Modelling a cell, dynamics to modify the surface

1.
Create a polygon cube, turn of interactive creation. Make the cube have 5 subdivisions in Width and Depth, but 2 subdivisions in height.
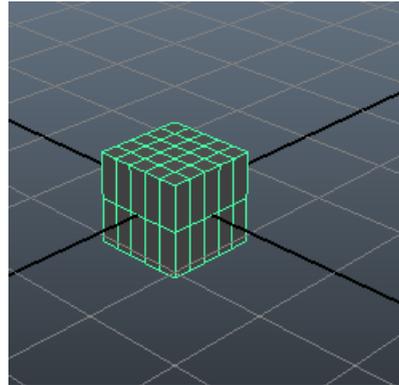
Scale out the middle vertices.
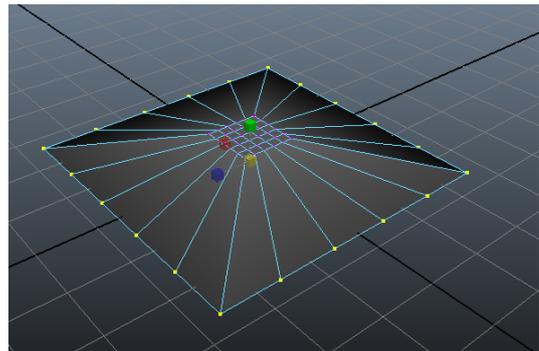
Looking from the top, move the vertices out in a star-like shape.
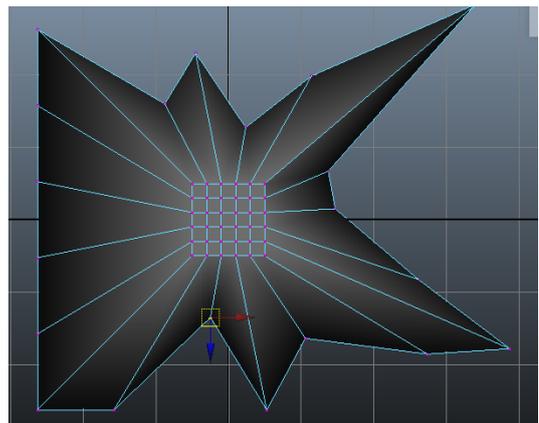
Move the middle vertices down to the same level as the bottom vertices
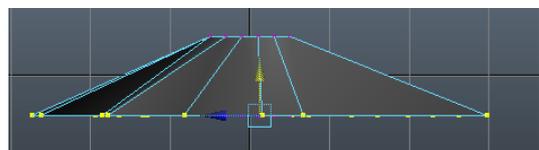
In the top view, spread out the vertices in the center, evenly.
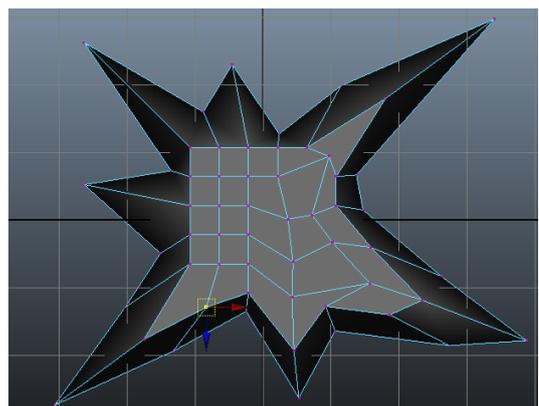
In the Polygons menu-set, do Edit Mesh, Insert Edge Loop Tool and insert an edge loop along the side of the cell.

Move the newly created vertices down towards the bottom by selecting them in the side view.
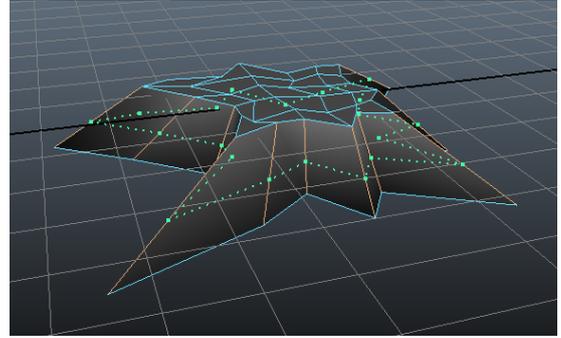
Turn on camera based selection, select the outermost vertices of the top part of the cell.
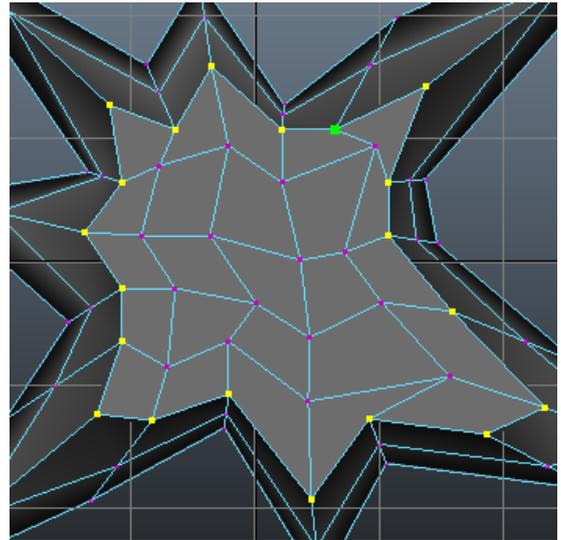
Move these vertices down as well
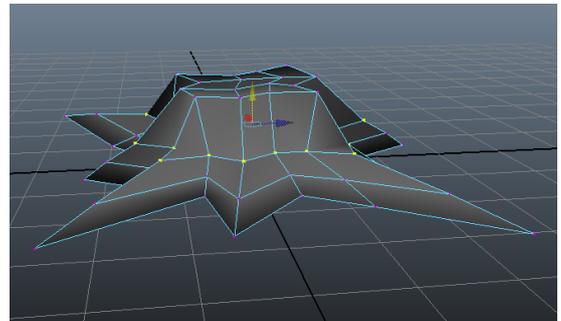
Select the top vertices and move those down as well
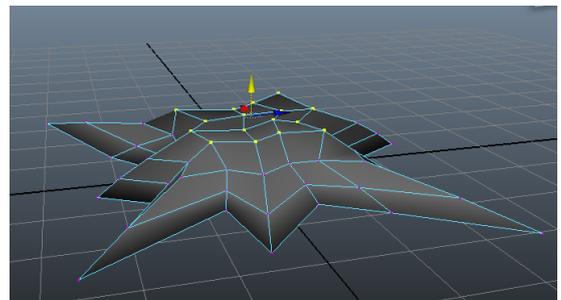
Press 3 to get a preview of how the smoothed lattice would look like. Edit the vertices if you are not happy with the look.
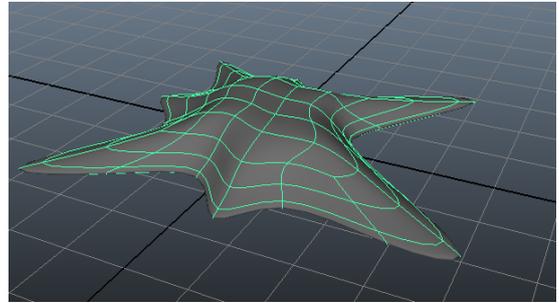
Do one smoothing using Polygons - Mesh -> Smooth
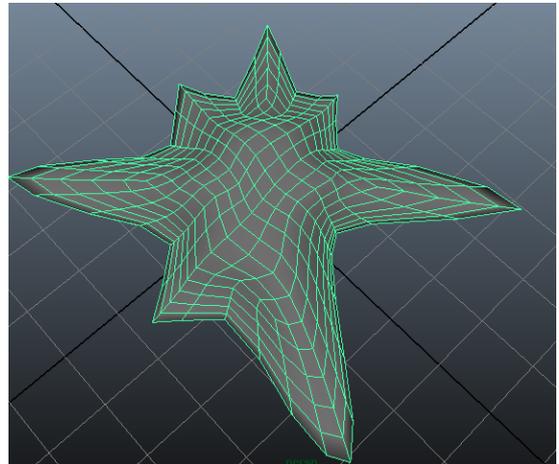
With the polygon mesh selected, go to the Dynamics menu-set and do Soft/Rigid Bodies -> Create Soft Body and press the options square. ☐

In the dialogue that appears change the parameters to this:

Press Create
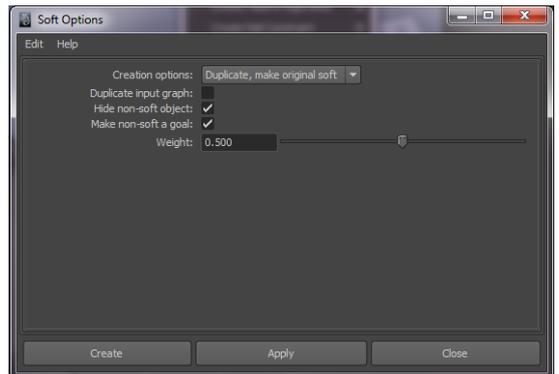
With the soft-body you just created selected:
Still in the Dynamics menu-set, do Fields -> Turbulence and press the options icon. Change the parameters for the Magnitude to 50 and the Frequency to 50 and press create.
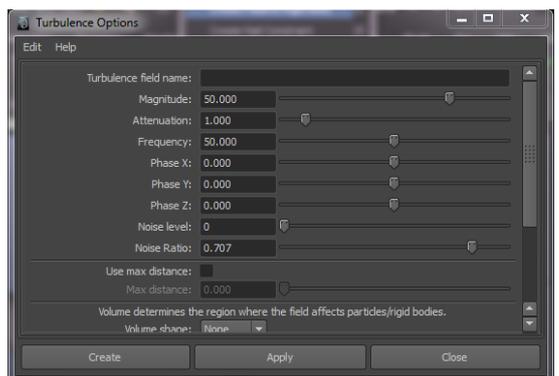
Now when you press the play button to the right of the timeline, you should get a nice random ondulation in the cell surface.

Do Polygons menu-set, Mesh -> Smooth on the cell to finalize the cell surface.

Plank DNA

Turn of interactive creation by unchecking Polygon Primitives -> Interactive Creation. Create a Polygon cube. Change its Scale Y to 0.2

In the top view, create a Nurbs Circle (with interactive creation turned off to get it exactly at radius = 2).

Make the polygon cube elongated by scaling (press R) and position it on the X-axis. Duplicate the polygon and position the new copy according to the image to the right.

Select both polygons. Group them (Ctrl+g) The new group should have its pivot right in the origin.

Double click the group in the outliner (should be named group1). Rename it basePair1

With the group selected, do Edit -> Duplicate Special and click the options box. In the options enter a Y translation of 0.33 and a Y rotation of 36 degrees, and 21 copies. Press Duplicate Special

You should see something like this in the viewport. Save the file as plankDNA.mb
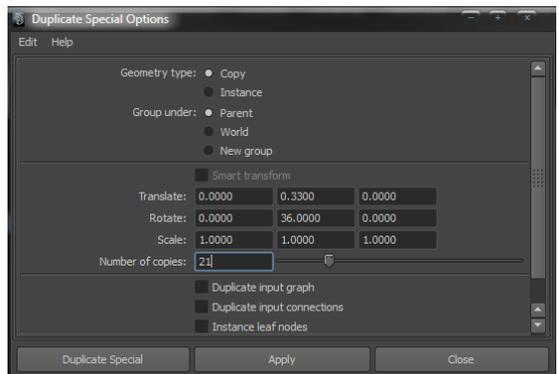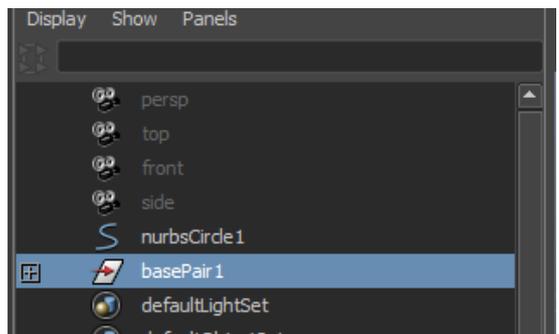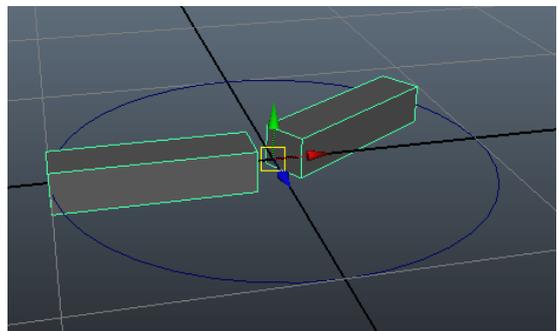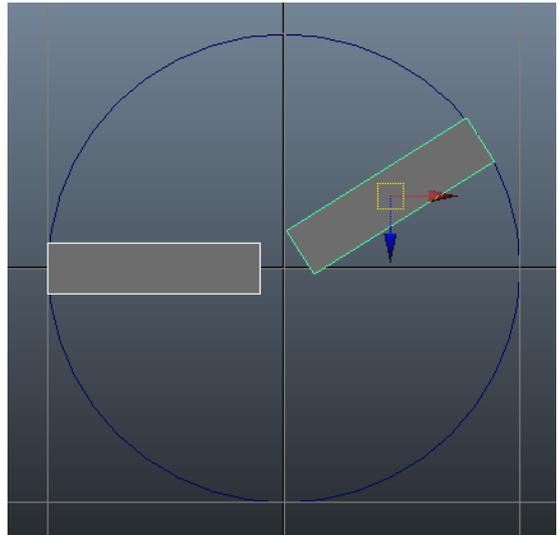
Spaghetti DNA

In the top view, create a Nurbs Circle (with interactive creation turned off to get it exactly at radius = 2).

Do Create -> CV Curve Tool and click the options box and check the Curve Degree = 1 Linear radio box.

Create a wedge using 3 CVs. The first two (the ones at x=-1 and in the origin) can be positioned exactly by keeping the X-key pressed while adding CVs (this will snap to grid). Place the third point anywhere. After placing the CV, hover the mouse over the circle, press C and press and hold the MMB and drag the CV in place (C will enable snap to curve).

Switch to side view and make a linear CV-curve with two CVs use X while drawing to make the length exactly = 1 unit

21 bp of DNA is 21 x 0.33 = 6.93 nm long so select the curve and change the Y scale to 6.93

With the new curve selected, in the Surfaces menu-set do Edit Curves -> Rebuild Curves options box. Use the settings shown here and press Rebuild

Go back in the perspective view, select first the wedge and then the new curve. Do Surfaces -> Extrude click the options and enter the following parameters:

21 bp of DNA takes 2 full turns, so the rotation shuold be 720 degrees.

Click Extrude to get a spiral surface.
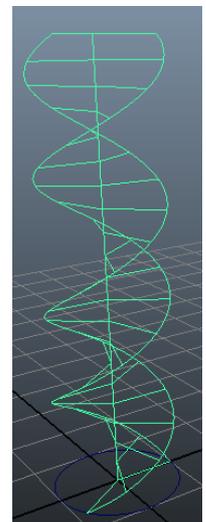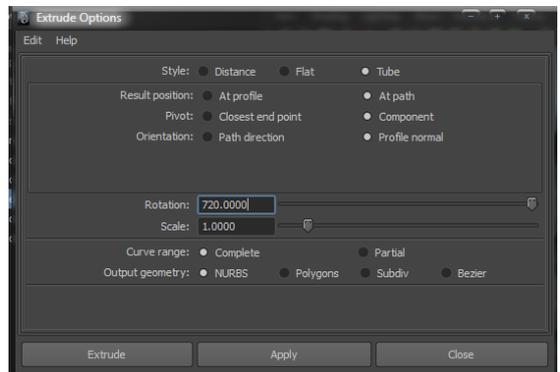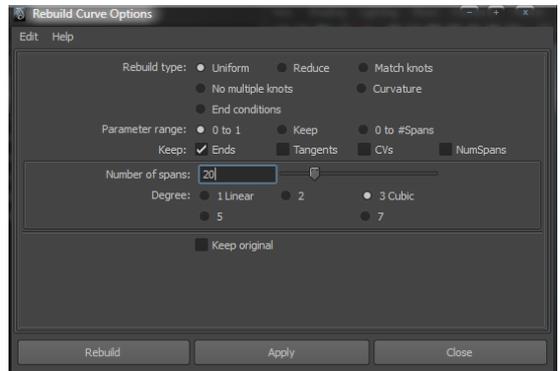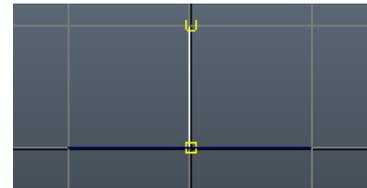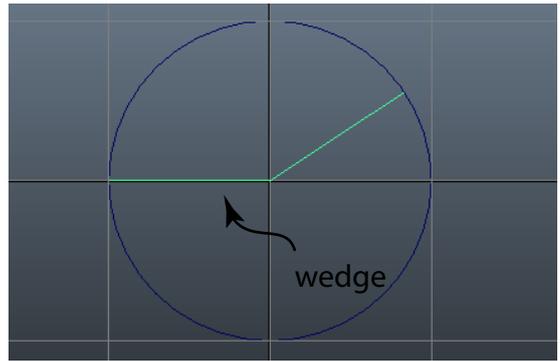
With the mouse on the extruded surface, RMB click and drag to Isoparm. Select both the outermost isoparms, the helical edges.

Do Edit Curves -> Duplicate Surface Curves to make two new curves that are copies of the selected isoparms.

With interactive creation turned off, create a NURBS circle. Scale all dimensions down to about 0.1

First select the circle, then one of the duplicated surface curves (should be called duplicatedCurve1 and 2 in the outliner). Do Surfaces -> Extrude options box, remove the rotation we used earlier and press Extrude.

Select the circle, and then shift select the other duplicated curve and press G (re-do the previous action) to extrude again.

Hide the first extruded surface by selecting it and pressing Ctrl+h
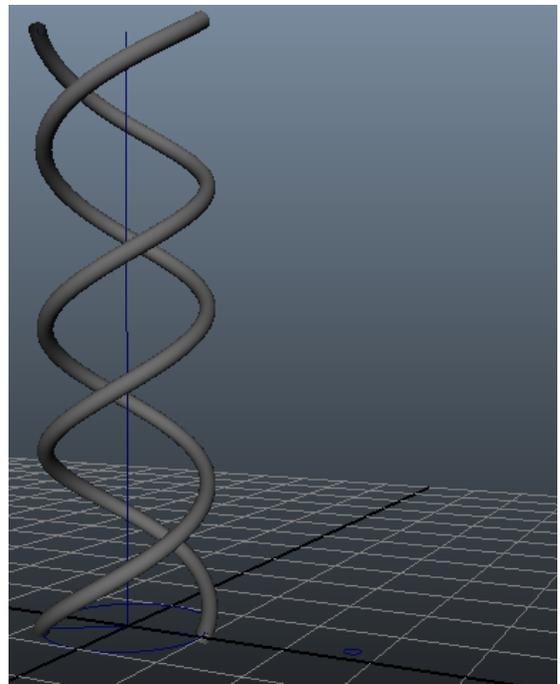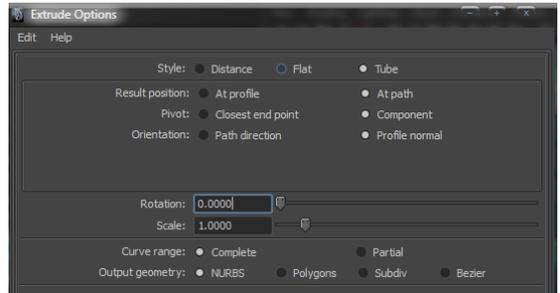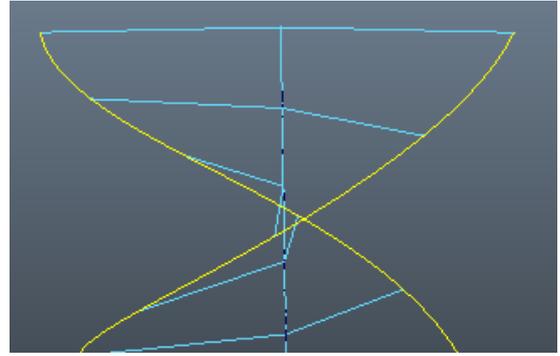
Animated Cadherin Structure using mMaya

In the mMaya Molecule Editor - the Import tab, enter the PDB ID: 1L3W in the download section and press download, then import.

Go to the Main tab of the mMaya Molecule Editor, expand the ribbon / cartoon backbone section and check the backbone vis, caps vis, wire trace vis boxes, press the display res: high button.
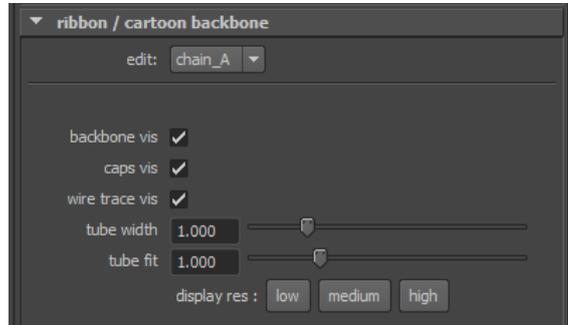
Select the cadherin tube geometry and duplicate it (ctrl+d). Hide the original mMaya molecule by going to the mMaya Editor, in the Main tab, under global uncheck Show Structure.

Switch to the Top view. In the Animations menu set, do Skeleton -> Joint Tool
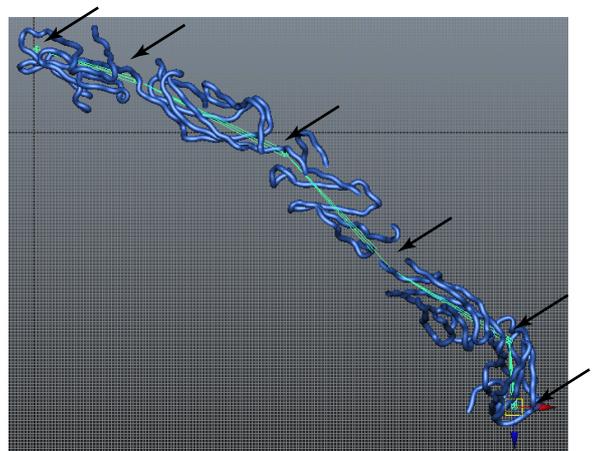
Using the joint tool place 6 joints at the edges between the different cadherin sub-units (as indicated by the arrows)

Switch back to perspective view and, starting with the first joint, move the joints up in the Y-direction so that the skeleton line up nicely with the cadherin structure.
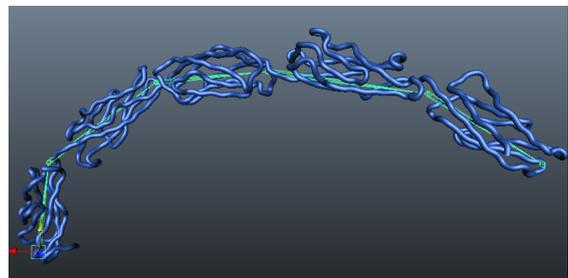
Do Skeleton -> IK Handle tool, with the tool first click the first joint in the skeleton chain, then the last to create an IK handle.
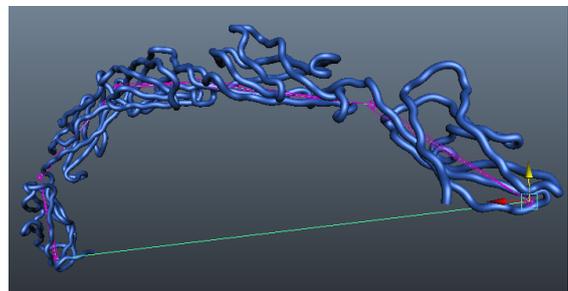
Select the joint1 in the outliner, shift select the cadherin geometry, do Skin -> Bind Skin -> Smooth Bind

Try moving around the handle.

Save the file as cadherin.001.mb

Holliday junctions in DNA using vHelix

vHelix is a plug-in for Maya developed in our lab to simplify the construction of DNA-nanostructures. Besides that, it can also be of use for anyone who wants to model DNA in an easy way.

Go to www.vhelix.net and download the plug-in file for your operating system. Save the file somewhere on your hard-drive where you can easily find it in the future.

In Maya, go to Window -> Settings/Preferences -> Plug-in Manager. In the Plug-in Manager, press the 'Browse' button and find the file you downloaded above. (On PC it will be called vHelix.mll, on Mac vHelix.bundle, on Linux libvHelix.so) Then close the Plug-in Manager.

You should now have access to a new menu called 'Helix'

In the 'Helix' menu, press the options-box of the 'Create helix'-command. In the pop-up, type 42 bases and press 'OK'. You should get something like this:
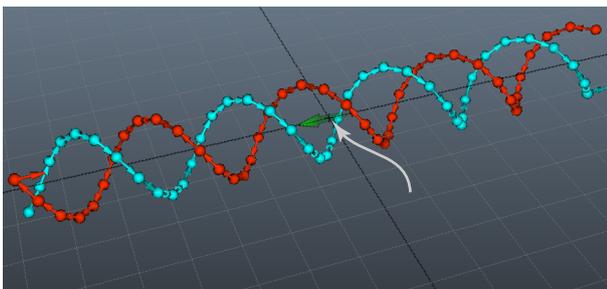
The little cross in the middle (arrow above) can be used as a handle to select the entire double-helix. Use the handle to select the first helix, move it to the side, and create a new 42 base-pair helix next to it.

In vHelix, DNA directionality in the phosphate backbone is represented as arrows along each strand.

Position the two helices close to each other, rotate them around their axis, to position two strands of opposite directionality so that they almost touch near the center of the helix.

Select two bases, each on a strand in a different helix. The selection order is important - the new connection will go *from* the base you select first, *to* the base you select second.

Do: Helix -> Connect bases

You should see the bases flip connections and the newly combined strand (that is now part of two helices) take a new color.

Aligning two strands of opposite directionality so that they almost touch

Selection, before 'Connect bases'
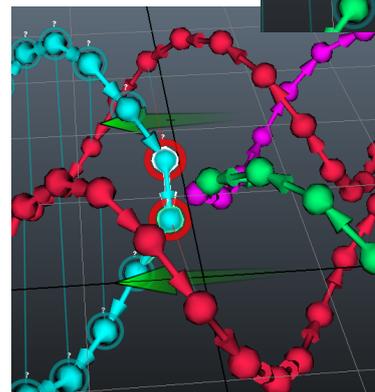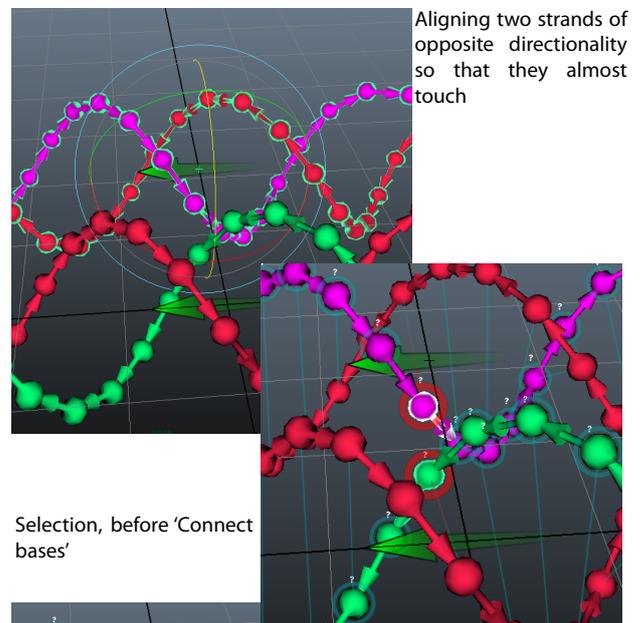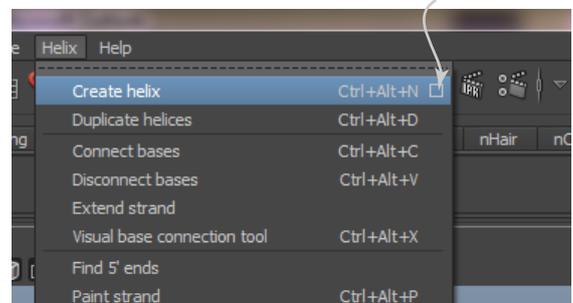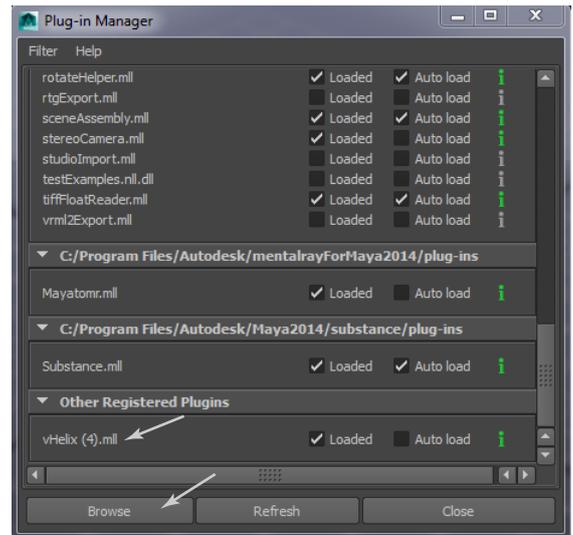
The same bases as above, after doing 'Connect bases'.

Now, select the two bases that were previously disconnected when performing the first 'Connect bases'-operation, again keep in mind to shift-select the bases in the same direction as you would like the new connection to occur.

Again, do 'Helix' -> 'Connect bases' to create the Holliday junction (double crossover).

In conditions where the Mg2+ concentration is relatively high, Holliday junctions are known to take the form of two stacked cylinders oriented approximately at an angle of about 60° between them. Lets try to re-create that conformation.

Rotate and translate one of the helices so that the two helices form this x-like conformation:
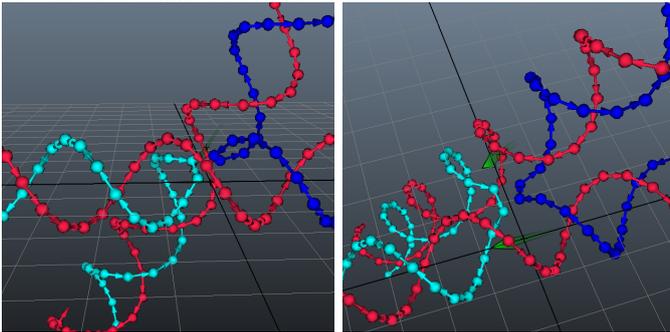
You will notice that you cannot render the vHelix objects themselves. To make something renderable we'll first create CV-curves out of the strands:

Select the two helices (not the bases, select the actual helix objects in the outliner or use the + handles in the center of the helices). With those selected, do: 'Helix' -> 'Create curves from strands'.

You won't see the strands, they will be right inside the vHelix objects, select all curves in the outliner and drag them out.

Using a small NURBS circle, make extrusions along each strand curve and take some renders, here an occlusion pass:

Selecting the bases for the other crossover.

The completed double-crossover after the second 'Connect bases'