Building and Animating Amino Acids and DNA Nucleotides in ShockWave Using 3ds max

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1 Introduction

1.1 Purpose

This document describes how to take a text file describing an amino acid or DNA nucleotide and create a model of that amino acid or nucleotide in *3ds max*[1], using a Max script written for that purpose, with animation as desired. We then describe how to export those models into the *ShockWave* format, and how to then use *Director* to create an animation of the amino acid or nucleotide that can be placed on the web.

1.2 Names and Abbreviations for the Amino Acids

	Name	Symbols		Formula
1.	Alanine	Ala	A	C_3O_2N
2.	ARginine	Arg	R	$C_6O_2N_4$
3.	AsparagiNe	Asn	N	$C_4O_3N_2$
4.	Aspartic AciD	Asp	D	C_4ON_4
5.	Cysteine	Cys	C	C_3O_2NS
6.	Glutamic Acid	Glu	E	C_5O_4N
7.	Glutamine	Gln	Q	$C_5O_3N_2$
8.	Glycine	Gly	G	C_2O_2N
9.	Histidine	His	H	$C_6O_2N_3$
10.	Isoleucine	Ile	I	C_6O_2N
11.	Leucine	Leu	L	C_6O_2N
12.	Lysine	Lys	K	$C_6O_2N_2$
13.	Methionine	Met	M	C_5O_2NS
14.	Phenylalanine	Phe	F	C_9O_2N
15.	Proline	Pro	P	C_5O_2N
16.	Serine	Ser	S	C_3O_3N
17.	Threonine	Thr	T	C_4O_3N
18.	Tryptophan	Trp	W	$C_{11}O_2N_2$
19.	Tyrosine	Tyr	Y	C_9O_3N
20.	Valine	Val	V	$C_5O_2NH_{11}$

1.3 Names and Abbreviations for the Nucleotides

1.3.1 The Sugar Deoxyribose

All nucleotides have in common the sugar and the phosphate group. The five-carbon sugar component of DNA (deoxyribonucleic acid) is known as deoxyribose (see Figure 1.3-1). This sugar alternates with phosphate groups to form the "backbone" of the DNA polymer. It binds to the four different nitrogenous bases G, A, C, T shown below.

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[1] AutoDesk *3ds max* 8.0, Service Pack 3

The binding between the sugar and the phosphate group occurs either with the sugar 5' carbon or with the sugar 3' carbon, as indicated in the figure. The bond between one of the nitrogen atoms in the nitrogenous base and the sugar occurs at the 1' carbon.

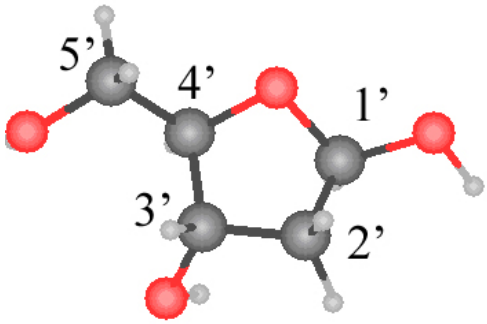

Figure 1.3-1: Deoxyribose

1.3.2 Guanine (G)

Guanine consists of the nitrogenous base Guanine (see Figure 1.3-2) with the sugar and phosphate group (see Figure 1.3-3 below). In Figure 1.3-3 the phosphate group is bound to the 5' carbon in the sugar.

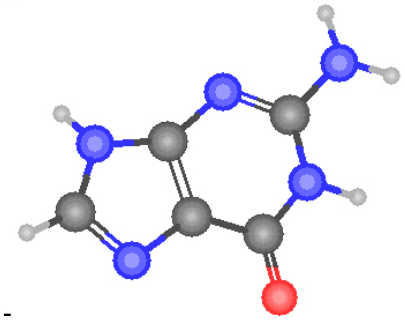

Figure 1.3-2: The Nitrogenous Base Guanine (G)

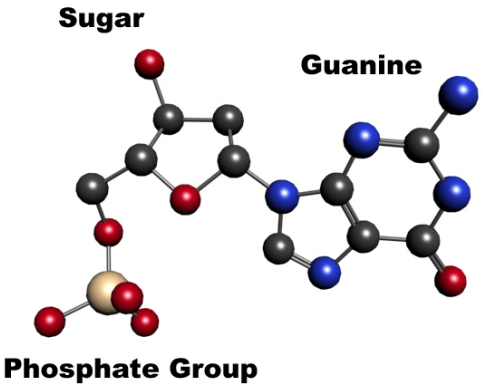

Figure 1.3-3: Guanine (G) with Phosphate Group

1.3.3 Adenine (A)

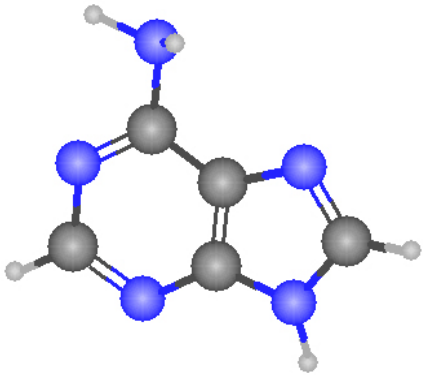

Figure 1.3-4: The Nitrogenous Base Adenine (A)

1.3.4 Cystocine (C)

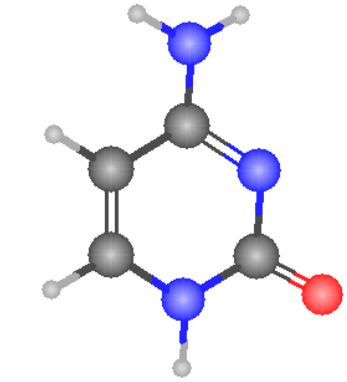

Figure 1.3-5: The Nitrogenous Base Cystocine (C)

1.3.5 Thymine (T)

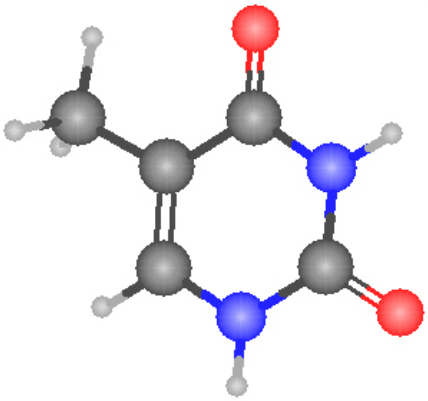

Figure 1.3-6: The Nitrogenous Base Thymine (T)

1.4 Files Used In This Document

This document and the *3ds max* files, *ShockWave* Director files etc. described herein can be found in a folder at

http://web.mit.edu/viz/soft/visualizations/biochemistry/

Figure 1.4-1 shows the directory structure of that folder.

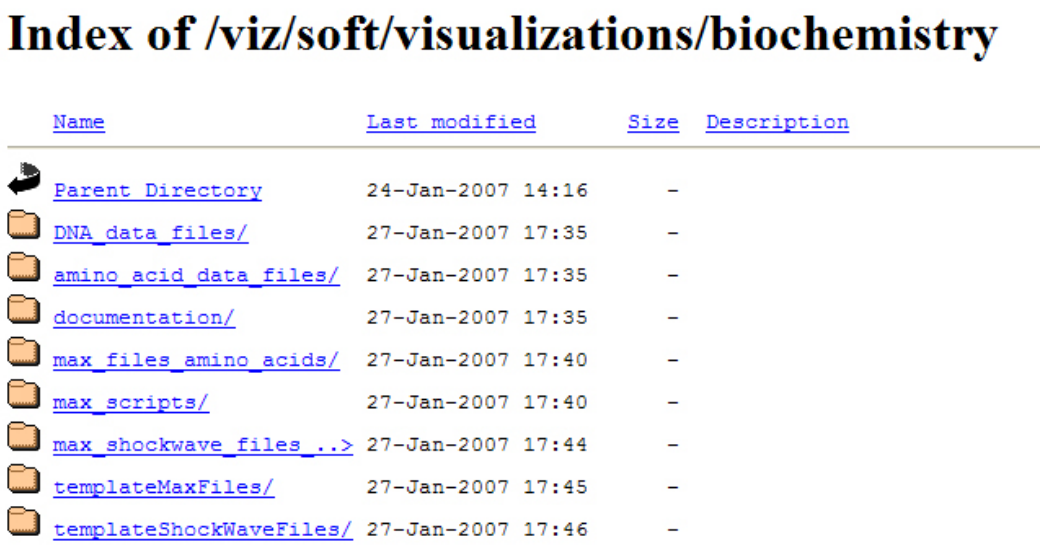

Figure 1.4-1: The structure of the *viz/soft/visualizations/biochemistry* folder

2 The Amino Acid File Format

2.1 Basic File Format: Example

The text file below describes the structure of the amino acid *Valine*. This file and files for the other 19 amino acids can be found in the folder *amino_acid_data_files* described above. The first line of the file gives the name of the amino acid, the number of atoms (19) and the number of bonds (18) for this amino acid.

```
6 Valine 19 18
1 C 2.395 -0.117 -0.531
2 H 2.72 0.05 0.496
3 H 2.735 0.707 -1.159
4 H 2.817 -1.052 -0.896
5 C 0.387 -1.345 0.311
6 H 0.71 -1.171 1.336
7 H 0.809 -2.283 -0.05
8 H -0.702 -1.401 0.278
9 C 0.866 -0.192 -0.575
10 H 0.542 -0.366 -1.602
```

```
11 H 0.604 1.946 -0.702
12 O -1.889 2.079 0.266
13 H -2.818 1.787 0.144
14 C -1.161 1.05 -0.121
15 O -1.709 0.038 -0.53
16 C 0.268 1.128 -0.067
17 H 0.308 2.283 1.603
18 H 1.72 1.473 1.303
19 N 0.7 1.38 1.315
1 1 2 Single
2 1 3 Single
3 1 4 Single
4 1 9 Single
5 5 6 Single
6 5 7 Single
7 5 8 Single
8 5 9 Single
9 9 10 Single
10 9 16 Single
11 11 16 Single
12 12 13 Single
13 12 14 Single
14 14 15 Double
15 14 16 Single
16 16 19 Single
17 17 19 Single
18 18 19 Single
```

2.2 Information in the File

The information in the file above is used to build the model shown in Figure 2.2-1, where we have annotated the figure with the numbers of the non-H atoms from the file above. There are a total of eight non-H atoms. The bonds are drawn using the information in the lower half of the file above. For example, the first bond is between carbon atom 1 and hydrogen atom 2, and is a single bond; the 14th bond is between carbon atom 14 and oxygen atom 15, and is a double bond.

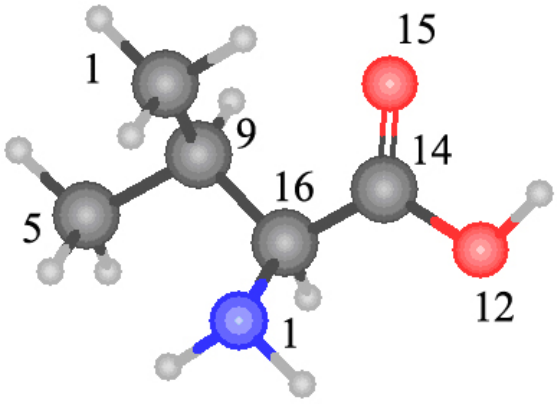

Figure 2.2-1: Valine

The bond colors are determined by the identity of the atoms they connect (red is oxygen, blue is nitrogen, dark gray is carbon, and light gray is hydrogen).

3 The Nucleotide File Format

The files for the nucleotides are very similar in structure to the files for the proteins. The files for the four nucleotides can be found in the folder *DNA_data_files* described above (see Figure 1.4-1).

4 The *ConstructAndRotateAminoAcid* Rollout

4.1 Creating the Rollout

Go to the *templateMaxFiles* folder in Figure 1-3.1 and open the *.max* file entitled *templateCreateAminoAcid.max*. In the panel on the right hand side click on the hammer icon to the far right of the second control bar from the top (see Figure 4.1-2 below). Click on the *MAXScript* label in the *Utilities* list. Click on the *Open Listener* box. You will see a window open up that will show you the progress as you construct your amino acid.

Then use the *Open Script* label under *MAXScript* to open the script *constructAndRotateAminoAcid.ms* contained in the *scripts* folder of Figure 1-4.1. Once that file is opened, select the *File* > *Evaluate All* command as shown in Figure 4.1-1.

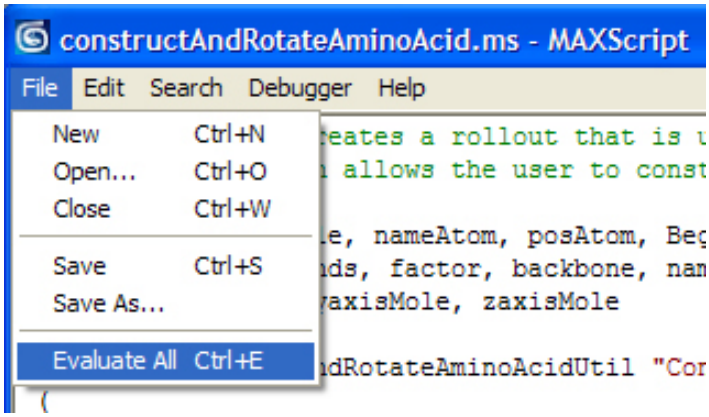

Figure 4.1-1: Creating the Rollout

You should now see the screen shown in Figure 4.1-2. Note that there are a number of atoms already present in this file, in a group named *individualAtoms*. The amino acid we will build always copies the atoms for that amino acid from this group. We use different individual atoms depending on whether the atom is in the backbone or the side chain. We do this so that these atoms will have different textures assigned to them, so that when we create the *ShockWave* animation we can make the side chain atoms semi-transparent, to distinguish them from the backbone atoms.

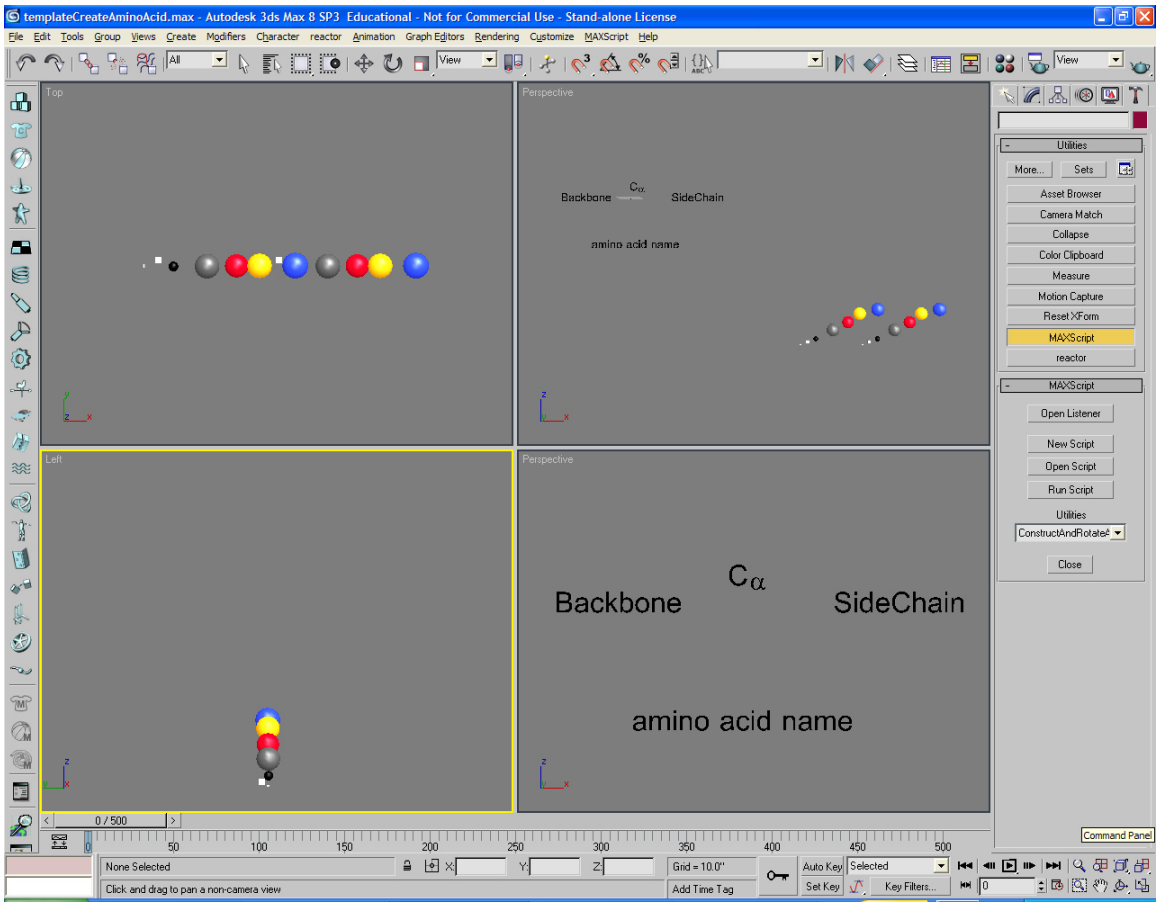

Figure 4.1-2: Screen Shot of *templateCreateAminoAcid.max*

4.2 Using the Rollout

To open the rollout panel, select *ConstructAndRotateAminoAcid* under *MAXScript > Utilities*. Once you have done that you will see the panel shown in Figure 4.2-1. Click on the *Select Amino Acid Data File.* A dialog box will open up which will allow you to navigate to one of the files contained in the *amino_acid_data_files* folder. Let's assume you choose the file named *Arginine.txt*. Once you double click on that file you will see in the *Max Listener* window the text

```
First line of data file selected
"8 Arginine 26    25"
```

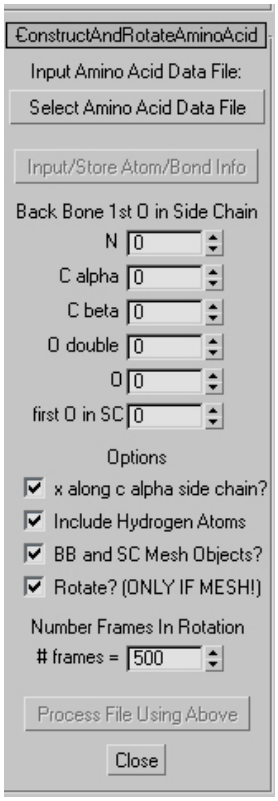

Figure 4.2-1: The Rollout Panel for the *ConstructAndRotateAminoAcid* Rollout

If you have gotten the correct file, click on *Input/Store Atom/Bond Info*. This will read in the data file and display the numbers of the atoms for the various components of the amino acid (for example, the number of the carbon alpha atom, and so on). You then have a number of options to choose from.

1. *x along c side chain:*
   If checked we construct the *xyz* coordinate axes so that the direction from the carbon alpha to the first side chain atom is the *x*-direction, the *y*-direction is perpendicular to the plane formed by the *x*-direction and the direction from the carbon alpha to the nitrogen atom in the backbone, and the *z*-direction completes the right handed system. If it is not checked, we construct the *xyz* axes so that the direction from the oxygen with the single bond in the backbone to the nitrogen atom in the backbone is the *z*-direction, the *y*-direction is perpendicular to the plane formed by the *z*-direction and the direction from the carbon alpha to the first atom in the side chain, and the *x*-direction completes the right handed system. The carbon alpha atom is always placed at the origin.
2. *Include Hydrogen Atoms:*
   If checked we include *H* atoms.
3. *BB and SC Mesh Objects?*:
   If checked, the atoms in the backbone and the side chain are collapsed into mesh objects, one for the side chain and one for the backbone. If not checked, all the

atoms are left as individual objects. For transfer into *ShockWave*, it is best to check this option.

4. *Rotate? (ONLY IF MESH!)*:
   If checked the amino acid is rotated about its *x*-axis (if you have chosen the first coordinate system above) or about its *z*-axis (if you have chosen the second coordinate system above) with a complete rotation in the number of frames specified in the box. ***You can only choose this option if you are forming meshes.***

After choosing your options, click on *Process File Using Above*. You should now see Figure 4.2-2 in your *Perspective* window of max. Note that we have changed the text in the *amino_acid_name* text field in *max*, so that the text correctly identifies the amino acid.

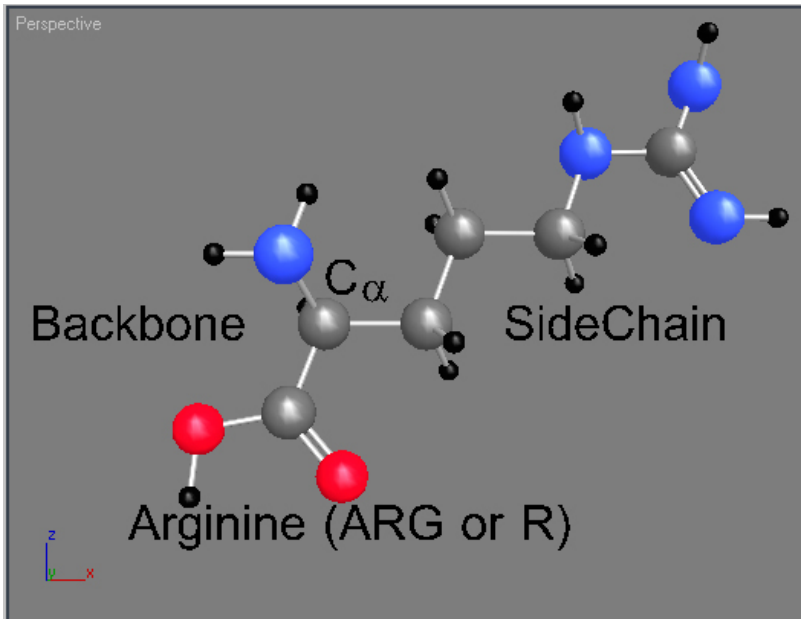

Figure 4.2-2: The amino acid *Arginine* as built using *constructAndRotateAminoAcid*.

5 The *ConstructAndRotateNucleotide* Rollout

5.1 Creating the Rollout

Go to the *templateMaxFiles* folder in Figure 1-3.1 and open the *.max* file entitled *templateCreateDNA.max*. As described in Section 4.1 above, use the *Open Script* label under *MAXScript* to open the script *constructAndRotateDNA.ms* contained in the *scripts* folder of Figure 1-4.1. Once that file is opened, select the *File > Evaluate All* command as shown in Figure 4.1-1.

You should now see the screen shown in Figure 5.1-1. Note that there are a number of atoms already present in this file, in a group named *individualAtoms*. The DNA we will build always copies the atoms from this group. We use different individual

atoms depending on whether the atom is sugar, the nitrogenous base, or the phosphate group. We do this so that these atoms will have different textures assigned to them, so that when we create the *ShockWave* animation we can make the various groups of atoms semi-transparent with different levels of transparency, to distinguish them from the other groups of atoms. Typically we have the nitrogenous base atoms totally non-transparent, the sugar atoms at 50% transparency, and the phosphate group atoms at 30% transparency in the ShockWave.

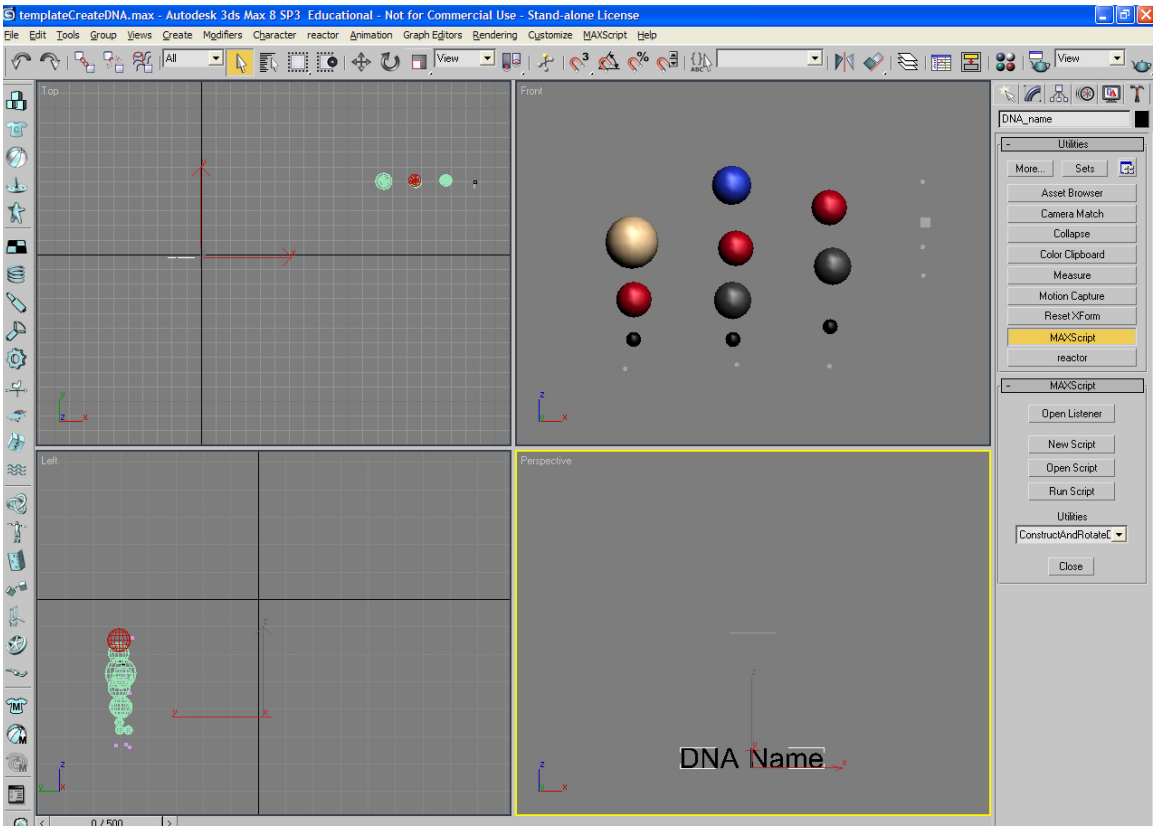

Figure 5.1-1: Screen shot of *templateCreateDNA.max*

5.2 Using the Rollout

To open the rollout panel, select *ConstructAndRotateDNA* under *MAXScript* > *Utilities*. Once you have done that you will see the panel shown in Figure 5.2-1. Click on the *Select DNA Data File.* A dialog box will open up which will allow you to navigate to one of the files contained in the *DNA_data_files* folder. Let's assume you choose the file named *Thymine.txt*. Once you double click on that file you will see in the *Max Listener* window the text

```
First line of data file selected
      "7 Thymine 37    38"
```

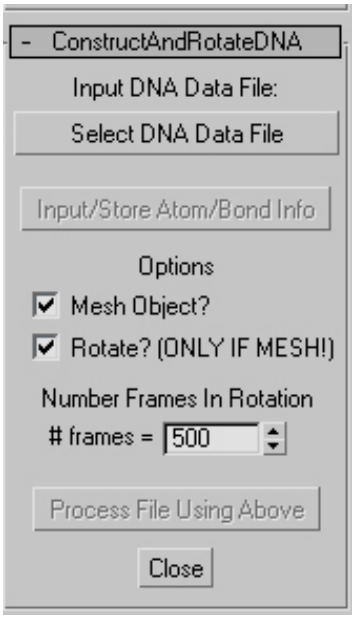

Figure 5.2-1: The Rollout Panel for the *ConstructAndRotateDNA* Rollout

If you have gotten the correct file, click on *Input/Store Atom/Bond Info*. This will read in the data file. You then have two options to choose from.

1. *Mesh Object?*:
   If checked, the atoms in the molecule are collapsed into one mesh object. If not checked, all the atoms are left as individual objects. For transfer into *ShockWave*, it is best to check this option.
2. *Rotate? (ONLY IF MESH!)*:
   If checked the amino acid is rotated about its *z*-axis, which is an axis more or less perpendicular to the plane of the nitrogenous base(s) in the DNA. ***You can only choose this option if you are forming a mesh.***

After choosing your options, click on *Process File Using Above*. You should now see Figure 5.2-2 in your *Perspective* window of max. Note that we have changed the text in the *DNA_name* text field in *max*, so that the text correctly identifies the molecule.

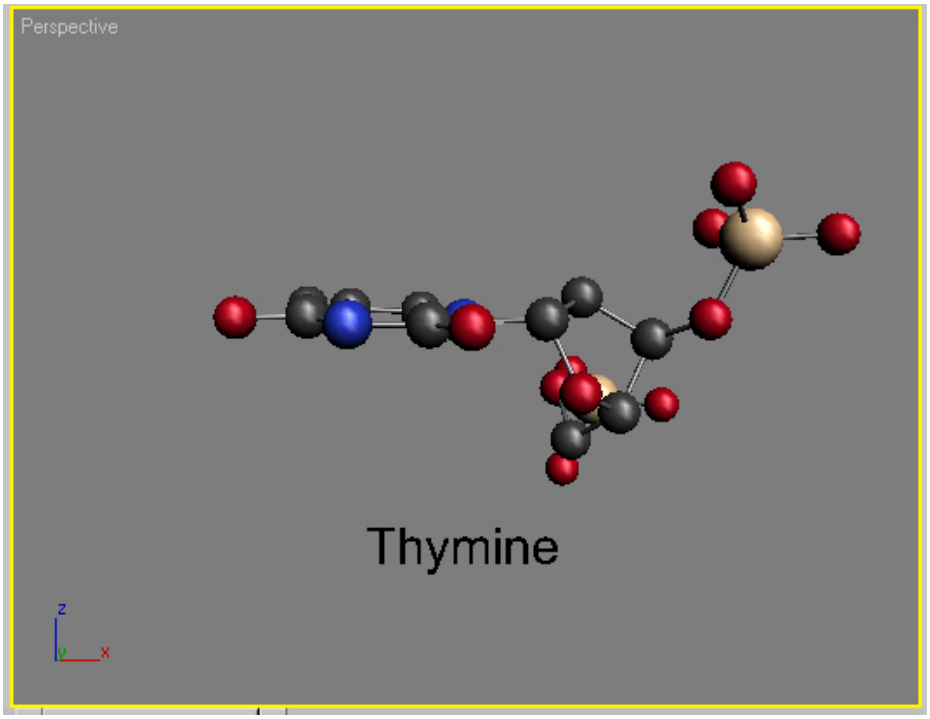

Figure 5.2-2: The nucleotide *Thymine* as built using *ConstructAndRotateDNA*.

6 Creating a *ShockWave* Animation for an Amino Acid

6.1 Exporting the *.W3D ShockWave* File From *Max*

We explain how to export using the amino acid *Arginine* created in Section 4.2 above. We assume you have the *3ds max* file open and have created the *Arginine* amino acid as shown in Figure 4-2.2. Make sure your active viewport is *Perspective* and not any other viewport (e.g. front), otherwise your amino acid will export in a "flat" orthographic projection. Delete the *individualAtoms* group.

Now look at your amino acid in the Perspective viewport, and make sure that when it rotates (if you have chosen rotation), you can see all of the atoms of the amino acid at every part of the rotation, and that the amino acid fits into the window in a reasonable way (e.g. it does not appear small in the viewport).

Go to *File > Export*. In the *Select File to Export* dialog box that comes up, chose *ShockWave 3D Scene Export (*.W3D)*. Choose the file name *arginine.W3D*. Take all the standard options in the *Shockwave 3D Scene Export Options* dialog box. Export the file.

6.2 Importing the *.W3D* File into a Director *.dir* File

Go to the folder *templateShockWaveFiles* and open the Director File *templateAminoAcidDirector.dir*. You will see something resembling Figure 6.2-1. If you do not see the *Cast* and *Stage* windows, go to *Window* in the main toolbar and select them. We have already imported the *Methionine .W3D* file into this Director file. If you hit the "*play*" icon in the upper tool bar of Director, this animation will play. Hit pause. We will now show you how to replace *Methionine* with *Arginine*.

Left click on the *methionine* in the Cast window, and hit delete. Chose *File* > *Import*, navigate to where you stored the *arginine.W3D* file, and import it. After you do this, it will now appear in the *Cast* window. Double left click on the *initialize* script in the *Cast* window to open that file.

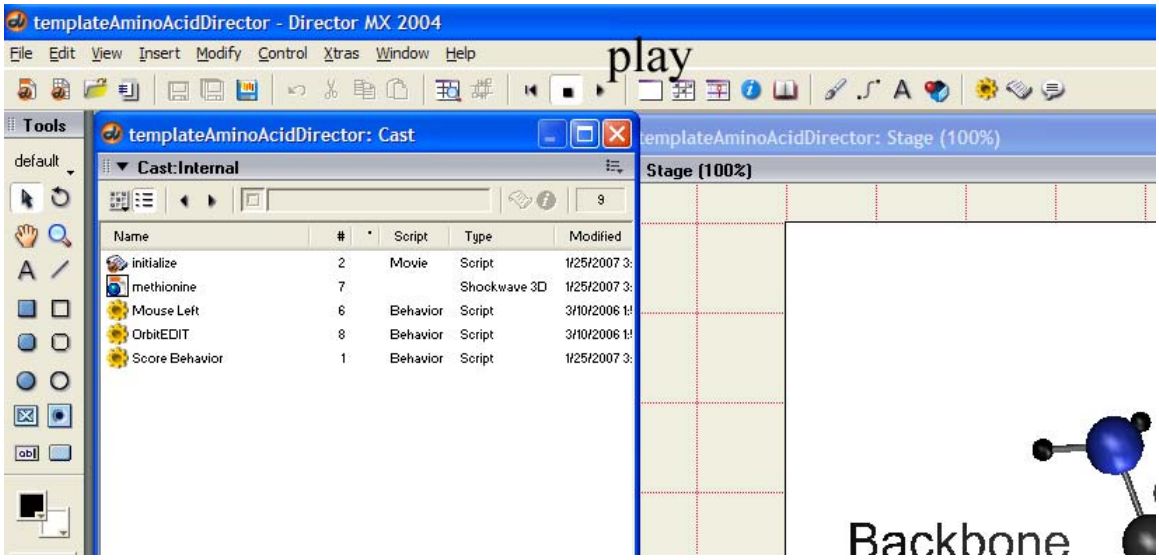

Figure 6.2-1: The Director Window for *Methionine*

In the fourth line down in that file, you will see a line:

```
scene = member("methionine")
```

Change the *methionine* to *arginine*. Navigate a little further down in the *initialize* file until you come to:

```
scene.shader("bondSC").blend = 50
scene.shader("carbonSC").blend = 50
scene.shader("hydrogenSC").blend = 50
scene.shader("sulfurSC").blend = 50
--  scene.shader("oxygenSC").blend = 50
--  scene.shader("nitrogenSC").blend = 50
```

For *methionine*, the side chain only has carbon, hydrogen, and sulfur atoms, so we cannot set the transparency of oxygen and nitrogen—thus these statements are commented out above (--). For *arginine*, the side chain has carbon, hydrogen, and nitrogen, and no sulfur or oxygen, so the statements above should be changed to:

```
scene.shader("bondSC").blend = 50
scene.shader("carbonSC").blend = 50
scene.shader("hydrogenSC").blend = 50
-- scene.shader("sulfurSC").blend = 50
-- scene.shader("oxygenSC").blend = 50
scene.shader("nitrogenSC").blend = 50
```

Then hit the "*lightning*" symbol in the tool bar of the edit window for *initialize* to save these changes.

Finally, left click in the *Stage* window on the panel containing the *arginine* model. Make sure you have your *Window* > *Property Inspector* window open, and in the tabs at the top of that window, choose *Behavior*. You will see Figure 6.2-2. Double left click on *OrbitEDIT*, and choose *parameters*. In the dialog box that comes up, choose *ARG_backbone*. If you now hit "*play*" in the upper tool bar (see Figure 6.2-1), you should now see the *arginine* model animating. If you left click in the player window you can change perspective.

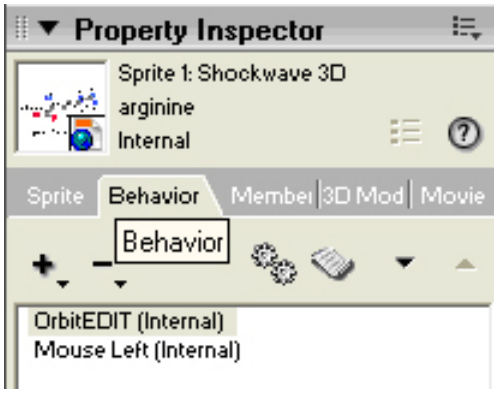

Figure 6.2-2: The Director *Property Inspector* window.

6.3 Publishing the Animation on the Web

Go to *File* > *Publish*. This will create a *ShockWave .dcr* file. This can be referenced in an *.htm* document such as the one found in your *templateShockWaveFiles* folder, and will play over the web. When you create the *.dcr* file, it will open a web browser and play a preview of the animation.

7 Creating a *ShockWave* Animation for a DNA Molecule

7.1 Exporting the *.W3D ShockWave* File From *Max*

We explain how to export using the nucleotide *Thymine* created in Section 5.2 above. We assume you have the *3ds max* file open and have created the *Thymine* as shown in Figure 5-2.2. Make sure your active viewport is *Perspective* and not any other

viewport (e.g. front), otherwise your molecule will export in a "flat" orthographic projection. Delete the *individualAtoms* group.

Now look at your molecule in the Perspective viewport, and make sure that when it rotates (if you have chosen rotation), you can see all of the atoms of the molecule at every part of the rotation, and that the molecule fits into the window in a reasonable way (e.g. it does not appear small in the viewport).

Go to *File > Export*. In the *Select File to Export* dialog box that comes up, chose *ShockWave 3D Scene Export (*.W3D)*. Choose the file name *thymine.W3D*. Take all the standard options in the *Shockwave 3D Scene Export Options* dialog box. Export the file.

7.2 Importing the *.W3D* File into a Director *.dir* File

Go to the folder *templateShockWaveFiles* and open the Director File *templateDNADirector.dir*. You will see something resembling Figure 6.2-1. If you do not see the *Cast* and *Stage* windows, go to *Window* in the main toolbar and select them. We have already imported the *adenine .W3D* file into this Director file. If you hit the "*play*" icon in the upper tool bar of Director, this animation will play. Hit pause. We will now show you how to replace *Adenine* with *Thymine*.

Left click on the *adenine* in the Cast window, and hit delete. Chose *File > Import*, navigate to where you stored the *thymine.W3D* file, and import it. After you do this, it will now appear in the *Cast* window. Double left click on the *initialize* script in the *Cast* window to open that file. In the fourth line down in that file, you will see a line:

```
scene = member("adenine")
```

Change the *adenine* to *thymine*. For the DNA files, you do not need to change any of the transparencies in the initialize file, e.g.

```
scene.shader("Osugar").blend = 50
```

unless you want to change the basic level of transparency. Then hit the "*lightning*" symbol in the tool bar of the edit window for *initialize* to save the changes.

Finally, left click in the *Stage* window on the panel containing the *thymine* model. Make sure you have your *Window > Property Inspector* window open, and in the tabs at the top of that window, choose *Behavior*. You will see something similar to Figure 6.2-2. Double left click on *OrbitEDIT*, and choose *parameters*. In the dialog box that comes up, choose *T* If you now hit "*play*" in the upper tool bar (see Figure 6.2-1), you should now see the *Thymine* model animating. If you left click in the player window you can change perspective.

7.3 Publishing the Animation on the Web

Go to *File > Publish*. This will create a *ShockWave .dcr* file. This can be referenced in an *.htm* document such as the one found in your *templateShockWaveFiles* folder, and will play over the web. When you create the *.dcr* file, it will open a web browser and play a preview of the animation.

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