AR Protein Visualization

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The Team

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- Computer Science with a Minor in Communication

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- Princeton, NJ
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- Computer Engineering with minor Computer Science

Motivation

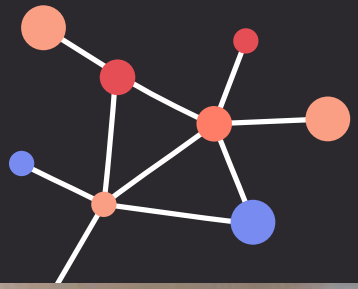
- What is Augmented Reality?
  - Computer-generated image on a user's view of the real world
- Why Augmented Reality?
  - Viewing 3D data on a 2D screen hides many details
  - Immersive and interactive exploration of complex datasets

Project and Technology Overview

Goal: Develop an interactive Augmented Reality (AR) solution to visualize and analyze molecular proteins, enhancing understanding.

- Data Source: Rutgers Protein Data Bank
- Technology: Unity Game Engine with C# scripting, Microsoft Hololens 2

RCSB PDB
PROTEIN DATA BANK



Program Breakdown

Input code: "*6PHQ*"

RCSB PDB PROTEIN DATA BANK

OR

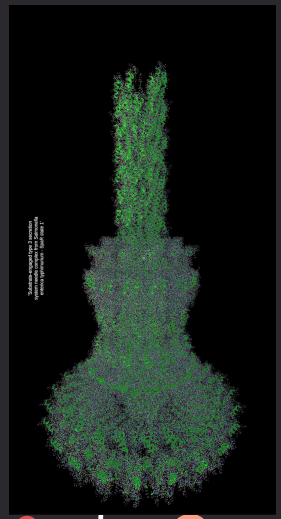
PDB

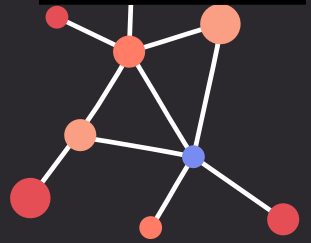
CIF

CSV

→ Color Atoms

→ Combine Meshes

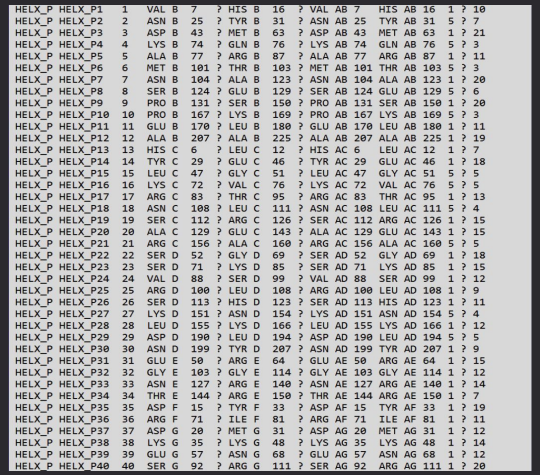




Web Scraping and CSV

- Downloads file from database
- Filters important information
- Autonomous

Original File:



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HELX_P HELX_P2   2   ASN B  25  ? TYR B  31  ? ASN AB 25  TYR AB 31  5 ? 7
HELX_P HELX_P3   3   ASP B  43  ? MET B  63  ? ASP AB 43  MET AB 63  1 ? 21
HELX_P HELX_P4   4   LYS B  74  ? GLN B  76  ? LYS AB 74  GLN AB 76  5 ? 3
HELX_P HELX_P5   5   ALA B  77  ? ARG B  87  ? ALA AB 77  ARG AB 87  1 ? 11
HELX_P HELX_P6   6   MET B  101 ? THR B  103 ? MET AB 101 THR AB 103 5 ? 3
HELX_P HELX_P7   7   ASN B  104 ? ALA B  123 ? ASN AB 104 ALA AB 123 1 ? 20
HELX_P HELX_P8   8   SER B  124 ? GLU B  129 ? SER AB 124 GLU AB 129 5 ? 6
HELX_P HELX_P9   9   PRO B  131 ? SER B  150 ? PRO AB 131 SER AB 150 1 ? 20
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HELX_P HELX_P19  19  SER C  112 ? ARG C  126 ? SER AC 112 ARG AC 126 1 ? 15
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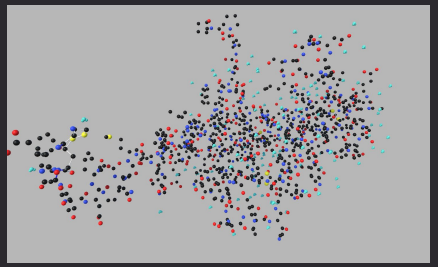
HELX_P HELX_P40  40  SER G  92  ? ARG G  111 ? SER AG 92  ARG AG 111 1 ? 20
```

CSV File:

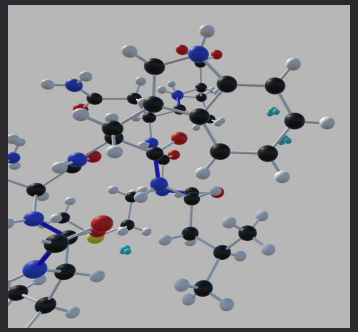
HELIX	7	16 AB
HELIX	25	31 AB
HELIX	43	63 AB
HELIX	74	76 AB
HELIX	77	87 AB
HELIX	101	103 AB
HELIX	104	123 AB
HELIX	124	129 AB
HELIX	131	150 AB
HELIX	167	169 AB
HELIX	170	180 AB
HELIX	207	225 AB
HELIX	6	12 AC
HELIX	29	46 AC
HELIX	47	51 AC
HELIX	72	76 AC
HELIX	83	95 AC
HELIX	108	111 AC
HELIX	112	126 AC
HELIX	129	143 AC
HELIX	156	160 AC
HELIX	52	69 AD

Generation and Interaction

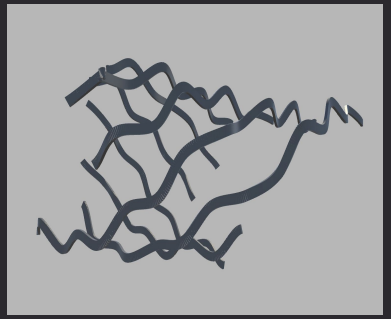
- Protein features from CSV
- Colors and Scales atoms
- Interaction Scripts attached



Atoms

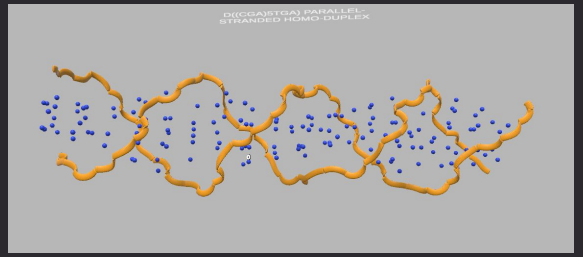


Bonds



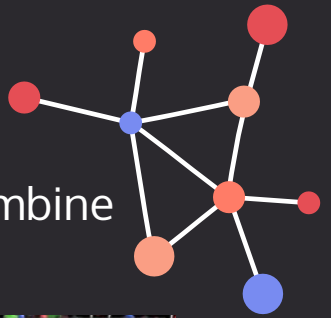
Beta Sheets

Helices

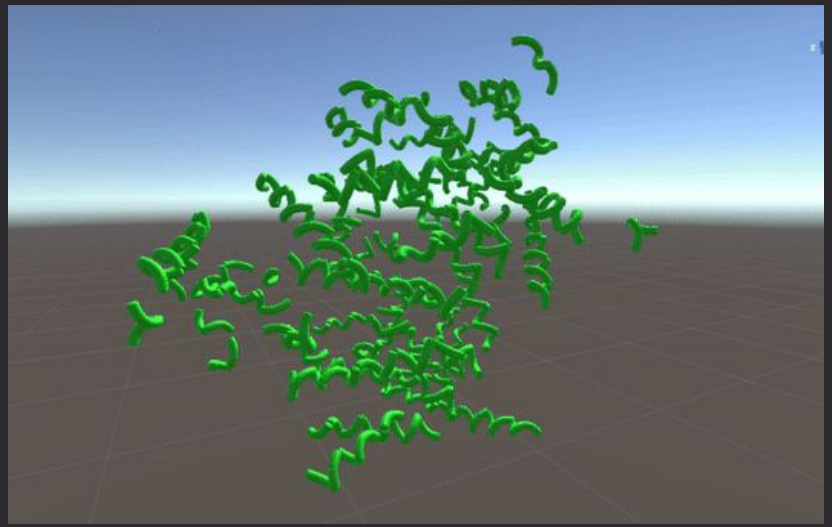


RNA

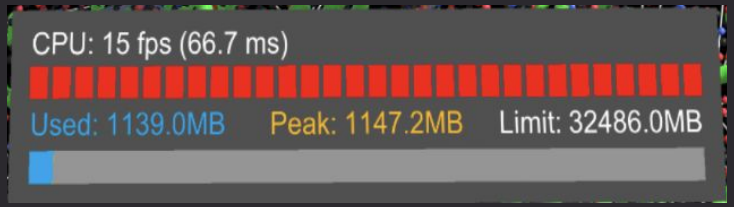
Challenges and Optimization Efforts



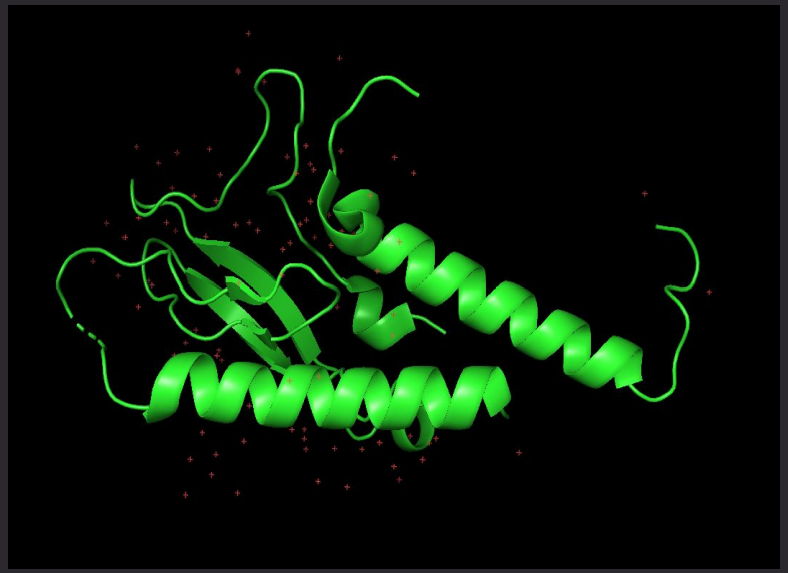
Jagged curved structures → use splines to smooth out



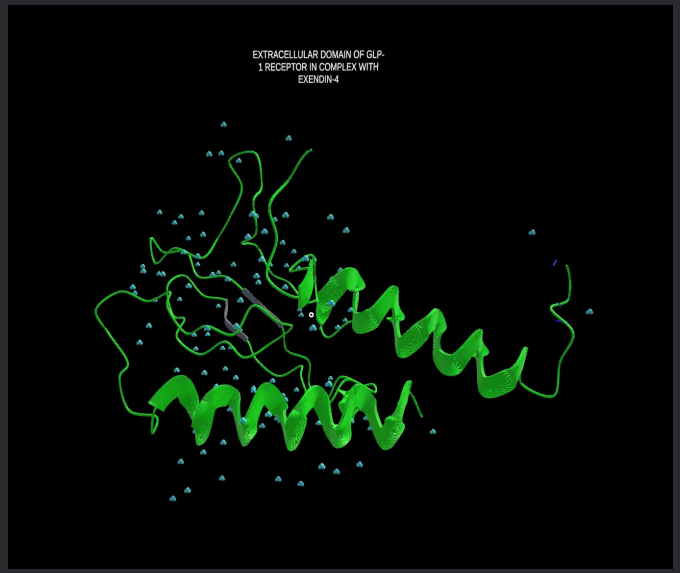
Slow model rendering → combine meshes of similar objects



Results

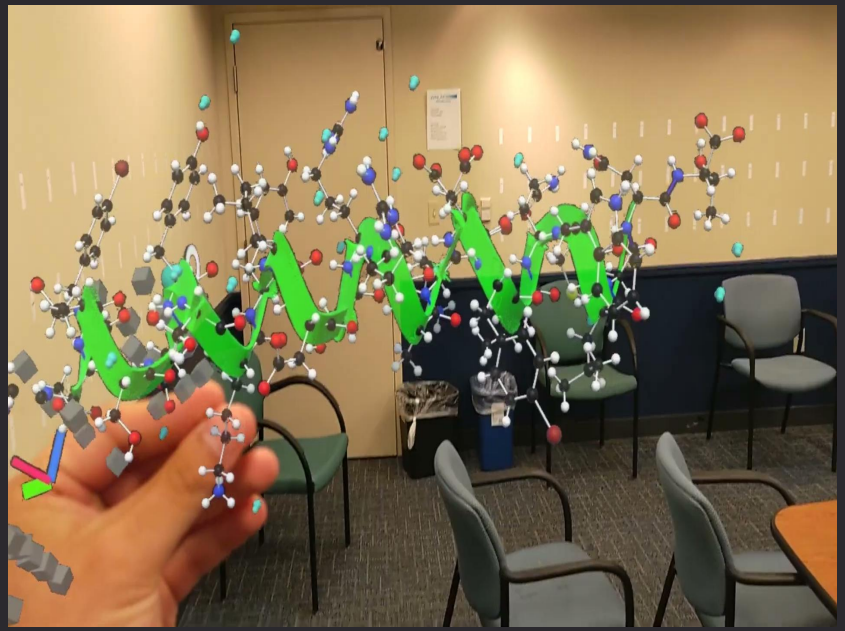


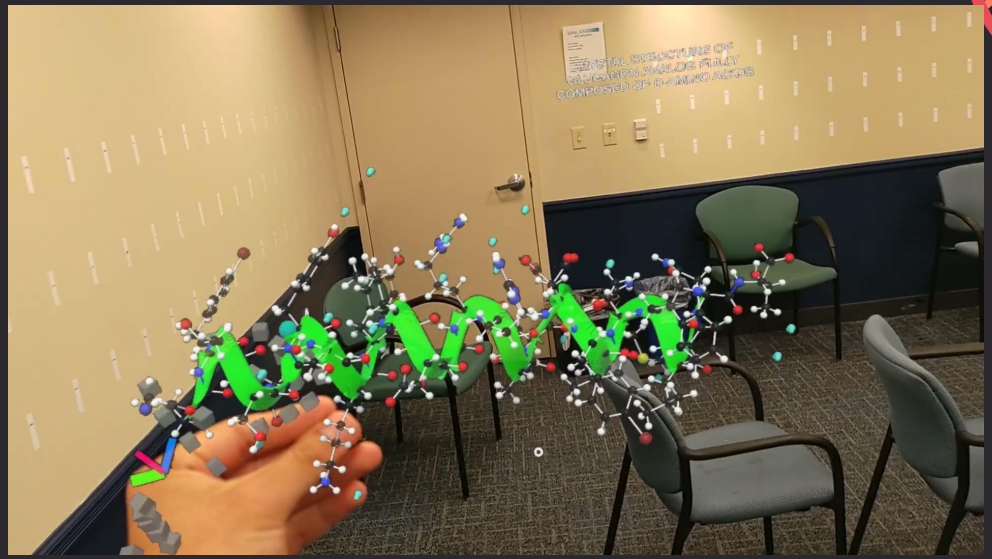
5OTT PyMol Model



5OTT Model in Unity

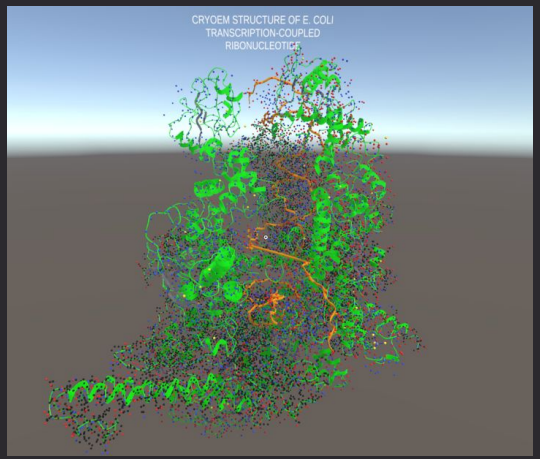
Voice Command Feature





Future Plans

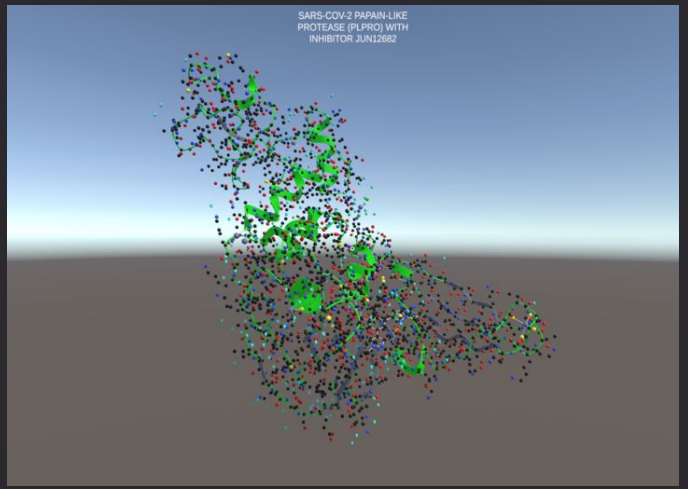
- Greater detail in RNA and Beta-Sheets implementation
- Optimized rendering for large proteins
- Faster 3D model generation and loading time of proteins
- Deploy visualizations to a mobile application
- Feedback from professionals



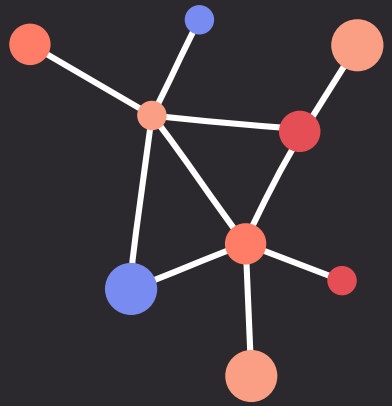
CryoEM Structure of E.Coli

Potential Project Applications

- Interactive Learning Experiences
- Drug Discovery and Manipulation
- Medical Training
- Public Health Awareness



SARS-CoV-2



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Thank You!