

“Building Your Own 3D Puzzle”

by Craig Lollin [UserName: clollin] ~ 3/21/2022

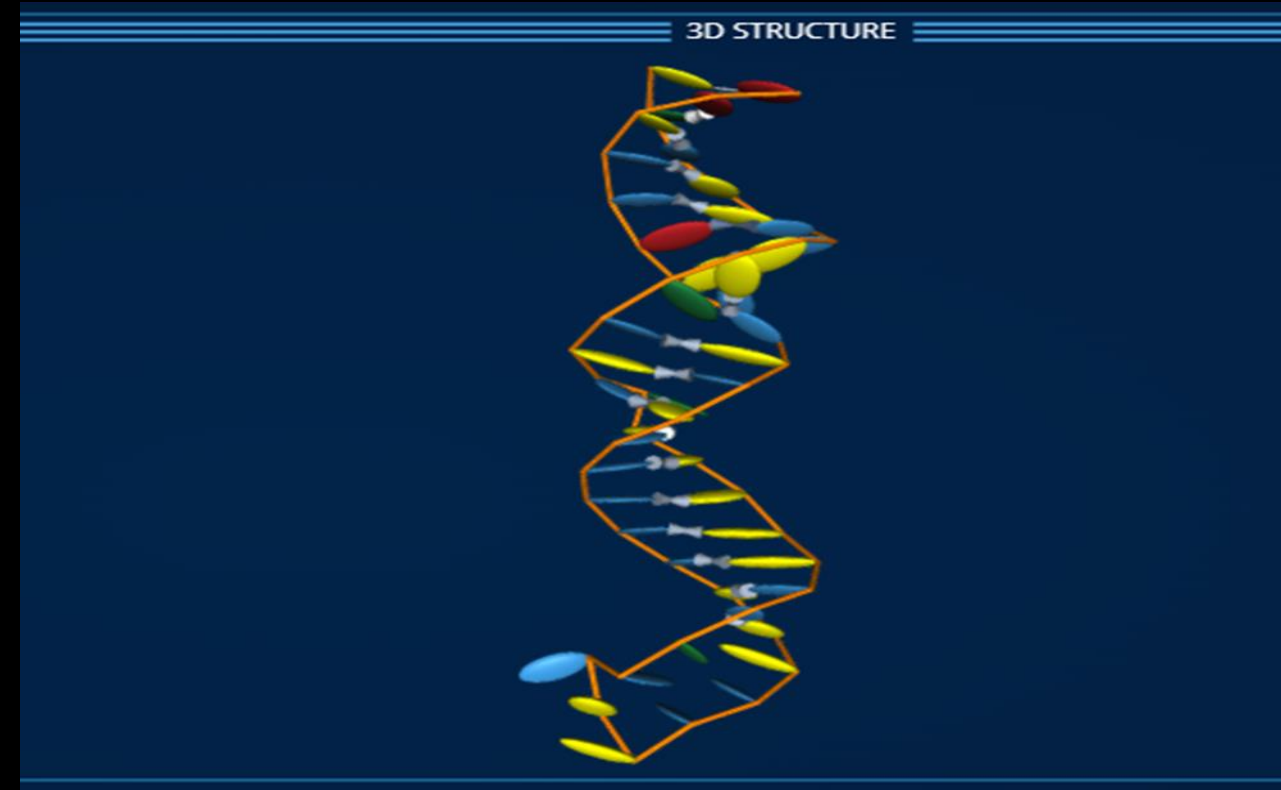
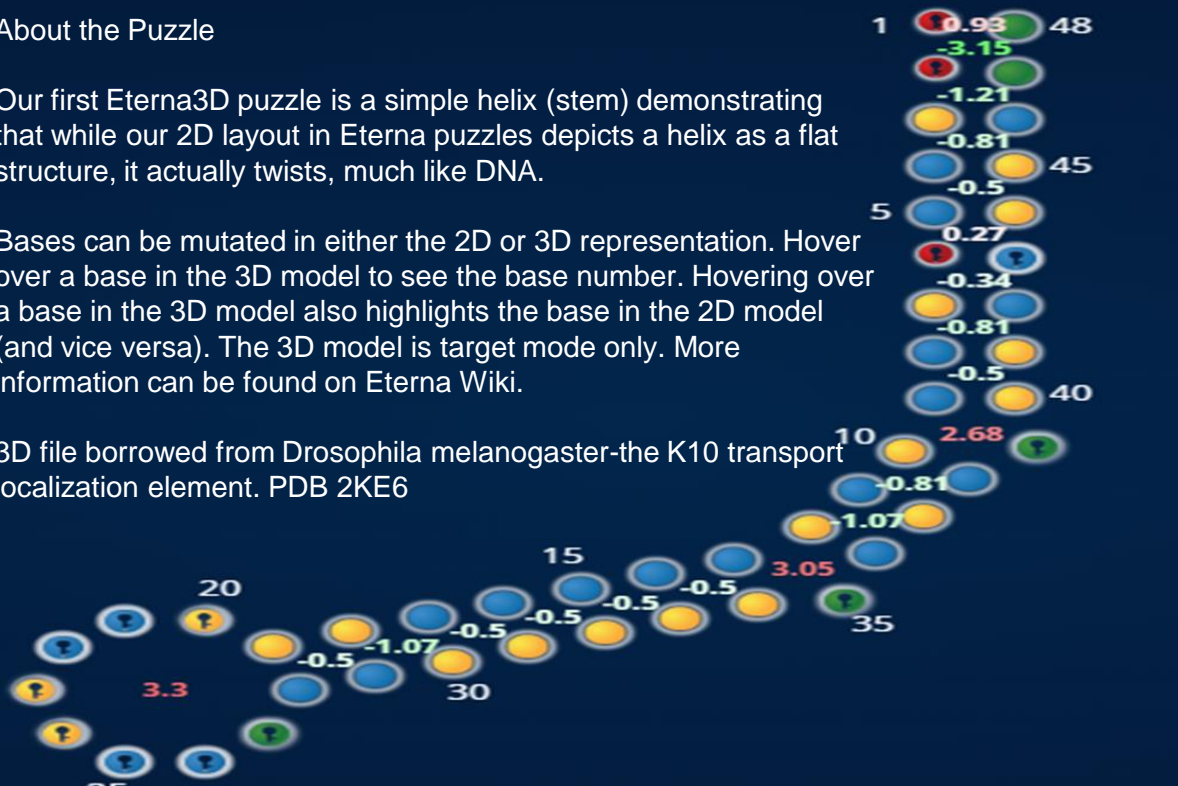
This looks pretty cool...How can I create a 3D Eterna puzzle?

About the Puzzle

Our first Eterna3D puzzle is a simple helix (stem) demonstrating that while our 2D layout in Eterna puzzles depicts a helix as a flat structure, it actually twists, much like DNA.

Bases can be mutated in either the 2D or 3D representation. Hover over a base in the 3D model to see the base number. Hovering over a base in the 3D model also highlights the base in the 2D model (and vice versa). The 3D model is target mode only. More information can be found on Eterna Wiki.

3D file borrowed from *Drosophila melanogaster*-the K10 transport localization element. PDB 2KE6



The First Eterna3D Puzzle - <https://eternagame.org/puzzles/11213497>

What are the steps to creating a 3D Eterna puzzle?

Overview

DigitalEmbrace

15 Feb 2022

@clollin Are you going to be the first player to create an Eterna3D player puzzle?

- My intro to this was: “**The First Eterna3D Puzzle**” - <https://eternagame.org/puzzles/11213497>
- I suggest you go there and read “**About the Puzzle**” as well as the “**Discussion**” section for a thorough background.
- **Summary – I solved the puzzle and posted** *“I like being able to see that 3D interface! Not that this is a challenging puzzle, but with the PDB accession number listed, the FASTA file and sequence is easily accessible to solve (or at least get close).”*
- DigitalEmbrace provided a sort of challenge to me – see above...
- *Well...I can't let a good challenge go unaddressed, so I was off to figure it out.*

Research – How did they do this? I want to be able to do this! How am I going to do this?

- Beam to PuzzleMaker – what did they do?

The screenshot displays the EternaFold web interface for a puzzle titled "The First Eterna3D Puzzle". The interface is dark-themed and includes several key components:

- Top Left:** A home icon and the puzzle title. Below it are two goal boxes: "14 OR MORE" (with a value of 0) and "2 OR FEWER" (with a value of 0 and a green checkmark). A red puzzle diagram is also visible.
- Top Right:** A chat icon and a help icon.
- Center Left:** Energy metrics showing "Total 1.11 kcal" and "Natural/Target Delta 2.91 kcal". Below these is the "EternaFold" logo.
- Center:** A vertical menu with options: "Preferences", "Specs", "Reset", "Copy Sequence", "Paste Sequence", and "Beam to PuzzleMaker". A large blue arrow points to the "Beam to PuzzleMaker" option.
- Center Right:** A 3D structure viewer window titled "3D STRUCTURE" with a "Rotate" dropdown menu. It shows a 3D ribbon model of a protein structure.
- Bottom Left:** A sequence visualization showing a circular arrangement of colored beads (blue, yellow, green, red) with numerical values (e.g., 1.43, -1.21, -0.81, -0.5, 0.27, -0.34, -0.81, -0.5, 2.68, -0.81, 1.07, 3.05, -0.5, -0.5, -0.5, -1.07, -0.5, 3.3, 2.5, 30, 35) and position numbers (1, 5, 10, 15, 20, 25, 30, 35, 40, 45, 48).
- Bottom:** A toolbar with various icons for navigation and editing, including a menu icon, a lightning bolt, a puzzle icon, a leaf, a target, and nucleotide symbols (A, U, G, C).

Research – How did they do this? I want to be able to do this! How am I going to do this?

- Beam to PuzzleMaker – “Load 3D Model”
- “WHAT 3D Model are they loading???” – basically asking for a file



Research – How did they do this? I want to be able to do this! How am I going to do this?

- Beam to PuzzleMaker – what did they do?
- “WHAT 3D Model are they loading???” –
- “3D file borrowed from Drosophila melanogaster - the K10 transport localization element. PDB 2KE6”

PDB is the Protein Data Bank - <https://www.rcsb.org/>

RCSB PDB (Research Collaboratory for Structural Bioinformatics PDB) operates the US data center for the global PDB archive, and makes PDB data available at no charge to all data consumers without limitations on usage



I am familiar with the PDB due to my involvement in the Waksman Student Scholars Program - WSSP <https://wssp.rutgers.edu/>

Originally 2Y9A – Now Obsolete and entered under 4WZJ – Spliceosomal U4 snRNP core domain

<https://www.rcsb.org/structure/4WZJ>

My WSSP (Piscataway High School, NJ) students identified one of the seven “ring” proteins of this snRNP complex and when we went to model it using jMol, we discovered there was RNA within the structure. We decided to go ahead a model it, but needed permission from WSSP to go ahead with this since they had not modelled anything with RNA to date...so we were the first to do that within the program.

Honestly, we were very proud of ourselves!

smE U4 snRNP Homolog: The Nested Doll

Conserved Basefamily

Abstract

The spliceosome is a ribonucleoprotein complex responsible for removing the intron from the pre-mRNA sequence. The U4 snRNP is one of the six snRNPs that assemble to create the spliceosome. Each complex is composed of seven protein subunits. In order to accommodate individual snRNPs, each of the U4 proteins is responsible for binding to specific regions of the pre-mRNA and performing the appropriate function on the snRNA strand. The U4 complex, in particular, is composed of the seven snRNP subunits: B, P, X, C1, C2, and B1. The specific protein being investigated in this preliminary research is the B1 subunit of the U4 complex. The structure for this protein was determined through X-ray crystallography and its structure was determined through a comparison to a similar homolog in silico. The structure was found to consist of the seven snRNP subunits binding in a ring to create a regular structure. The ring structure is composed of the B, P, and C1 units creating a ring. The B and C2 forming a base, and the C1 and C2 forming another base.

Phylogeny

Molecular Construction

The overall structure of the U4 snRNP is a complex of the seven subunits of the snRNP. The protein subunits are arranged in a ring, with the protein subunits and bases of the snRNA strand. The B1 subunit is a conserved region of the snRNA strand. The B1 subunit is a conserved region of the snRNA strand. The B1 subunit is a conserved region of the snRNA strand.

Hypothesized snE Binding Site

In order to support this hypothesis, a global alignment was performed in order to test the similarity of these three specific amino acids among various organisms. The results illustrate that throughout many different classes of organisms, the 3 amino acids of smE that surround the free nucleotide appear to be highly conserved. This could potentially support this idea that these amino acids are responsible for interacting with the nucleotide as high conservation in this case correlates with the structural similarities that determine function.

Substructural Analysis

RNA Binding

In addition to the hypothesized binding site, there is one known region within 528A in which the substructure. This region, referred to as an oligonucleotide, is the region of pre-mRNA in which the snRNP assembles around. It is also important to note that this sequence recognized for binding is identical throughout many RNA sequences. Upon recognition of the sequence (highlighted green), each of the six units of the snRNP assemble as two dimers and a trimer around this specific sequence.

Piscataway High School Research Team

Pravita Acharya, Roma Patel, Aubrey Zhou, Agnieszka Tkacz, Anika Thakur, Daniela Coman, Gavin McKim, Jordan Bennett, Malvika Ghoshal, Tyler DeFazio

Supervising Advisors

Ms. Lesley Wilson, Dr. Greg Lullin

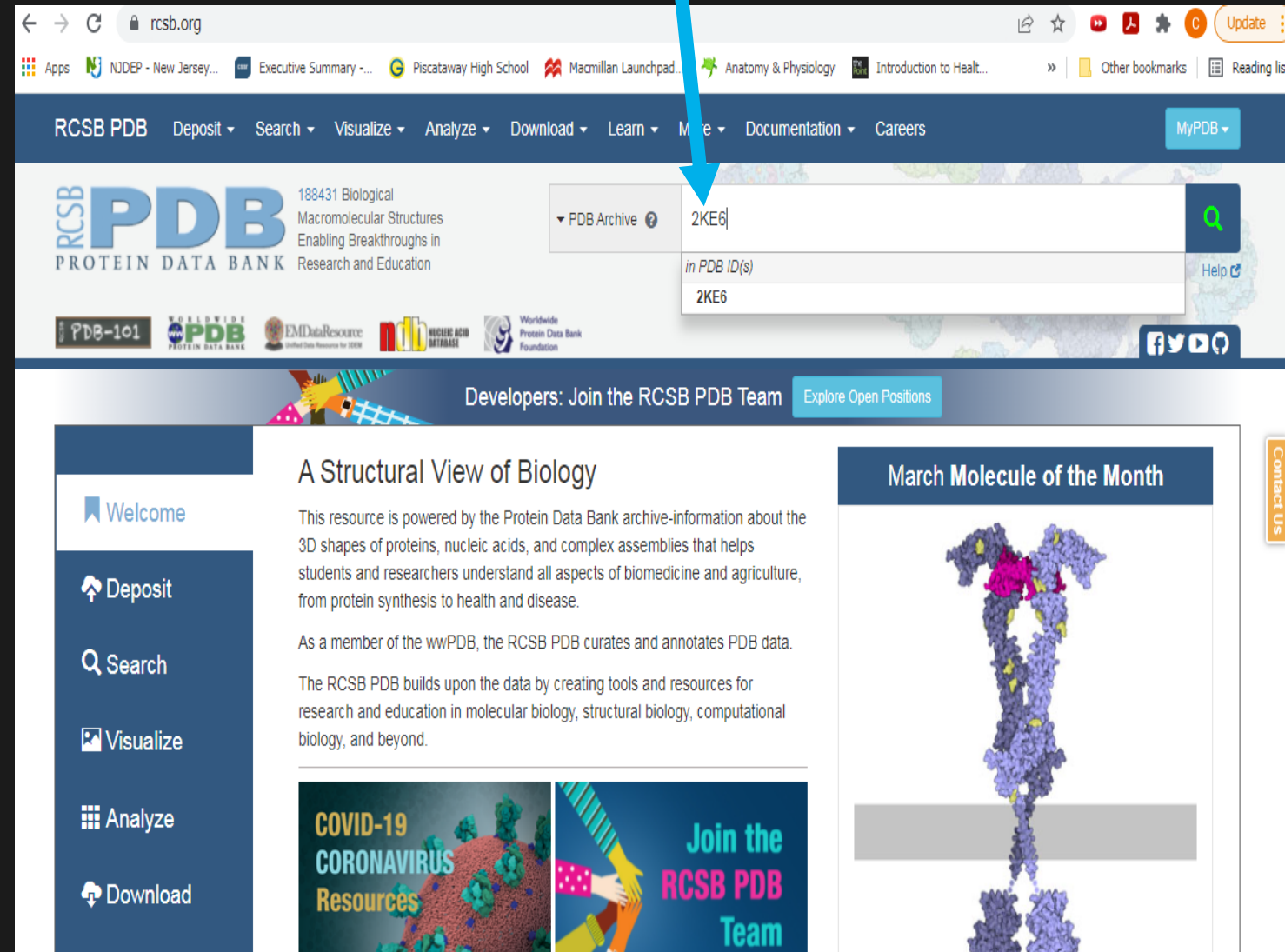
So how do we use PDB?

Every molecular model (atomic coordinate file) in the Protein Data Bank (PDB) has a unique accession or identification code. These codes are always 4 characters in length. The first character is a numeral in the range 1-9, while the last three characters can be either numerals (in the range 0-9) or letters (in the range A-Z in the Latin alphabet). Plans for an expanded identification code system that handle more entries have been announced.

Just paste in the PDB Accession # into this field and usually it will show you a drop down of the Accession # - just click it.

This will take you to the main PDB page for that entry.

This is where you will find all the relevant details and files.



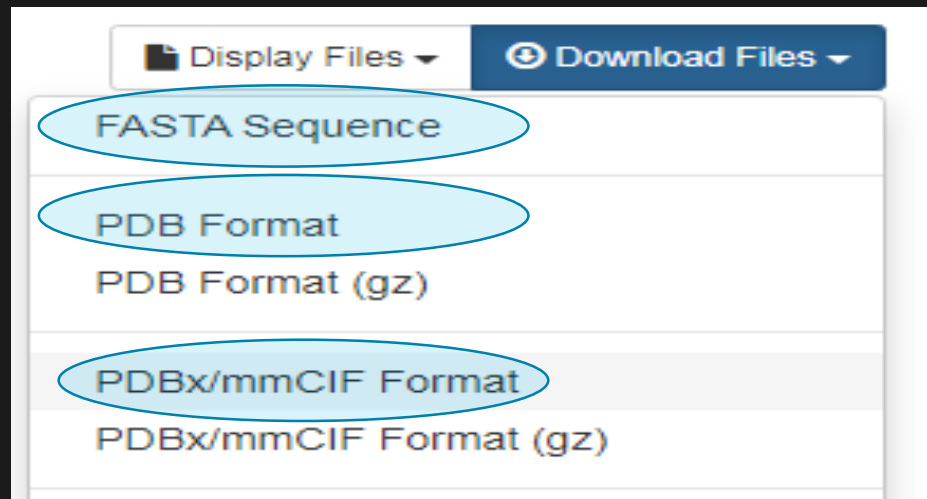
The screenshot shows the RCSB PDB website interface. At the top, there is a navigation bar with links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. A search bar is located in the top right, with the text '2KE6' entered. A blue arrow points from the text above to the search bar. Below the search bar, a dropdown menu shows '2KE6' as a result. The main content area features a sidebar on the left with links for Welcome, Deposit, Search, Visualize, Analyze, and Download. The main content area has a header 'A Structural View of Biology' and a section 'March Molecule of the Month' with a 3D molecular model. There are also banners for 'COVID-19 CORONAVIRUS Resources' and 'Join the RCSB PDB Team'.

So how do we use PDB?

These are the files associated with the PDB entry.

You will want the FASTA sequence file, the PDB format file, possibly the CIF file...

I recommend you download them into a folder for use and possible later research.



A screenshot of the PDB website showing the entry for 2KE6. The page title is '2KE6 Solution Structure of K10 TLS RNA'. The page includes a 3D visualization of the RNA structure, a search bar, and navigation tabs for 'Structure Summary', '3D View', 'Annotations', 'Experiment', 'Sequence', 'Genome', and 'Versions'. A blue arrow points from the text on the left to the 'Download Files' button in the top right corner of the page. The 'Download Files' button is also highlighted in the inset image on the left.

RCSB PDB
188431 Biological Macromolecular Structures
Enabling Breakthroughs in Research and Education

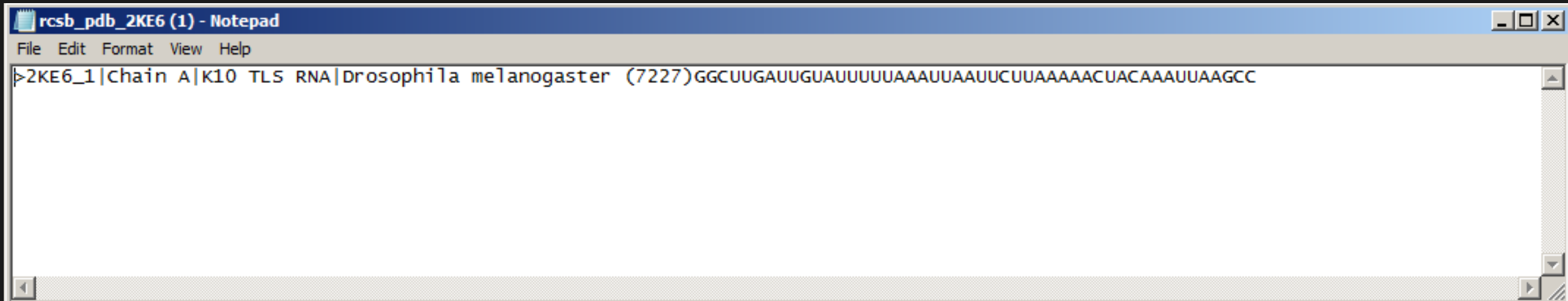
10.2210/pdb2KE6/pdb NDB: 2KE6

Classification: RNA
Organism(s): Drosophila melanogaster
Mutation(s): No

Deposited: 2009-01-23 Released: 2010-01-26
Deposition Author(s): Bullock, S.L., Ringel, I., Ish-Horowicz, D.

Method: SOLUTION NMR
Conformers Calculated: 200

Files – FASTA Sequence file



A screenshot of a Notepad window titled "rcsb_pdb_2KE6 (1) - Notepad". The window has a menu bar with "File", "Edit", "Format", "View", and "Help". The main text area contains a single line of FASTA format text: ">2KE6_1|Chain A|K10 TLS RNA|Drosophila melanogaster (7227)GGCUUGAUUGUAUUUUUAAAUAUUUCUAAAAACUACAAAUUAAGCC". The text is left-aligned and the window has standard Windows window controls (minimize, maximize, close) in the top right corner and a scroll bar on the right side.

```
>2KE6_1|Chain A|K10 TLS RNA|Drosophila melanogaster (7227)GGCUUGAUUGUAUUUUUAAAUAUUUCUAAAAACUACAAAUUAAGCC
```

Files – PDB Format file



2ke6.pdb

```
HEADER      RNA                      23-JAN-09   2KE6
TITLE       SOLUTION STRUCTURE OF K10 TLS RNA
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: K10 TLS RNA;
COMPND      3 CHAIN: A;
COMPND      4 ENGINEERED: YES;
COMPND      5 OTHER_DETAILS: K10 TRANSPORT AND LOCALISATION SIGNAL (TLS)
SOURCE      MOL_ID: 1;
SOURCE      2 SYNTHETIC: YES;
SOURCE      3 ORGANISM_SCIENTIFIC: DROSOPHILA MELANOGASTER;
SOURCE      4 ORGANISM_COMMON: FRUIT FLY;
SOURCE      5 ORGANISM_TAXID: 7227;
SOURCE      6 OTHER_DETAILS: PREPARED BY IN VITRO TRANSCRIPTION USING T7
KEYWDS      RNA TRANSPORT, RNA HAIRPIN, RNA
EXPDTA      SOLUTION NMR
NUMMDL      12
AUTHOR      S.L.BULLOCK, I.RINGEL, D.ISH-HOROWICZ
REVDAT      5 16-MAR-22 2KE6 1 REMARK
REVDAT      4 16-JUN-10 2KE6 1 JRNL
REVDAT      3 26-MAY-10 2KE6 1 JRNL
REVDAT      2 19-MAY-10 2KE6 1 JRNL REMARK COMPND AUTHOR
REVDAT      1 26-JAN-10 2KE6 0
JRNL        AUTH  S.L.BULLOCK, I.RINGEL, D.ISH-HOROWICZ, P.J.LUKAVSKY
JRNL        TITL  A'-FORM RNA HELICES ARE REQUIRED FOR CYTOPLASMIC MRNA
JRNL        TITL 2 TRANSPORT IN DROSOPHILA
JRNL        REF   NAT.STRUCT.MOL.BIOL.          V. 17  703 2010
JRNL        REFN                ISSN 1545-9993
JRNL        PMID  20473315
JRNL        DOI   10.1038/NSMB.1813
REMARK      2
```

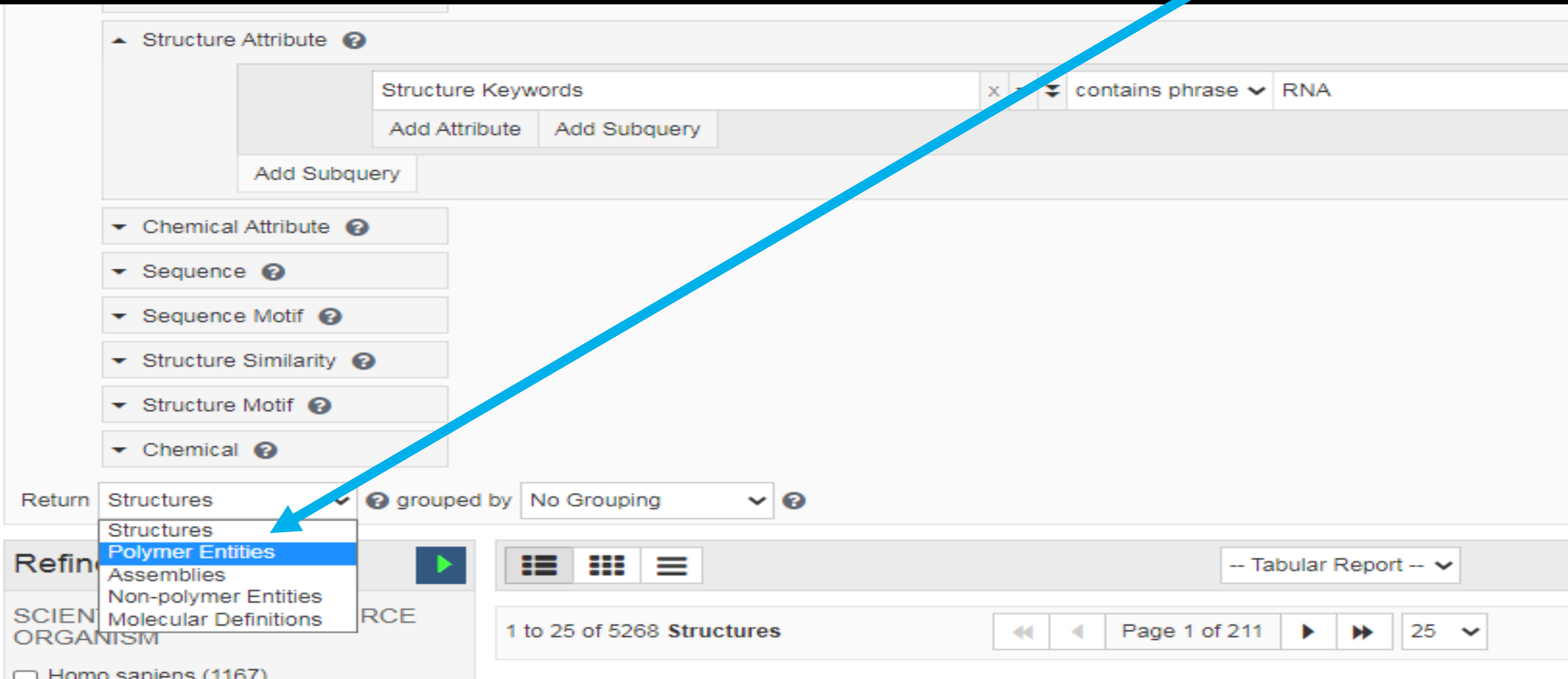
```
ORIGX2      0.000000  1.000000  0.000000      0.000000
ORIGX3      0.000000  0.000000  1.000000      0.000000
SCALE1      1.000000  0.000000  0.000000      0.000000
SCALE2      0.000000  1.000000  0.000000      0.000000
SCALE3      0.000000  0.000000  1.000000      0.000000
MODEL       1
ATOM        1  O5'  G A  1  -5.468 -1.296 32.261 1.00 0.00 O
ATOM        2  C5'  G A  1  -4.486 -0.267 32.420 1.00 0.00 C
ATOM        3  C4'  G A  1  -3.080 -0.845 32.551 1.00 0.00 C
ATOM        4  O4'  G A  1  -3.049 -1.792 33.625 1.00 0.00 O
ATOM        5  C3'  G A  1  -2.767 -1.610 31.277 1.00 0.00 C
ATOM        6  O3'  G A  1  -1.926 -0.827 30.423 1.00 0.00 O
ATOM        7  C2'  G A  1  -2.016 -2.848 31.740 1.00 0.00 C
ATOM        8  O2'  G A  1  -0.610 -2.730 31.506 1.00 0.00 O
ATOM        9  C1'  G A  1  -2.322 -2.970 33.231 1.00 0.00 C
ATOM       10  N9   G A  1  -3.091 -4.201 33.500 1.00 0.00 N
ATOM       11  C8   G A  1  -4.426 -4.349 33.764 1.00 0.00 C
ATOM       12  N7   G A  1  -4.803 -5.585 33.943 1.00 0.00 N
ATOM       13  C5   G A  1  -3.628 -6.316 33.786 1.00 0.00 C
ATOM       14  C6   G A  1  -3.402 -7.719 33.868 1.00 0.00 C
ATOM       15  O6   G A  1  -4.221 -8.606 34.098 1.00 0.00 O
ATOM       16  N1   G A  1  -2.068 -8.034 33.645 1.00 0.00 N
ATOM       17  C2   G A  1  -1.077 -7.116 33.377 1.00 0.00 C
ATOM       18  N2   G A  1   0.144 -7.609 33.183 1.00 0.00 N
ATOM       19  N3   G A  1  -1.280 -5.801 33.300 1.00 0.00 N
ATOM       20  C4   G A  1  -2.575 -5.473 33.515 1.00 0.00 C
ATOM       21  H5'  G A  1  -4.718  0.310 33.315 1.00 0.00 H
ATOM       22  H5'' G A  1  -4.520  0.394 31.553 1.00 0.00 H
ATOM       23  H4'  G A  1  -2.349 -0.054 32.716 1.00 0.00 H
ATOM       24  H3'  G A  1  -3.686 -1.891 30.761 1.00 0.00 H
```

So how did I make it a **new one**?

- Go to PDB and search for anything that has RNA, but I ran into problems immediately.
 - Many PDB entries have RNA and Protein and the PDB Format files have ALL the coordinate data for both (ALL) and so it will not work in ETERNA when trying to upload the 3D file in PuzzleMaker. (basically it needs to be just 1 sequence).
 - My options at this point are to edit the PDB Format file and delete away any non-relevant sequence data – either from protein or other RNA or even hetero atoms like HOH (water).
 - I tried this but when saving the file it cannot be saved as a PDB file extension (or at least I can't do that) – soooo, this may be a dead end!!!
 - So the other option is to search for polymer entities, which restricts your search to entries with just 1 type of sequence.
-

So how did I make it a **new one**?

- Within PDB, search for RNA, but restrict your search to Polymer Entities



The screenshot displays the PDB search interface. At the top, under 'Structure Attribute', there is a search box containing 'Structure Keywords' with a search filter set to 'contains phrase' and the search term 'RNA'. Below this are buttons for 'Add Attribute', 'Add Subquery', and 'Add Subquery'. A list of search categories is shown on the left, including 'Chemical Attribute', 'Sequence', 'Sequence Motif', 'Structure Similarity', 'Structure Motif', and 'Chemical'. At the bottom left, the 'Return' dropdown menu is open, showing options: 'Structures', 'Structures', 'Polymer Entities' (highlighted in blue), 'Assemblies', 'Non-polymer Entities', and 'Molecular Definitions'. A blue arrow points from the top right towards the 'Polymer Entities' option. The 'grouped by' dropdown is set to 'No Grouping'. The bottom right shows a 'Tabular Report' dropdown and pagination information: '1 to 25 of 5268 Structures', 'Page 1 of 211', and '25' items per page.

- DNA (841)
- NA-hybrid (157)
- Other (4)

REFINEMENT RESOLUTION (Å)

- 0.5 - 1.0 (24)
- 1.0 - 1.5 (487)
- 1.5 - 2.0 (1378)
- 2.0 - 2.5 (1699)
- 2.5 - 3.0 (2403)
- 3.0 - 3.5 (2295)
- 3.5 - 4.0 (1662)
- 4.0 - 4.5 (644)
- > 4.5 (766)

RELEASE DATE

- 1975 - 1979 (2)
- 1985 - 1989 (14)
- 1990 - 1994 (69)
- 1995 - 1999 (337)
- 2000 - 2004 (784)
- 2005 - 2009 (2101)
- 2010 - 2014 (2383)
- 2015 - 2019 (4223)
- 2020 - 2024 (2726)



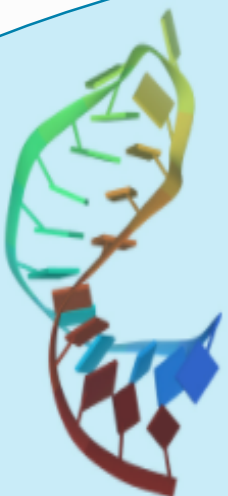
[3D View](#)

DUPLEX CONTAINING TWO G(ANTI).A(ANTI) BASE-PAIRS

Leonard, G.A., McAuley-Hecht, K.E., Ebel, S., Lough, D.M., Brown, T., Hunter, W.N.

(1994) *Structure* **2**: 483-494

Released 1994-05-31
Method X-RAY DIFFRACTION 1.8 Å
Chain IDs A, B
Macromolecule RNA (5'-R>(*CP*GP*CP*GP*AP*AP*UP*UP*AP*GP*CP*G)-3')



[3D View](#)

17RA: Entity 1

[Download File](#) [View File](#)

BRANCHPOINT HELIX FROM YEAST AND BINDING SITE FOR PHAGE GA/MS2 COAT PROTEINS, NMR, 12 STRUCTURES

Nikonowicz, E.P., Smith, J.S.

(1998) *Biochemistry* **37**: 13486-13498

Released 1999-04-20
Method SOLUTION NMR
Chain ID A
Organism
Macromolecule RNA



1A3M: Entity 1

[Download File](#) [View File](#)

PAROMOMYCIN BINDING INDUCES A LOCAL CONFORMATIONAL CHANGE IN THE A SITE OF 16S RRNA, NMR, 20 STRUCTURES

About the Puzzle

@DigitalEmbrace
Suggested I create the first 3D player made puzzle. Obtained from PDB entry 17RA - BRANCHPOINT HELIX FROM YEAST AND BINDING SITE FOR PHAGE GA/MS2 COAT PROTEINS, NMR, 12 STRUCTURES

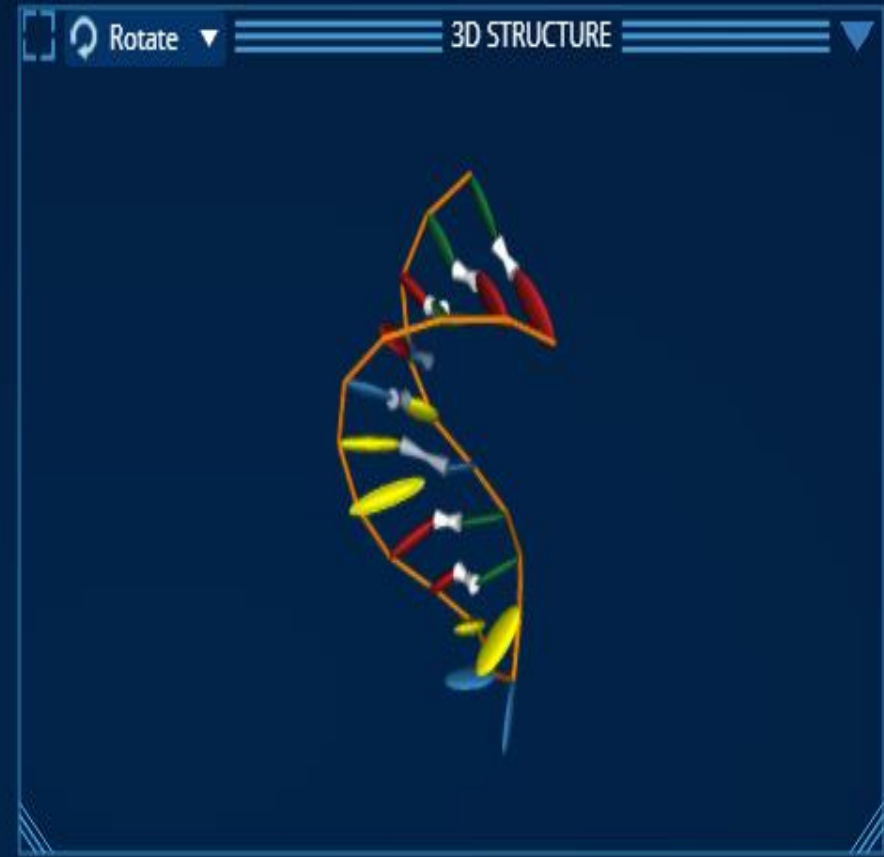
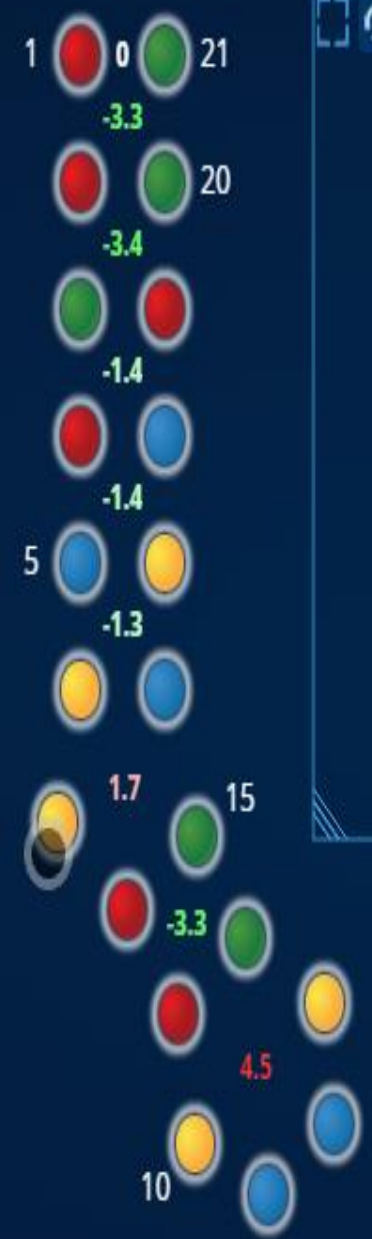
This is a very small, very simple RNA entity that I thought could have a clean PDB file so it would work in the Eterna 3D model. It can be done!



Total
-7.9 kcal

Natural/Target Delta
0 kcal

Vienna2



About the Puzzle

PDB Entry 1A51 - LOOP D/LOOP E ARM OF E. COLI 5S RRNA, NMR, 9 STRUCTURES

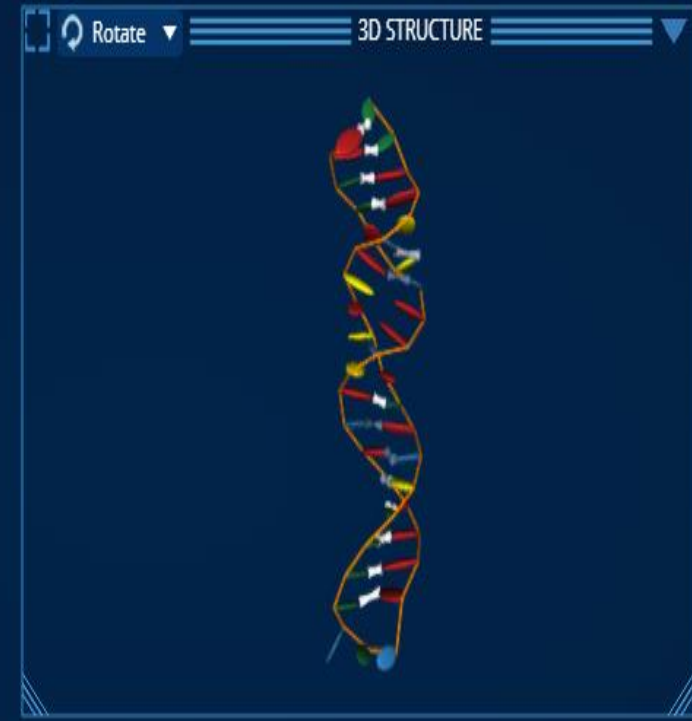
Locked the unpaired bases per the native sequence from PDB FASTA

LOOP D/LOOP E ARM



Total -19.4 kcal
Natural/Target Delta 0 kcal

Vienna



About the Puzzle

PDB Entry 1AFX - UGAA
EUKARYOTIC
RIBOSOMAL RNA
TETRALOOP, NMR, 13
STRUCTURES

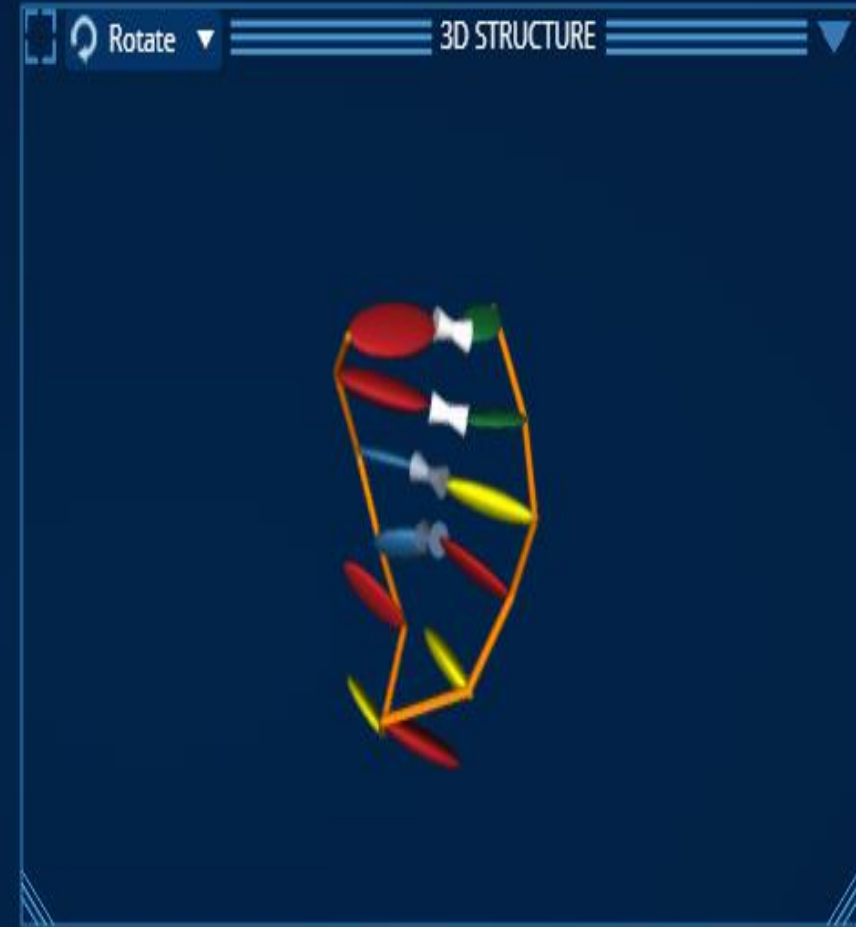
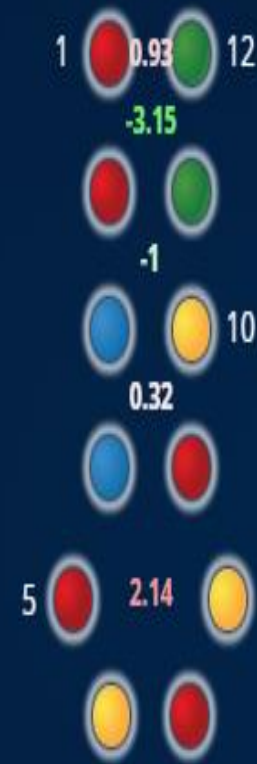
Home > [EFOLD]UGAA EUKARYOTIC RIBOSOMAL RNA TETRALOOP



Total
-0.76 kcal

Natural/Target Delta
0 kcal

EternaFold



About the Puzzle

PDB Entry 1B36 - SOLUTION STRUCTURE OF THE HAIRPIN RIBOZYME LOOP B DOMAIN RNA, NMR, 10 STRUCTURES

https://www.nature.com/articles/nsb0399_212

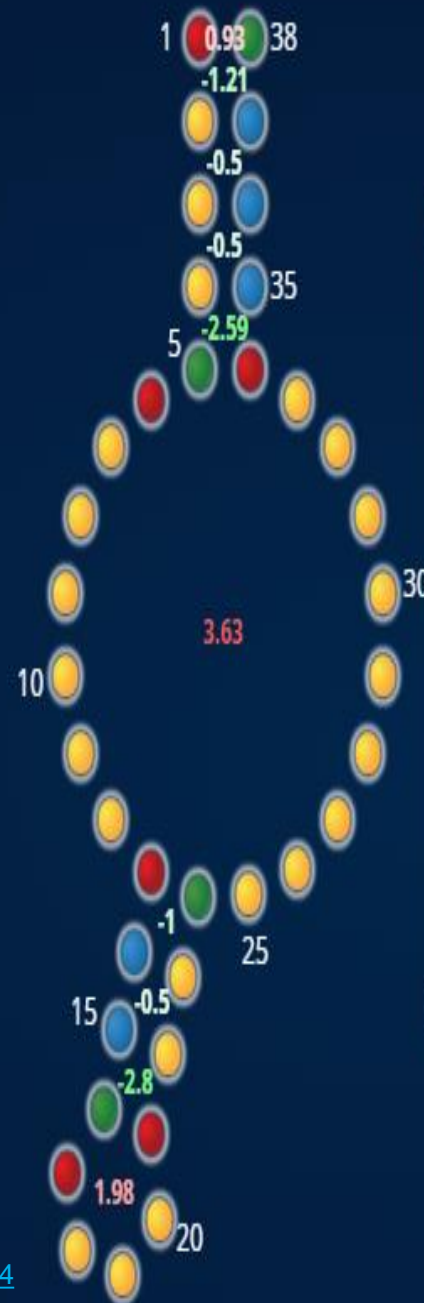
From the Abstract: "Here we present the solution structure of the loop B domain of the hairpin ribozyme, which contains most of the catalytically essential nucleotides. The 38-nucleotide domain contains a 16-nucleotide internal loop that forms one of the largest non-Watson–Crick segments of base pairing thus far determined by either NMR or crystallography. "

🏠 > [EFOLD]HAIRPIN RIBOZYME LOOP B DOMAIN RNA



Total
-2.56 kcal

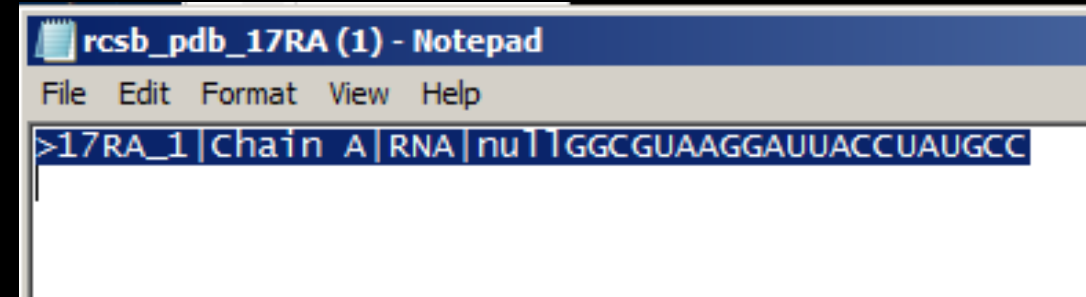
Natural/Target Delta
0 kcal



How do I get the Dot Bracket Structure for this sequence...?

RNA Fold

<http://rna.tbi.univie.ac.at/cgi-bin/RNAWebSuite/RNAfold.cgi>



Results for minimum free energy prediction

The optimal secondary structure in dot-bracket notation will be displayed below.

[color by base-pairing probability | color by positional entropy]

```
1      GGCGUAAGGAUUACCUAUGCC
```

```
1      ((((((.(.....)))))))))
```

You can download the minimum free energy (MFE) structure from the [server](#).

- CAN I DO THIS WITH MY EXISTING PUZZLES? And therefore with any other puzzle in ETERNA...
 - OKAY, I can get the Dot Bracket Structure for my created puzzles (RNA Fold), but my problem now is created puzzles don't have PDB Format files to create the 3D info for PuzzleMaker...sad face...stop now...never
 - Natural question...how do I create a PDB Format file?
-

About the Puzzle

This is awesome! Thanks owed to several people in the forum, but a little digging brought me to this site:

<https://rnacomposer.cs.put.poznan.pl/>

With the sequence from my puzzle and the dot-bracket code from puzzle maker, I was able to create a PBD text file which works perfectly in jMol and in this Eterna 3D puzzle.

What's even cooler, is that in 3D it looks a lot like the letter A.

🏠 > [Alpha - 3D](#)

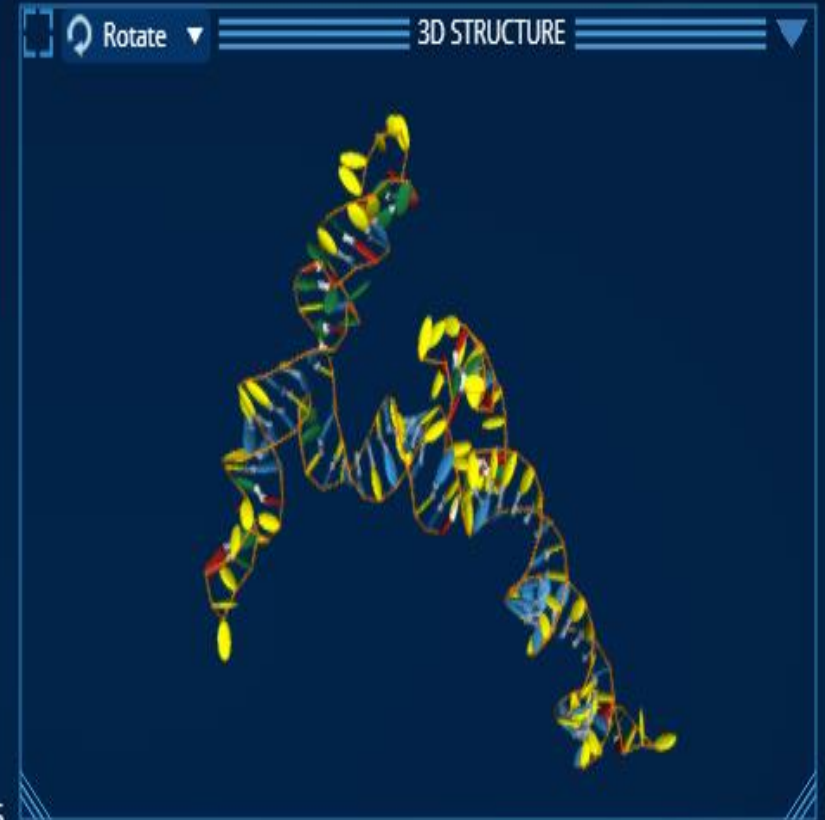


Total
-53.7 kcal

Natural/Target Delta
0 kcal

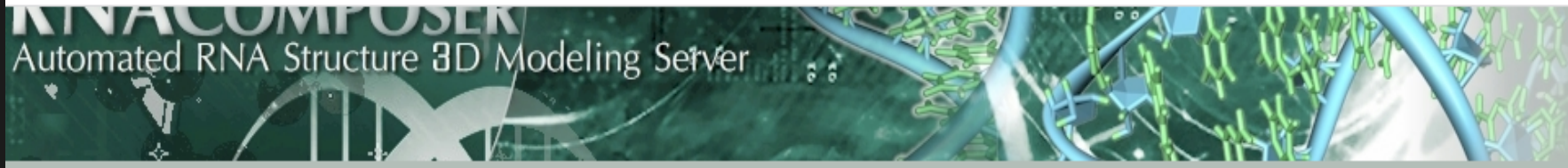


Vienna



Original Alpha Puzzle <https://eternagame.org/puzzles/451129>

5th - Alpha - 3D <https://eternagame.org/puzzles/11223535> 18 Feb 2022



- Home
- Tools
- Help
- About
- References
- Links
- Contact us

User ID:

Password:

[Forgot your password?](#)

[Create an account](#)

You are **1,817,428** visitor.

Visitors online: **8**



Welcome to RNAComposer, a fully automated RNA structure modeling server. (Mirror site: rnacomposer.ibch.poznan.pl)

The RNAComposer system offers a new user-friendly approach to the fully automated prediction of large RNA 3D structures. The method is based on the machine translation principle and operates on the [RNA FRABASE](#) database acting as the dictionary relating RNA secondary structure and tertiary structure elements.

RNAComposer works in two modes:

- **interactive mode** - allows to work on one RNA molecule of interest at a time; its use is limited up to 500 nt residues and results in a single 3D-RNA structure model. Input your RNA sequence and secondary structure ([Example 1](#) and [Example 2](#)) or sequence only ([Example 3](#)). Example 3 is offered for introductory purposes.
- **batch mode** - is designed for large-scale automated modeling of RNA structures up to 500 nt residues, based on user-defined RNA secondary structures. As an input a set of up to 10 RNA sequences can be used. This mode is available only for registered users.

You are in interactive mode

Enter RNA sequence and secondary structure in dot-bracket format ([Example 1](#) and [Example 2](#)) or sequence only ([Example 3](#)). A maximum sequence length is limited to 500 residues.

Load example: [1](#) [2](#) [3](#)

```
#HIV-2 DIS RNA hairpin
>example1
GCUCCUAGAAAGGCCGCGGGCCGAGGUACCAAGGCAGCGUGUGGAGC
((((.....(((.(.....)))..))))..))))
```

Select secondary structure prediction method

Email results to:

RNA COMPOSER

<https://rnacomposer.cs.put.poznan.pl/>

Info for RNA Composer site:

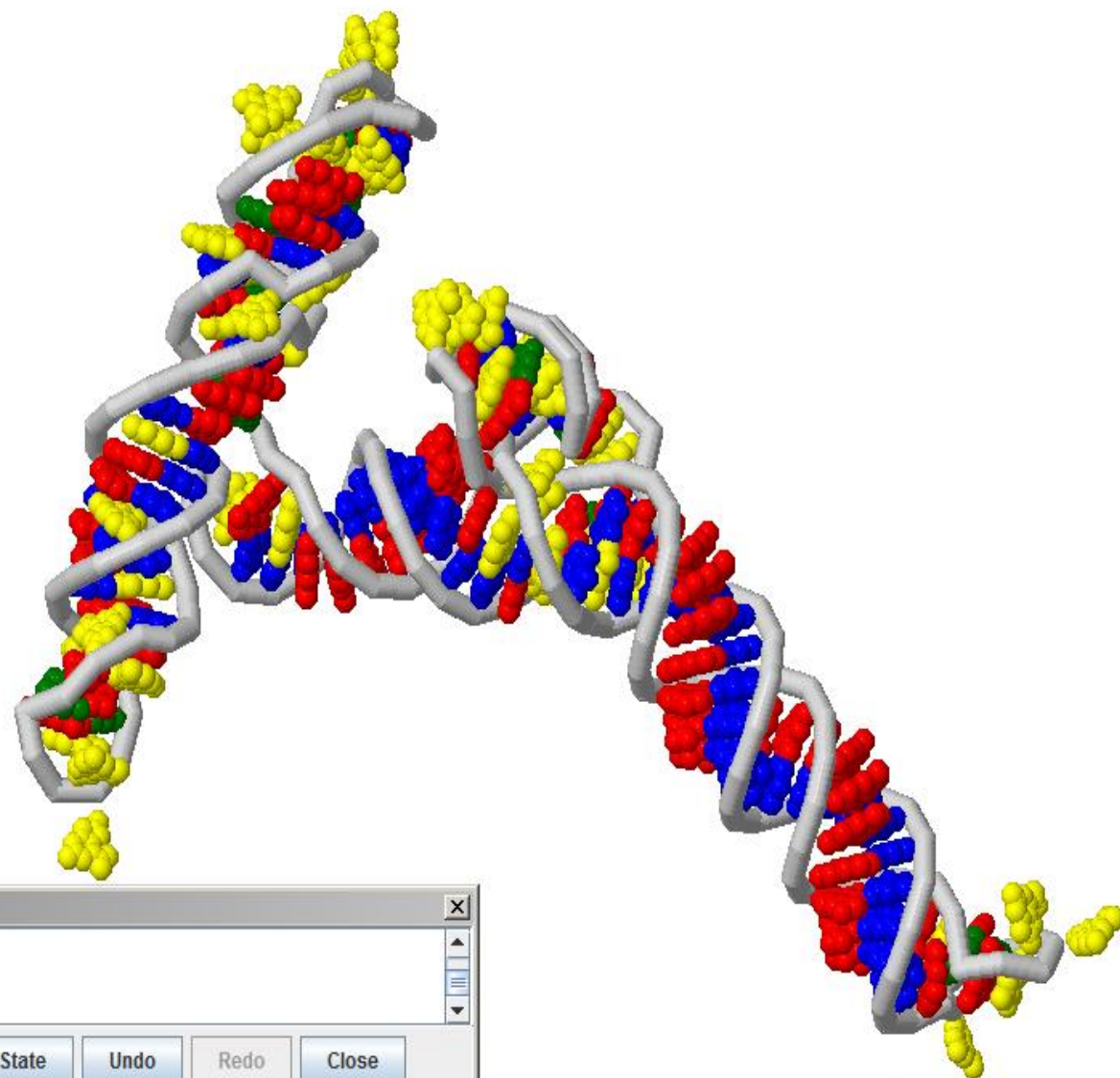
Alpha letter in clollin series Eterna

>ALPHA

AUGCAAGUGAAAGCAAGUUUUUUUUUUUUUAAGUUUAUGUGAGCAAAGCGAAGUAUGUGGAUGGUAAUCAGCGGAAUGGAAAAACACUGUAAUGAGCCGAGGGGGGGGG
GAUAUAUUUUUUUUUUUUUUUUUUUUUGAAGGCAAAGCAGGGGGGGGGGGGGGGGGGGGGUGAAGAGAAAUCAAGUAA

.(((..(.....))..((((((((((((((((..((((((((((..(.....)).....))))))))))(((..((((((((..(.....)))))..))))))))))))))
)))..((((((((((((((((((((((((((((.....((..))..))))))))))))))))))..(.....))..)))..

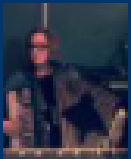
MODEL	1										
ATOM	1	HO5'	A	A	1	-0.433	-0.197	-1.235	1.00	0.00	H
ATOM	2	O5'	A	A	1	-0.072	0.491	-0.669	1.00	0.00	O
ATOM	3	C5'	A	A	1	1.303	0.175	-0.436	1.00	0.00	C
ATOM	4	H5'	A	A	1	1.930	1.007	-0.759	1.00	0.00	H
ATOM	5	H5''	A	A	1	1.576	-0.713	-1.004	1.00	0.00	H
ATOM	6	C4'	A	A	1	1.549	-0.091	1.031	1.00	0.00	C
ATOM	7	H4'	A	A	1	0.605	0.059	1.556	1.00	0.00	H
ATOM	8	O4'	A	A	1	2.089	-1.436	1.177	1.00	0.00	O
ATOM	9	C1'	A	A	1	3.156	-1.424	2.108	1.00	0.00	C
ATOM	10	H1'	A	A	1	2.991	-2.254	2.797	1.00	0.00	H
ATOM	11	N9	A	A	1	4.402	-1.671	1.384	1.00	0.00	N
ATOM	12	C4	A	A	1	5.594	-2.080	1.931	1.00	0.00	C
ATOM	13	N3	A	A	1	5.851	-2.340	3.225	1.00	0.00	N
ATOM	14	C2	A	A	1	7.119	-2.711	3.386	1.00	0.00	C
ATOM	15	H2	A	A	1	7.411	-2.943	4.410	1.00	0.00	H
ATOM	16	N1	A	A	1	8.086	-2.842	2.469	1.00	0.00	N
ATOM	17	C6	A	A	1	7.794	-2.572	1.179	1.00	0.00	C
ATOM	18	N6	A	A	1	8.758	-2.701	0.267	1.00	0.00	N
ATOM	19	H61	A	A	1	8.560	-2.503	-0.703	1.00	0.00	H
ATOM	20	H62	A	A	1	9.682	-2.992	0.552	1.00	0.00	H
ATOM	21	C5	A	A	1	6.483	-2.169	0.876	1.00	0.00	C
ATOM	22	N7	A	A	1	5.863	-1.825	-0.318	1.00	0.00	N
ATOM	23	C8	A	A	1	4.634	-1.540	0.037	1.00	0.00	C
ATOM	24	H8	A	A	1	3.873	-1.232	-0.665	1.00	0.00	H
ATOM	25	C2'	A	A	1	3.117	-0.070	2.813	1.00	0.00	C
ATOM	26	H2'	A	A	1	4.114	0.255	3.118	1.00	0.00	H
ATOM	27	O2'	A	A	1	2.209	-0.146	3.896	1.00	0.00	O
ATOM	28	HO2'	A	A	1	1.738	0.689	3.920	1.00	0.00	H
ATOM	29	C3'	A	A	1	2.577	0.815	1.698	1.00	0.00	C



Jmol Script Console 14.31.20 2020-12-16 21:21

```
3590 atoms selected  
$ color gainsboro  
$
```

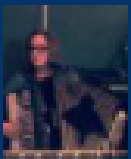
Editor Font Clear History State Undo Redo Close



DigitalEmbrace

19 Feb 2022

The 3D model must be purely a prediction since you used RNAComposer and no natural RNA would have straight helices. Great work!



DigitalEmbrace

18 Feb 2022

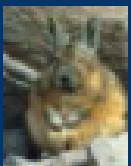
Is the PDB file based on the known 3D structure or is it a prediction based on the dot-bracket and sequence?



jnicol

18 Feb 2022

Nice!



Anamfija

18 Feb 2022

Whoa, that's super cool! I had seen RNApdbee before (which takes in a PDB ID or 3D structure and changes it into dot-bracket notation), but I hadn't come across RNAComposer yet. So many possibilities . . .

Conclusion

- 3D Puzzles can be made by anyone with a fairly straight forward series of steps...if you run into difficulty; I am more than happy to try and help!
- Try one and see!
- <https://forum.eternagame.org/t/testing-eterna3d-functionality/4144> - *DigitalEmbrace*

Problems

- Puzzles that we create are rarely representations of biologically valid sequences and are thus **NOT** verified regarding folding (3D)

How to control 3D puzzles

I just tried some things that work with Jmol and realized that you can use the shift button with the mouse and it will pan. So all three options for moving would be directly accessible if rotate was the default.

(For me anyway)

- Shift and left click = pan.
- Left click alone = rotate.
- Scroll wheel = zoom.

Try it out!

QUESTIONS?

Acknowledgments: So many Eterna players have helped me in ways they may never know; whether it comes to solving a puzzle or learning something new. Someone even recently helped my 5yr old daughter in the chat while she was playing on the site. Thanks to all, especially:

DigitalEmbrace, Iroppey, Eli Fisker, Anamfija, Astromon, jnicol, ETERNA DEV team and many others not mentioned...