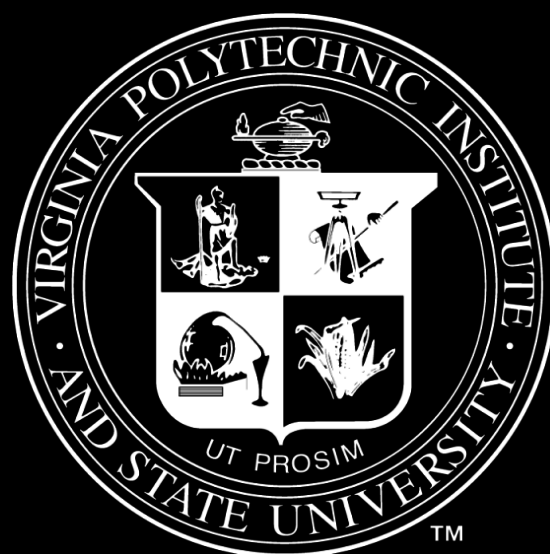


FUGUPOS—update

First **U**niversal **G**ranted **U**niformed **P**harmaceutical **O**ptimized **S**trategy

A Web 3.0 Interface Forefront for Human-AI Interaction in Pharmaceuticals

Gunnar Beck-Nelson



Human AI Interaction

Want to establish an initial framework

- Given the 3D molecular space
- We want to present a full surround knowledge and immersive experience for users who are within pharmaceuticals to design and deploy novel drug discoveries
- Give rapid combination and advancement for new pharmaceuticals

Improving from NCBI

- NCBI tabled out instructions for viewing the 3D molecular viewing model
- File formats are in mmCIF, which showcase the binary output for the protein molecular structure

Unreal Engine Framework

- Unreal vs Unity
- Unreal has shown for intuitive nature and high fidelity to be able to take on the file formats when improving them
- There has been a lot of work outside of Unreal with other VR devices, but sticking with mainstream conventions—Oculus is the go to for VR deployment
- Given mainstream appeal

Deploying for the oculus

- Challenges one would need to face
- The file formatting
- The 3D viewing of the molecular structure
- Since PDB already pushes for a 3D molecular structure
- Question===How can we improve the experience to help users understand the structure
- Can be utilized for education and research for further drug discoveries

VR Framework

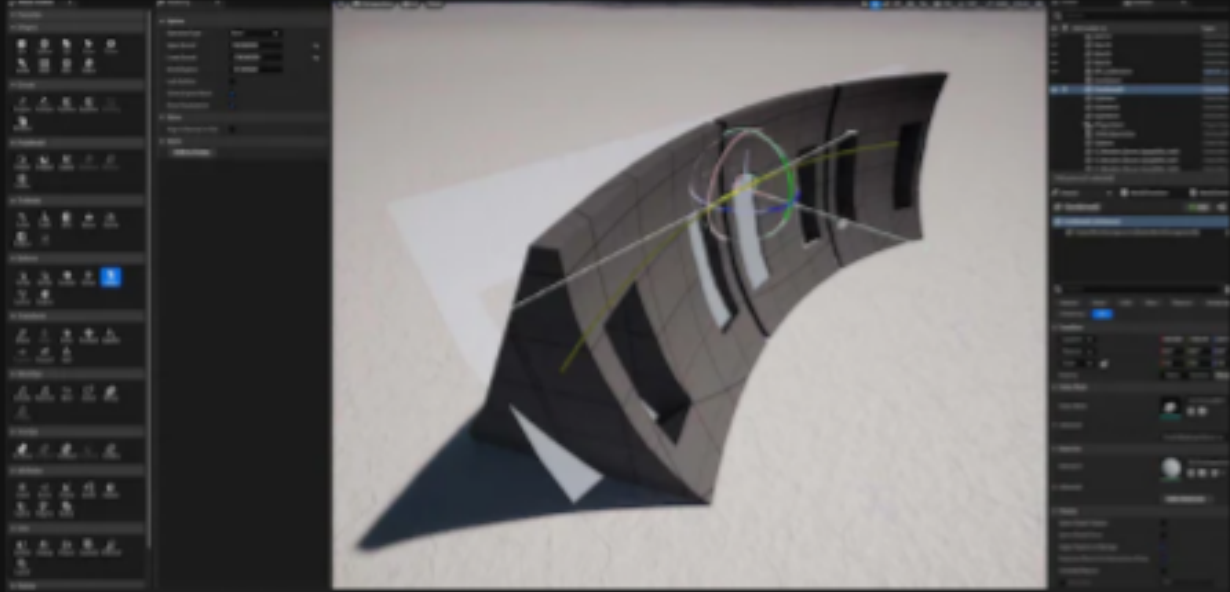
The screenshot shows the Unreal Engine 5.0.0 website interface. At the top left is the Epic Games logo. Below it is the Unreal Engine logo. The navigation bar includes 'News' (highlighted), 'Samples', 'Marketplace', 'Library', and 'Twinmotion'. A yellow 'Launch Unreal Engine 5.0.0' button is in the top right. The main content area is titled 'Featured Content' and contains two articles. The left article is 'Exploring Geometry Tools in UE5' with a thumbnail showing a 3D model in a software interface. The right article is 'Featured free Marketplace content—April 2022' with a thumbnail of a tavern interior. A sidebar on the left contains 'Downloads', 'Settings', and a user profile 'GChief_117'. The bottom of the page features two horizontal image banners.

Epic Games

Unreal Engine

News Samples Marketplace Library Twinmotion **Launch Unreal Engine 5.0.0**


Featured Content



Exploring Geometry Tools in UE5

The official release of Unreal Engine 5 has brought with it a ton of incredible features and tools that we're excited to explore, so this week we kick it off with a demo and discussion of the Geometry Tools! Between UE5's native modeling tool suite and geometry scripting, there is a ton of information to crack into. We've got the experts coming on to answer your questions - so tune in

Inside Unreal




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News

Downloads Settings GChief_117

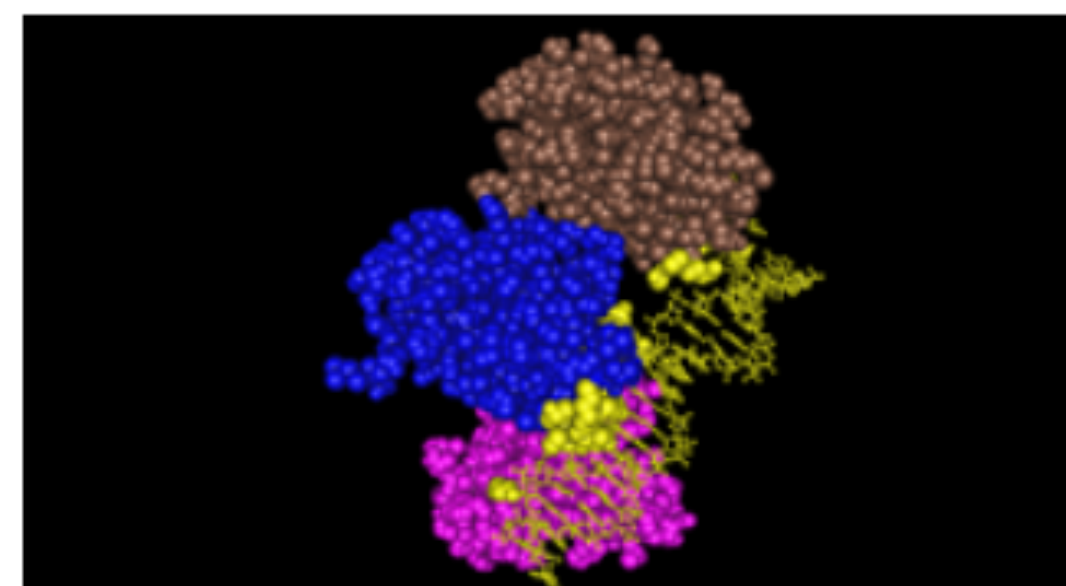
Structure

Structure 

Search

[Advanced](#)

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Structure

Three dimensional structures provide a wealth of information on the biological function and the evolutionary history of macromolecules. They can be used to examine sequence-structure-function relationships, interactions, active sites, and more.

Using Structure

[Search](#)

[How to \(Quick Start\) Guides](#)

[Help](#)

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[Publications](#)

[Discover](#)

Structure Tools

[Macromolecular Resources Overview](#)

[iCn3D \(web-based 3D viewer\)](#)

[Cn3D \(3D viewer application\)](#)

[IBIS](#)

[VAST](#)

[VAST+](#)

More Resources

[PDB](#)

[Protein](#)

[CDD](#)

[PubChem](#)

[NCBI Structure Group Resources & Research](#)

7Q0Y

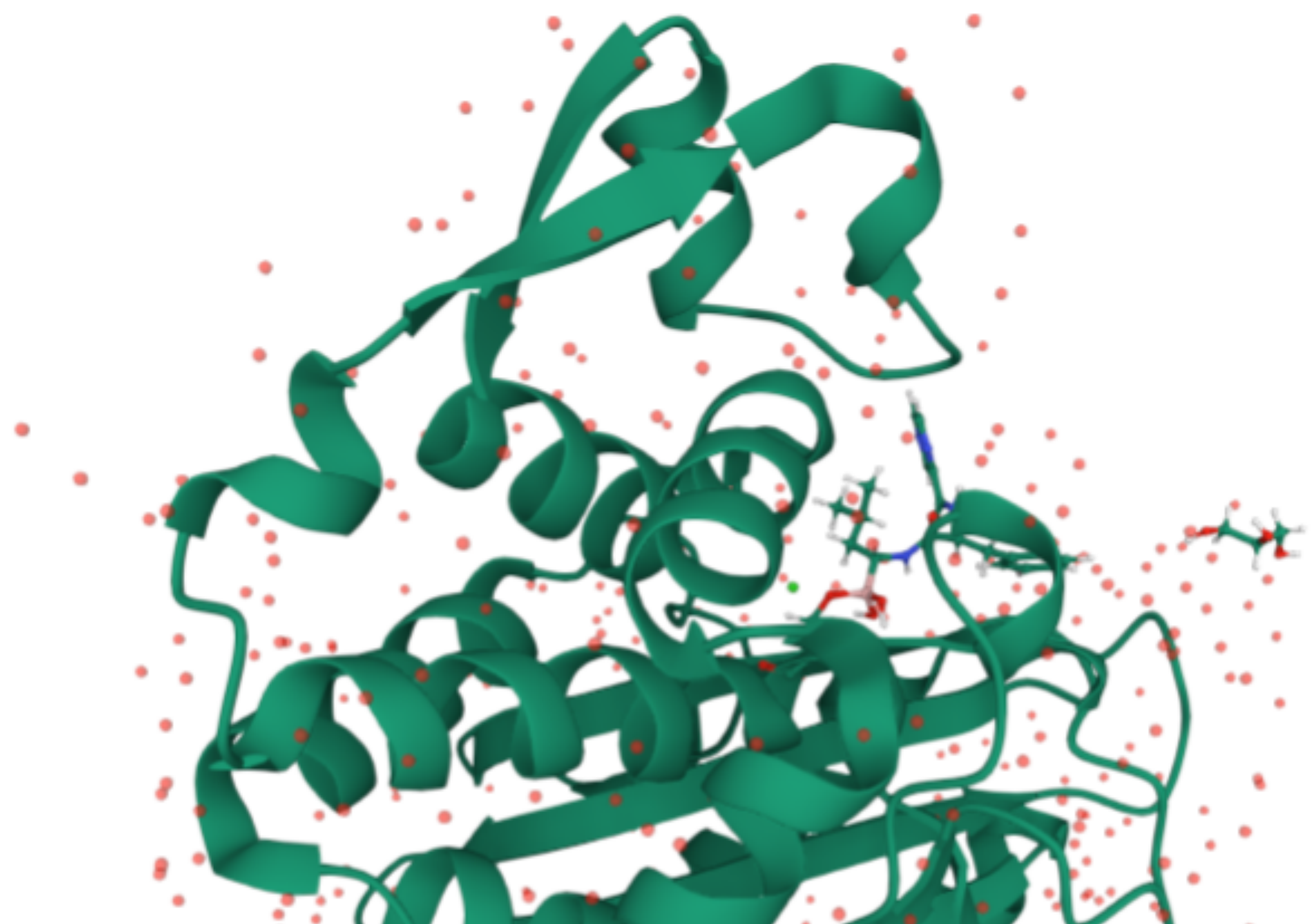
Crystal structure of CTX-M-14 in complex with Bortezomib

Display Files Download Files

Help

Sequence of 7Q0Y | Crystal ... Chain 1: Beta-lactam... A

```
25      35      45      55      66      76      86      96      106      116      126      136
ETSAVQOKLAALEKSSGGRLGVALIDTADNTQVLYRGDERFPMCSTSKVMAAAVVKQSETQKQLLNQPVVEIKPADLVNYPNPIAEKHVNGTMTLAELSAAALQYSDNTAMNKL
146      156      166      176      186      196      206      216      226      236      247
IAQLGGPGGVTAFAARAIGDETFRDLRTEPTLNTAIPGDPRDTTTPRAMAQTLRQLTLGHALGETQRAQLVTWLKGNITGAASIRAGLPTSWTVGDKTGSGDYGTTNDIAVIWP
257      267      277      287
QGRAPLVLVITYFTQPQNAESRRDVLASAARIIAEGL
```



Structure

7Q0Y | Crystal structure of CTX-M-1...

Type	Assembly
Asm Id	1: Author Defined Asse...
Dynamic Bonds	Off

Nothing Focused

Measurements

Structure Motif Search

Components

Preset	Add			
Polymer	Cartoon	Eye	Trash	...
Ligand	Ball & Stick	Eye	Trash	...
Water	Ball & Stick	Eye	Trash	...
Ion	Ball & Stick	Eye	Trash	...

Unit Cell P 21 21 21

Density



Epic Games

News

Samples

Marketplace

Library

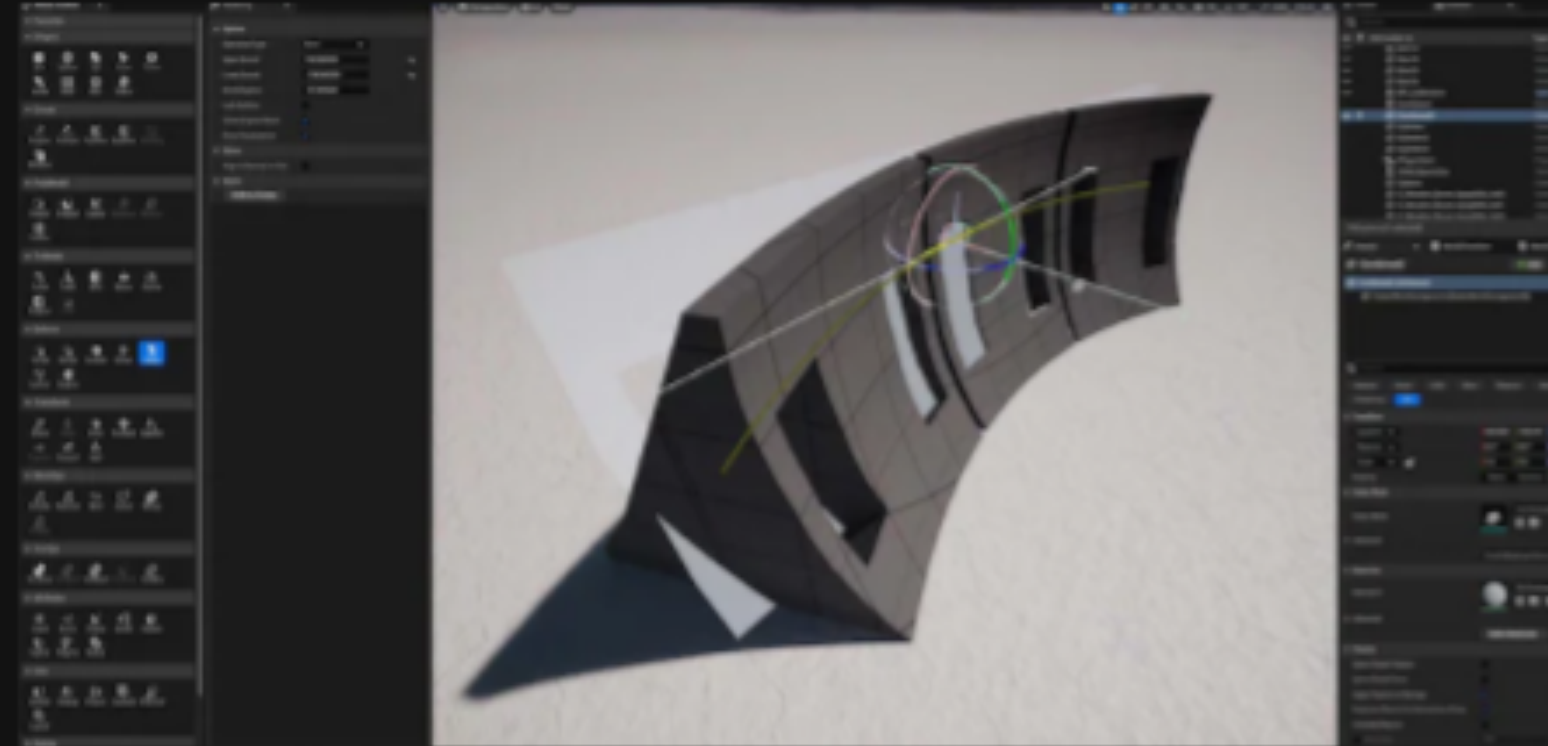
Twinmotion

Launch
Unreal Engine 5.0.0



Unreal Engine

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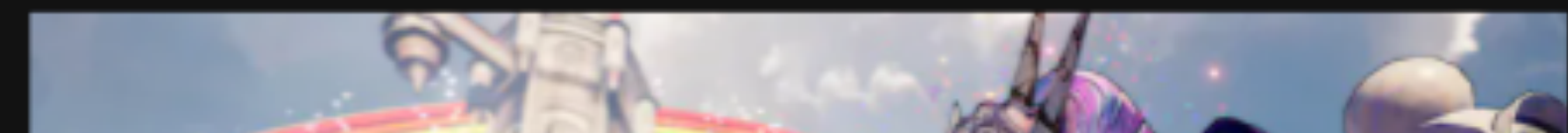
Downloads



Settings



GChief_117



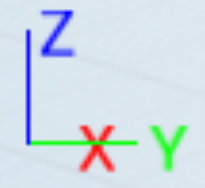
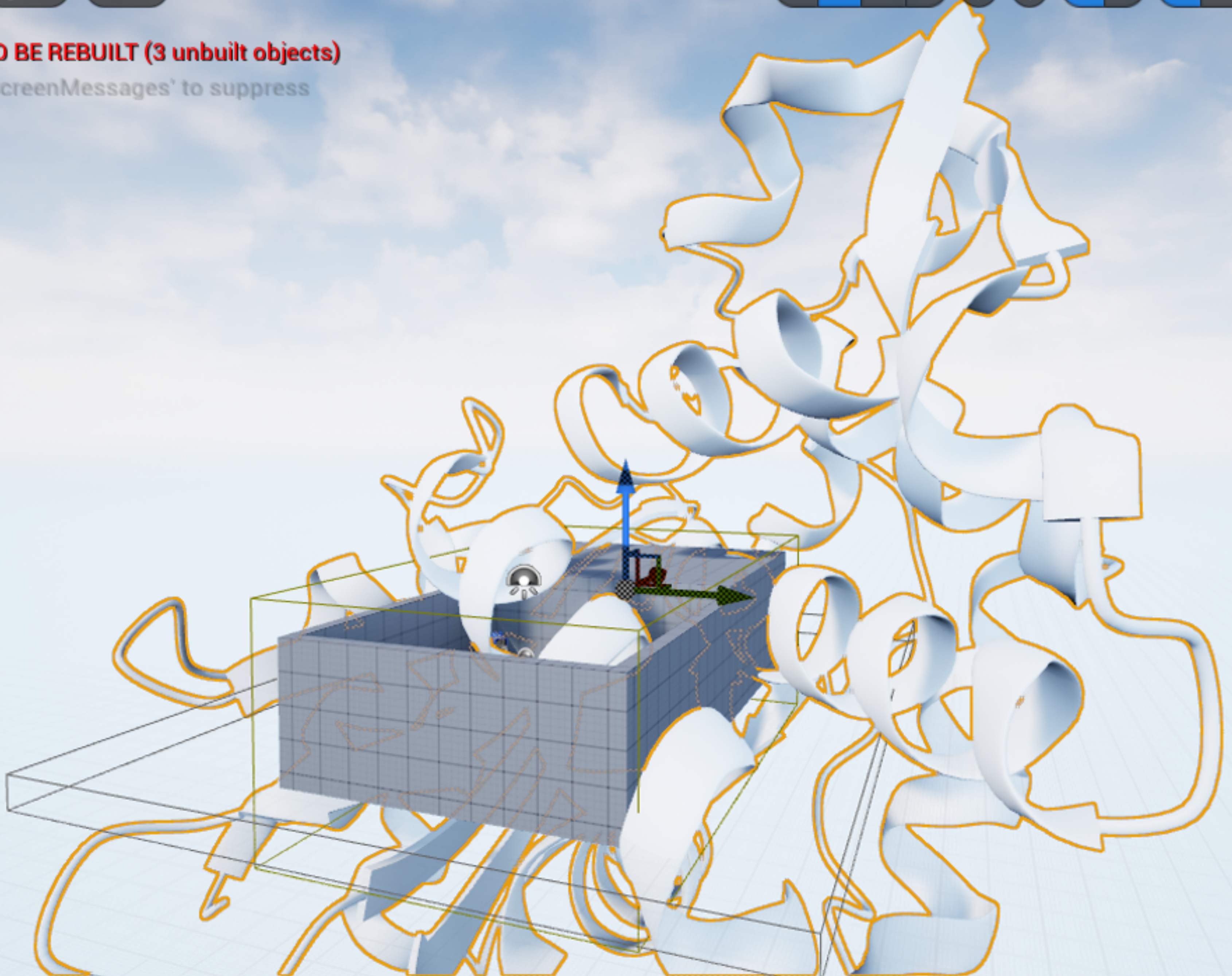
Understanding further prediction to be set in place

- There must be a library set in place to allow users to collect from protein data bank
- And recall from the other
- There is currently a 1 way method
- Improving the geometry of the PDB file and then have further augmentation in Blender to Unreal Engine

Technical Challenges

- Updates
- The following updates we faced issues related to Android SDK deployment and Oculus integration
- Unity and Oculus have had further partnership for hand tracking on the inside
- Coloration and segmentation of such protein formats to know when the structure is organized in what fashion
- Smoothing of the files
- Size augmentation

LIGHTING NEEDS TO BE REBUILT (3 unbuilt objects)
'DisableAllScreenMessages' to suppress



DEMO