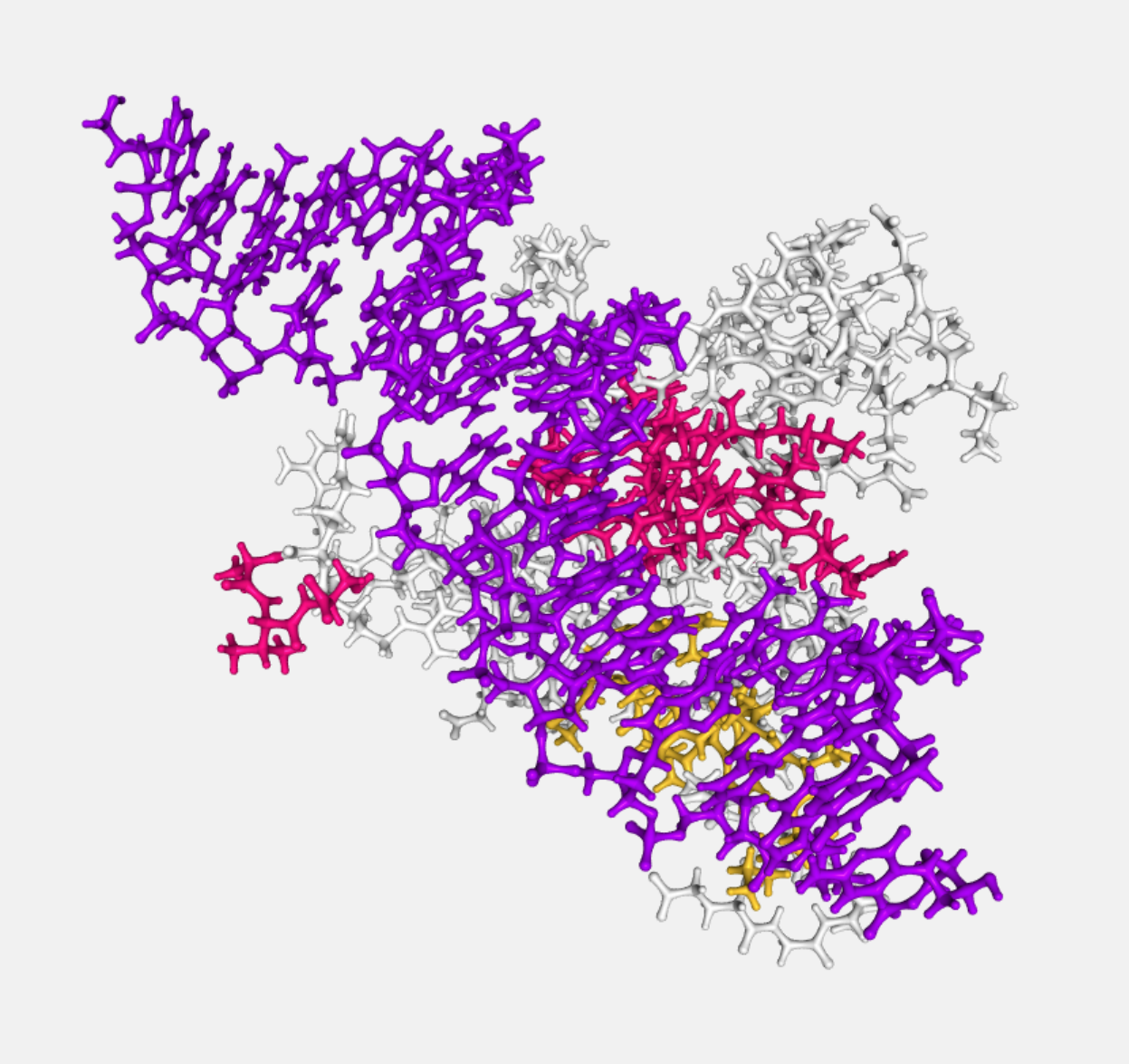
The main backbone atoms (see backbone) of successive residues in unbroken chains are connected by a smooth trace. The trace is expanded perpendicular to its tangent with an elliptical cross-section. The major axis points from **.CA** in the direction of the .O in case of proteins and from the **C1'/C3'** to **C2'/O4'** for RNA/DNA, respectively.

If RNA/DNA an **additional base representation** is added: simplified display of RNA/DNA nucleotides, best used in conjunction with a cartoon representation. Here, a stick is drawn connecting the sugar backbone with a nitrogen in the base (**.N1** in case of adenine or guanine, **.N3** in case of thymine or cytosine).



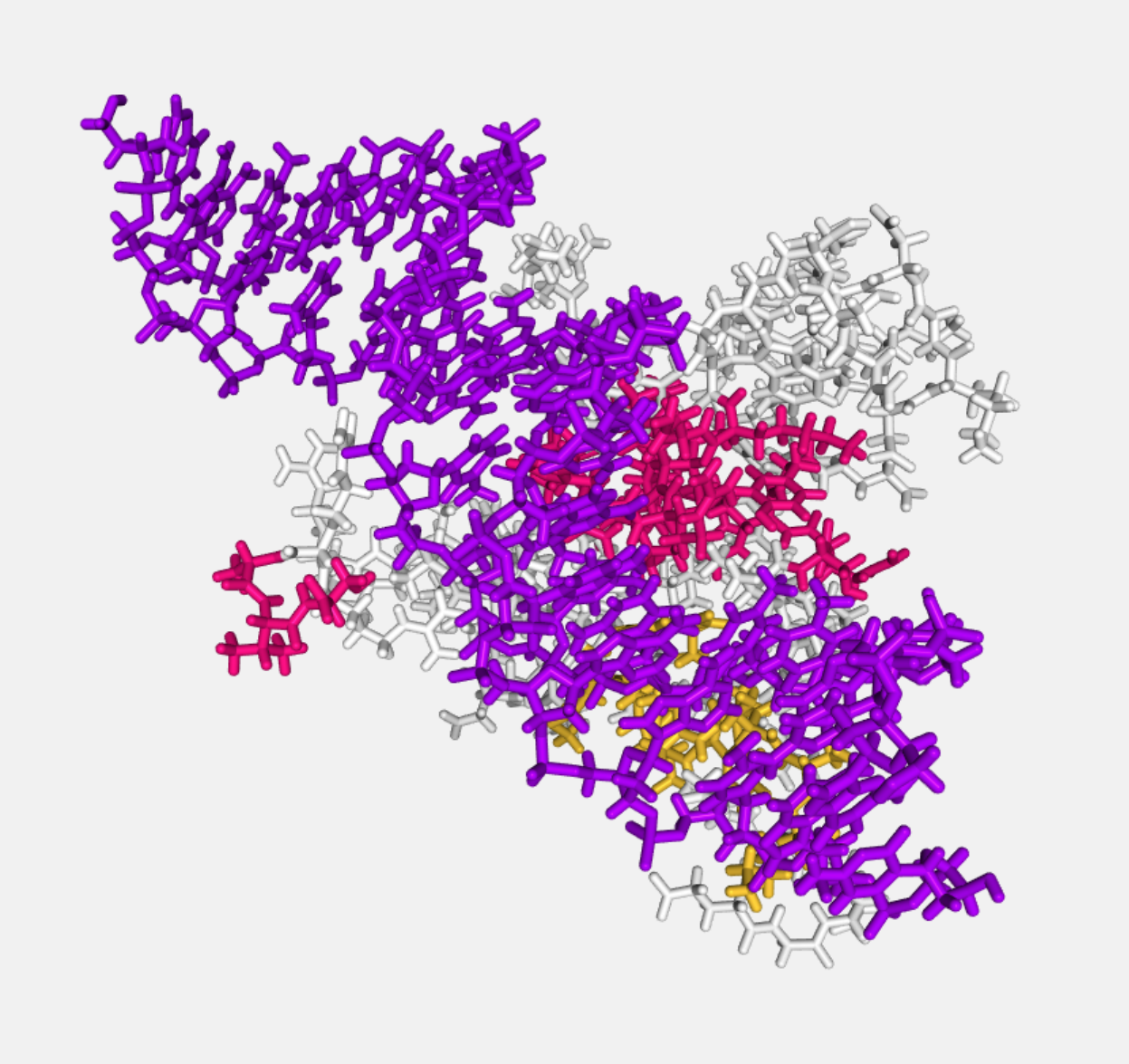
### Hyperball

A derivate of the ***ball+stick*** representation (pioneered by HyperBalls project) in which atoms are smoothly connected by an elliptic hyperboloid.



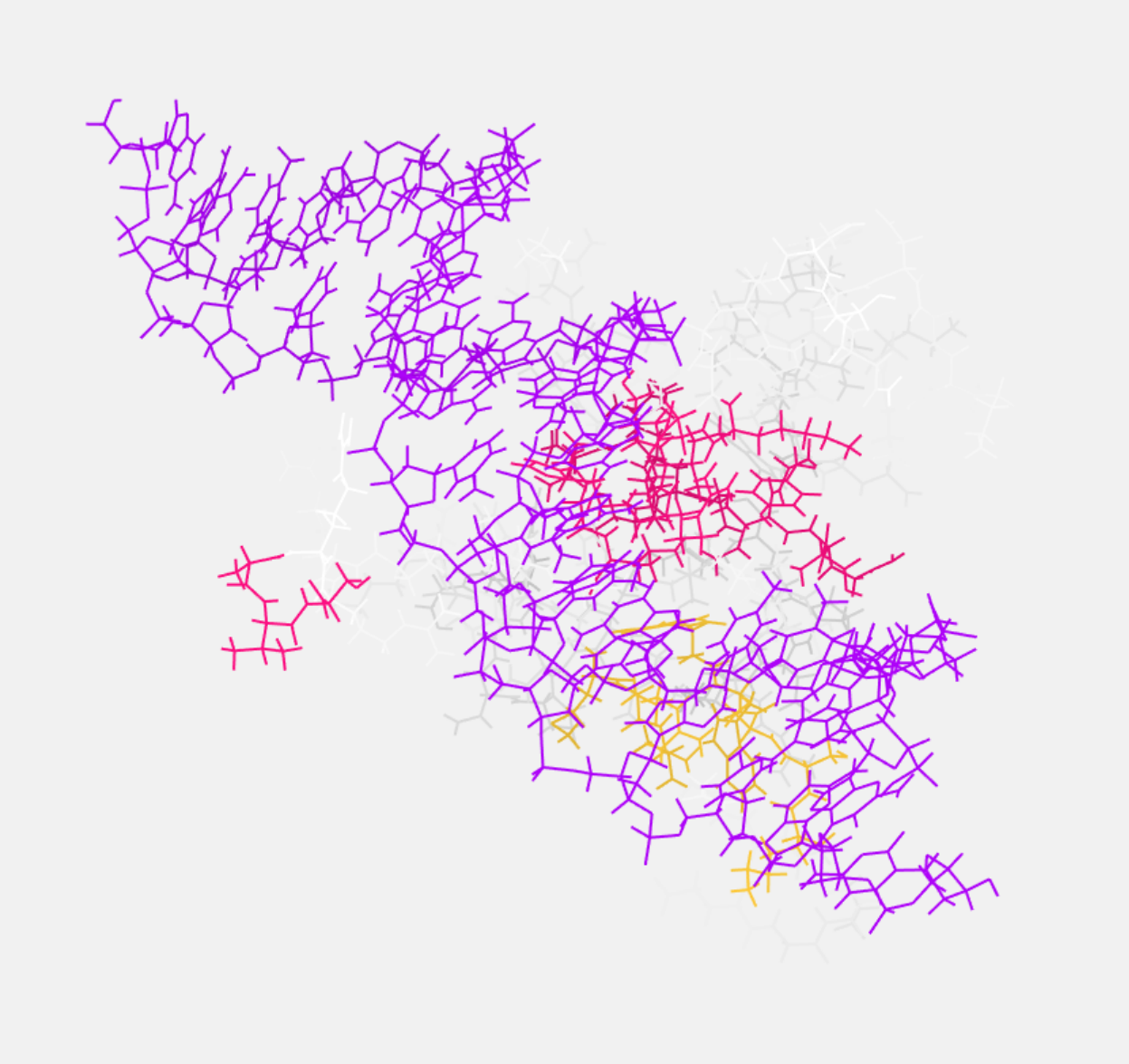
### Licorice

A variant of the ***ball+stick*** representation where balls and sticks have the same radius.



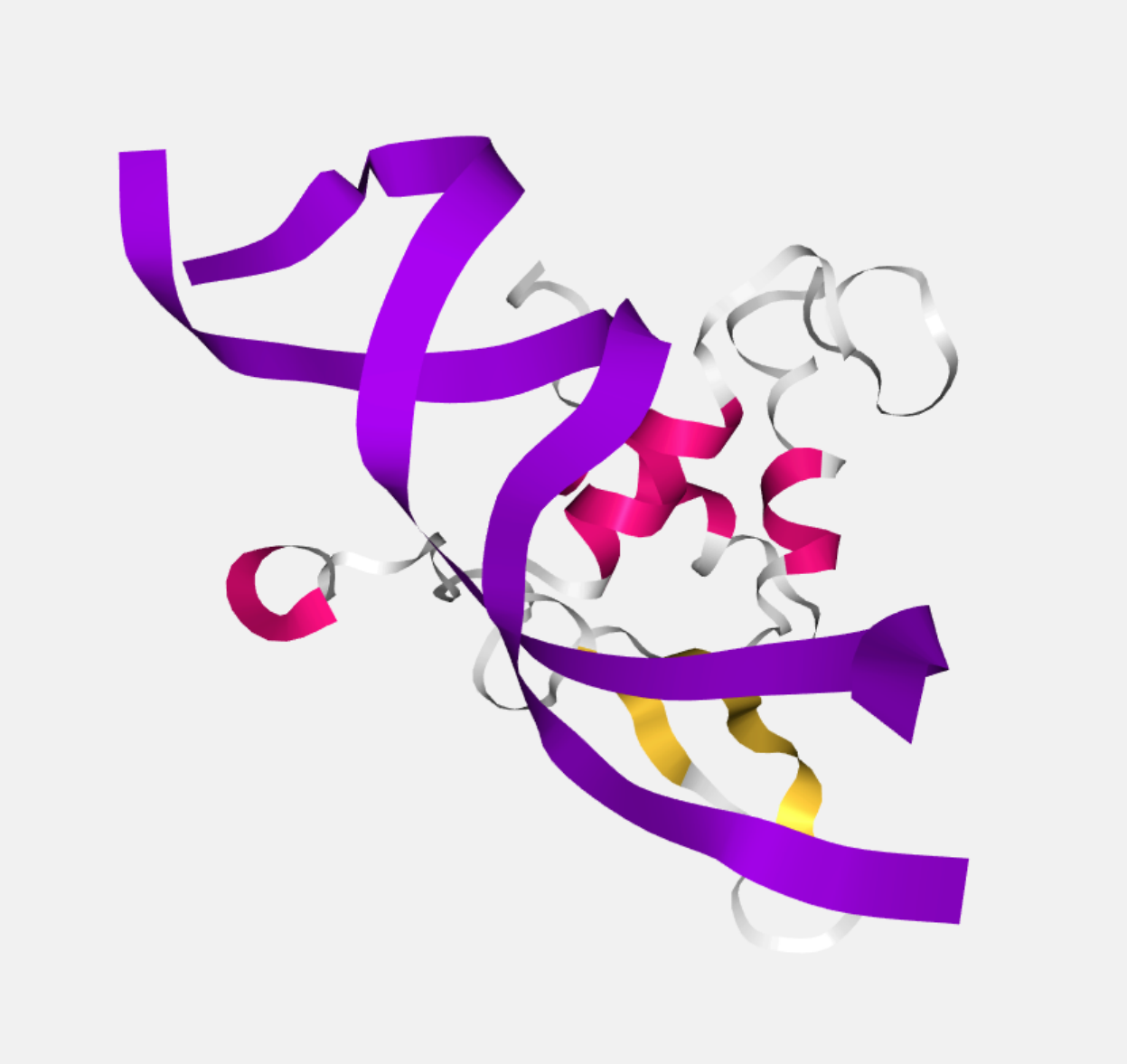
### Line

Bonds are displayed by a flat, unshaded line.



### Ribbon

A thin ribbon is displayed along the main backbone trace.

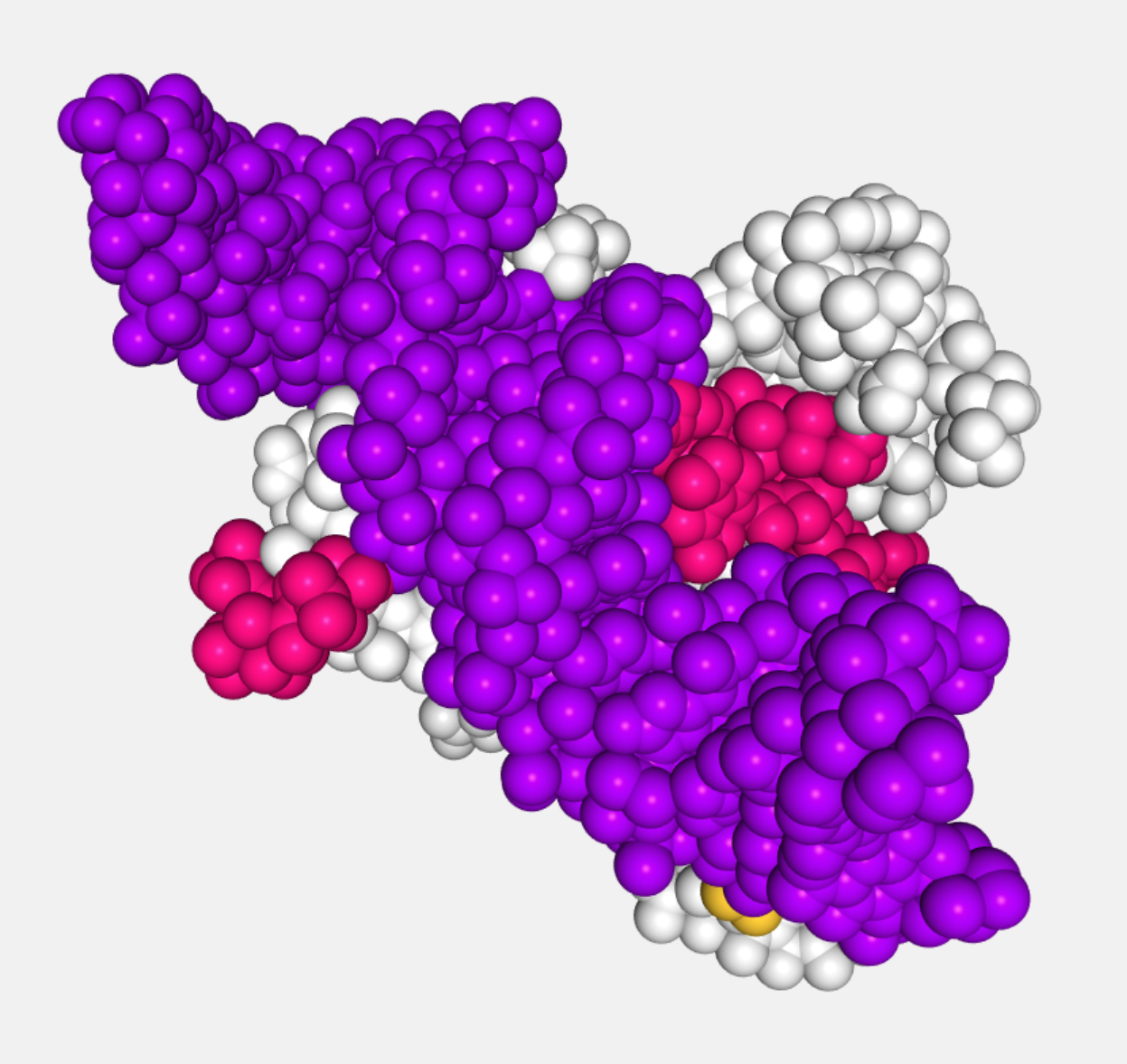


### Rope

A rope-like protein fold abstraction well suited for coarse-grained structures. In this representation a tube follows the center points of local axes. The result is similar to what is shown by the Bendix tool.

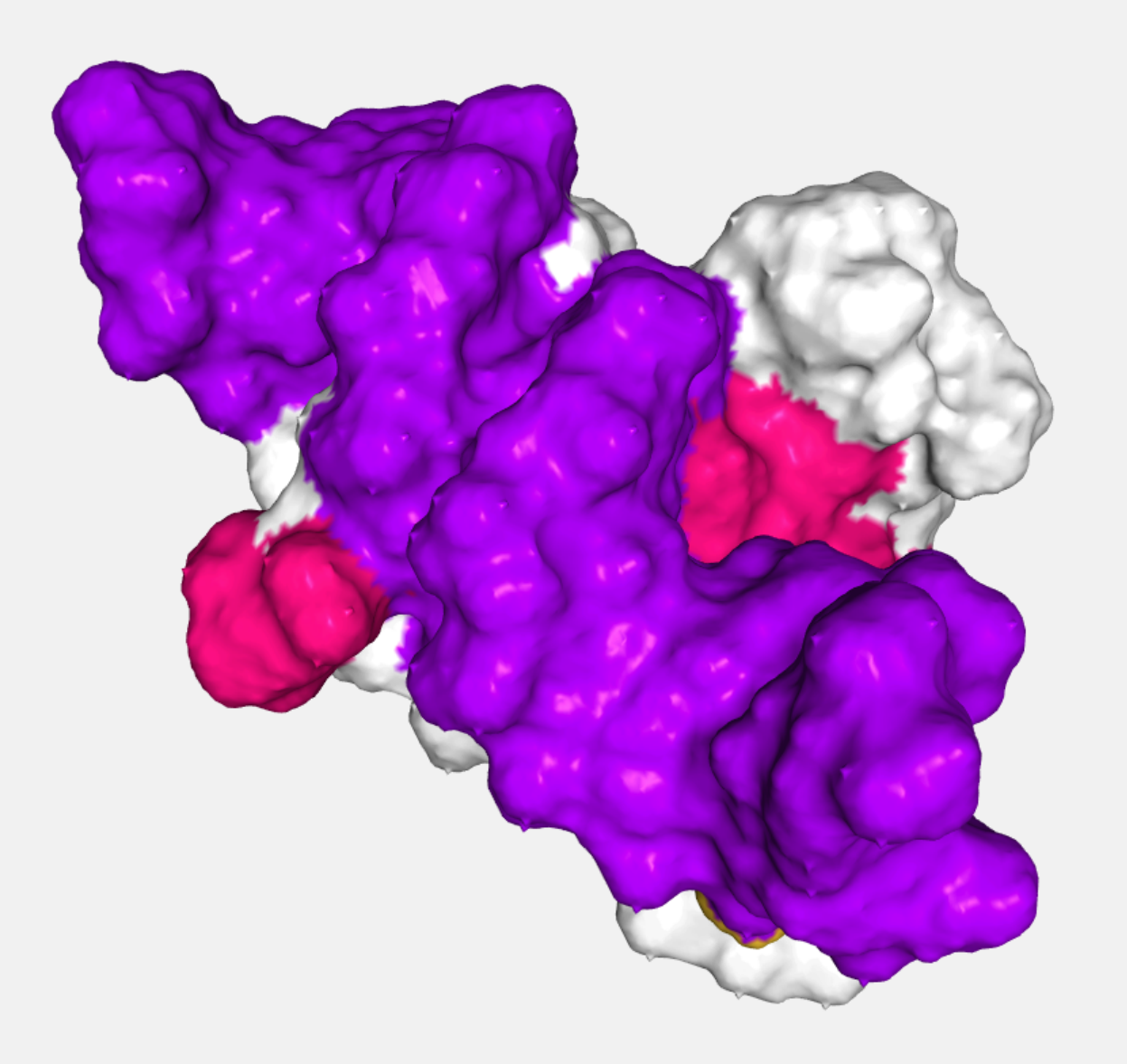
### Spacefill

Atoms are displayed as a set of space-filling spheres.



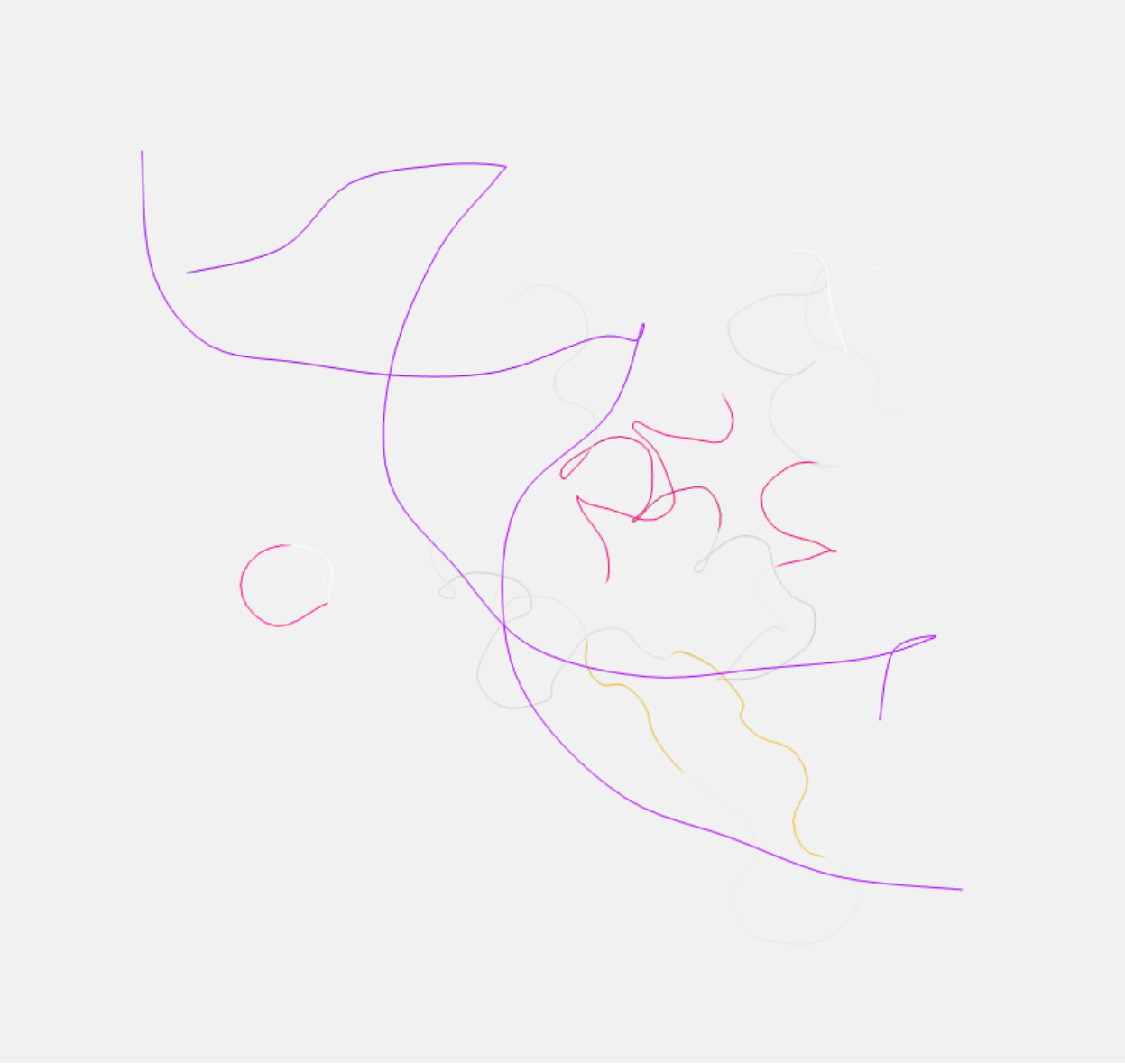
### Surface

Displays the molecular surface and its variants.



### Trace

A flat, unshaded line is displayed along the main backbone trace.



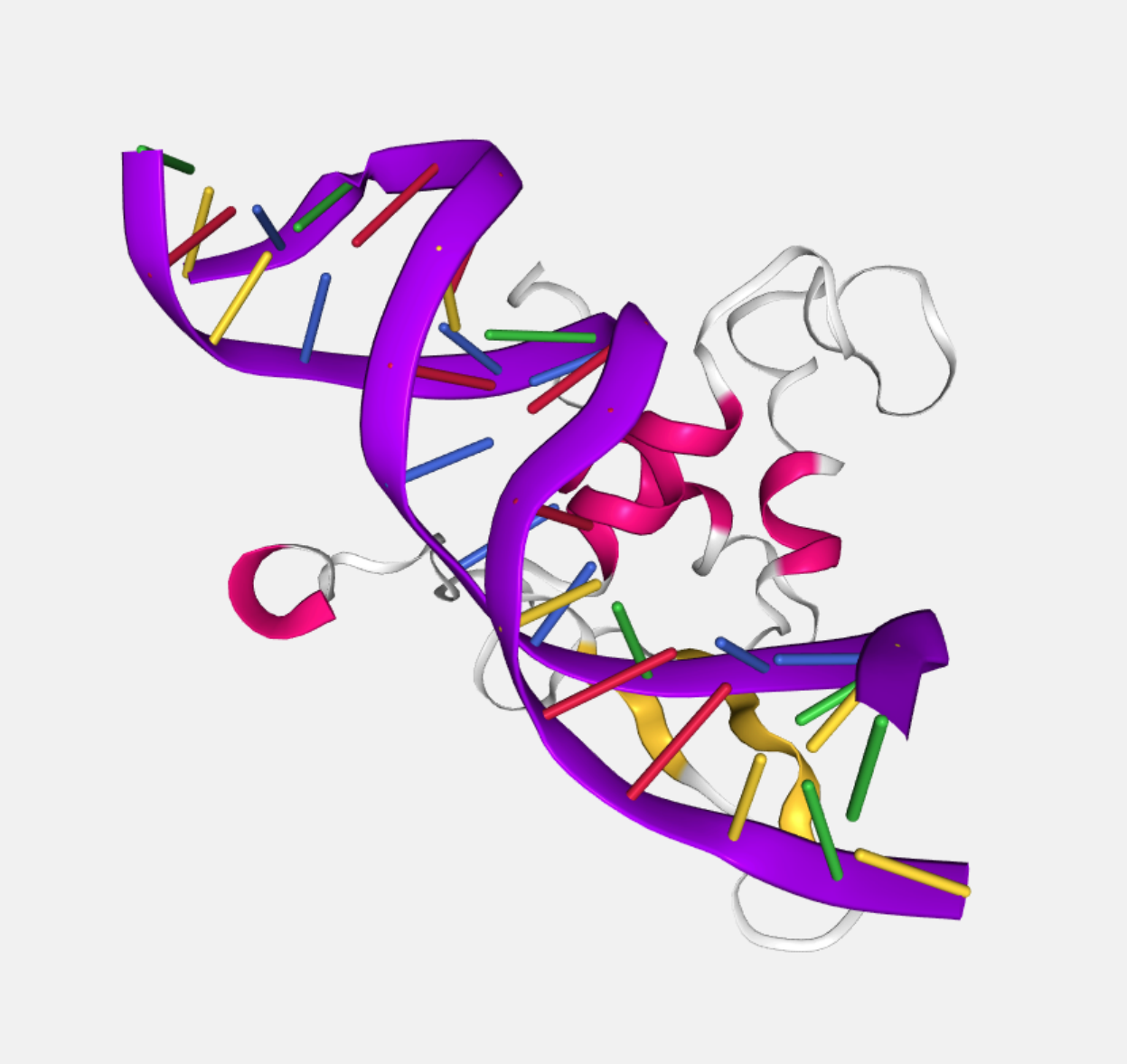
### Tube

Essentially like ***cartoon*** but with the aspectRatio fixed at a value of 1.0.

Due to a shortcoming of NGL Viewer, the **cartoon** and **ribbon** representations only can show **four or more** consecutive residues.

The **Default** representation can't be edited but represents the structure in a standard way:

- Backbone: **Cartoon** representation.
- NA bases (if present): **Base** representation.
- Heteroatoms: **Ball and stick** representation.
- Ions: **Ball and stick** representation.
- Waters: **Ball and stick** representation.



So take into account that if for example there is an heteroatom with **ATOM** instead of **HETATM** in the PDB file, it won't be shown in this **Default** representation.

### Radius


Through this slider, the **radius** can be modified in the next molecular representations:

- Backbone
- Ball and stick
- Cartoon
- Licorice

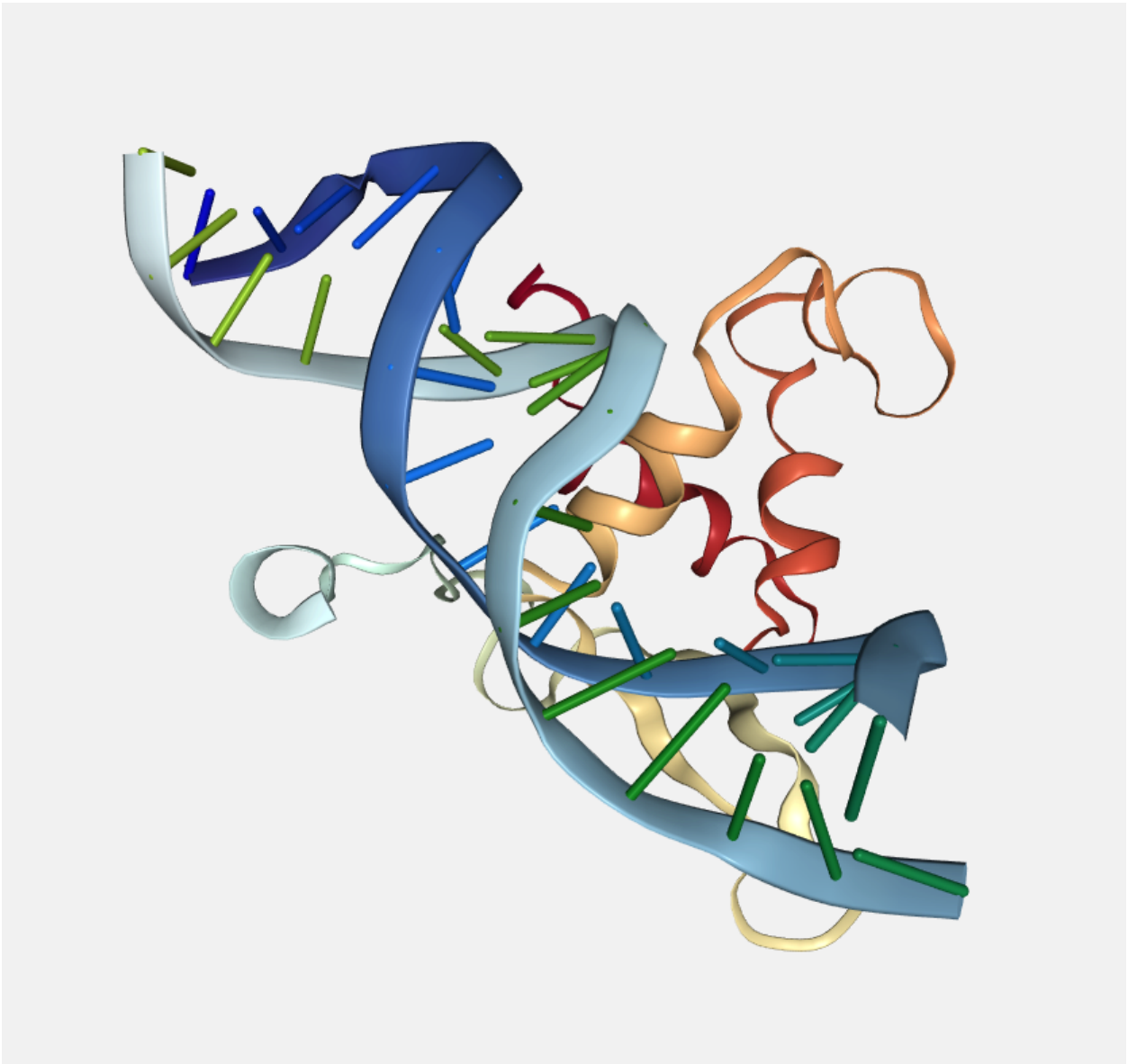
- Spacefill

### Color scheme


Each loaded structure can be displayed using a variety of **color schemes**:

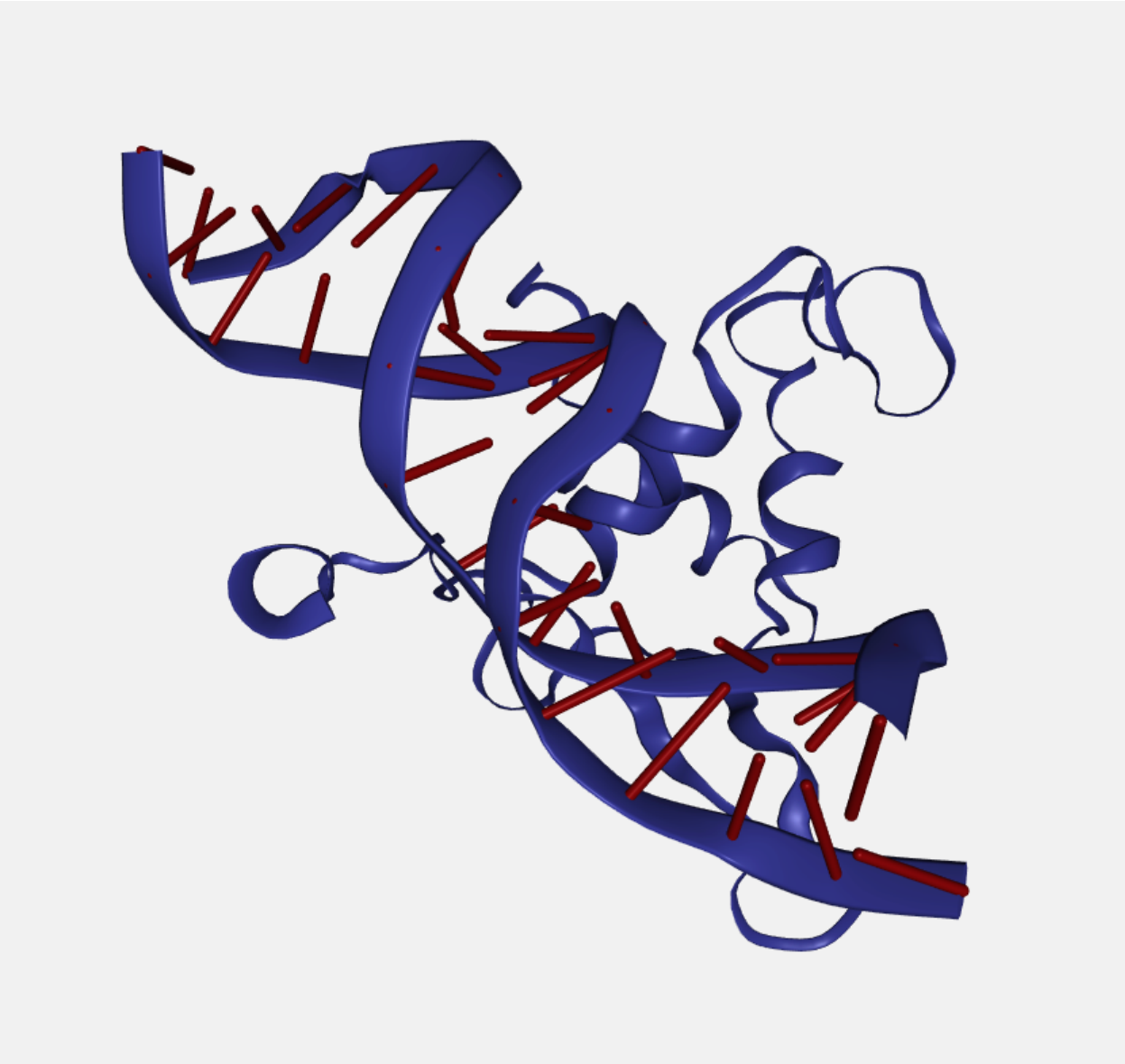
### Atom index

Color by atom index.



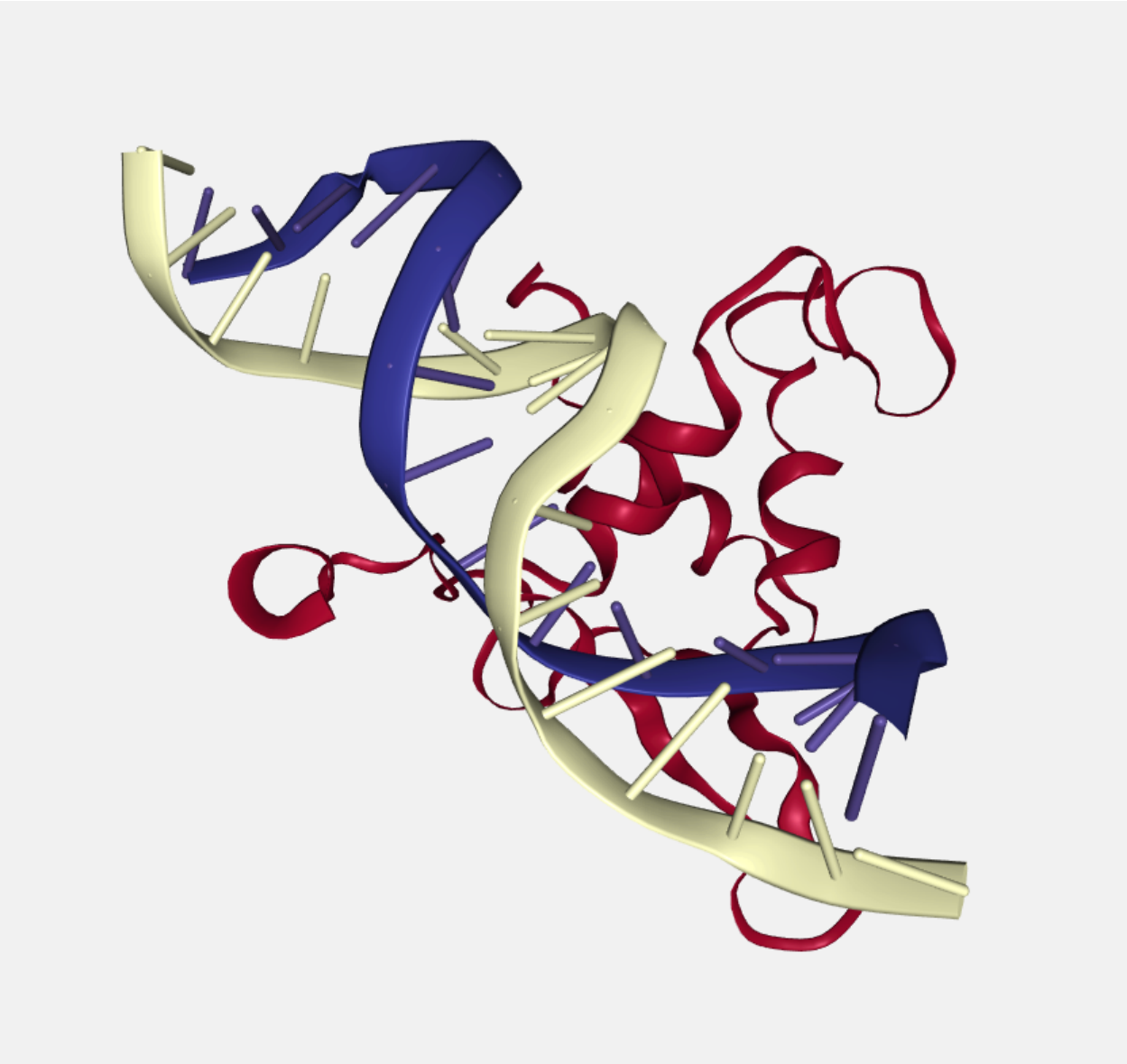
### B-factor

Color by b-factor.



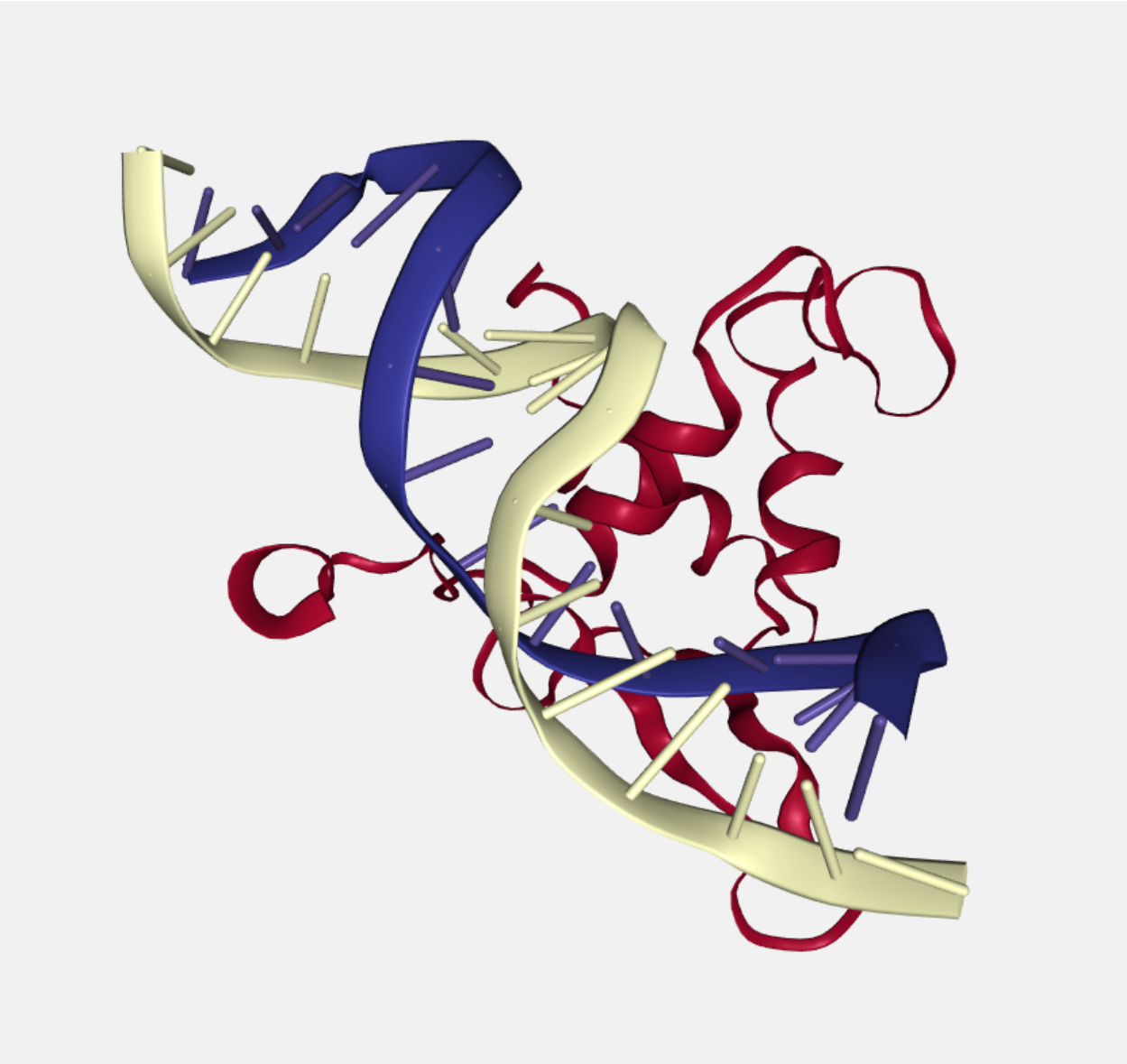
### Chain id

Color by chain id.



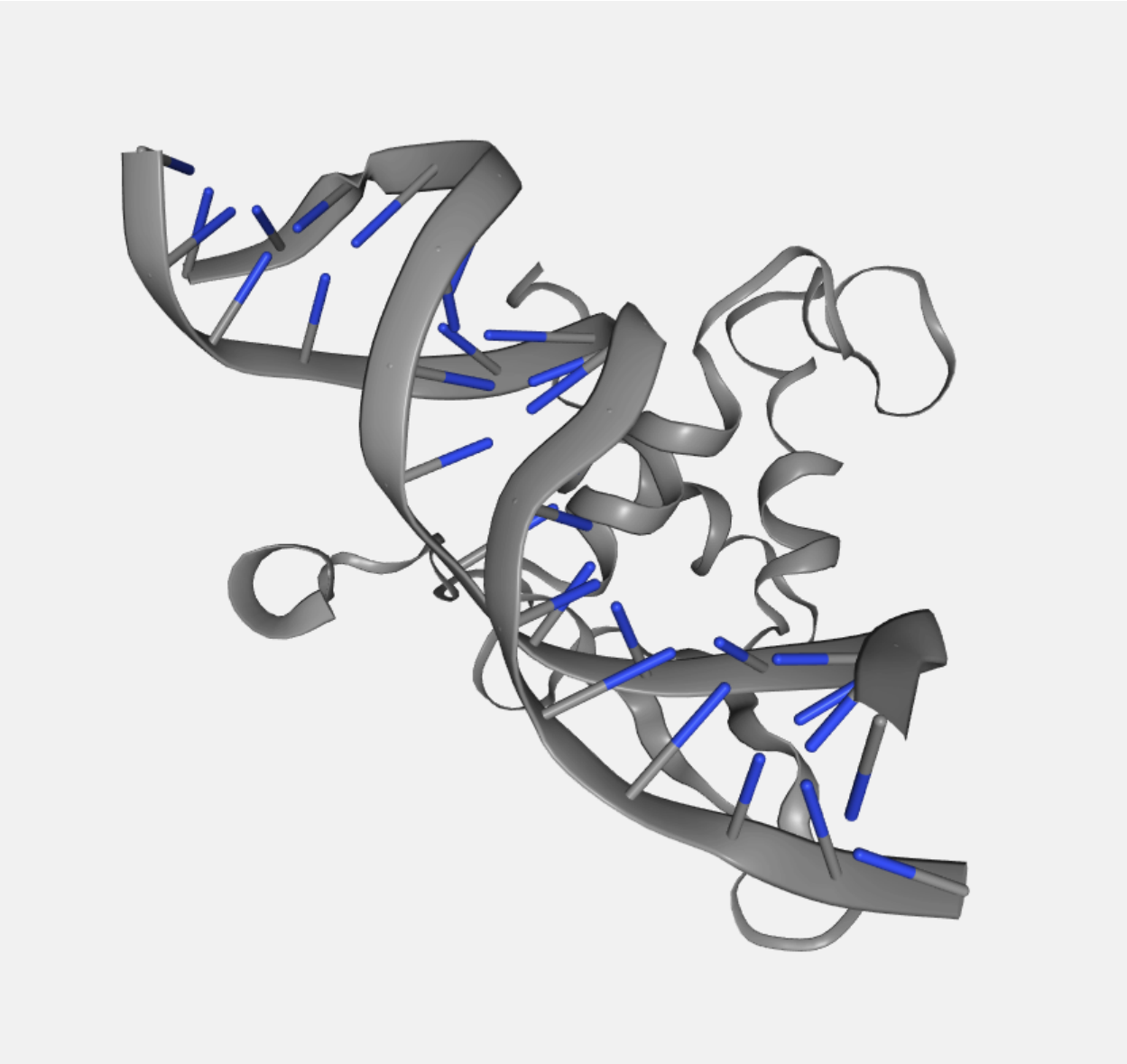
### Chain index

Color by chain index.



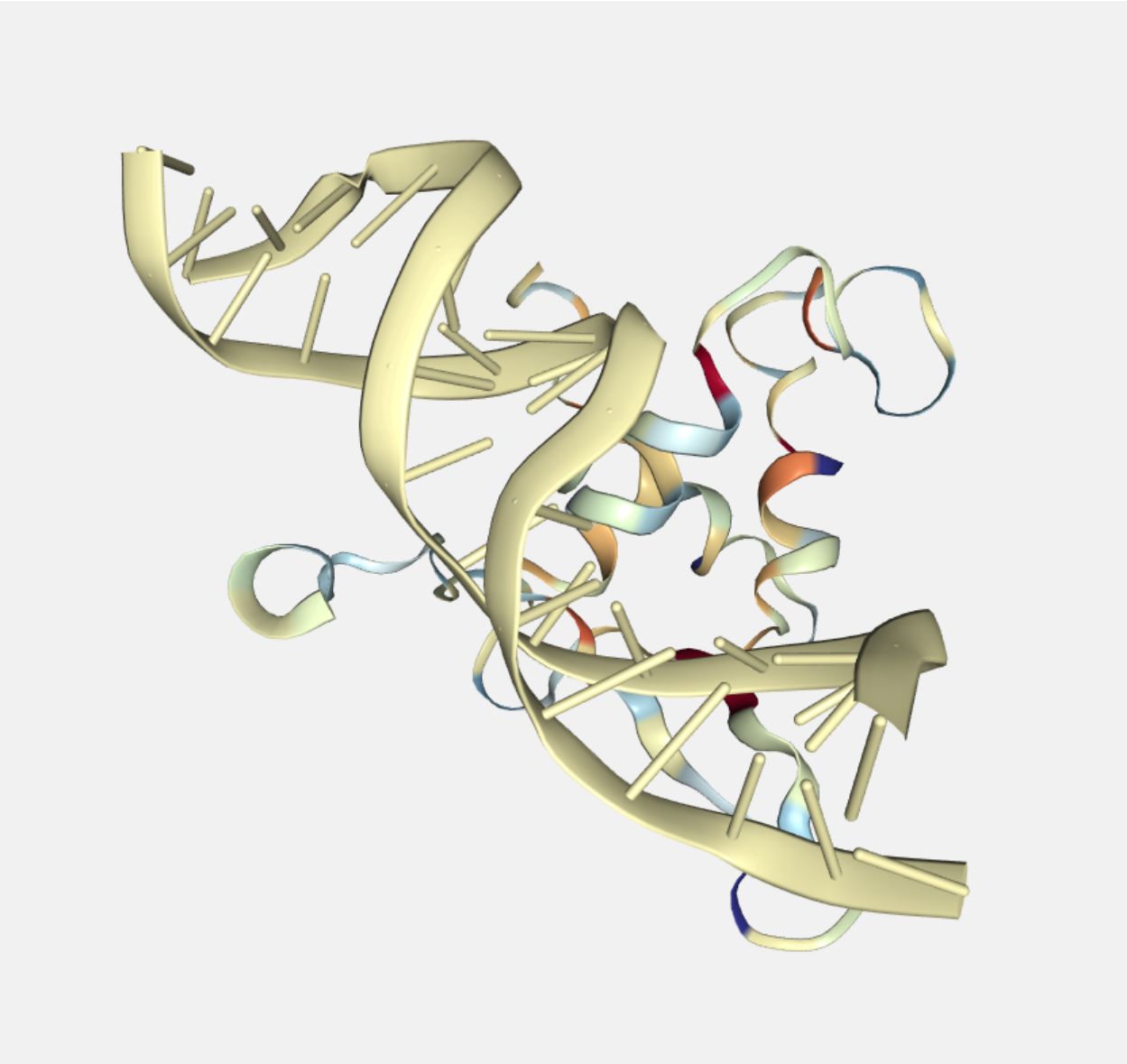
### Element

Color by chemical element.



### Hydrophobicity

Color by hydrophobicity.

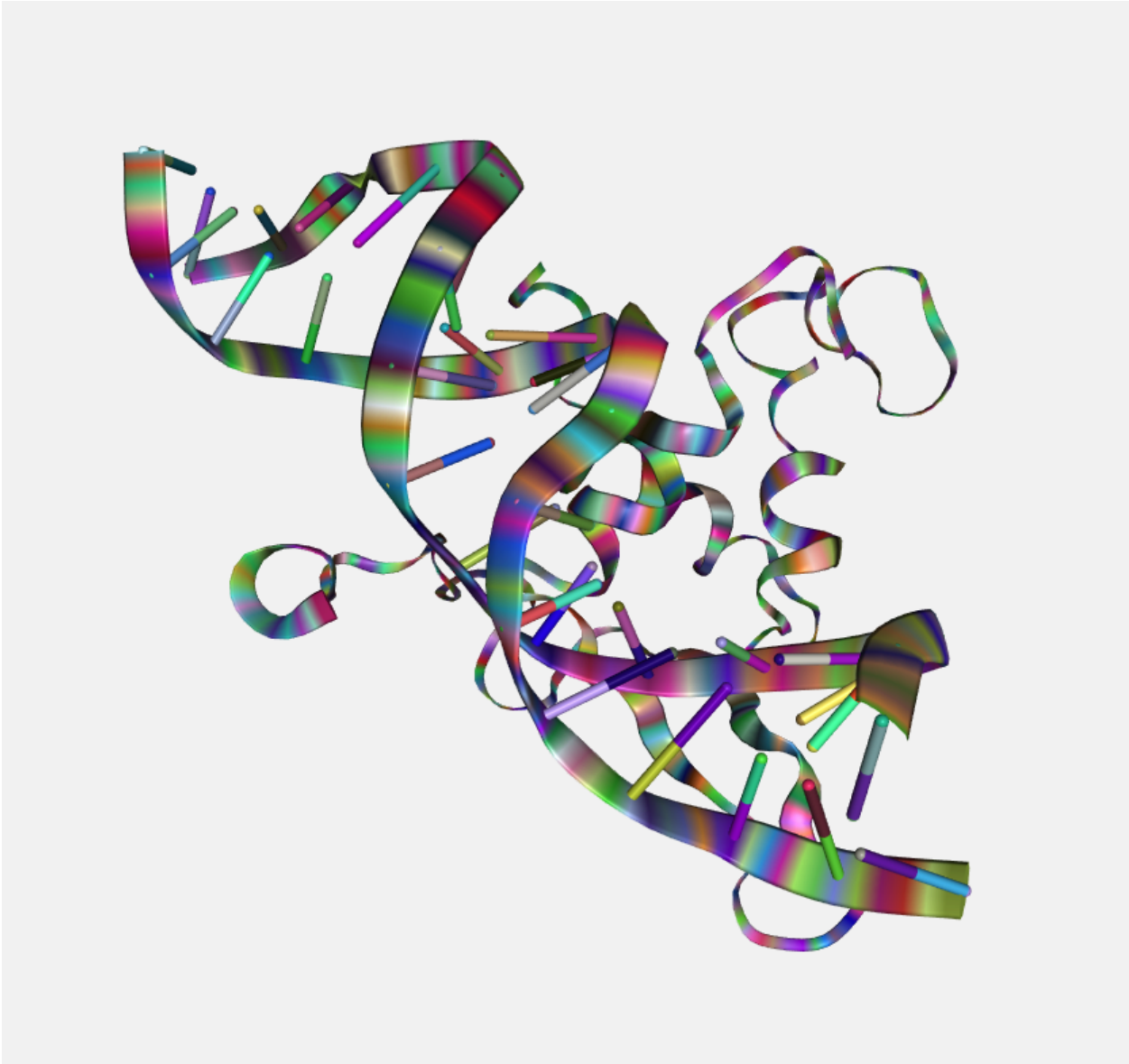


### Model index

Color by model index.

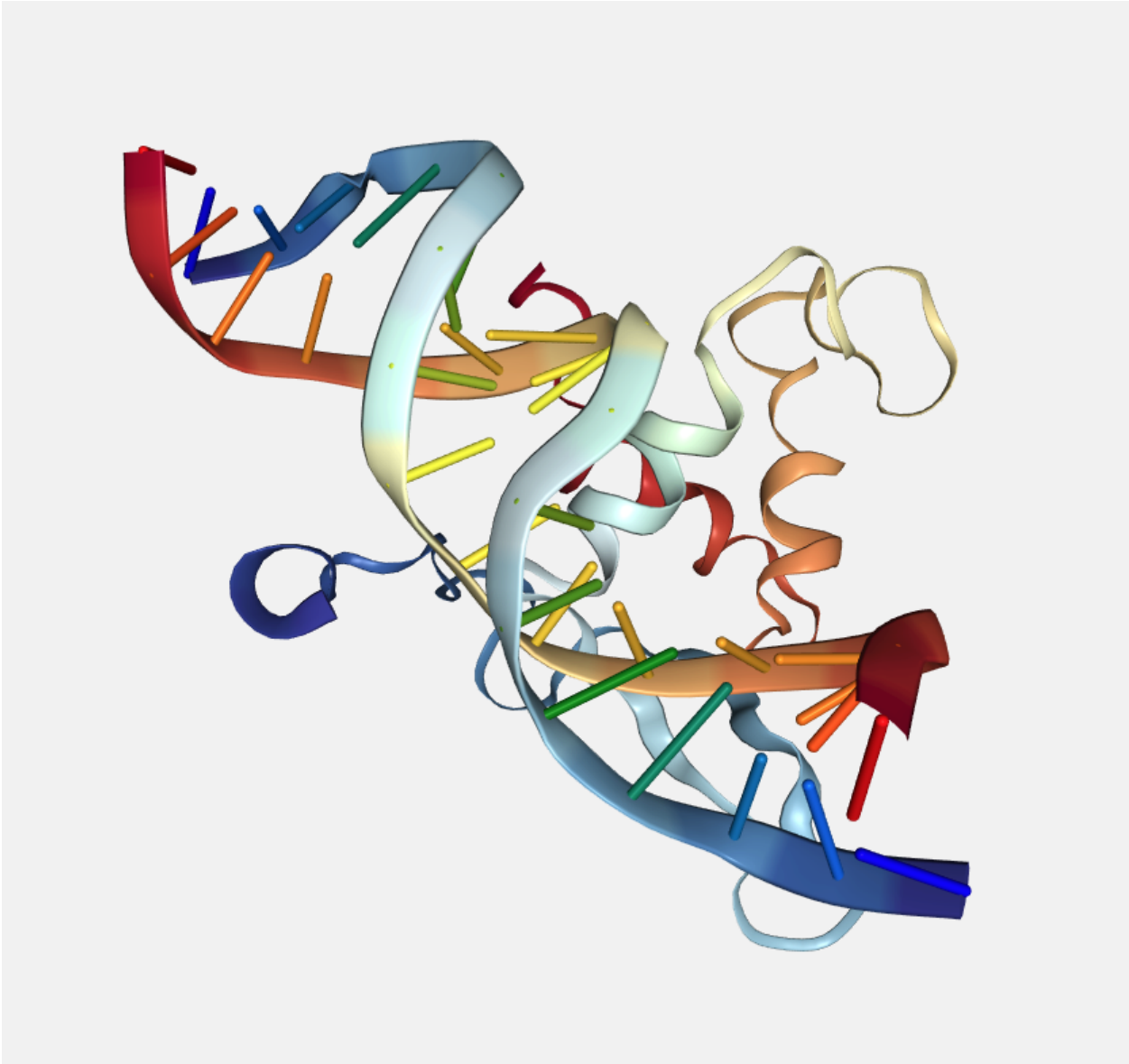
### Random

Class by random color.



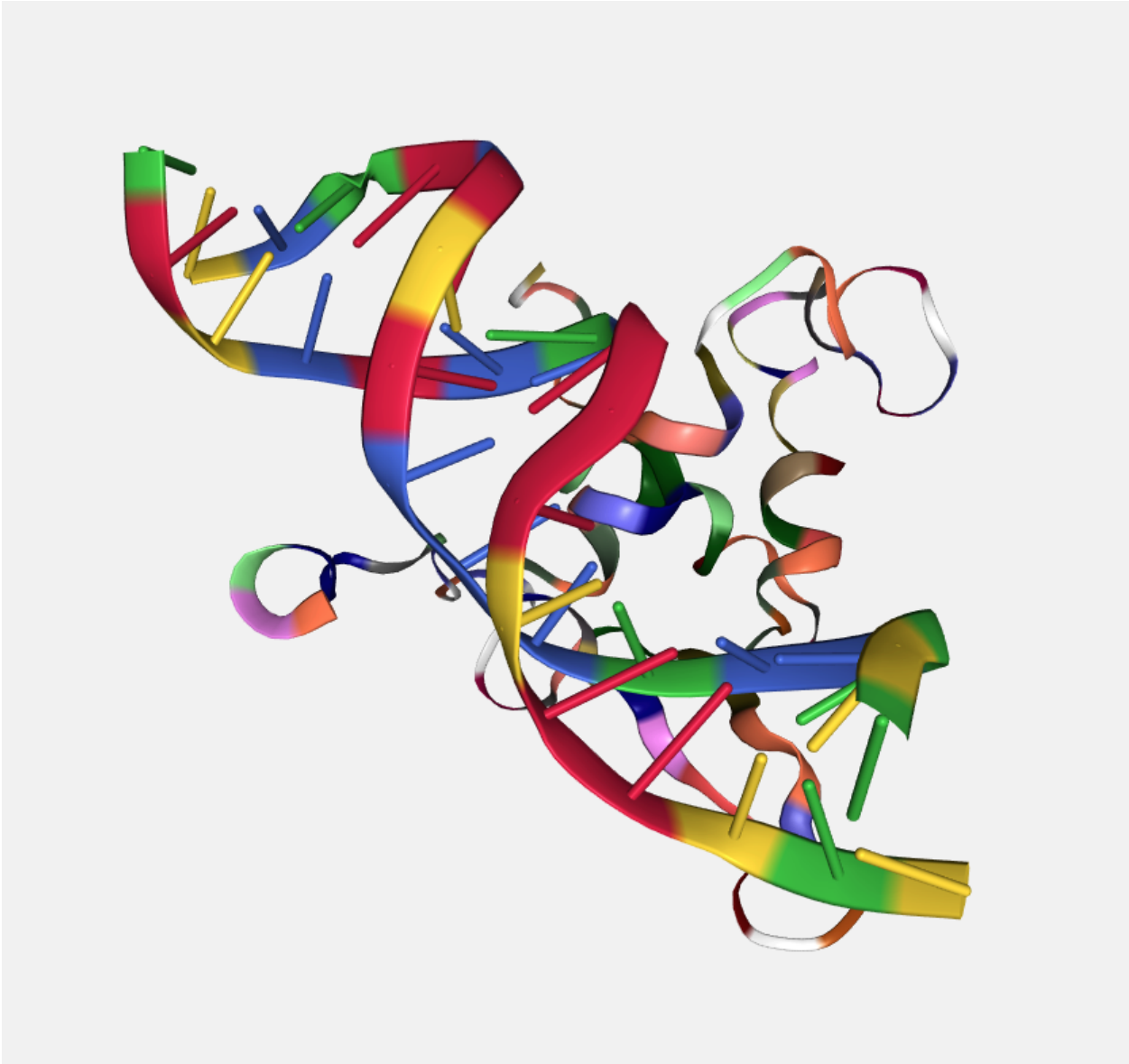
### Residue index

Color by residue index.



### Residue name

Color by residue name.

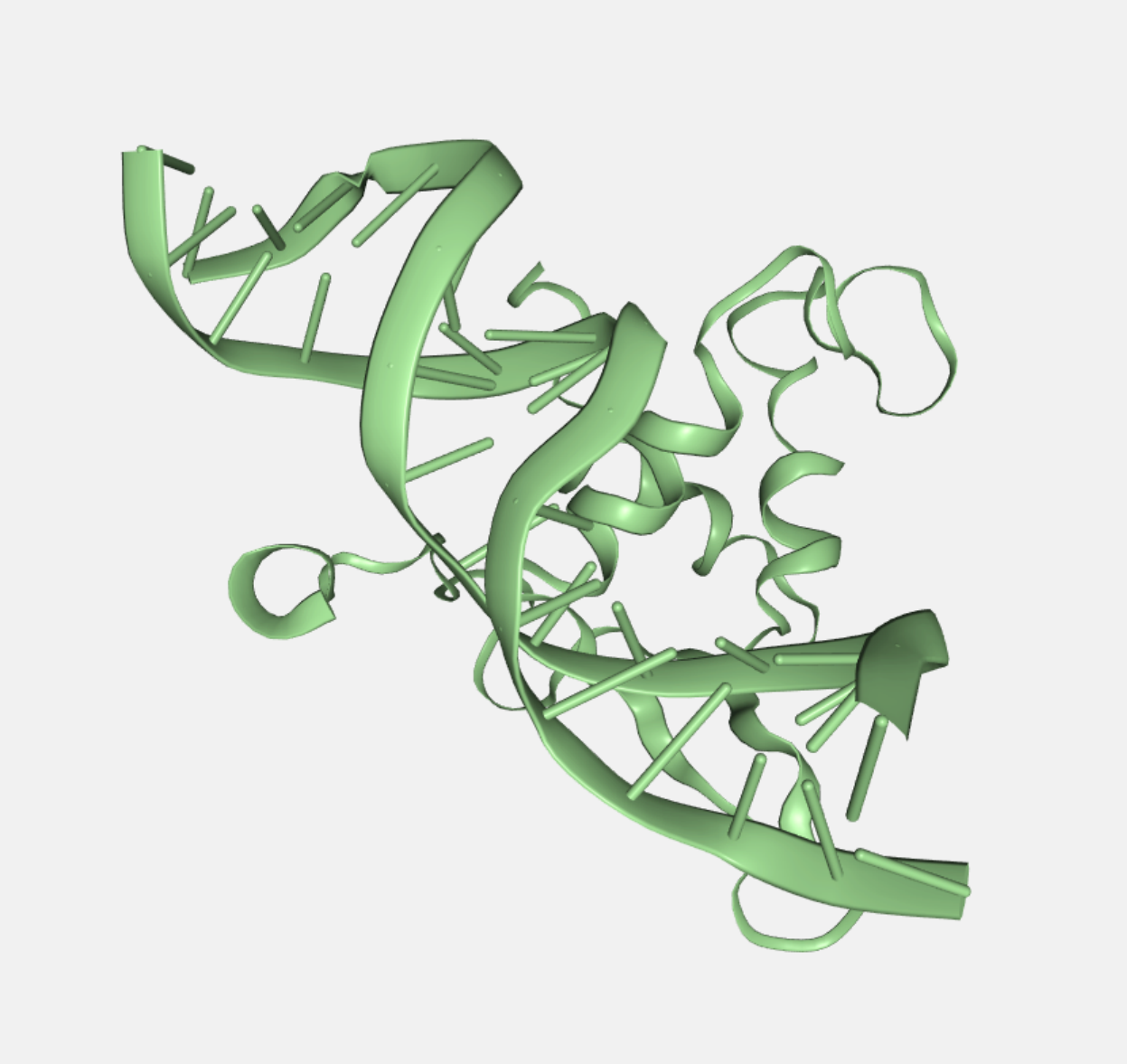


### Secondary structure

Color by secondary structure.

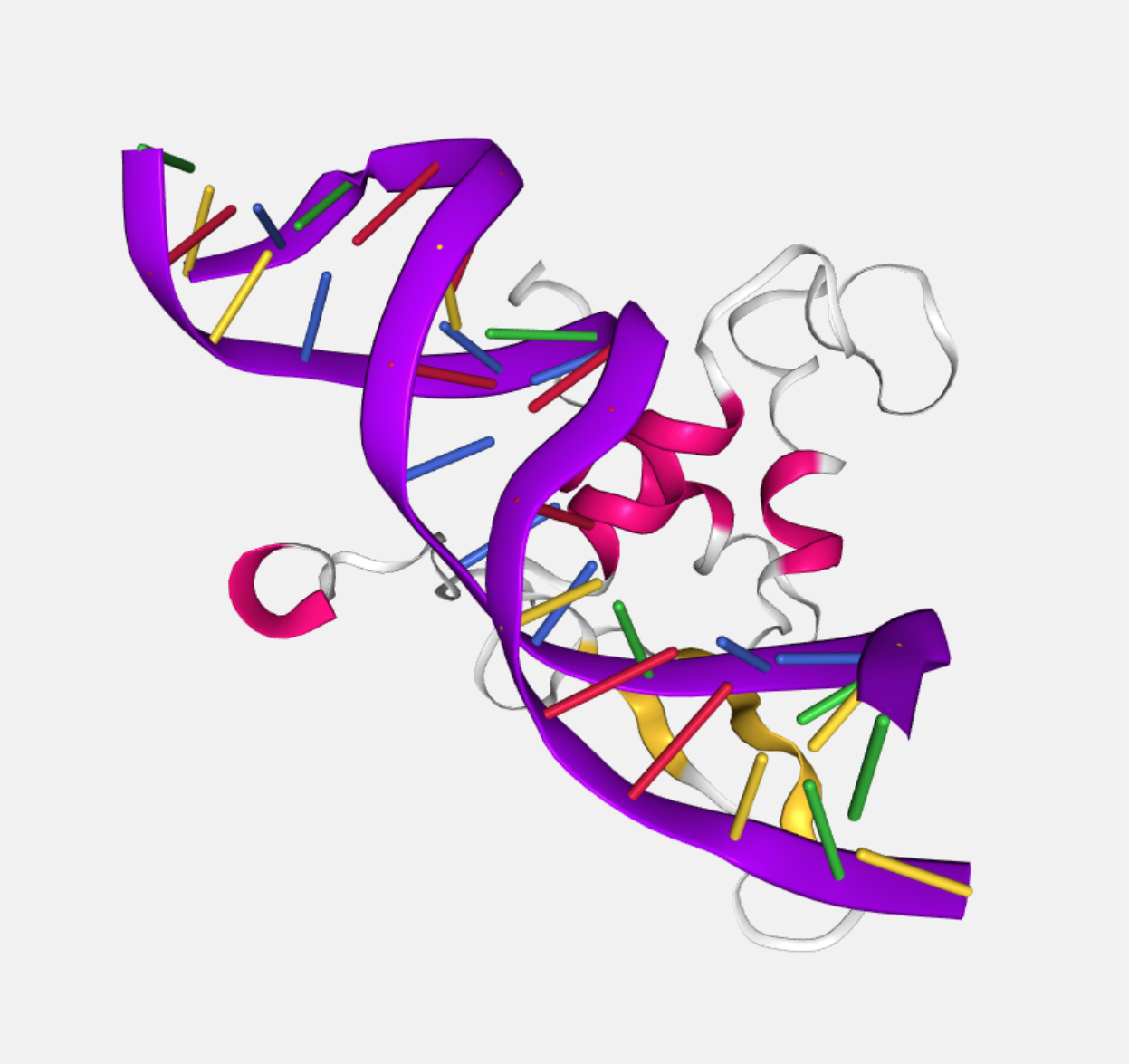
### Uniform

Color by uniform color selected from the color picker that appears at right of the dropdown menu when this option is selected.



The colors for the **Default** representation are as follows:

- Backbone: **Secondary structure** color scheme.
- NA bases (if present): **Residue name** color scheme.
- Heteroatoms: **Element** color scheme.
- Ions: **Element** color scheme.
- Waters: **Element** color scheme.

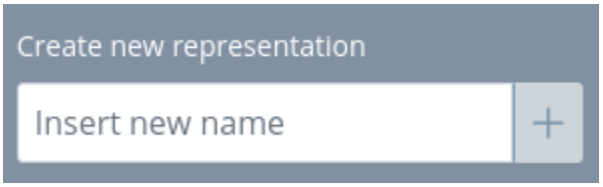


### Opacity

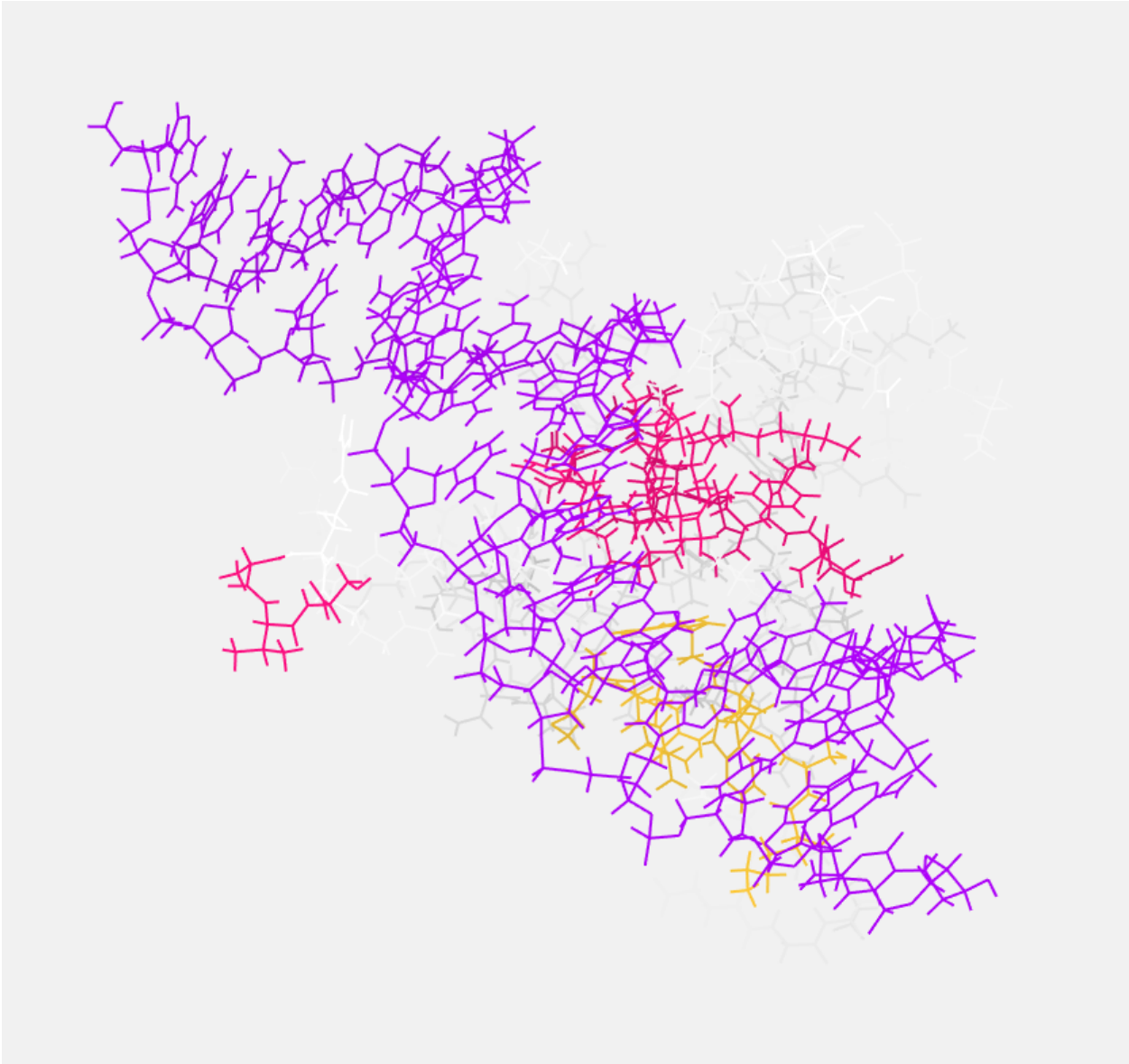

Through this slider, the **opacity** of the representation varies. Note that due to an incompatibility of NGL Viewer, opacity in multilayer projects can generate some **issues**. So creating multiple representations with different degrees of opacity can give **non desired outcomes**.

Moreover, if the opacity of a representation is **less than 30** it won't be possible to select the residues from the stage. Due to a WebGL problem, the threshold for allowing selections from stage is set to **greater than 30**.

### New representation




In this text box, users should insert the name for **creating a new representation**. For the sake to clearly see all the items that can be selected in the representation, **initially a line representation will be shown** (see image below). But at the moment that some molecule is selected, the rest of molecules will **disappear** from the stage. See ***next section*** for a more detailed description of this behavior.



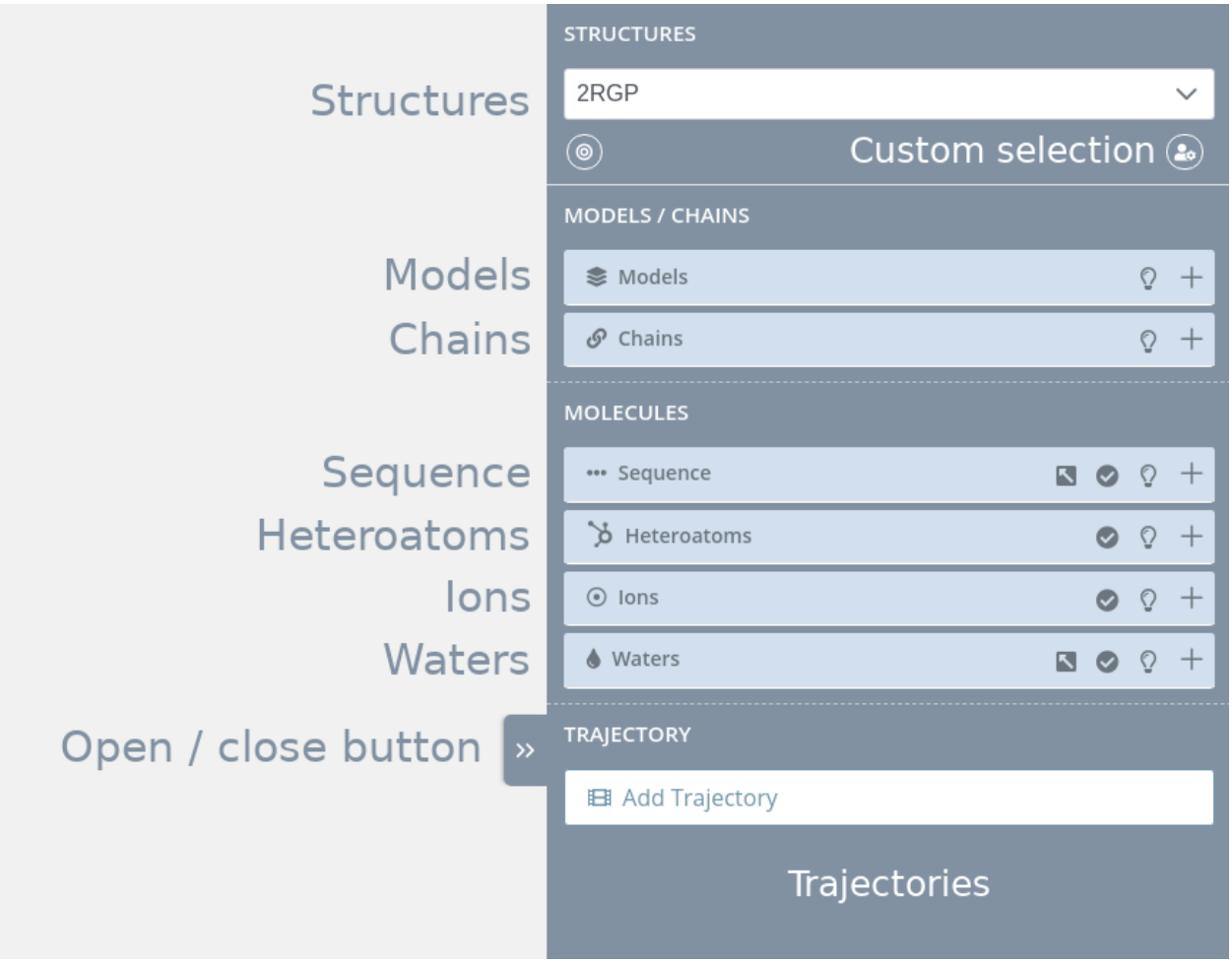
### 1.3.4 Selections

The **Selections** panel is at the right side of the stage and is used for applying selections to the current representation selected in the ***Representations*** panel.

Note that if the current representation is the **Default** one, this panel will be disabled. Once users create a new representation, the **Representations** panel will open automatically though it can be closed clicking the open / close button.

When a **new representation** is created, all the items in the stage will be selected by default with a **Line** representation and **Secondary structure** color scheme. The meaning of this is to easily glimpse **all the molecules** contained in the representation. Once the **first molecule** (one of Sequence, Heteroatoms, Ions or Waters) is selected, this one will be the only one selected.

The **Selections** panel is divided into ten parts:




- ***Open / close button***
- ***Structures***
- ***Custom selection***
- ***Models***
- ***Chains***
- ***Sequence***
- ***Heteroatoms***

- *Ions*
- *Waters*
- *Trajectories*

### Open / close button

This button, located at the left part of the **Selections** panel, allows to **open or close** it.

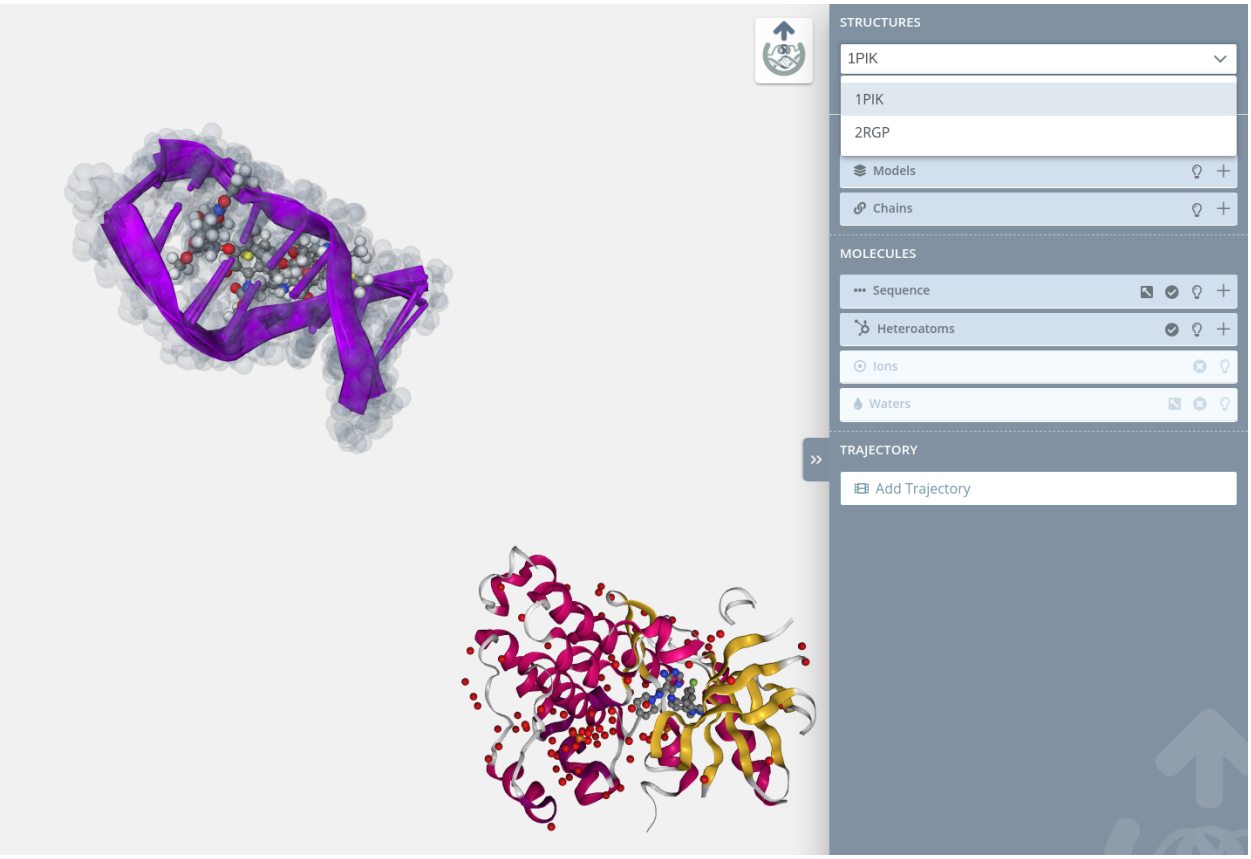
In the default representation this feature is disabled.

### Structures

### Select structure


In this dropdown menu, users can switch between the different structures uploaded in the **Launch project** page.

Opening the dropdown menu and **passing the mouse** over the structures contained on it will **highlight** them in the stage:




If there is only a **single structure**, this dropdown menu will be disabled:


### Structures menu

Below the dropdown menu there are a couple of buttons:

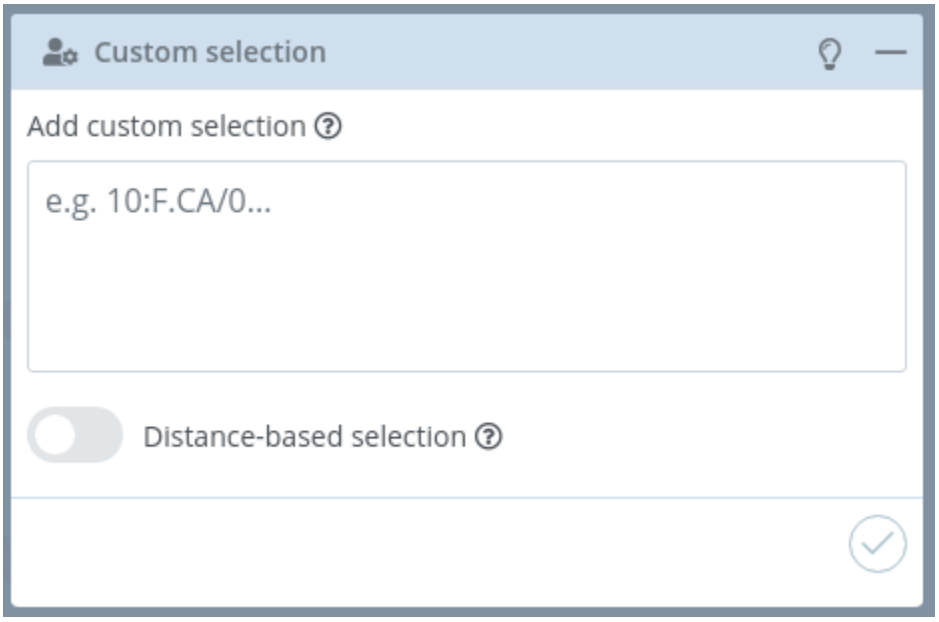
### Center structure

Centers the **stage** view in the currently **selected structure**. Note that if there is only a portion of the structure selected, the view will center around **this portion**.

### Custom selection / Manual selection

As explained ***later on***, advanced users can make custom selections using NGL viewer Selection Language. When custom selection is clicked, **only this panel will be shown** in the molecules part of the **Structures panel**. For coming back to the **manual selection** just click the same button again:

### Custom selection




For accessing this section, the **Custom selection** button of the **Structures menu** must be clicked.

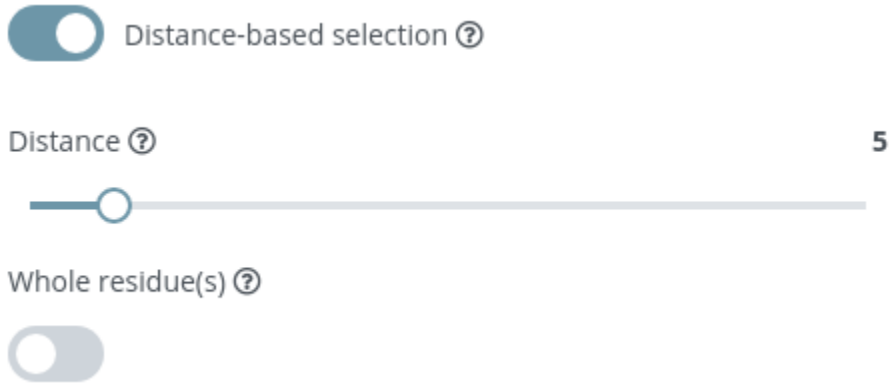
In this block, users can add a custom selection written in NGL viewer Selection Language. Please visit the Selection language section of the NGL Viewer manual **before starting** with this section.

There is a mini menu at the right side of the block header:

- **Show tips:**  opens a modal dialog with a short help for this section
- **Show / hide block:**  allows to open or collapse the panel.

### Distance-based selection

If enabled, a selection of atoms that are within a certain distance of the selection will be given instead of the selection itself.




After enabling this option, two new parameters are shown:

### Distance

Distance from selection in Ångstroms.

### Whole residue(s)

Whether to select or not the whole residue from the selected atoms.

Two actions can be performed after writing the custom selection:

### Save

Clicking this button the **custom selection** is added to the **current representation**.

### Remove

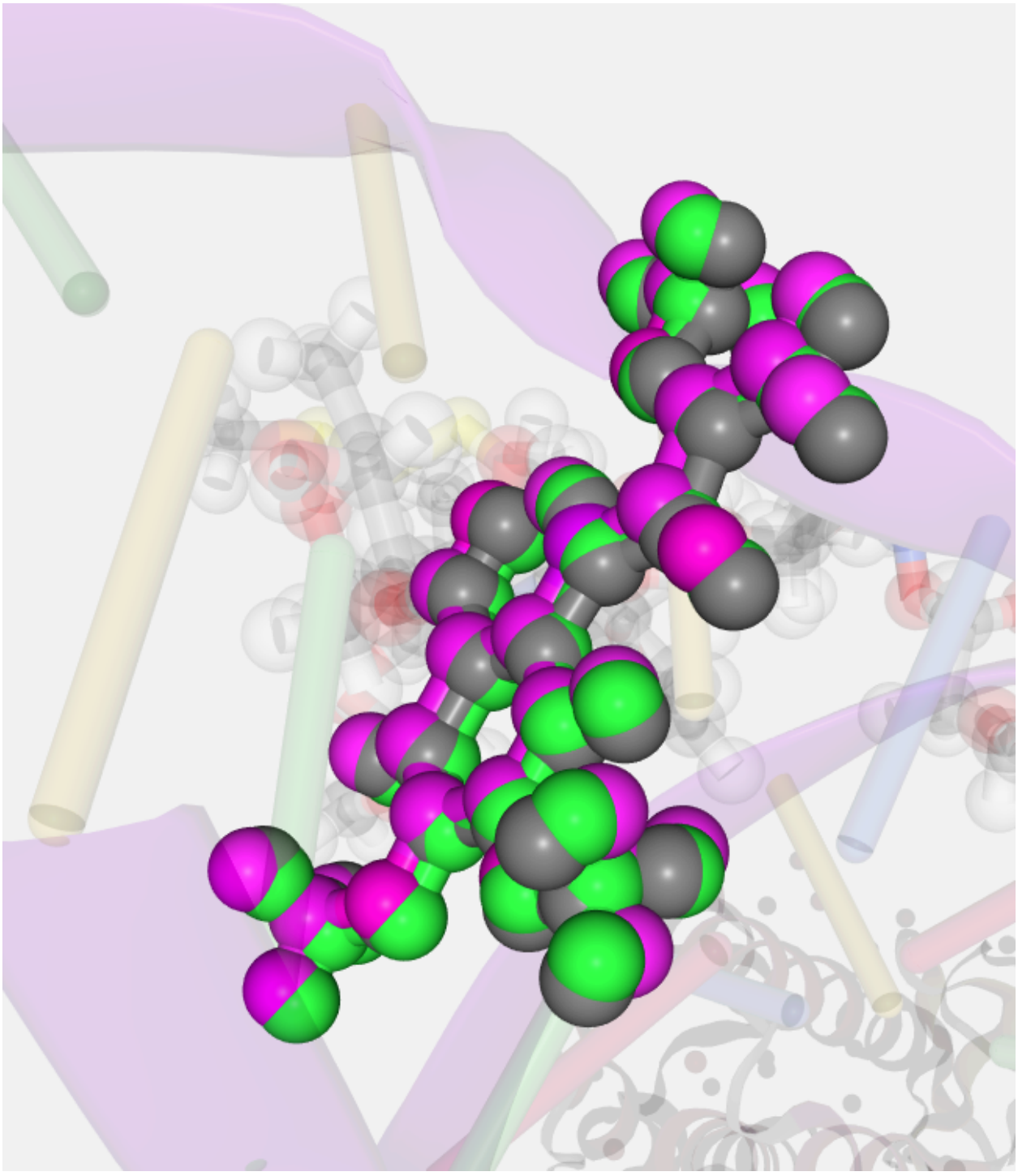
Clicking this button the **custom selection** is removed from the **current representation**.

Note that **custom selection is not compatible with manual selection**, so even though the selections made in the manual selection section will not be removed, they won't be visible in the stage. If users want to **restore a previously made manual selection**, just removing the custom selection will do the trick.

### Models


If the selected structure has **more than one model**, this block will be enabled allowing users to **switch between the different models** of the structure.

Same heteroatom in **different models** represented in three different colors:



There is a mini menu at the right side of the block header:

- **Show tips:**  opens a modal dialog with a short help for this section
- **Show / hide block:**  allows to open or collapse the panel.

Note that **switching between models will change the succeeding panels** (i.e. if the Model 1 has two chains A and B

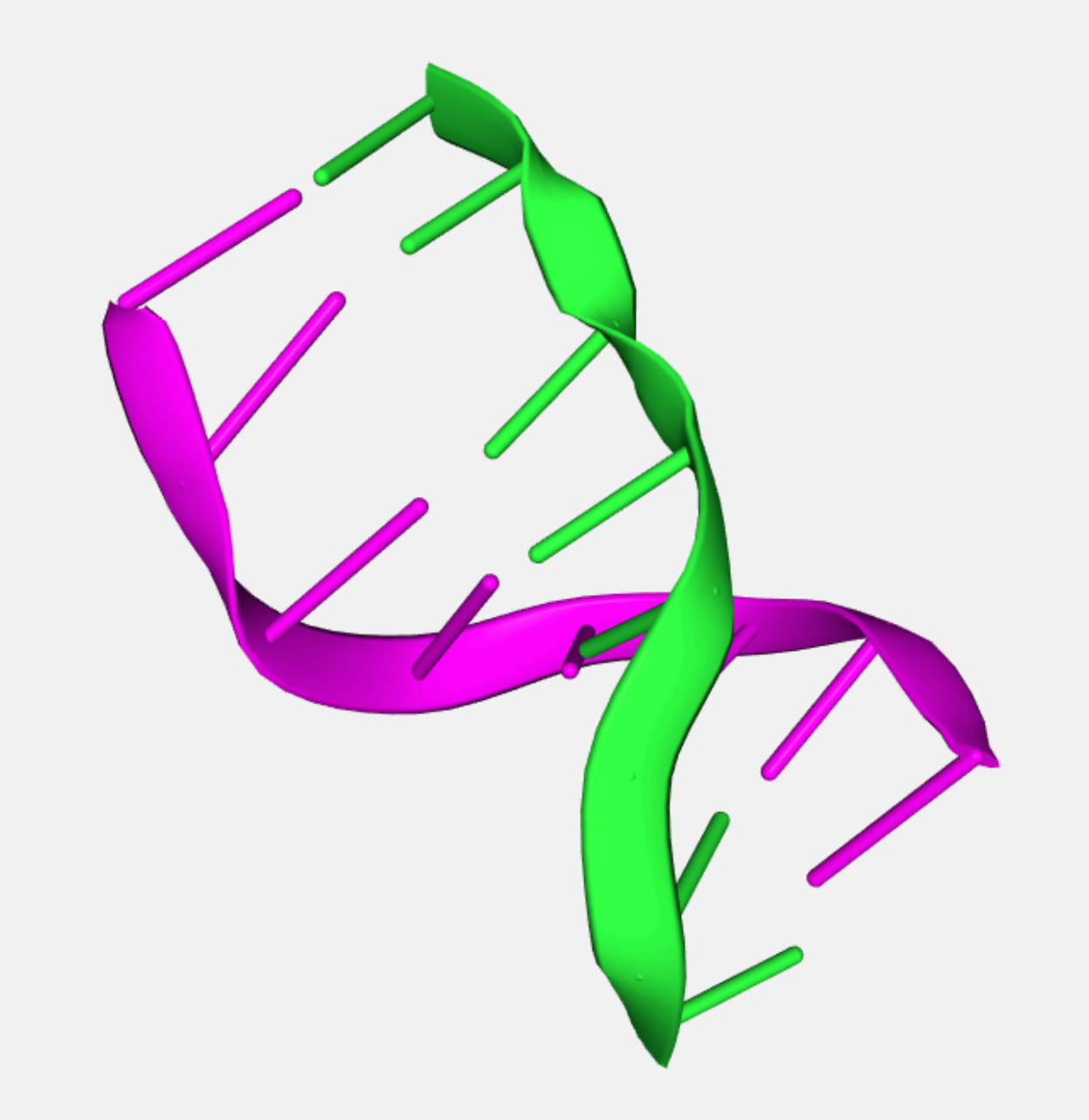
and the Model 2 has three chains A, B and C, the Chains block will change).

If there is only a **single model**, this block menu will be disabled:


### Chains


If the selected model of the current structure has **more than one chain**, this block will be enabled allowing users to **switch between the different models** of the structure.

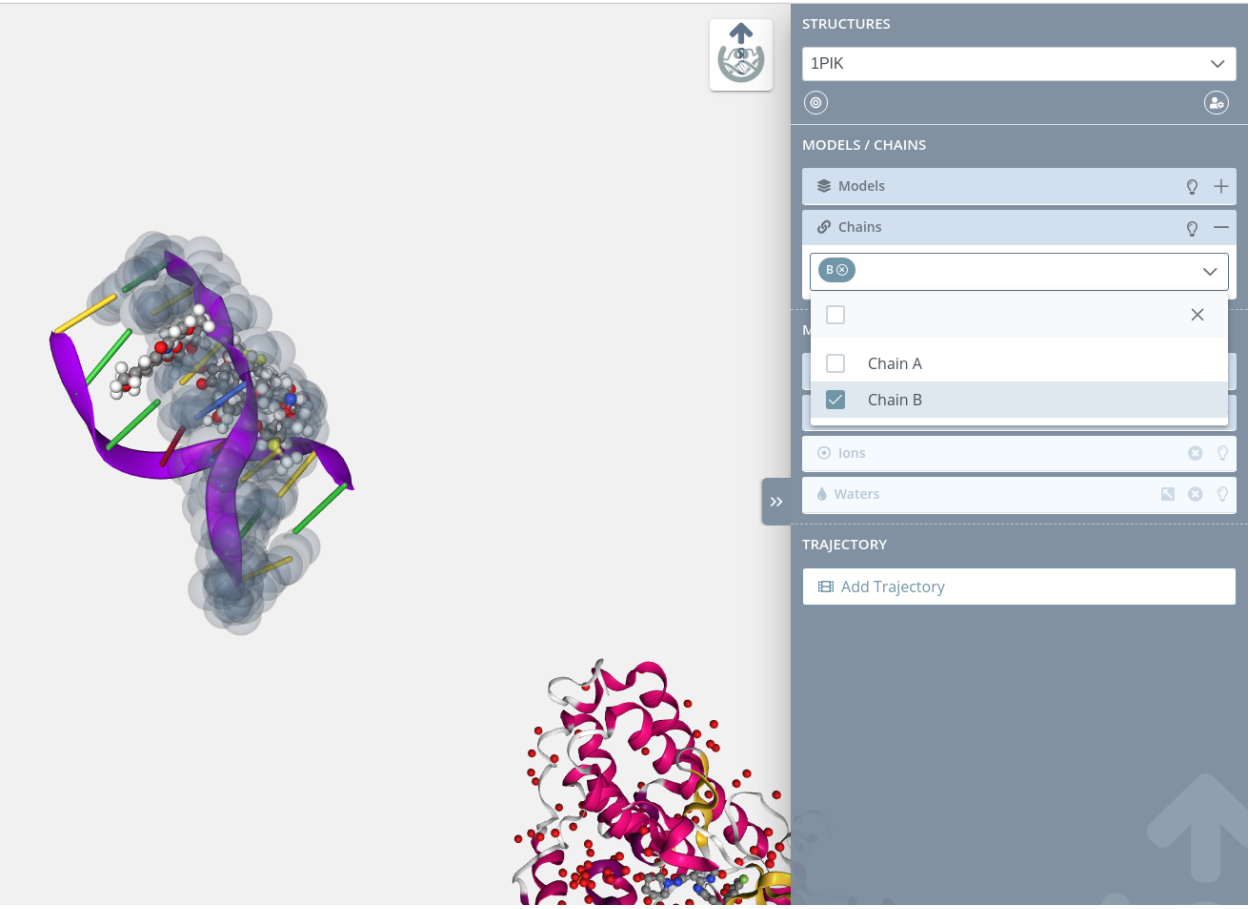
Two **different chains** represented in two different colors:



There is a mini menu at the right side of the block header:

- **Show tips:**  opens a modal dialog with a short help for this section
- **Show / hide block:**  allows to open or collapse the panel.

Opening the dropdown menu and **passing the mouse** over the chains contained on it will highlight them in the stage:



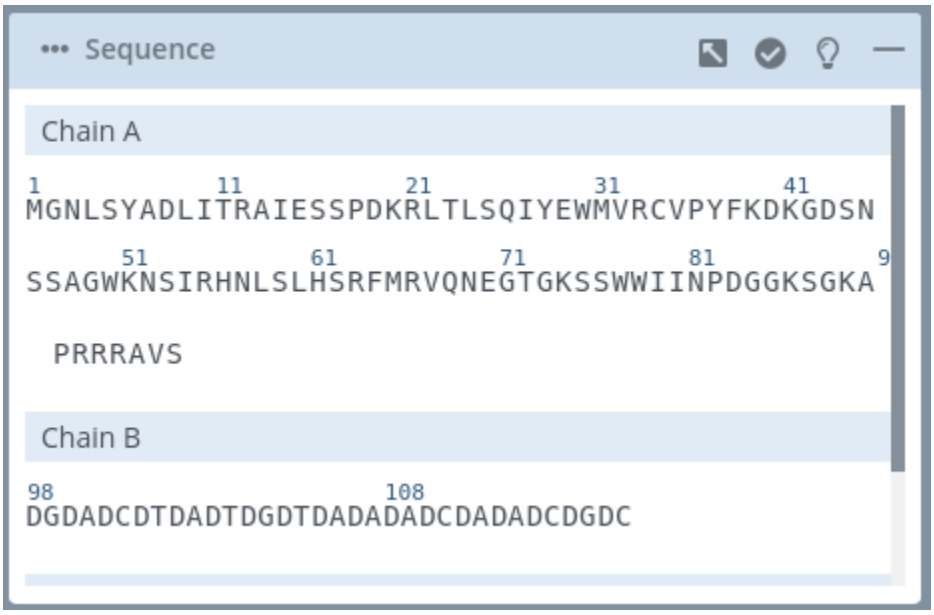

Note that if the structure has **no chains**, all the molecules will be automatically assigned to the **Chain A**. If the structure has **one or more chains** but some of its molecules have **no chain**, these "orphan" molecules will be assigned to a **mock Chain @**.

If there is only a single chain, this block menu will be disabled:


### Sequence

There are **two ways** to perform sequence residues selection: directly through ***the block in the Selection panel*** or though the ***Zoom window***:

### Selection panel block




This block shows **all the residues of the structure** classified by chains.

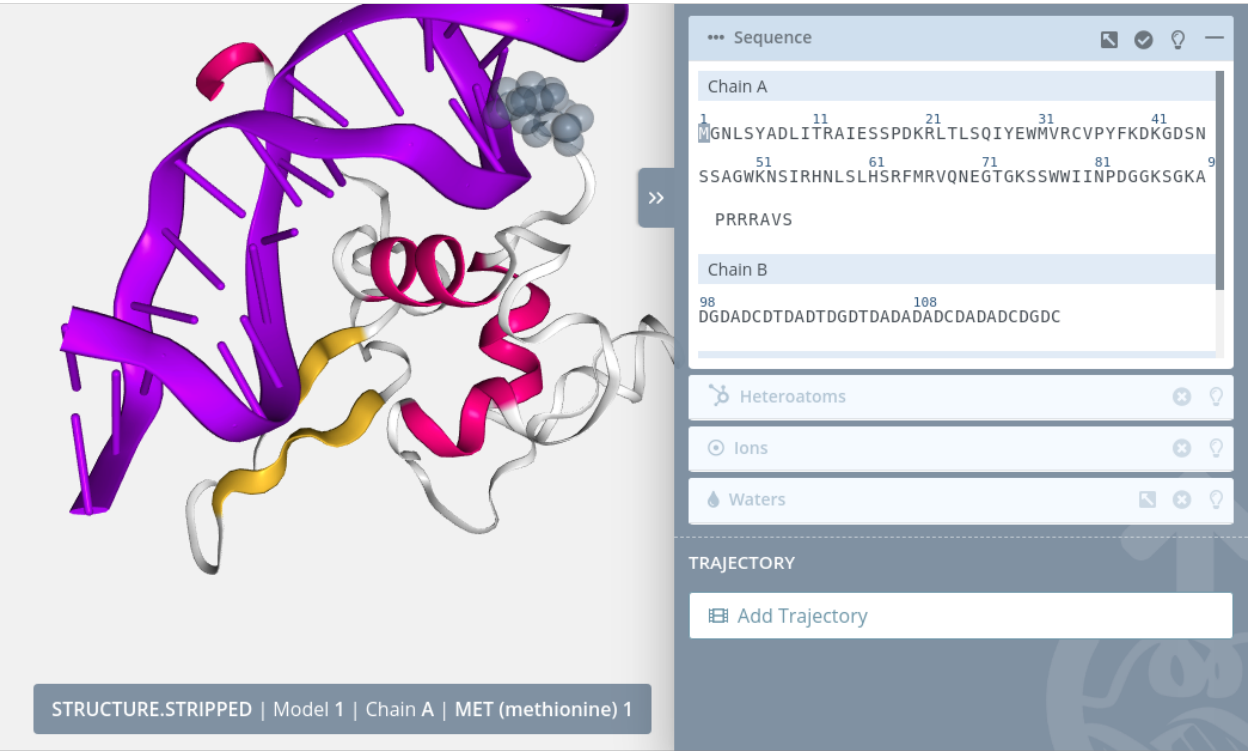
There is a mini menu at the right side of the block header:

- **Open / close external window:** allows to open or close the Zoom window for this section.
- **Select / unselect all:** allows to select or unselect all the molecules of this block with a single click.
- **Show tips:** opens a modal dialog with a short help for this section
- **Show / hide block:** allows to open or collapse the panel.

Different actions can be performed with the residues:

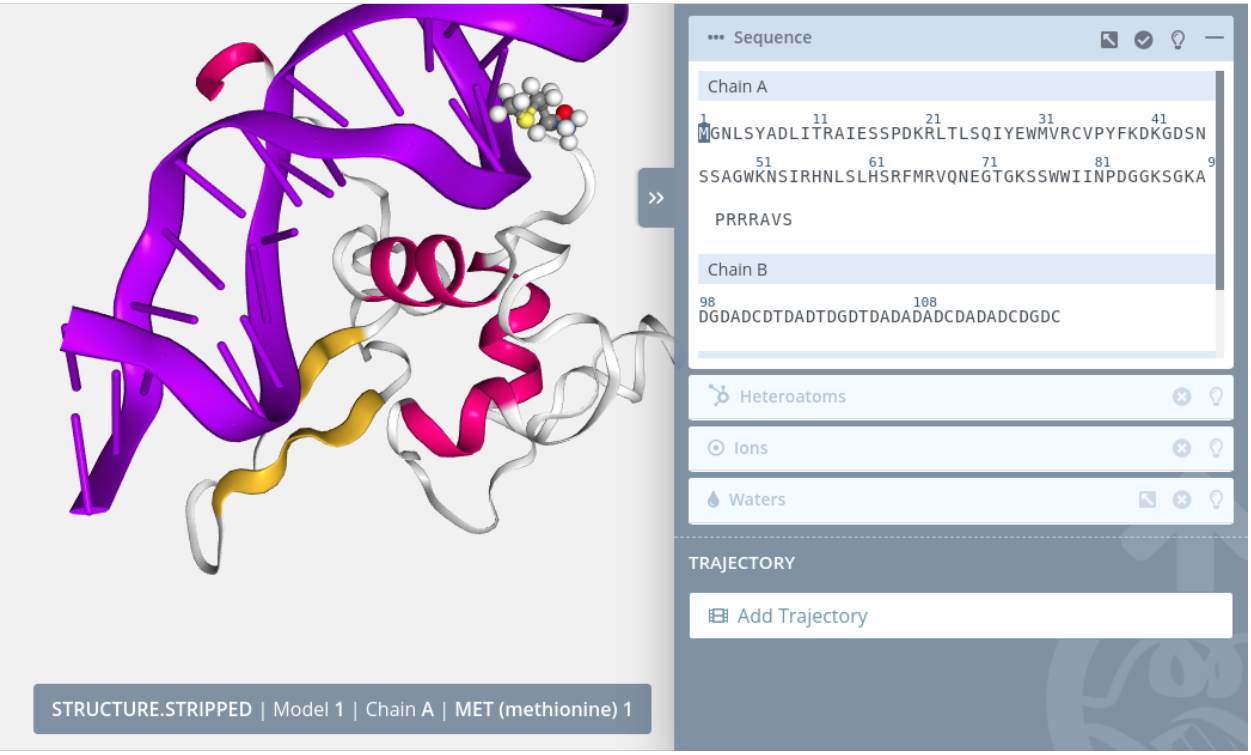
### Highlight

Passing the **mouse over** a residue will **highlight it** on the stage:




### Selection

**Clicking on a residue** will select it in the current selection **applying to it** the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:

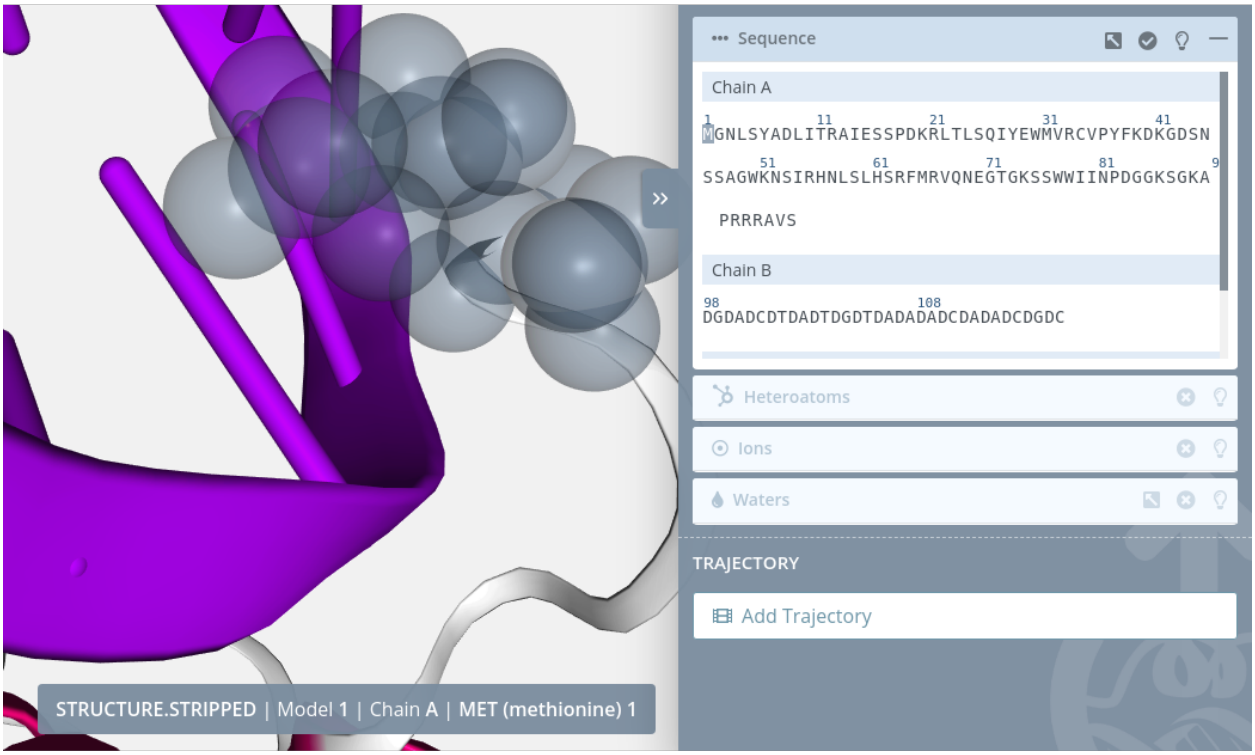



### Unselection

**Clicking on a selected residue** will unselect it from the current selection.

### Zoom

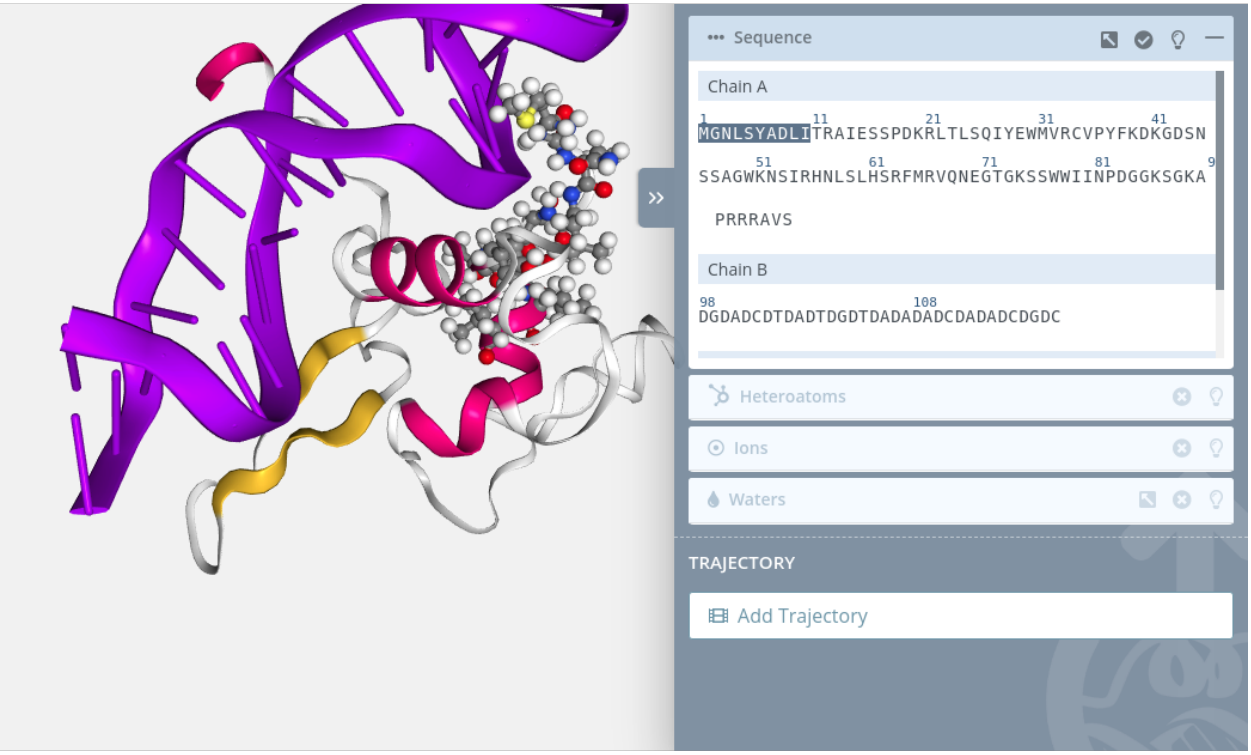
**Clicking on a residue** with the mouse **left button while pressing the Alt key** will do a zoom to the residue:




### Multiple selection

For **selecting multiple residues** just click the first residue of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

Then, click the last residue of the custom sequence again with the mouse **left button while pressing the Shift key**:

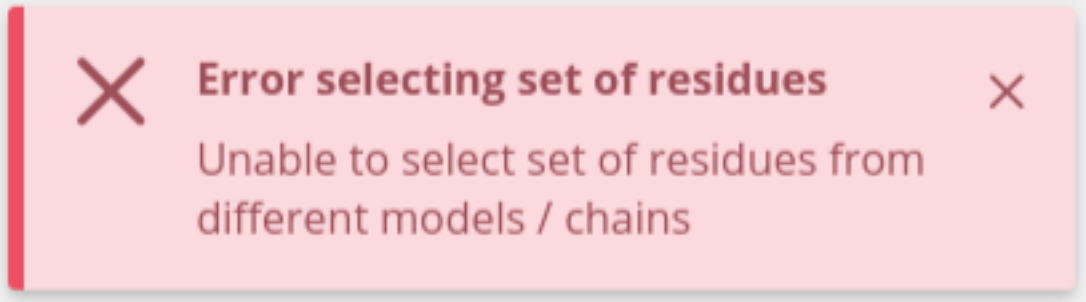



### Multiple unselection

For **unselecting multiple residues** is exactly the same process: just click the first residue of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

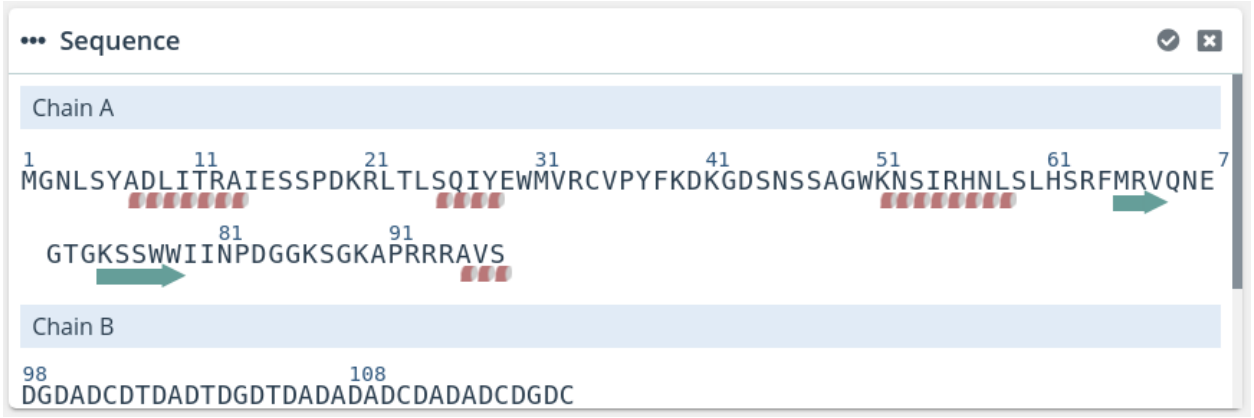
Then, click the last residue of the custom sequence again with the mouse **left button while pressing the Shift key**.

Note that **multiple selections** are only **allowed** between residues of the **same Model and Chain**. Trying to select multiple residues from **different Model and / or Chain** will show an **error notification**:




If there are **no residues** in the selected structure (i.e. an heteroatom), this block menu will be disabled:


### Zoom window




This window shows the same information of the ***Sequences block*** but in a little more detail, adding the **ability** of selecting **-helices** and **-sheets** if they are present in the structure.

There is a mini menu at the right side of the window:

- **Select / unselect all:**  allows to select or unselect all the molecules of this block with a single click.
- **Close window:**  closes the window.

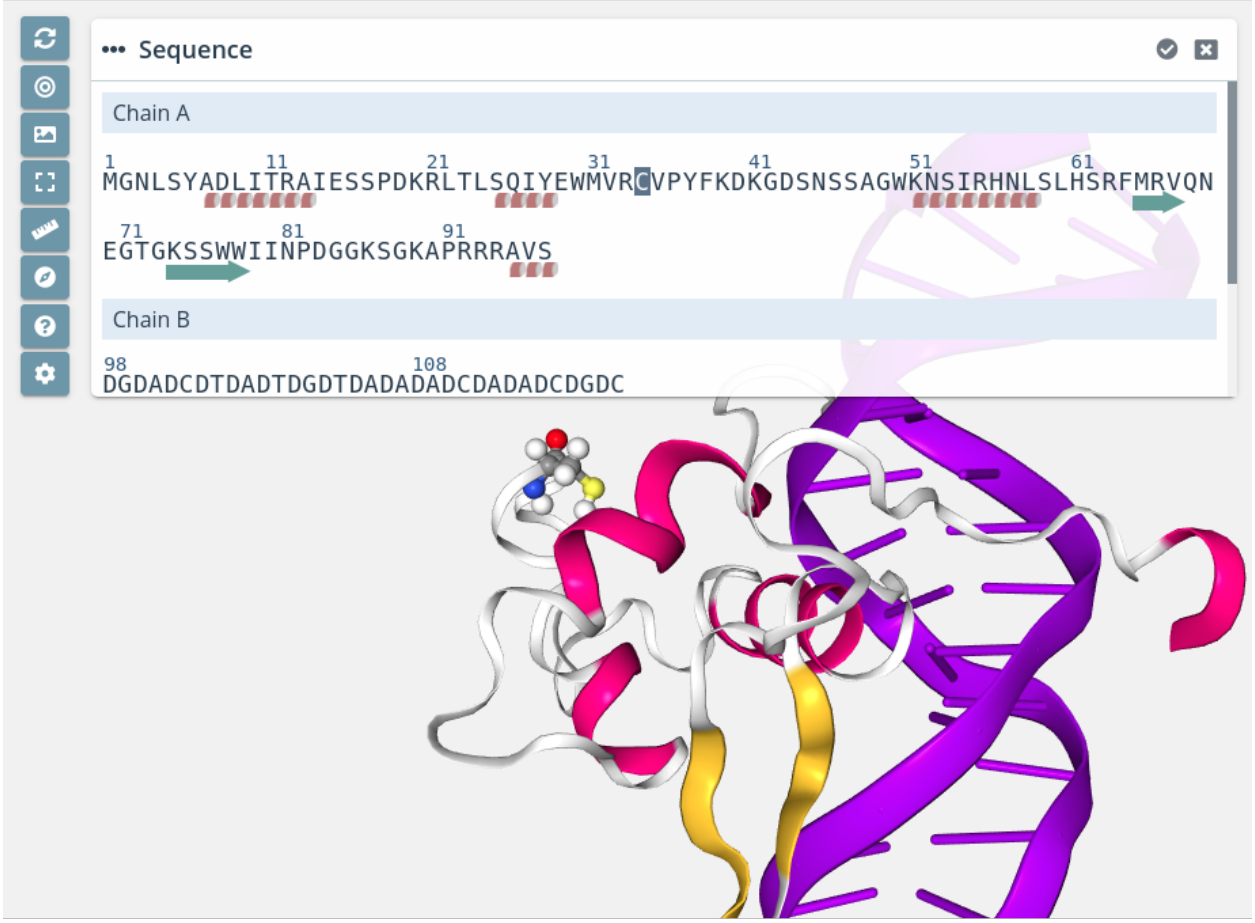
Different actions can be performed with the residues:

### Residue highlight

Passing the **mouse over** a residue will **highlight** it in the stage:


### Residue selection

**Clicking on a residue** will select it in the current selection **applying to** it the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:

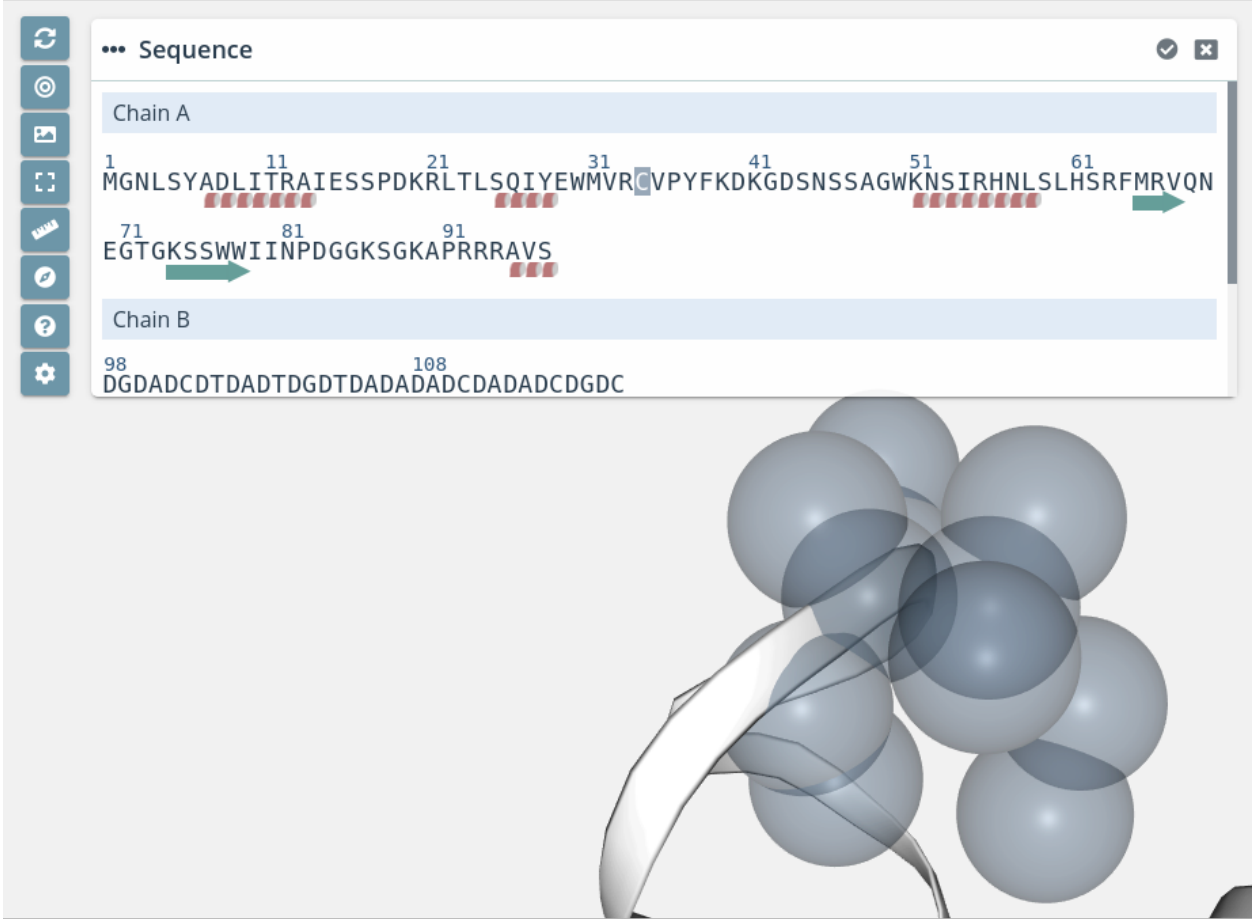



### Residue unselection

**Clicking on a selected residue** will **unselect** it from the current selection.

### Residue zoom

**Clicking on a residue** with the mouse **left button while pressing the Alt key** will do a zoom to the residue:




### Multiple residue selection

For **selecting multiple residues** just click the first residue of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

Then, click the last residue of the custom sequence again with the mouse **left button while pressing the Shift key**:

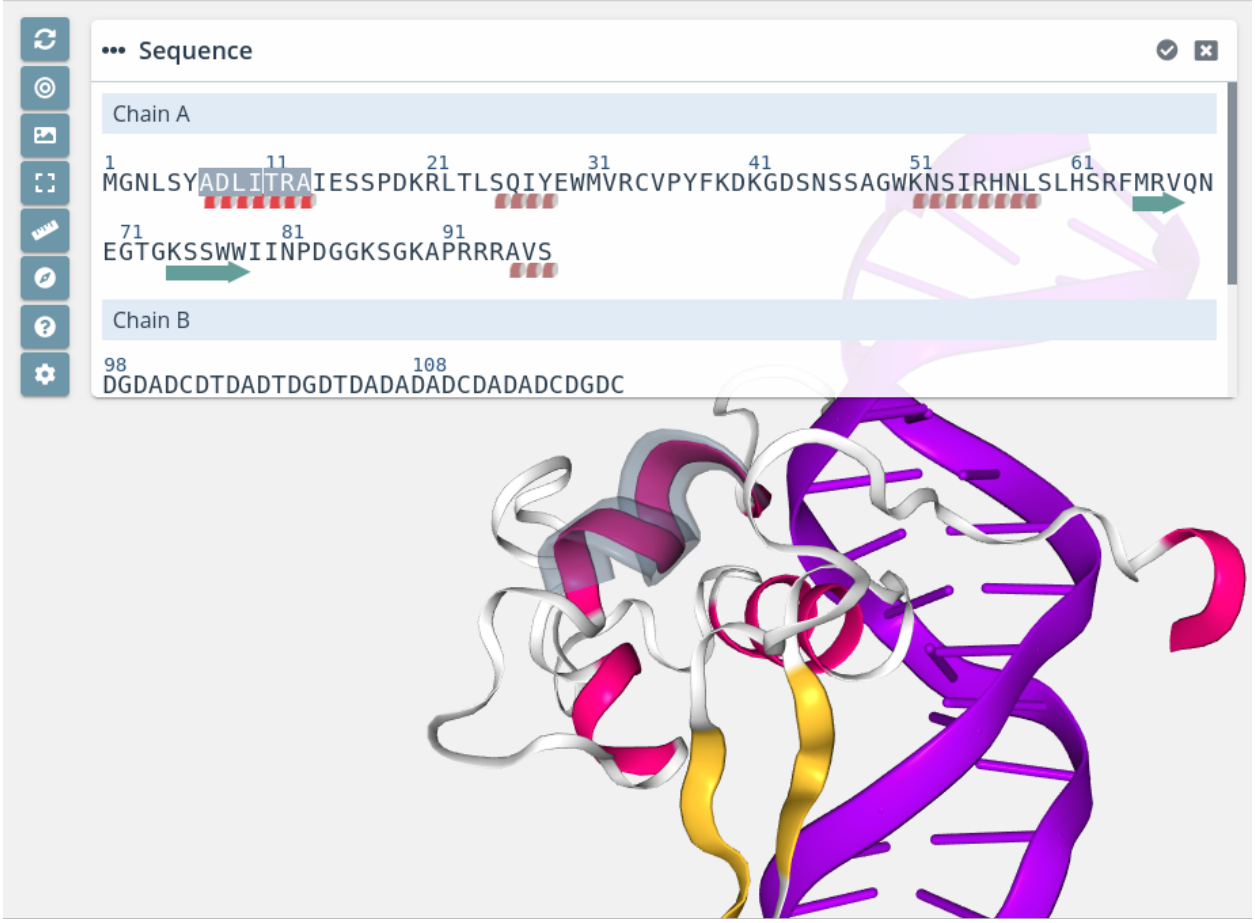

### Multiple residue unselection

For **unselecting multiple residues** is exactly the same process: just click the first residue of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

Then, click the last residue of the custom sequence again with the mouse **left button while pressing the Shift key**.

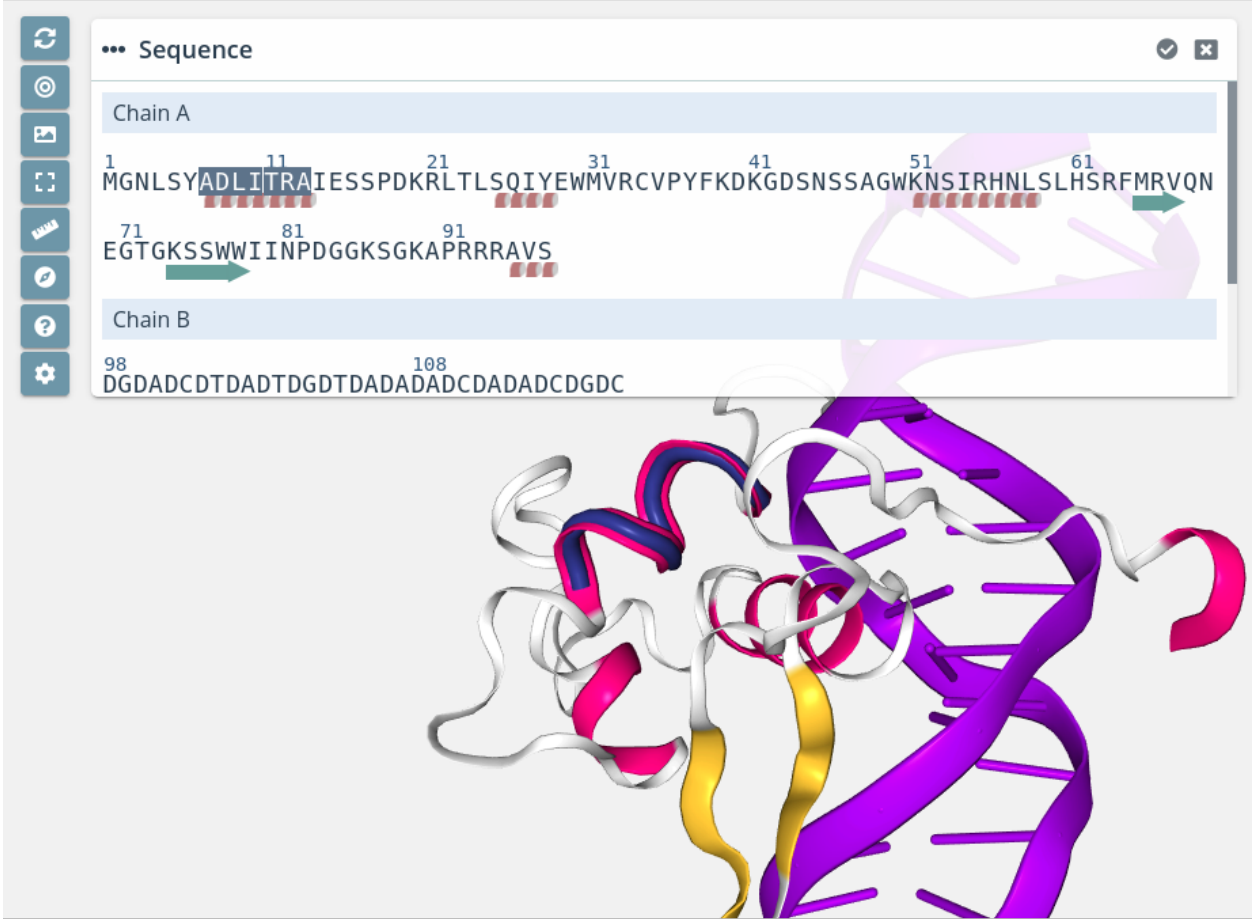
### -helix / -sheet highlight

Passing the **mouse over** an -helix or a -sheet will **highlight it** in the stage:




### -helix / -sheet selection

**Clicking on a -helix or a -sheet** will select it in the current selection **applying to it** the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:



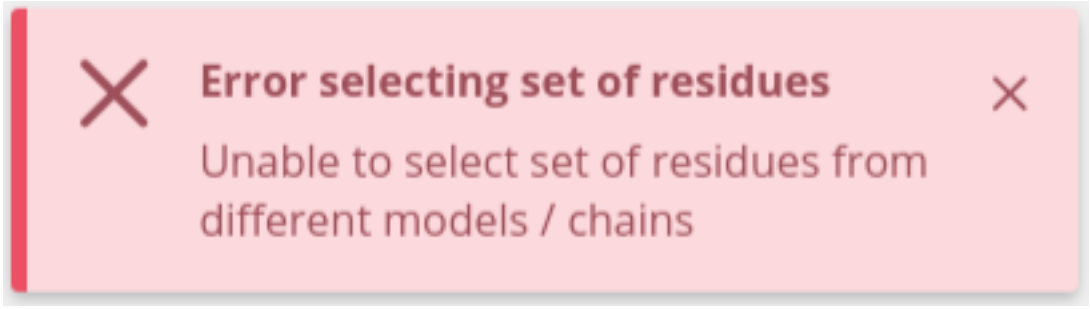

### -helix / -sheet unselection

**Clicking on a selected -helix or a -sheet** will **unselect** it from the current selection. Note that to unselect a **whole -helix or -sheet** all its residues must be selected.

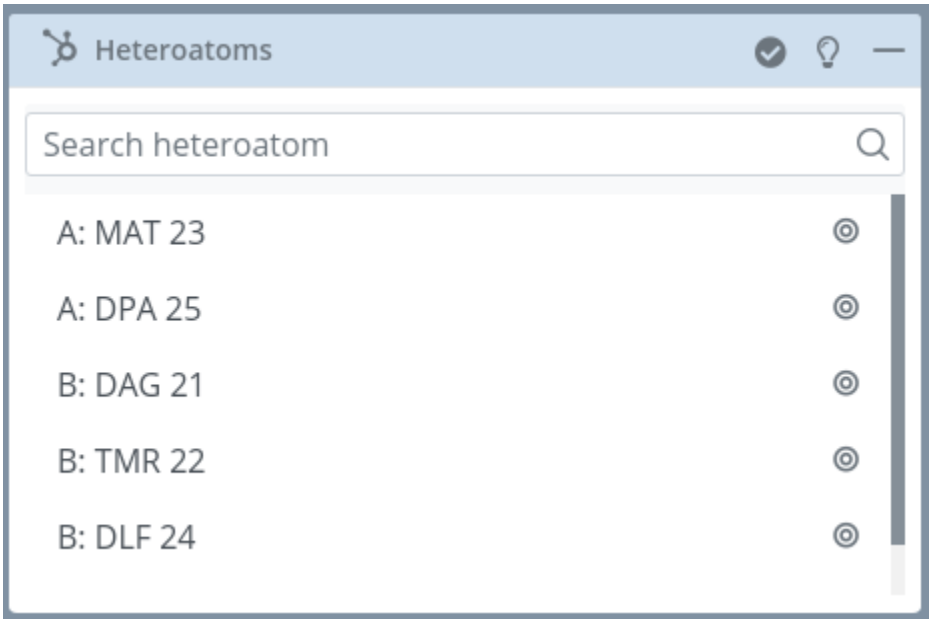
### -helix / -sheet zoom

- **Clicking on a -helix or a -sheet** with the mouse **left button while pressing the Alt key** will do a zoom to the ensemble of residues:


Note that **multiple selections** are only **allowed** between residues of the **same Model and Chain**. Trying to select multiple residues from **different Model and / or Chain** will show an **error notification**:



### Heteroatoms




This block shows **all the heteroatoms of the structure**.

There is a mini menu at the right side of the block header:

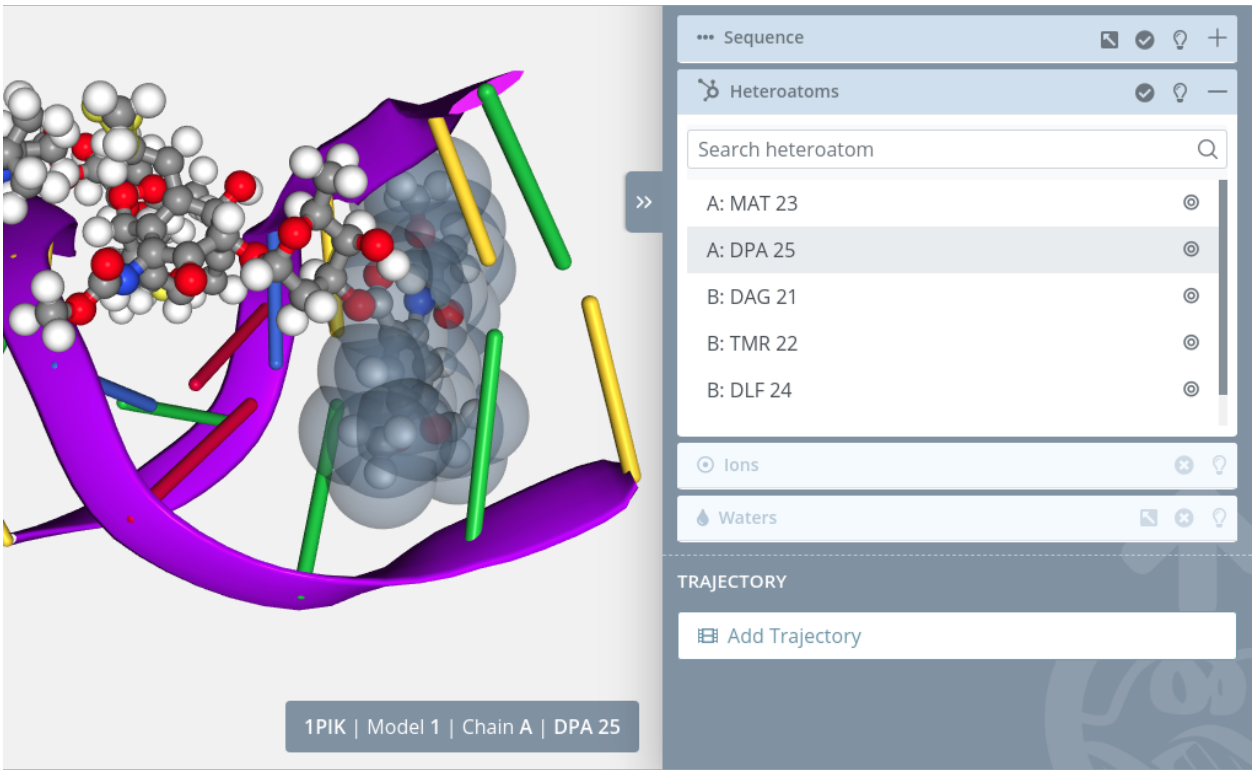
- **Select / unselect all:** allows to select or unselect all the molecules of this block with a single click.
- **Show tips:** opens a modal dialog with a short help for this section
- **Show / hide block:** allows to open or collapse the panel.

There is a **search box** on the top of the heteroatoms list that allows users to perform **searches** on this list.

Different actions can be performed with the heteroatoms:

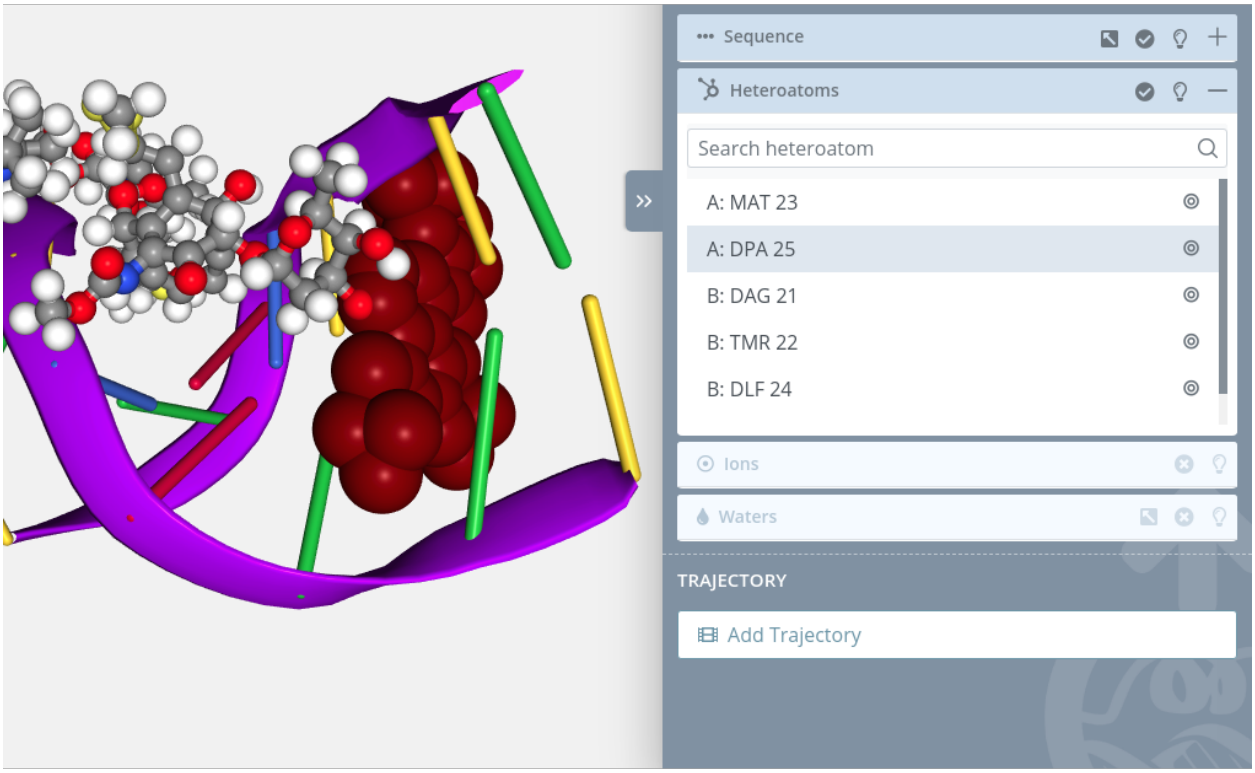
### Highlight

Passing the **mouse over** an heteroatom will **highlight** it in the stage:




### Selection

**Clicking on an heteroatom** will select it in the current selection **applying to it** the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:

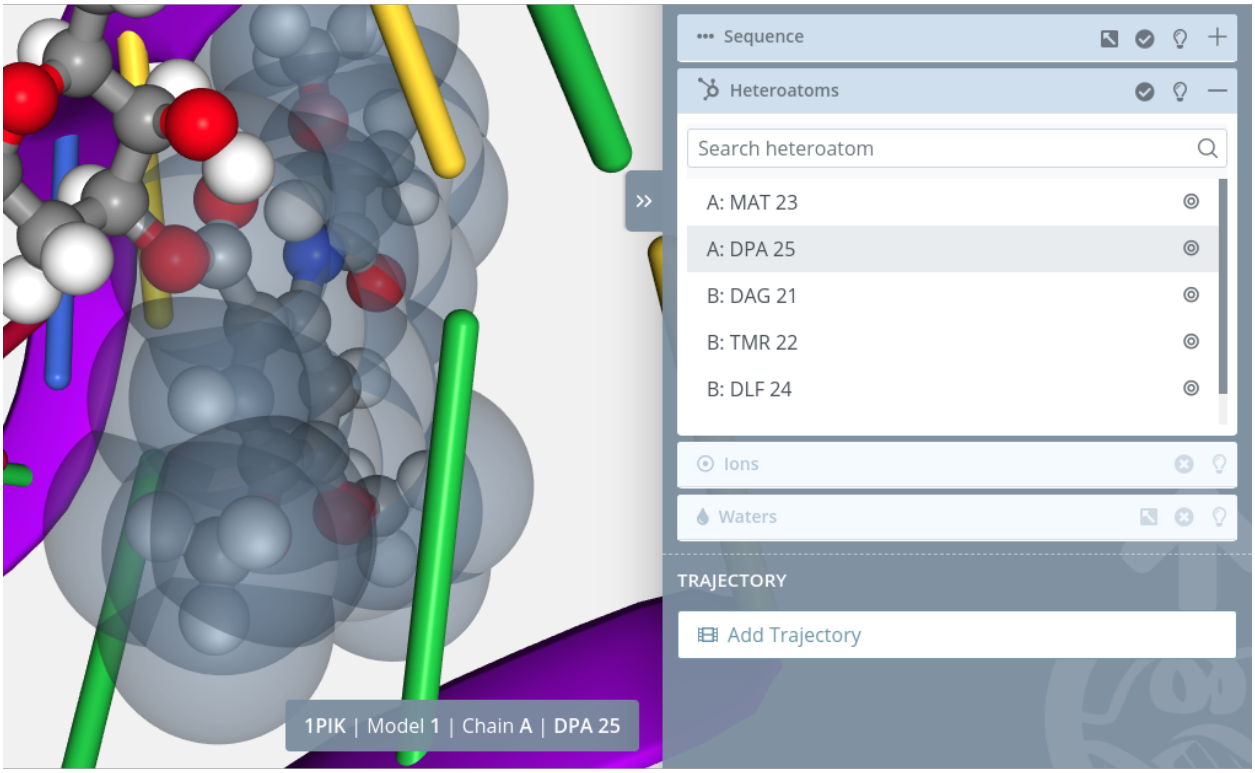



### Unselection

**Clicking on a selected heteroatom** will **unselect** it from the current selection.

### Zoom

**Clicking on the Center button**  of each heteroatom will do a zoom on it:




If there are **no heteroatoms** in the selected structure, this block menu will be disabled:


### Ions


This block shows **all the ions of the structure**.

There is a mini menu at the right side of the block header:

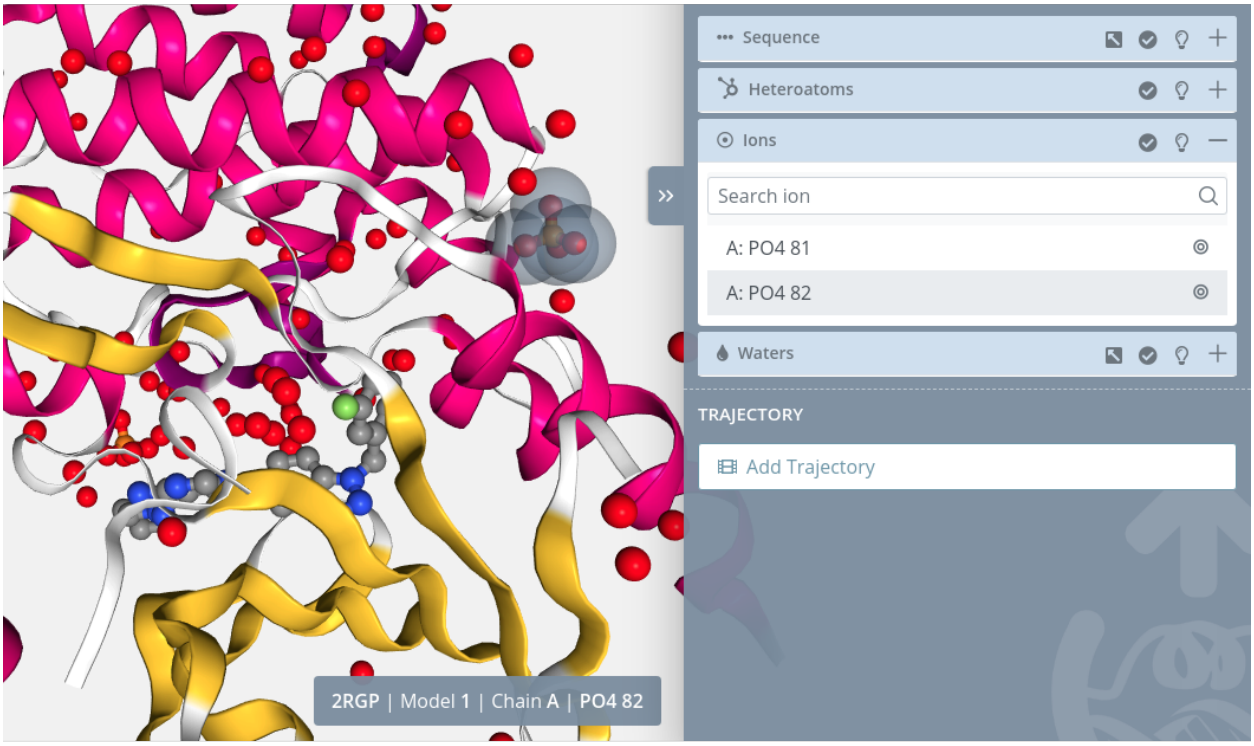
- **Select / unselect all:**  allows to select or unselect all the molecules of this block with a single click.
- **Show tips:**  opens a modal dialog with a short help for this section
- **Show / hide block:**  allows to open or collapse the panel.

There is a **search box** on the top of the ions list that allows users to perform **searches** on this list.

Different actions can be performed with the ions:

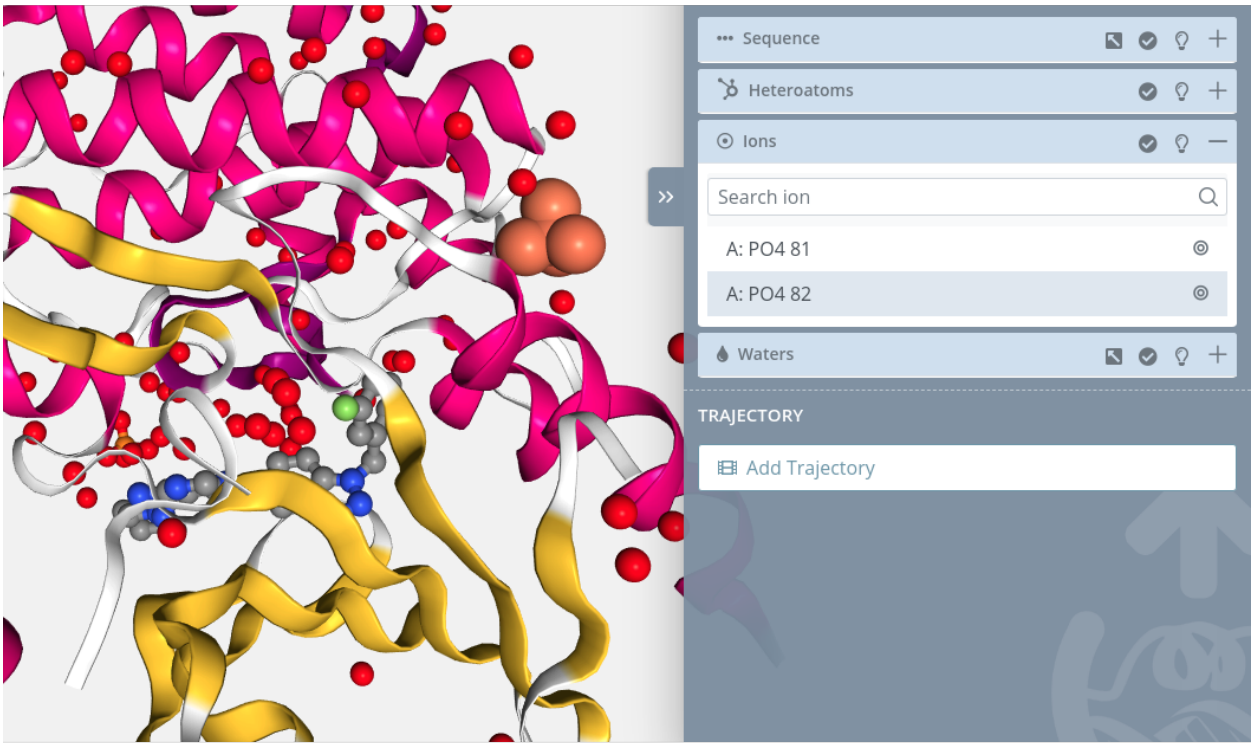
### Highlight

Passing the **mouse over** an ion will **highlight it** in the stage:



### Selection

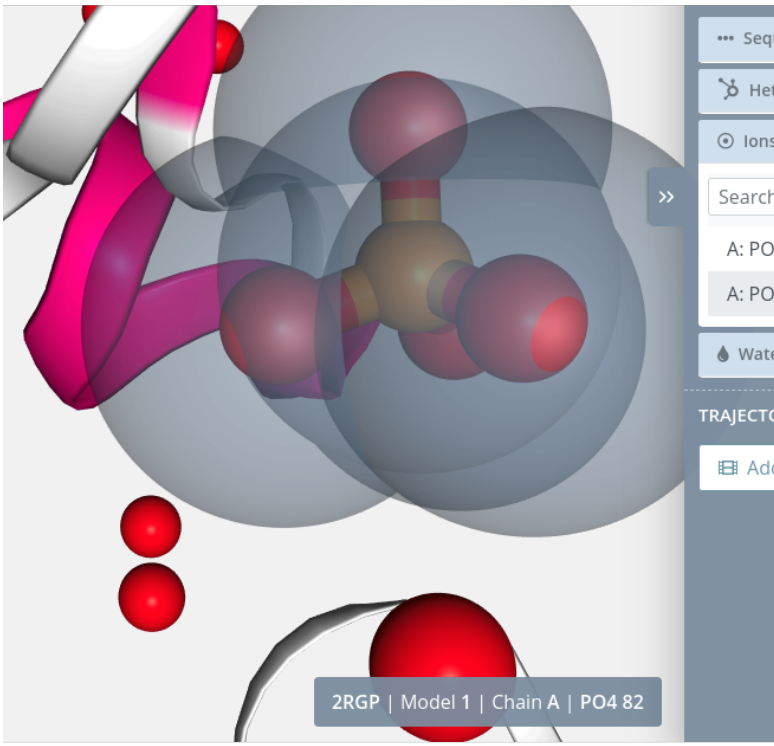
**Clicking on an ion** will select it in the current selection **applying to it** the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:




### Unselection

**Clicking on a selected ion** will **unselect** it from the current selection.

### Zoom




**Clicking on the Center button** of each ion will do a zoom on it:

If there are **no ions** in the selected structure, this block menu will be disabled:


### Waters

There are **two ways** to perform sequence waters selection: directly through ***the block in the Selection panel*** or though the ***Zoom window***:

### Selection panel block


This block shows **all the waters of the structure** classified by chains.

There is a mini menu at the right side of the block header:

- **Open / close external window:** allows to open or close the Zoom window for this section.
- **Select / unselect all:** allows to select or unselect all the molecules of this block with a single click.
- **Show tips:** opens a modal dialog with a short help for this section
- **Show / hide block:** allows to open or collapse the panel.

Different actions can be performed with the water molecules:

### Highlight

Passing the **mouse over** a water molecule will **highlight it** on the stage:


## Selection

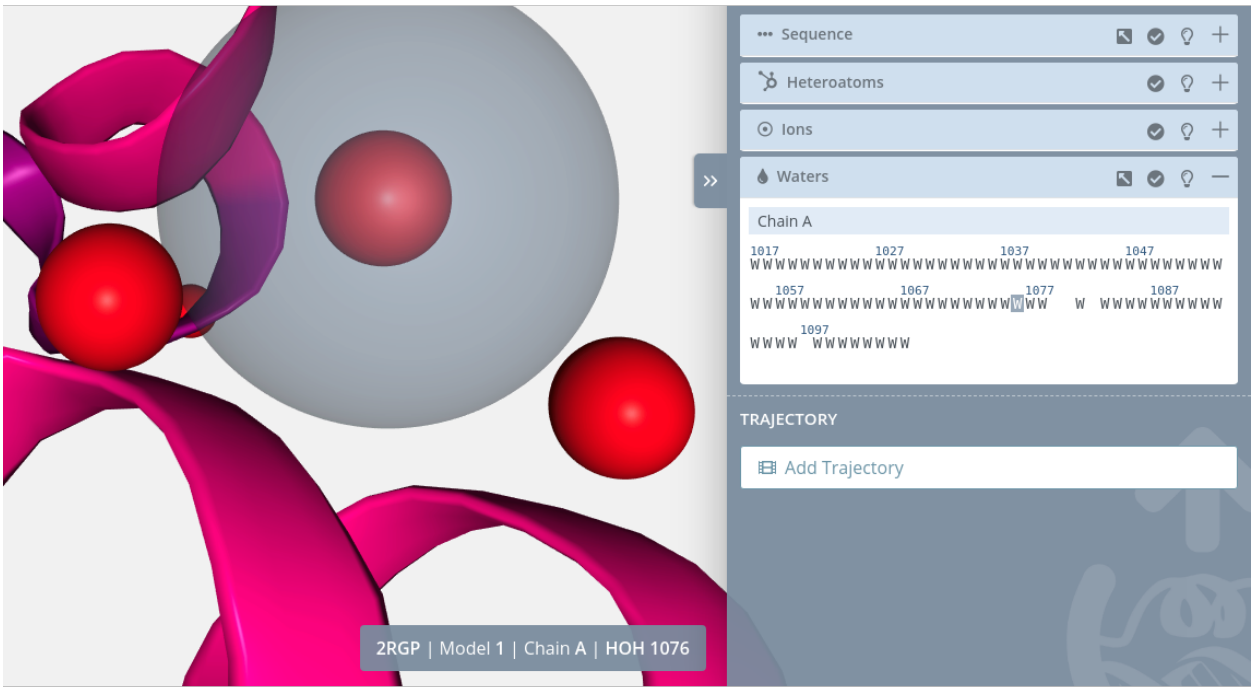
**Clicking on a water molecule** will select it in the current selection **applying to it** the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:


### Unselection

**Clicking on a selected water molecule** will **unselect** it from the current selection.

### Zoom

**Clicking on a water molecule** with the mouse **left button while pressing the Alt key** will do a zoom to the water molecule:




### Multiple selection

For **selecting multiple water molecules** just click the first water molecule of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

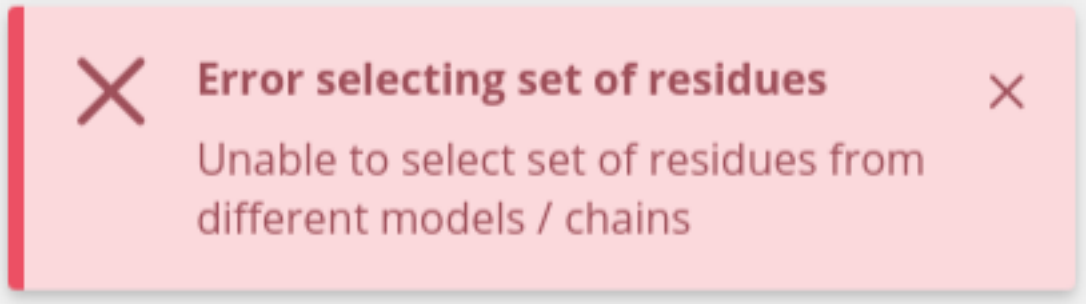
Then, click the last water molecule of the custom sequence again with the mouse **left button while pressing the Shift key**:


### Multiple unselection

For **unselecting multiple water molecules** is exactly the same process: just click the first water molecule of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

Then, click the last water molecule of the custom sequence again with the mouse **left button while pressing the Shift key**.

Note that **multiple selections** are only **allowed** between water molecules of the **same Model and Chain**. Trying to select multiple water molecules from **different Model and / or Chain** will show an **error notification**:




If there are **no water molecules** in the selected structure, this block menu will be disabled:


### Zoom window


This window shows the same information of the ***Waters block*** but in a little more detail.

There is a mini menu at the right side of the window:

- **Select / unselect all:** allows to select or unselect all the molecules of this block with a single click.
- **Close window:** closes the window.

The actions that can be performed are the same that in the **Waters block**:

### Highlight

Passing the **mouse over** a water molecule will **highlight it** on the stage:


## Selection

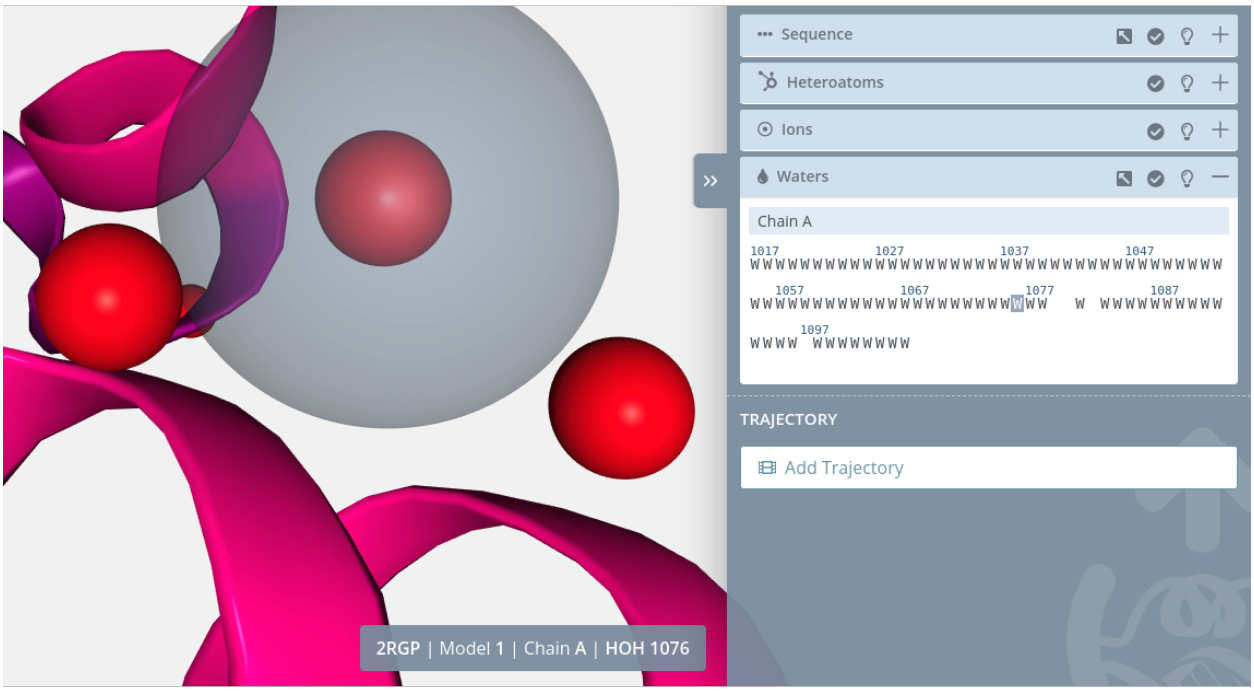
**Clicking on a water molecule** will select it in the current selection **applying to it** the molecular representation, radius, color scheme and opacity selected in the representations panel for the **current representation**:


### Unselection

**Clicking on a selected water molecule** will **unselect** it from the current selection.

### Zoom

**Clicking on a water molecule** with the mouse **left button while pressing the Alt key** will do a zoom to the water molecule:




### Multiple selection

For **selecting multiple water molecules** just click the first water molecule of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

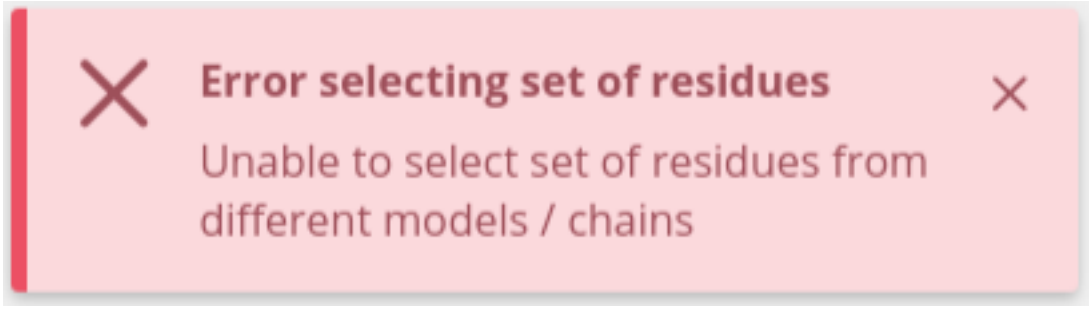
Then, click the last water molecule of the custom sequence again with the mouse **left button while pressing the Shift key**:


### Multiple unselection

For **unselecting multiple water molecules** is exactly the same process: just click the first water molecule of the custom sequence with the mouse **left button while pressing the Shift key**. A small cross will be shown next to the mouse pointer:

Then, click the last water molecule of the custom sequence again with the mouse **left button while pressing the Shift key**.

Note that **multiple selections** are only **allowed** between water molecules of the **same Model and Chain**. Trying to select multiple water molecules from **different Model and / or Chain** will show an **error notification**:

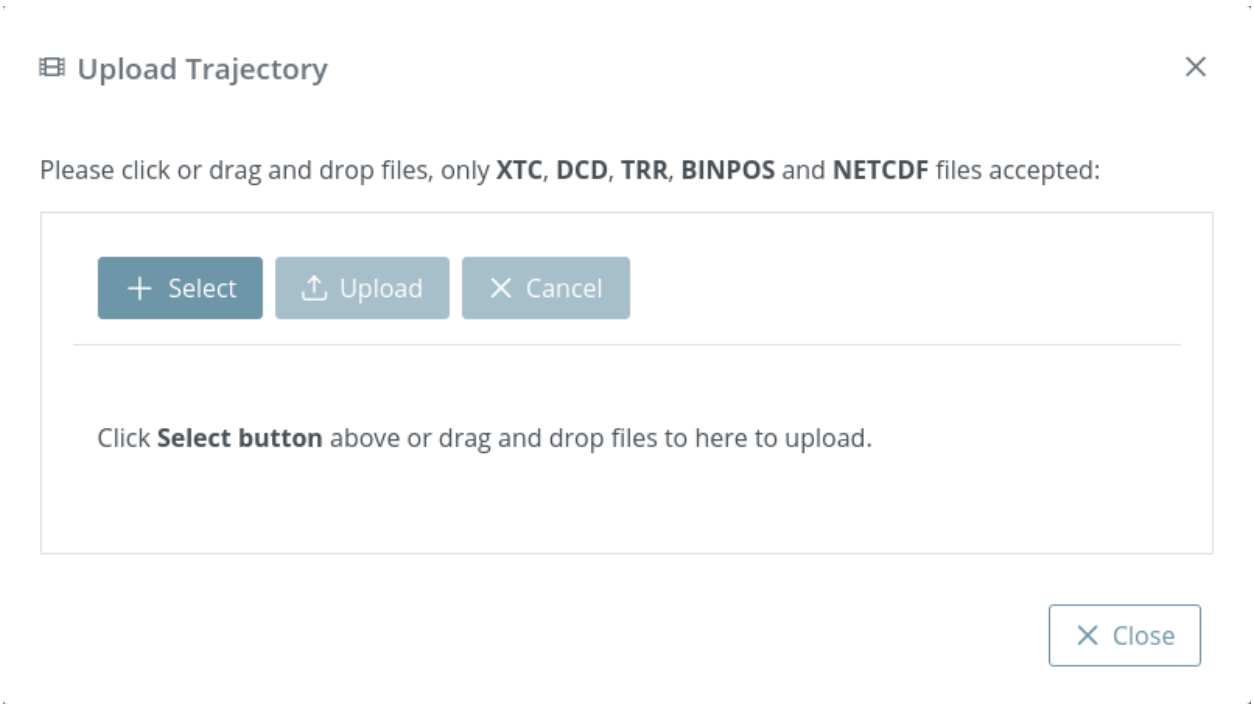


### Trajectories

Each structure can be linked to a **trajectory**. In this section, initially there is a button that opens a modal window for uploading this **trajectory** associated with the structure.

### Add trajectory

Clicking the button **Add trajectory** will open the modal window for uploading a trajectory:


This modal window allows **uploading a single trajectory**. Note that depending on the file size, **the process may take a while**. After uploading it to the server it will be processed through **MDsrv**.

As explained in the introduction, in the backend of this web application is running **MDsrv**, a powerful tool for viewing and sharing **molecular dynamics simulations** on the web. So once a trajectory is uploaded, MDsrv processes it in order to **stream it frame by frame**.

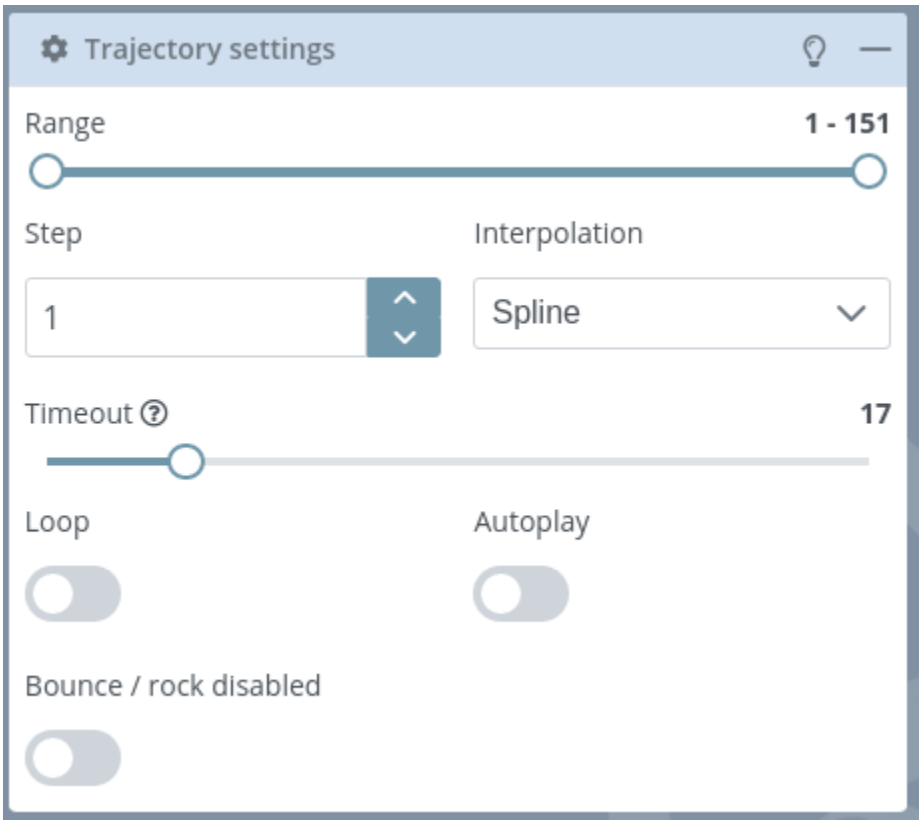
For further information about **MDsrv**, please visit the official website or the Nature Methods paper.

In the current version, only **XTC**, **DCD**, **TRR**, **BINPOS** and **NETCDF** (.netcdf / .nc) formats are accepted and the maximum file size is **500MB**.

### Player


Once the trajectory has been **uploaded and processed** in the backend, it can be played through the **trajectory player**. In this player, trajectories can be **played**, **paused** or played manually either **frame by frame** or **dragging the slider**.

### Settings




This block allows users to modify the **trajectory settings**.

There is a mini menu at the right side of the block header:

- **Show tips:**  opens a modal dialog with a short help for this section
- **Show / hide block:**  allows to open or collapse the panel.

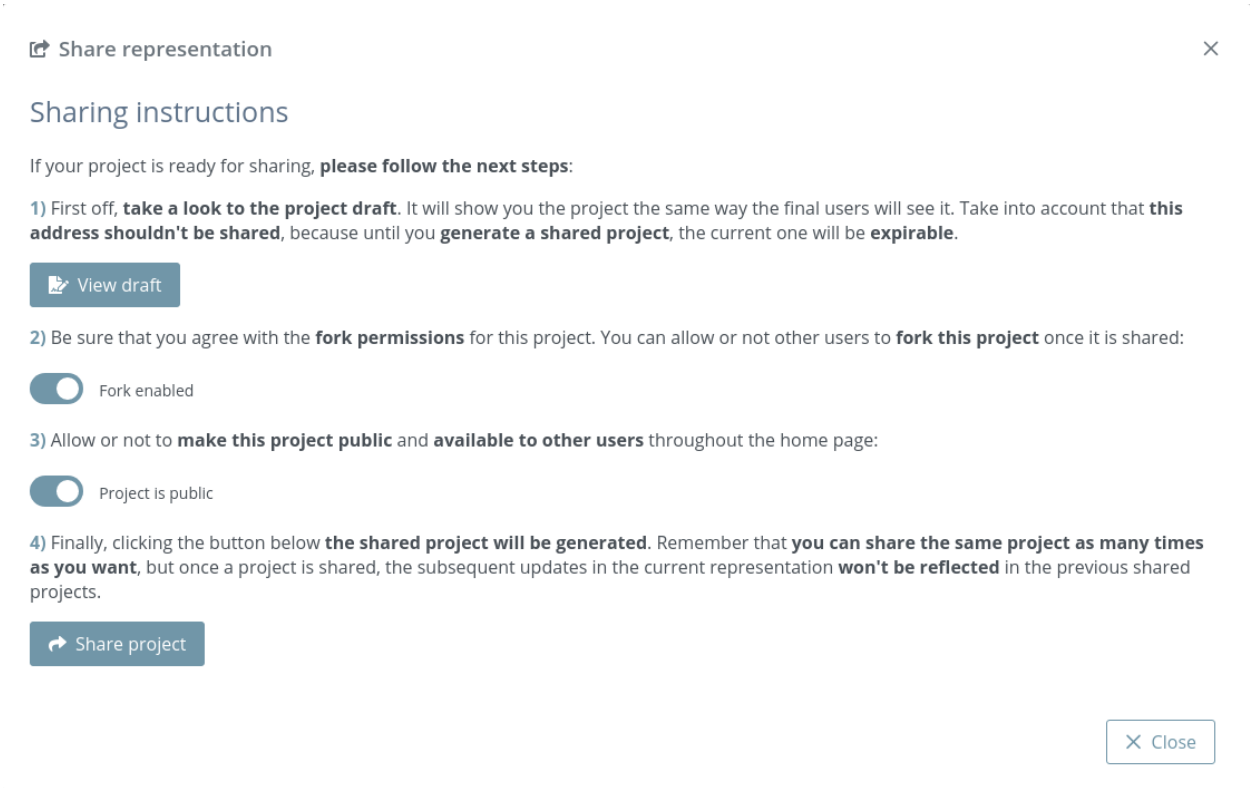
Different trajectory properties can be updated:

- **Range:** initially set from the first to the last frame of the trajectory, defines a **range of frames** with which the trajectory will be played.
- **Step:** defines the number of frames between playing steps.

- **Interpolation:** type of interpolation between steps. Possible values: None, Linear or Spline.
- **Timeout:** timeout between playing frames. Actually this slider is in a logarithmic scale from **50** to **10000** milliseconds, but it has been set from 0 to 100 for the sake of simplicity.
- **Loop:** if enabled plays the trajectory indefinitely.
- **Autoplay:** if enabled plays the trajectory automatically.
- **Bounce:** if enabled plays in rock / bounce mode (back and forth).

### 1.3.5 Share

The **Share button**, located at the top right of the **stage**, opens a modal window for creating a shared version of the current project.




In this window, users must follow four steps:

### Draft

Take a look at the **project Draft**. This Draft is an exact copy of the **Shared project** so it allows users to figure how the final project will look.

Note that as a **draft version** of the final **Shared page**, some of the actions are **disabled** in this draft page: **Embed code, QR code** generation and **fork project**. The rest of the actions are **exactly the same** as in the final Shared version.

### Fork

Be sure to agree with the **fork permissions**. Note that once the project is shared, if fork is enabled, every user with the Share representation link **will be able to fork and edit it**.

### Public

Be sure to agree with the **public permissions**. Note that once the project is shared, if public is enabled, the shared project will be available from the Last projects list in the home page.

### Share

Finally, clicking the **Share project button** will generate a new read-only project with a different identifier. Once the button is pressed, **three new sections** will appear in the modal window.

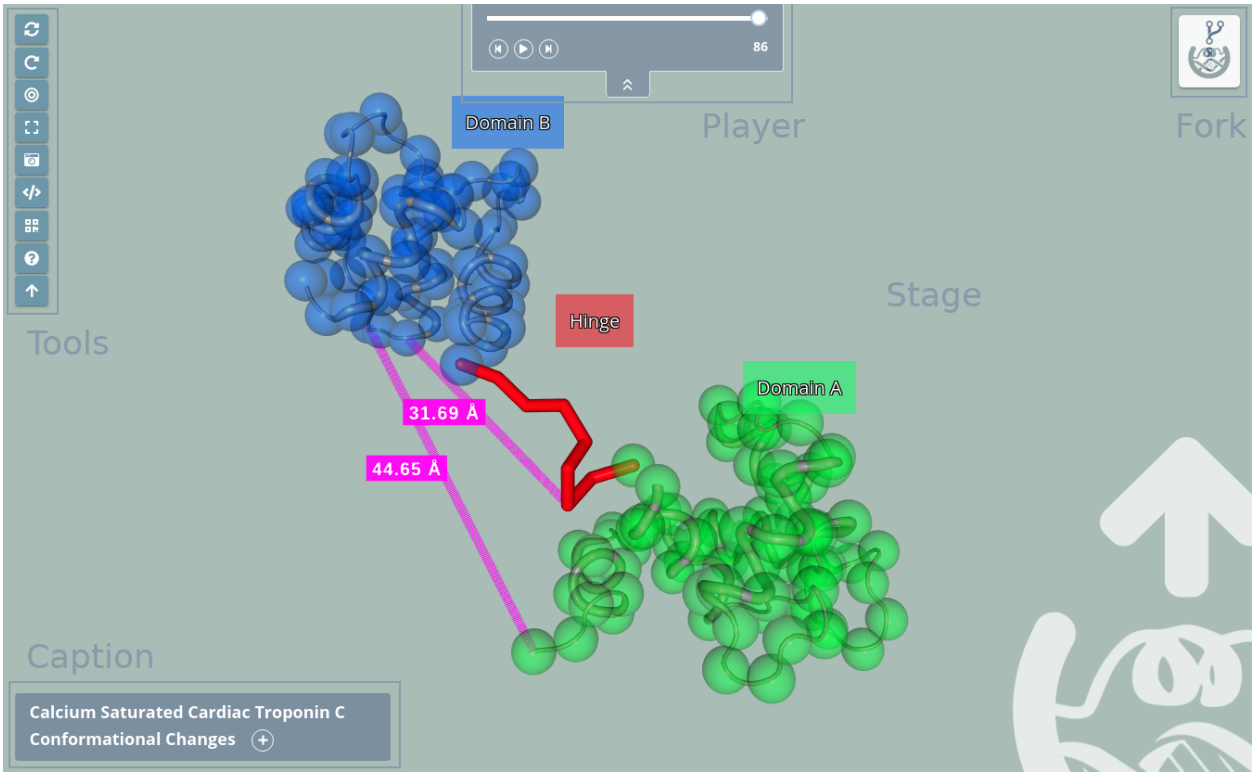

- A text box with the **new address** with a couple of buttons for copying or opening it.
- A text box with the **embed code**. Just copy and paste this code to a new website to embed it.
- A **QR code** that opens the new address.

It's very important to notice that **you can share the same project as many times as you want**, but once a project is shared, the subsequent updates in the current representation **won't be reflected** in the previous shared projects.

## 1.4 Share representation

Once the project is shared, a new **Share representation** will be created. This is a new address different from the **Edit representation** one. This page **doesn't expire** and we could say that it is a "read-only" version of the **Edit representation** page. That means that though it is an interactive page, the changes such as zoom or rotation are not saved.

This **Share representation page** can be splitted into five parts:




### 1.4.1 Stage

The **stage** covers the entire screen and the rest of the parts are on top of it. In the stage the **structure is loaded** and users can interact with it in several ways.

#### Zoom / Drag

Actions of **zoom in** and **zoom out** can be done with the scroll mouse or the trackpad of a notebook:

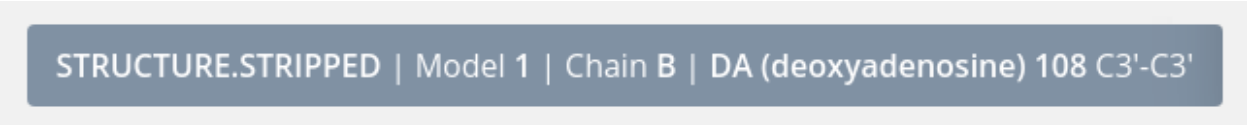
- Clicking **out of the structure** (that means in the "empty" part of the stage) with the **left button** and **dragging will rotate the view**.
- Clicking **out of the structure** (that means in the "empty" part of the stage) with the **right button** and **dragging will translate the view**.
- Double clicking **out of the structure** (that means in the "empty" part of the stage) with the **left button** will center the view.

#### Mouse actions

#### Mouse over actions

Passing the mouse over the molecules of the structure will **show their information** in the **legend** on the bottom right of the stage.

#### Legend

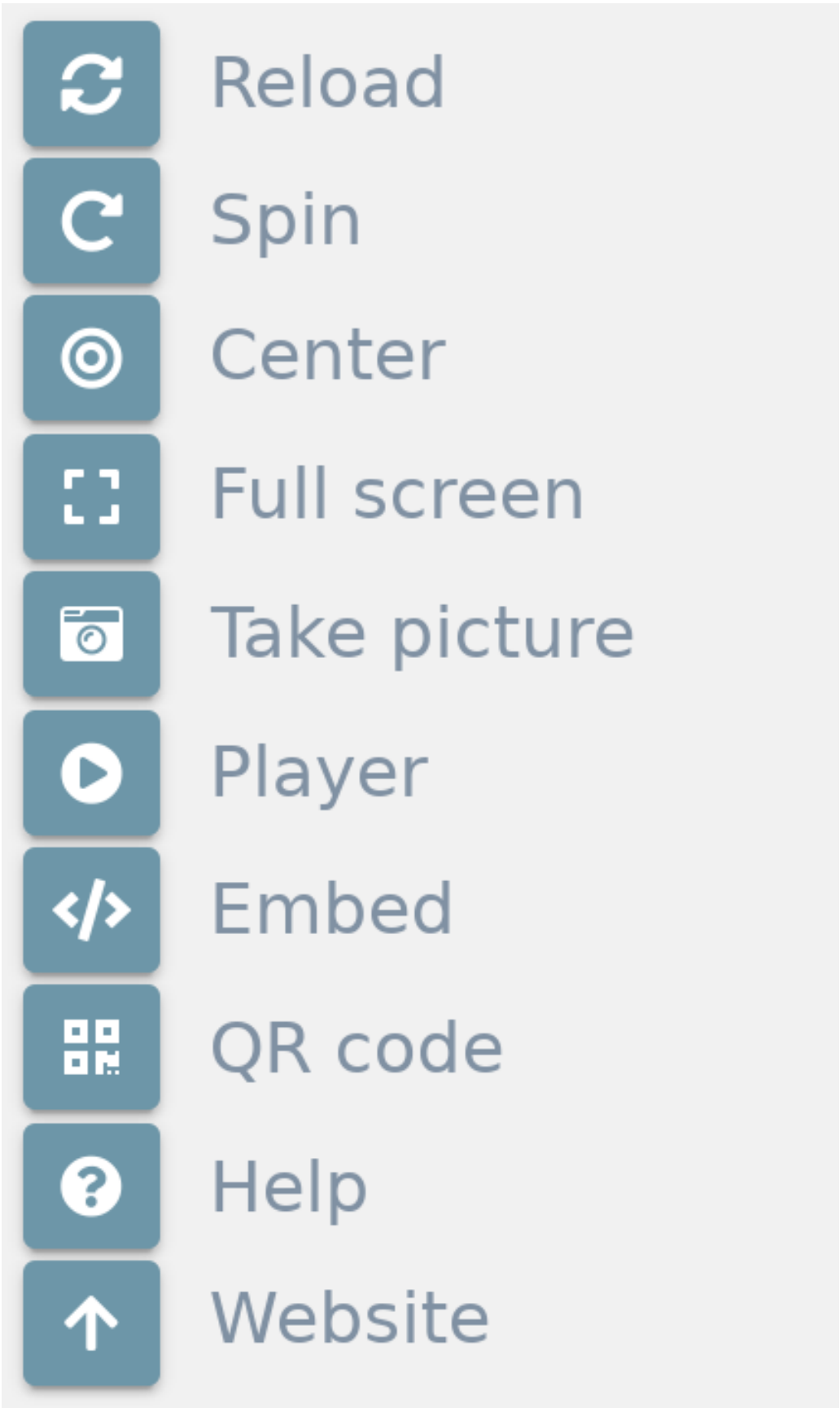



As explained in the previous section, passing the mouse over the molecules of the structure will **show their information** in the **legend** on the bottom right of the stage. This legend shows information about the molecule in the next format:

> **Structure file name |** Model **number |** Chain **ID | Residue name (Residue long name) Residue number**
> Atom name (or Bond)

### 1.4.2 Tools

The tools menu is at the top left of the **stage** and allows users to make some actions over it. Note that the tools of the **Shared representation** are different from the ones of the **Edit representation**.


Reload
Spin
Center
Full screen
Take picture
Player
Embed
QR code
Help
Website

- *Reload*
- *Spin*
- *Center*
- *Full Screen*
- *Take picture*
- *Player*
- *Embed*
- *QR code*
- *Help*
- *Website*

### Reload

Clicking this button **restores the view to the initial position** on the **stage**.

### Spin

Clicking this button starts / stops a **spinning animation** over the elements of the **stage**.

### Center

Clicking this button **centers** the structure(s) position on the **stage**.

### Full screen

Clicking this button opens the **fullscreen mode**. For **exiting** full screen mode, just **click the button again** or press the **Esc key**.

### Take picture

Clicking this button **takes a picture** of the **stage**. Depending on the zoom and the amount of molecules of the representation, **it can take a few seconds**. In order to get a **good resolution**, **the stage will move** during the process of taking the picture, though it will return to its **normal status** once this process is finished.

Note that if there are **representation labels** present, they will not be shown in the picture.

### Player

Only shown if there are **multiple trajectories** present in the representation, allows to **play / pause** them.

In case there is only one trajectory, it will be controlled through the ***Player panel***.

### Embed

Opens a modal dialog with the **embed code**. Just copy and paste this code to a new website to embed it.

Below you can find an example of an embed code:

```
<iframe width="500" height="500" src="https://mmb.irbbarcelona.org/3dRS/embed/
↪60c1ff158a6696.79962296" title="3dRS" frameborder="0" allowfullscreen></iframe>
```

And how it looks embedded in a HTML page:

### QR code

Opens a modal dialog with the **QR code** that opens the address of the current **Shared representation**:


Get QR code for this representation
Close

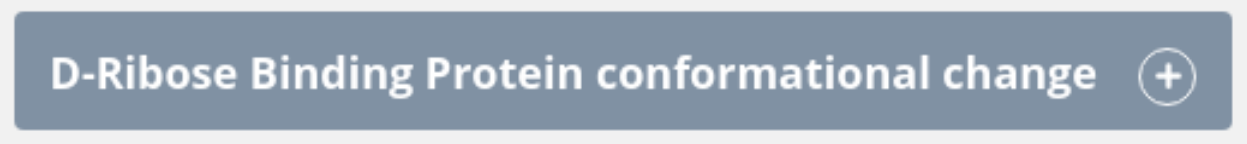
#### Help

Link to this same Read the Docs.

#### Website

Link to the **3dRS official web page**.

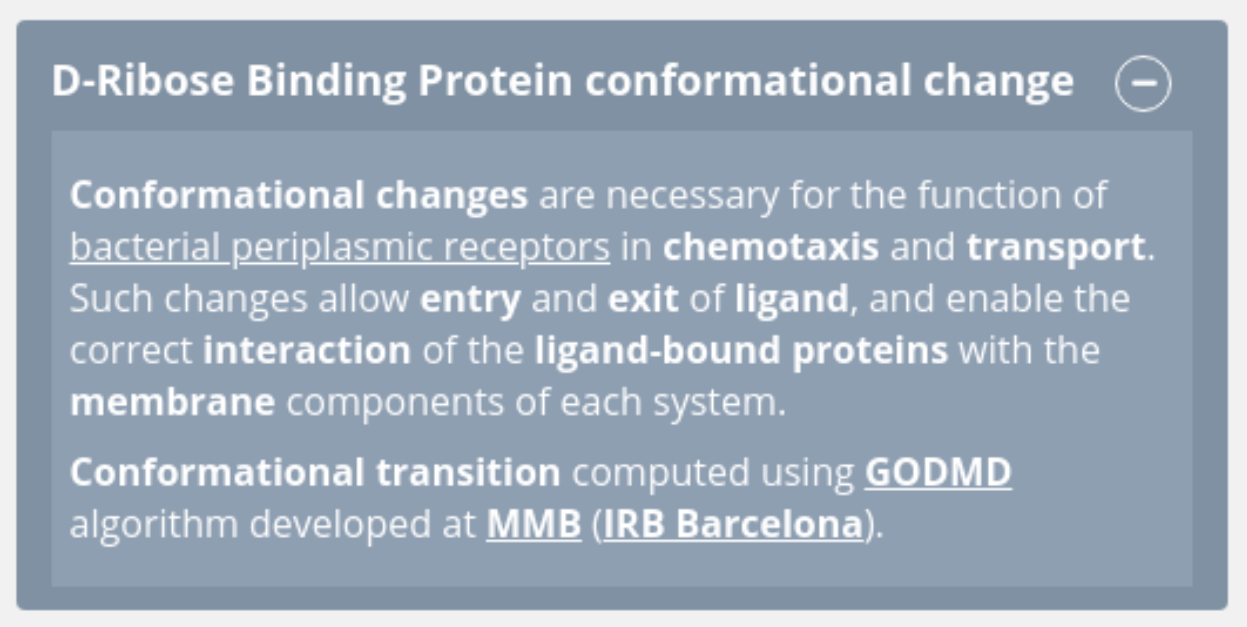
### 1.4.3 Caption




The **Caption** panel is at the bottom left of the stage and shows the project title and caption added in the **Project Settings** modal window.

If **no title** is added, the **Caption won't be shown**.

If **no caption** is added, only the **project title** will be shown, if it's added, a  **button** appears and allows **displaying the Caption**:




### 1.4.4 Player


The **Player** panel is at the top of the stage and allows to control the **trajectory**. In this **player**, trajectories can be **played**, **paused** or played manually either **frame by frame** or **dragging the slider**.

If **no trajectory** is added, the **Player won't be shown**.

In the other hand, if **more than one trajectory** is provided (in case there is more than one structure), this player **won't appear** and the control of **all the trajectories** will be performed through the Tools ***Player*** button.

### 1.4.5 Fork

If fork has been enabled in the **Project Settings** modal window or in the **Share** modal window, this button will appear in the top right of the stage. Clicking on it creates a new **Edit representation** page that allows editing **all the**

**representations and selections** present in the current **Shared project**. Once the new page is created, users will be automatically redirected to it.

Be aware that **some browsers block the opening of new tabs**, so in this case, users sould manually allow this browser feature.

## 1.5 Changelog

### 1.5.1 1.1.1

15/11/2021 - v1.1.1

- Added link to **publication**
- Bug fix in trajectories

### 1.5.2 1.1.0

30/07/2021 - v1.1.0

- Distance-based custom selection
- Minor improvements
- Minor bug fixes

### 1.5.3 1.0.1

15/06/2021 - v1.0.1

#### First stable release

- New gallery items
- UX bug fixes
- Allowing to disable labels in measurements

### 1.5.4 1.0.0

09/06/2021 - v1.0.0

#### First release

### 1.5.5 0.6.1

29/05/2021 - Beta v0.6.1

### 1.5.6 0.6.0

21/05/2021 - Beta v0.6.0

### 1.5.7 0.5.0

14/05/2021 - Beta v0.5.0

### 1.5.8 0.1.0

26/03/2021 - Alpha version

CHAPTER

TWO

# GITHUB REPOSITORY.