Leveraging the Protein Databank

Creating effective molecular 3D models for improving scientific communication

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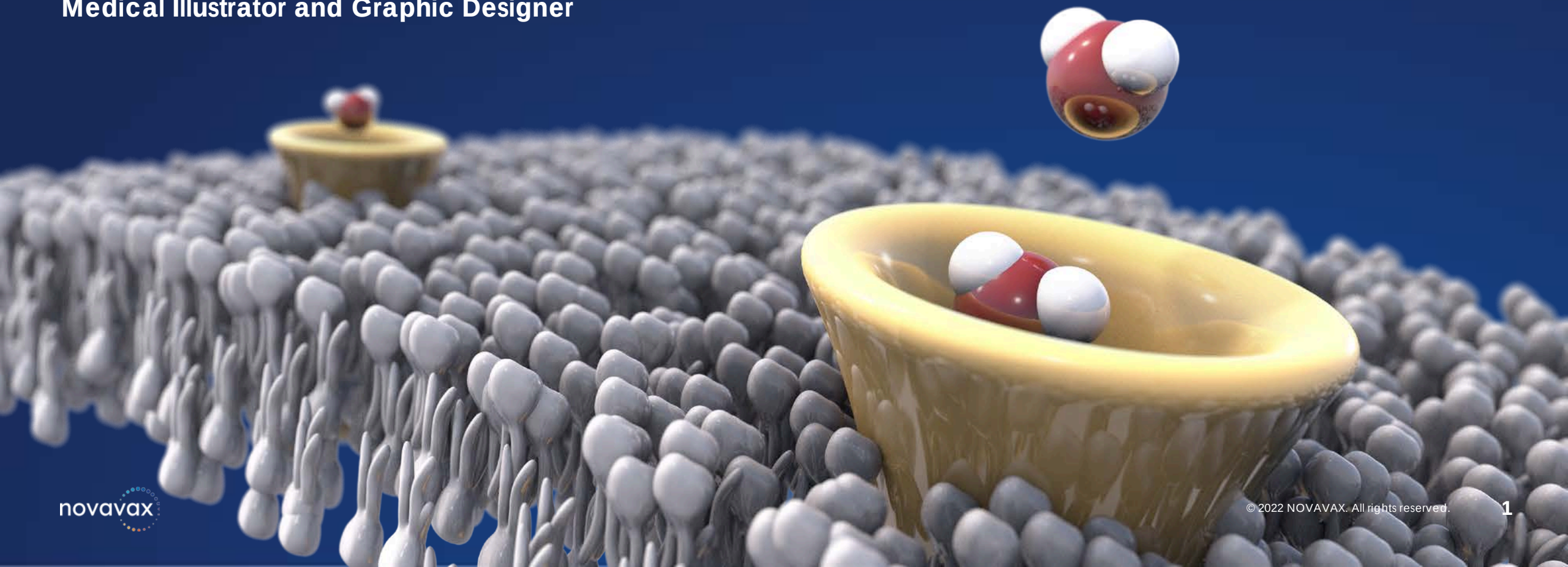


Downloads

Pymol

Molecular model editing

https://pymol.org/2/

Chimera

Molecular model editing

https://www.cgl.ucsf.edu/chimera/download.html

Blender

Whole 3D pipeline (modelling, animating, lighting, etc.)

https://www.blender.org/download/

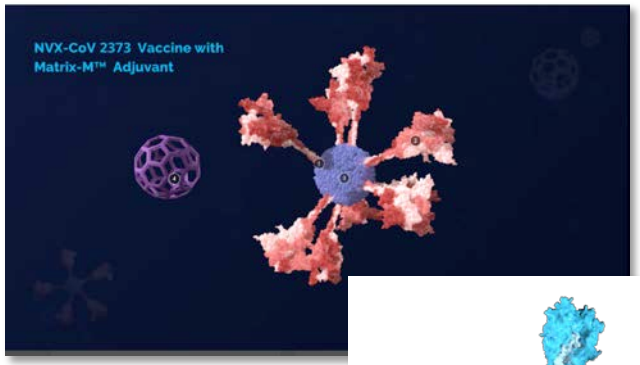
Overview

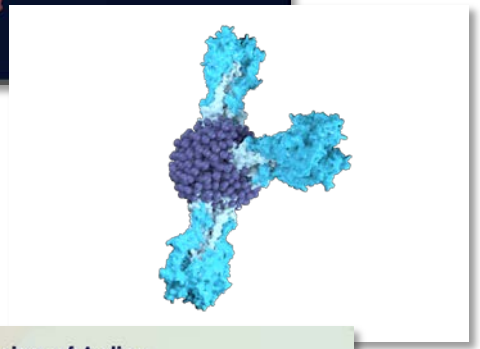
By the end of this workshop you should:

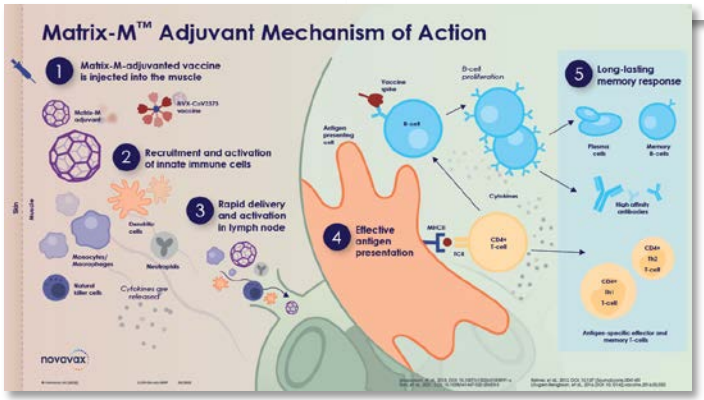
- Have a better understanding of what an accurate protein is and why different representations might be used
- How to export a file from the Protein Databank to use in 3D graphics software
- How to manipulate the file in other software to select and export different elements for use in 3D modeling

Why visualize molecular structures?

Communication with the public, subject matter experts, students and more







- Explain complex biological processes to a general audience, including patient communication
- Help people using the technology (ie. Healthcare providers, public) understand how it works
- Provide internal experts with visual materials they can use to explain the scientific concepts to external stakeholders
- Enhance understanding for employees, scientists and others for training and improved productivity

Image 1-Protein ID: 6VXX (Closed Spike Protein)
Image 2 -Protein ID: 21BX (HA protein)

What is the protein databank?

Public databank of molecularly accurate proteins:

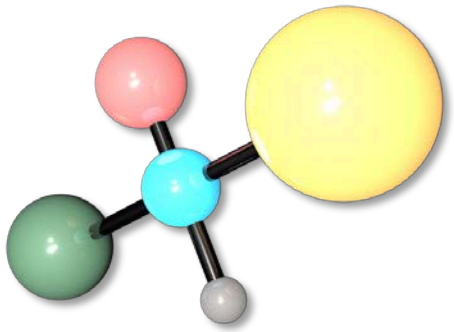
- **File Type:** PDBs (can be converted to other types of 3D data)
- **License:** CC0 1.0 Universal Public Domain Dedication
- **Number of available Files:** ~190,000
- Citation instructions are available on the website

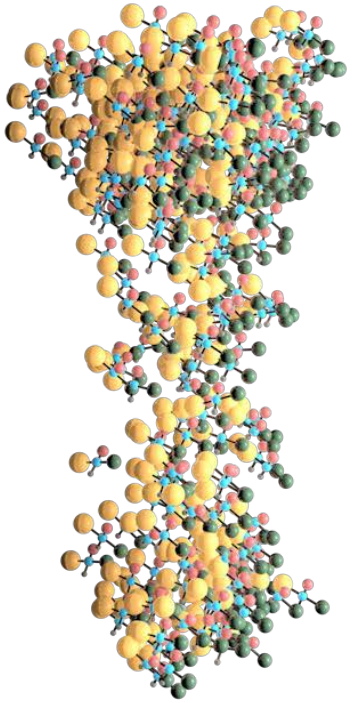
RCSB PDB: Homepage

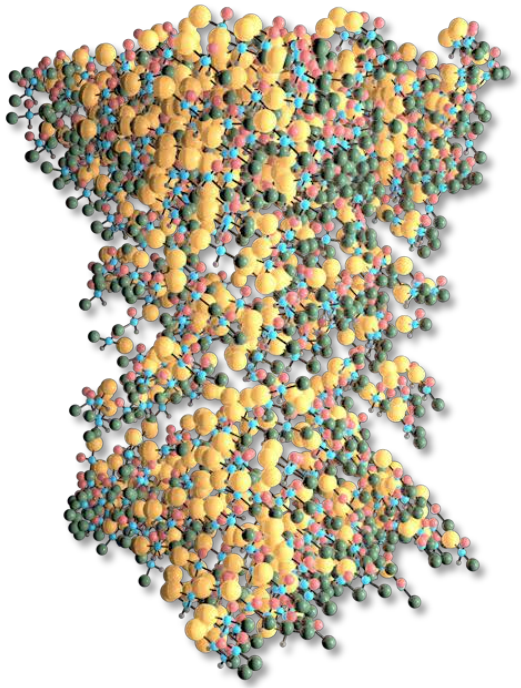
What is a protein?

Molecules that compose one or more long chains of amino acids

Amino Acid (AA) → **Protein (many AAs)** → **Oligomer (several of the same protein together)**







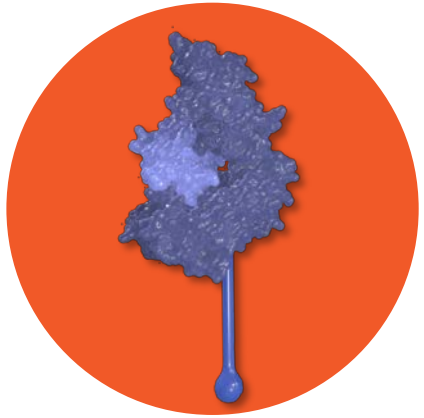
Proteins (of all sizes) do much of **the work of the cell**: growth, structure, signaling, transport, etc.

Visualizing Proteins

Ribbon Diagram

The overall path of the protein's backbone

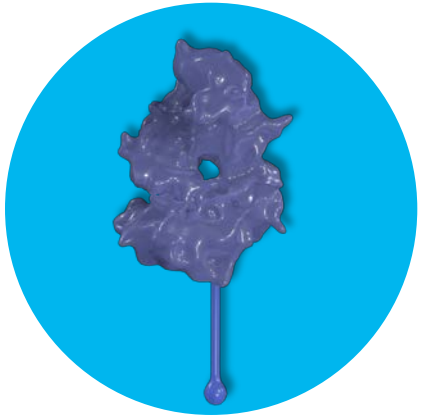
Allows you to include important features at key locations



Surface Structures

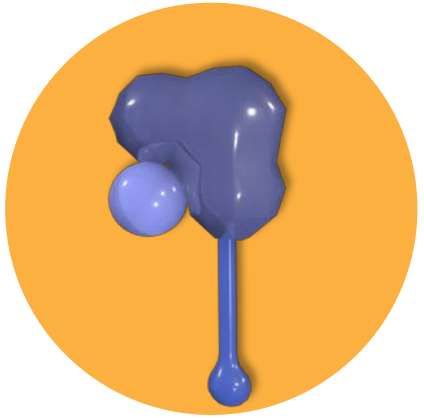
The combined shapes of the electrostatic potential of the molecules

Can help to show protein interactions and fit



Reduced

A less detailed surface diagram



Abstract

Represents subunits or important parts of a protein using generic shapes

Illustrating larger-scale pathways and mechanisms

Hands-on:

Go to the link below to access a PDB in the protein databank and work through the following slides to learn the basics of working in molecular editors such as the Protein Databank Editor, PyMol, and Chimera.

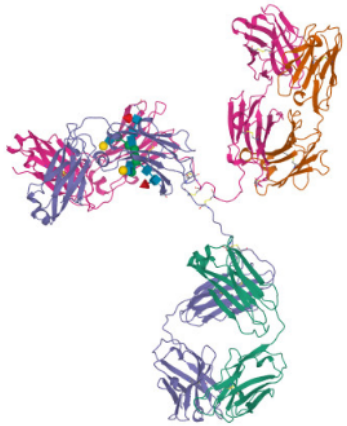
RCSB PDB - 1IGT: STRUCTURE OF IMMUNOGLOBULIN

Accessing the Structure in the Databank Editor

RCSB PDB | Deposit | Search | Visualize | Analyze | Download | Learn | More | Documentation | Careers | MyPDB

Structure Summary | 3D View | Annotations | Experiment | Sequence | Genome | Versions

Biological Assembly 1



3D View: Structure | 1D-3D View | Validation Report

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Hetero 4-mer - A2B2

Display Files | Download Files

1IGT

STRUCTURE OF IMMUNOGLOBULIN

PDB DOI: 10.2210/pdb1IGT/pdb

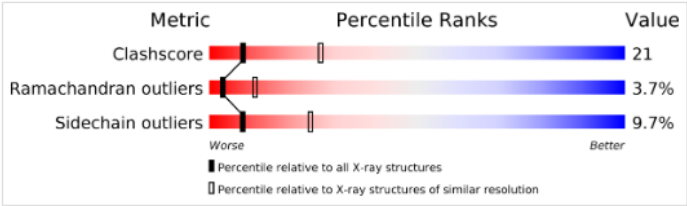
Classification: IMMUNOGLOBULIN
Organism(s): Mus musculus
Mutation(s): No

Deposited: 1996-10-25 **Released:** 1997-07-07
Deposition Author(s): Harris, L.J., Larson, S.B., Hasel, K.W., McPherson, A.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.80 Å
R-Value Free: 0.297
R-Value Work: 0.209
R-Value Observed: 0.209

wwPDB Validation | 3D Report | Full Report

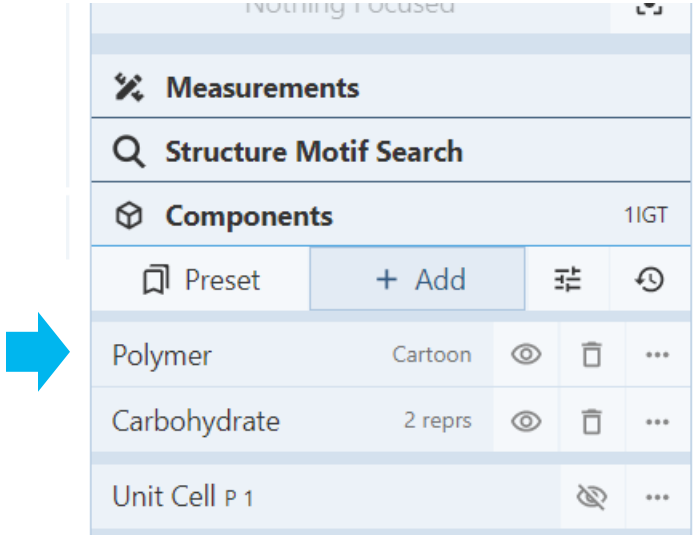


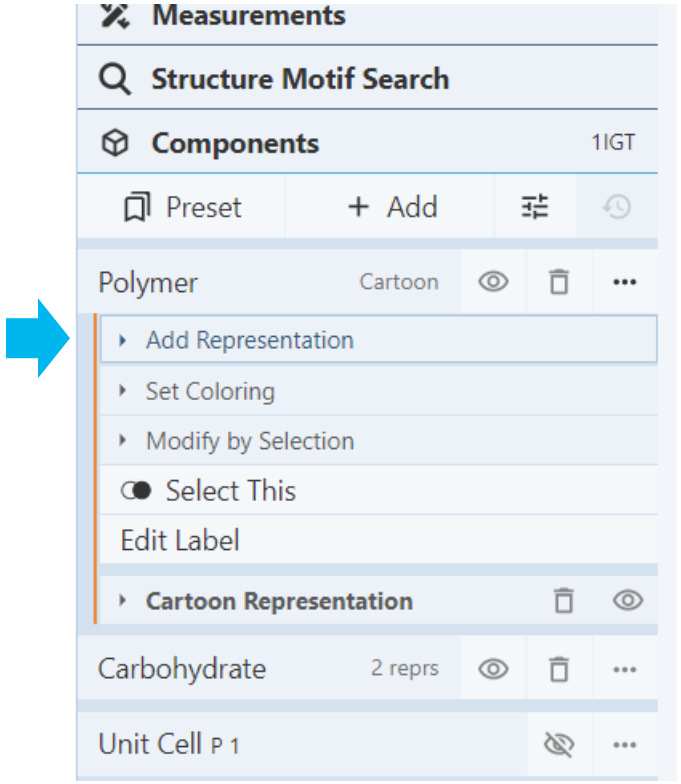
This is version 2.0 of the entry. See complete history.

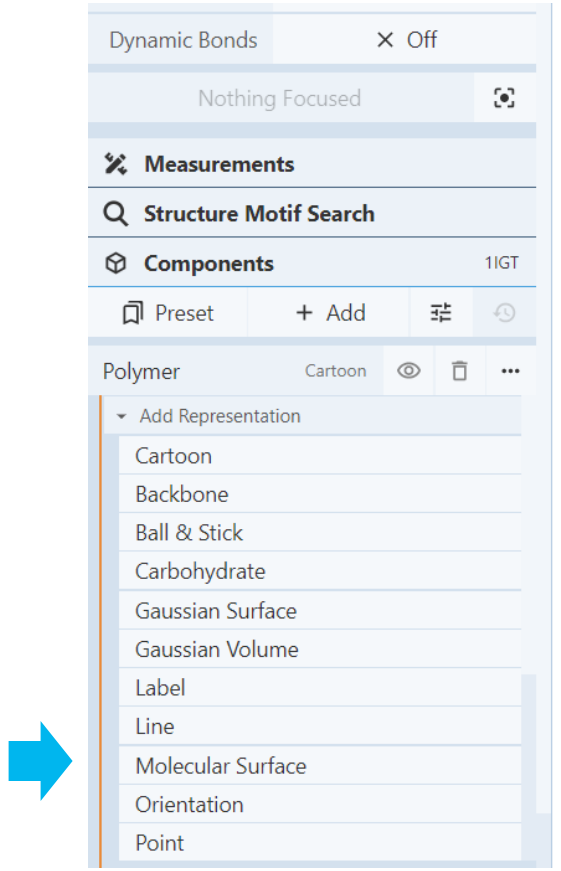
Protein ID: 1IGT (Immunoglobulin)
Berman, et al. 2000, The Protein Data Bank *Nucleic Acids Research*, 28: 235-242. rcsb.org

Adding a molecular surface in the PDB Editor

Instructions: Polymer > Add Representation > Molecular Surface







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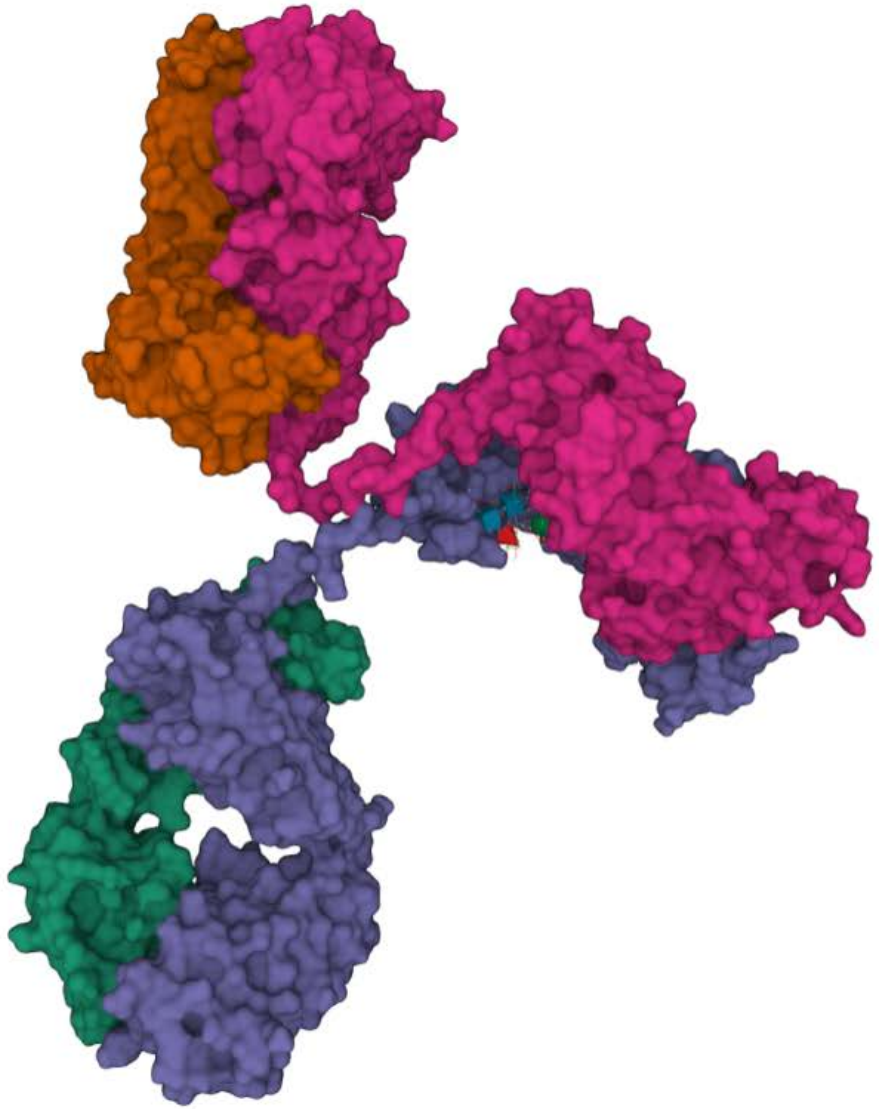
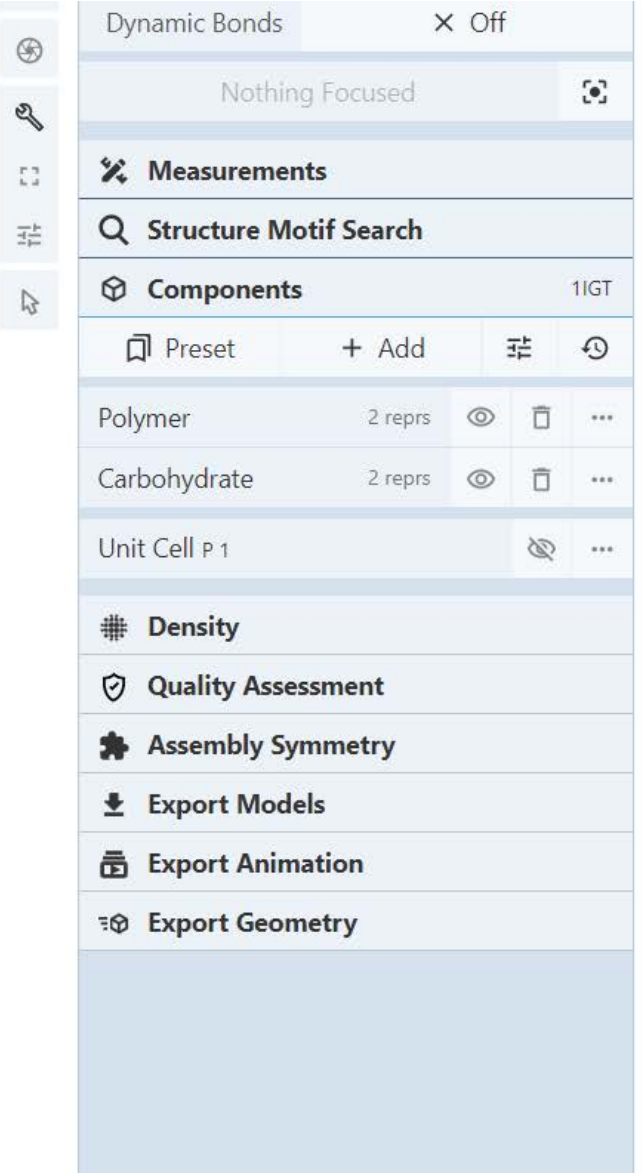
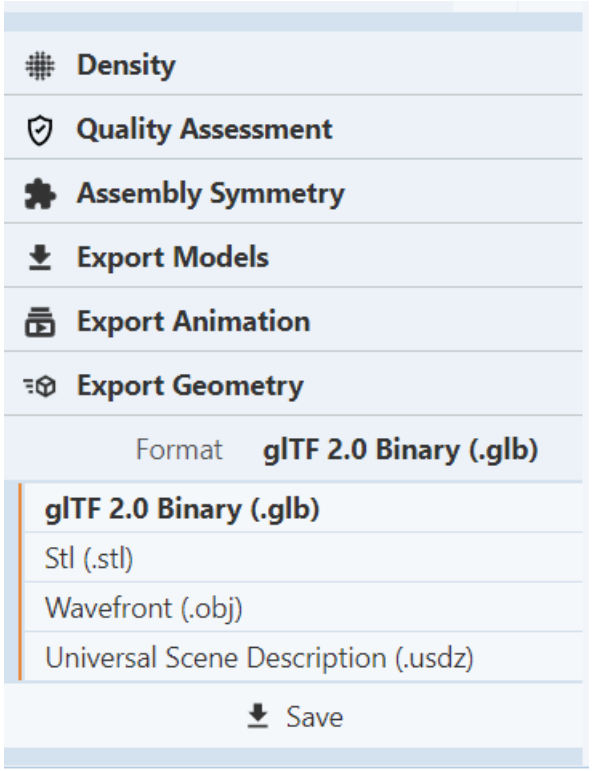




Protein ID: 1IGT (Immunoglobulin)
Berman, et al. 2000, The Protein Data Bank *Nucleic Acids Research*, 28: 235-242. rcsb.org

Downloading the Geometry

Instructions: Export Geometry > gITF 2.0 Binary > Select File Type > Save



gITF, STL, and OBJ

Compatible with Blender

Download a .glb

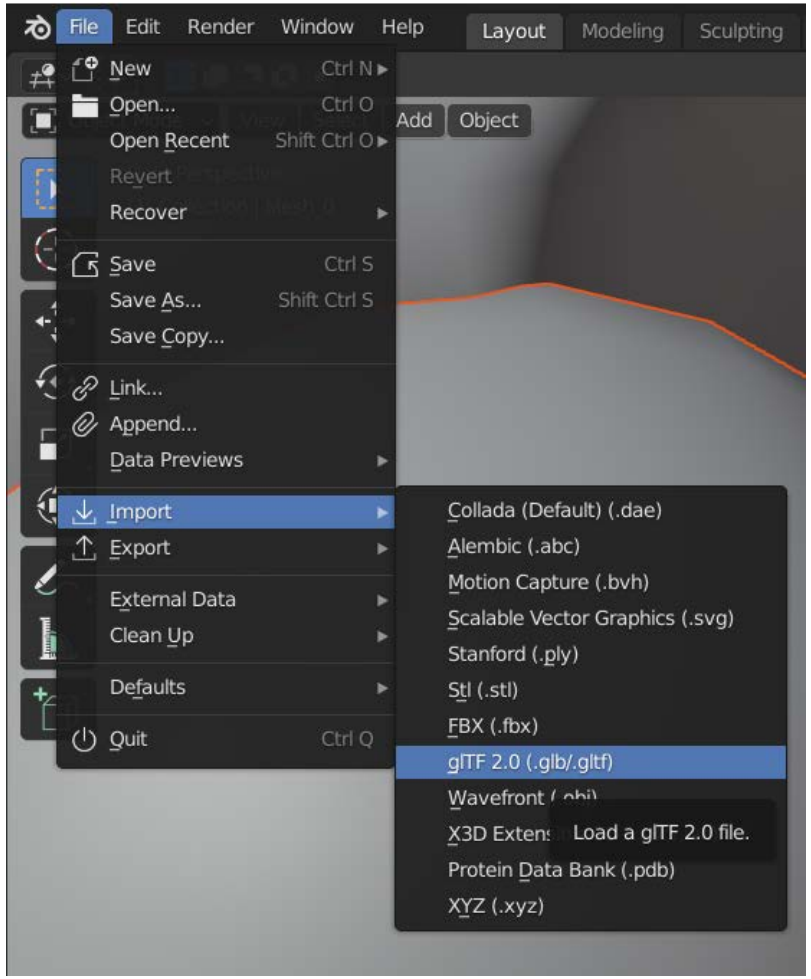
STL and OBJ

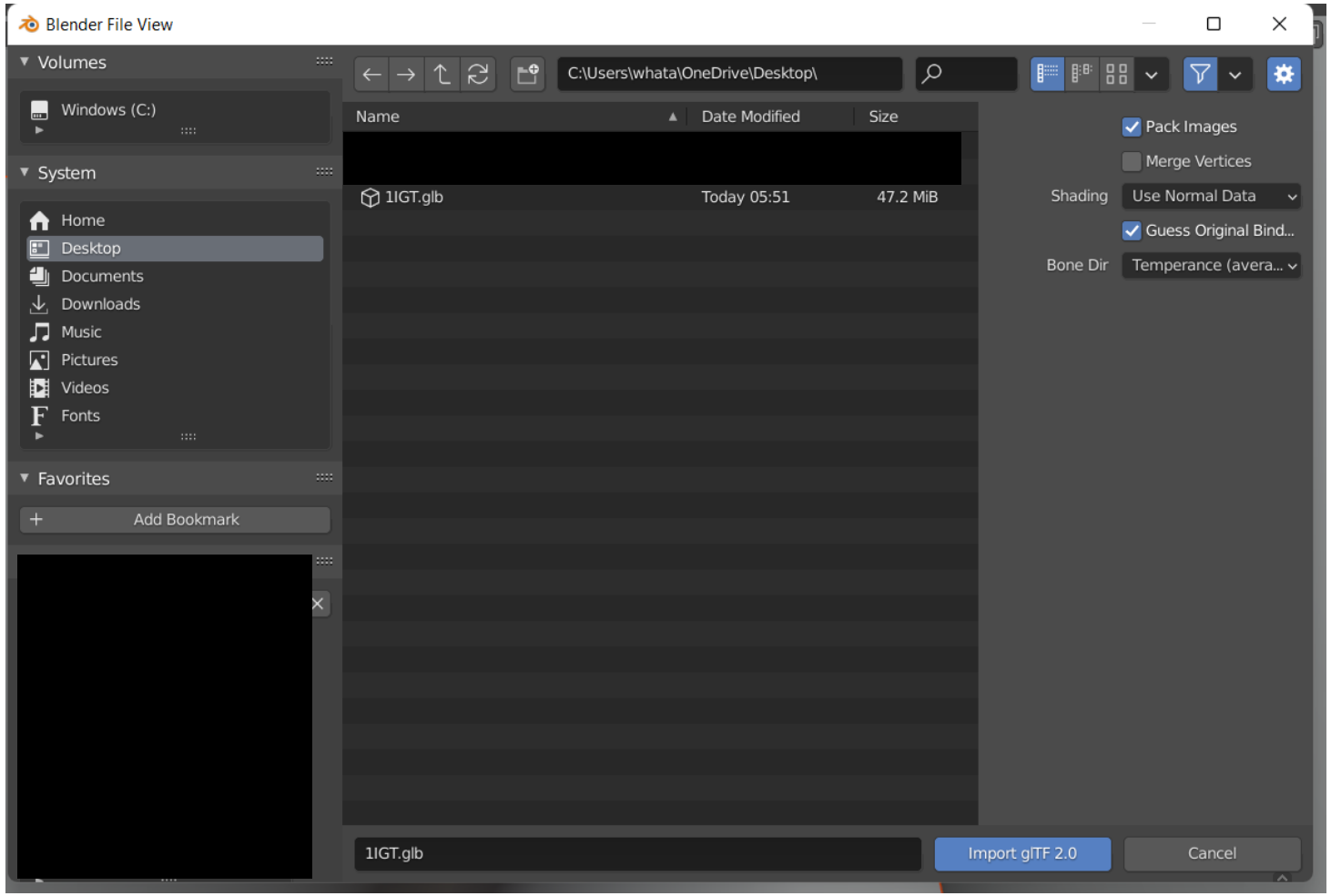
Compatible with Cinema 4D

Protein ID: 1IGT (Immunoglobulin)
Berman, et al. 2000, The Protein Data Bank *Nucleic Acids Research*, 28: 235-242. rcsb.org

Bringing a Protein Into Blender

Instructions: File > Import > [File Type] > Select File > Import

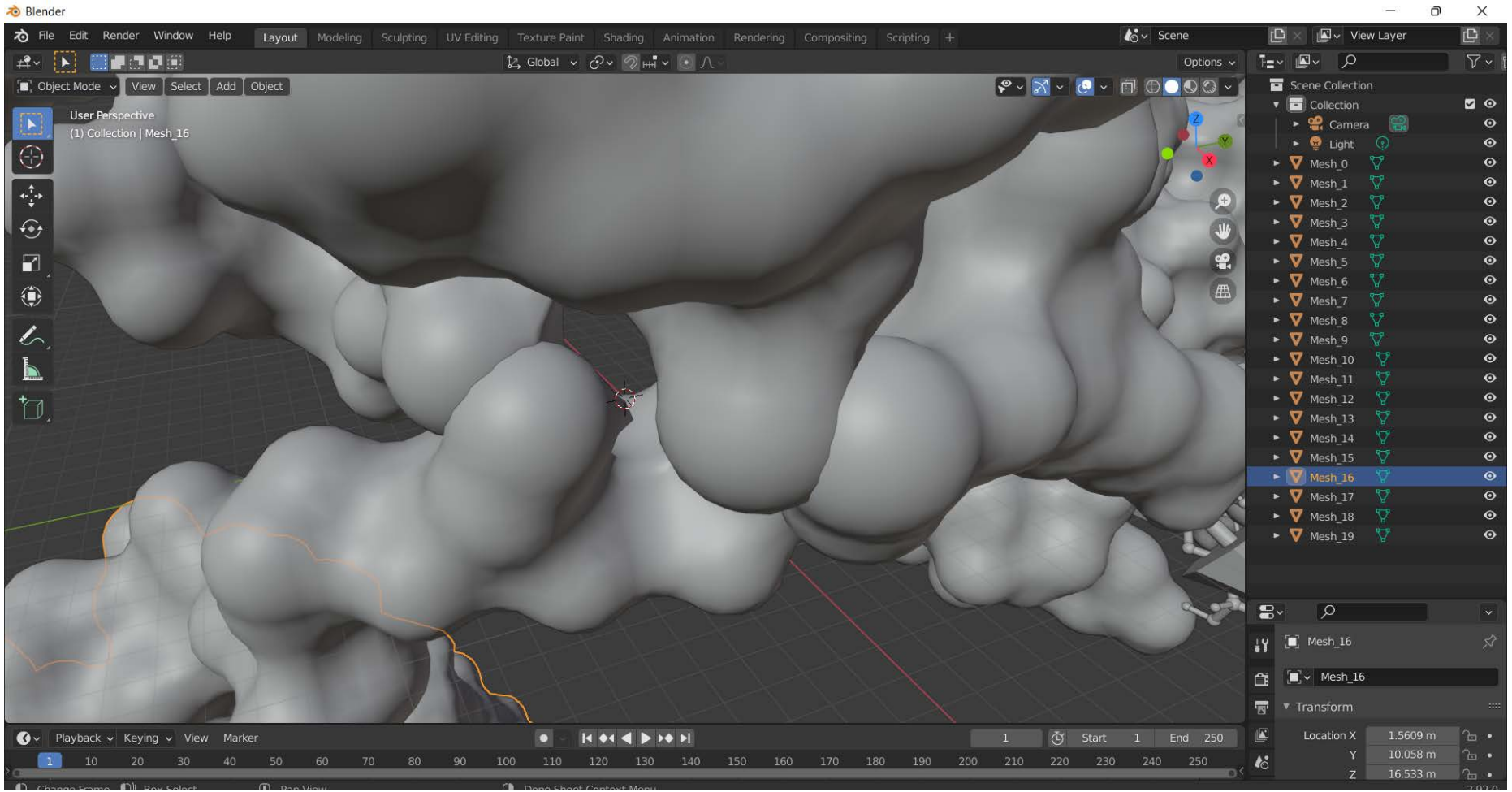




Protein ID: 1IGT (Immunoglobulin)
CC BY-SA 3.0 Blender Foundation – www.blender.org

Protein Enters Scene

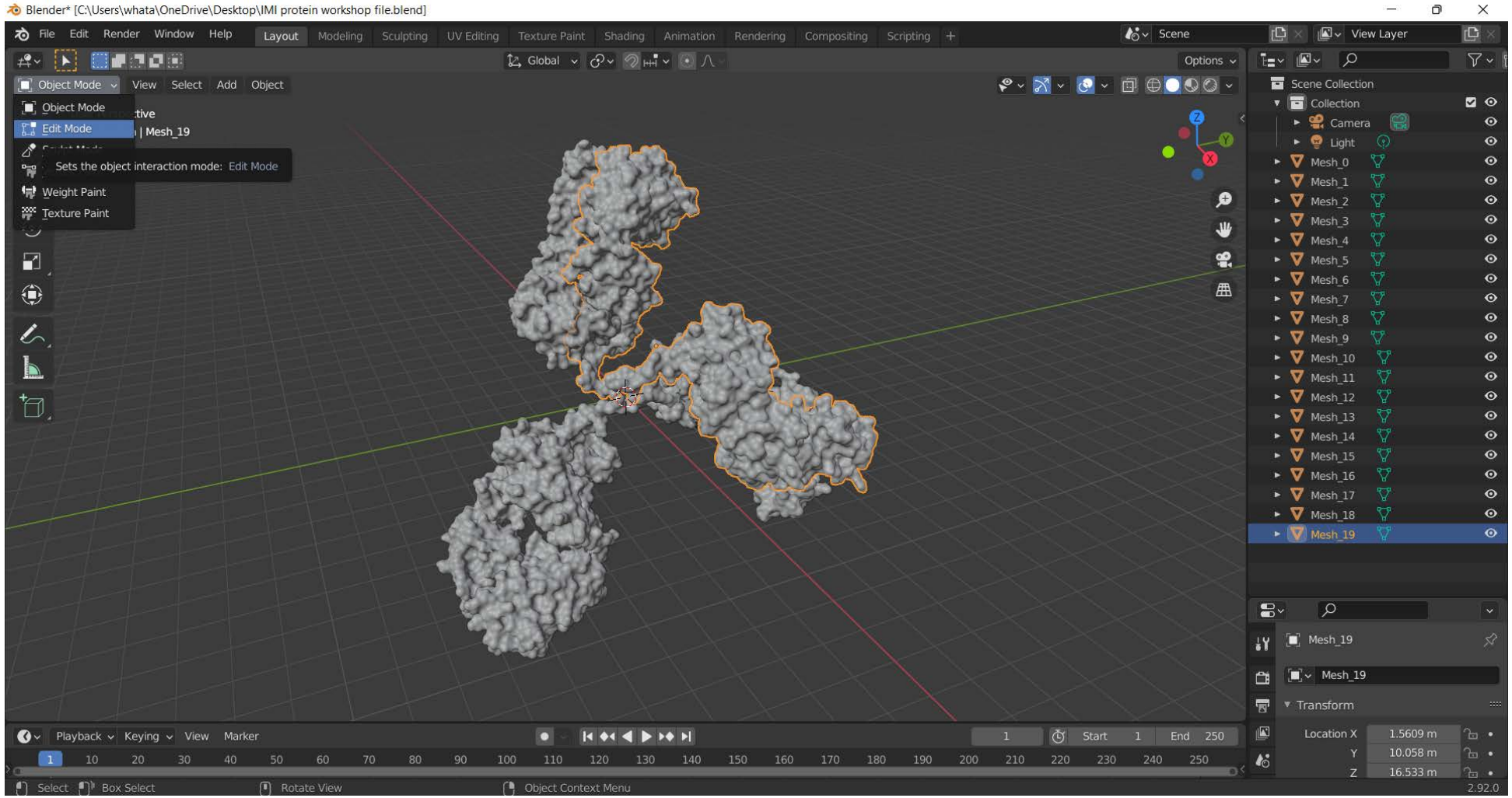
Protein may not be visible when it first comes into scene or may be very zoomed in



Protein ID: 1IGT (Immunoglobulin)

Object Mode to Edit Mode

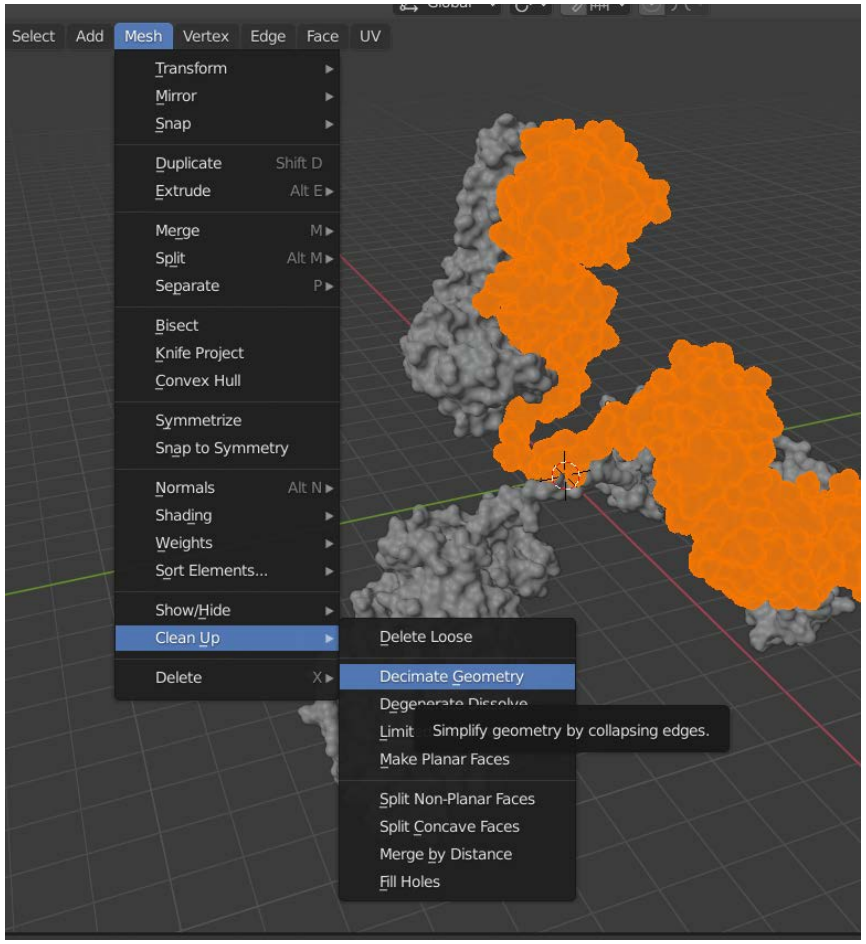
Instructions: Object Mode > Edit Mode

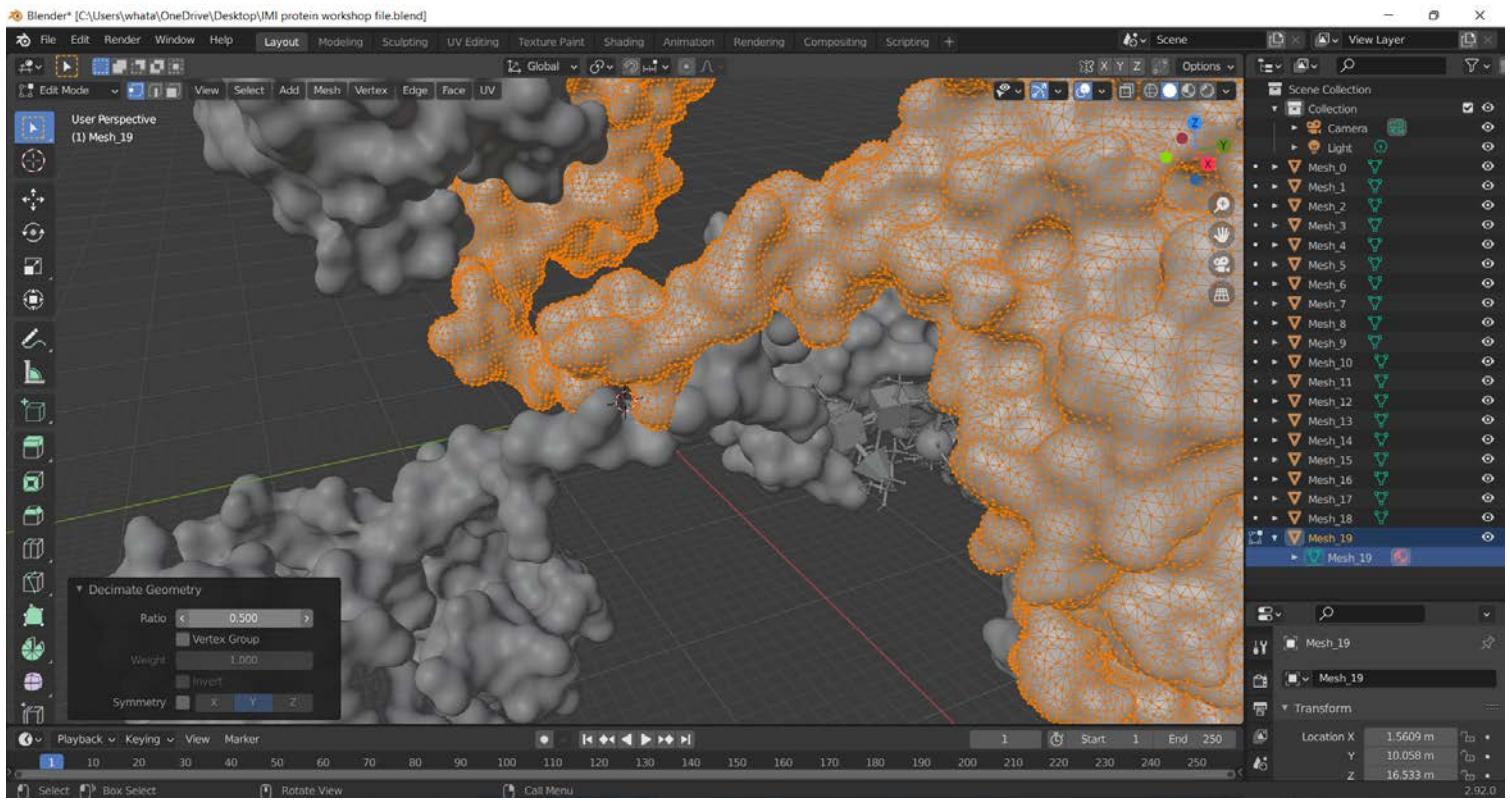


Protein ID: 1IGT (Immunoglobulin)
CC BY-SA 3.0 Blender Foundation – www.blender.org

Decimate Geometry

Instructions: Mesh > Clean Up > Decimate Geometry > Adjust number in ratio slider



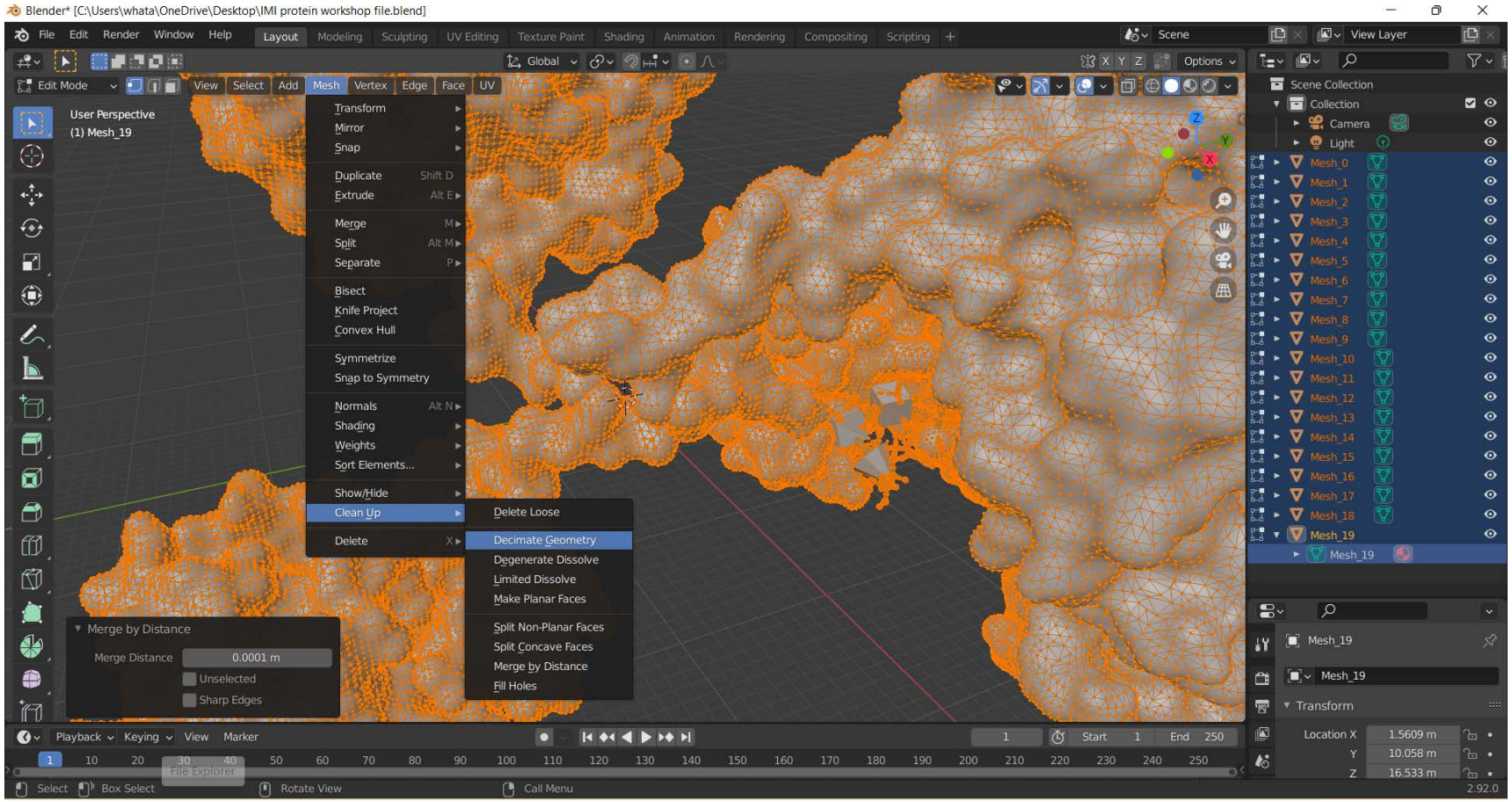


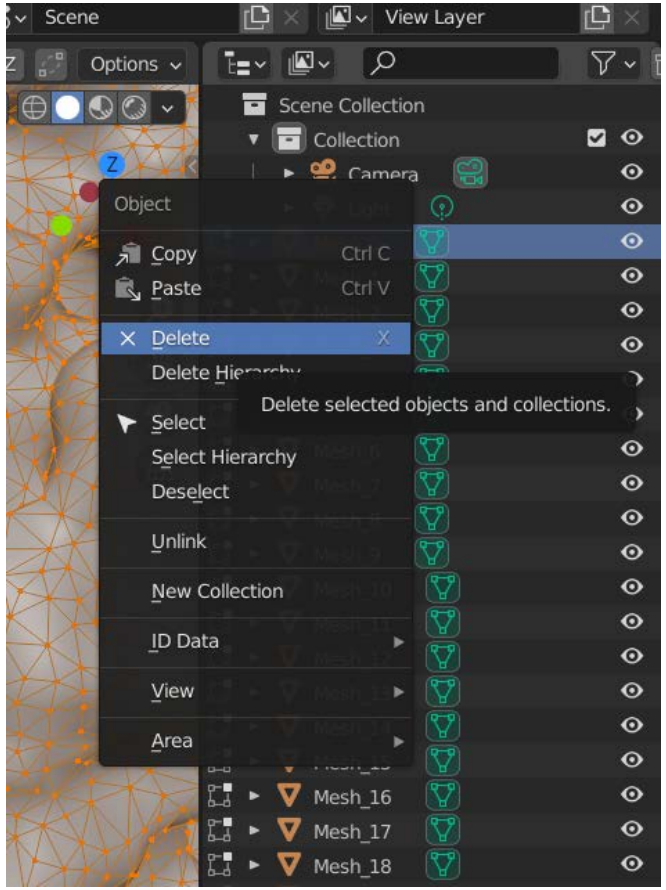
*you may need to zoom in to see the polygons, reduce it based on your needs

Protein ID: 1IGT (Immunoglobulin)
CC BY-SA 3.0 Blender Foundation – www.blender.org

Selecting > 1 Object and Deleting Objects

Instructions: Select one object > Shift > Select the number of objects you want
Right click > Select delete

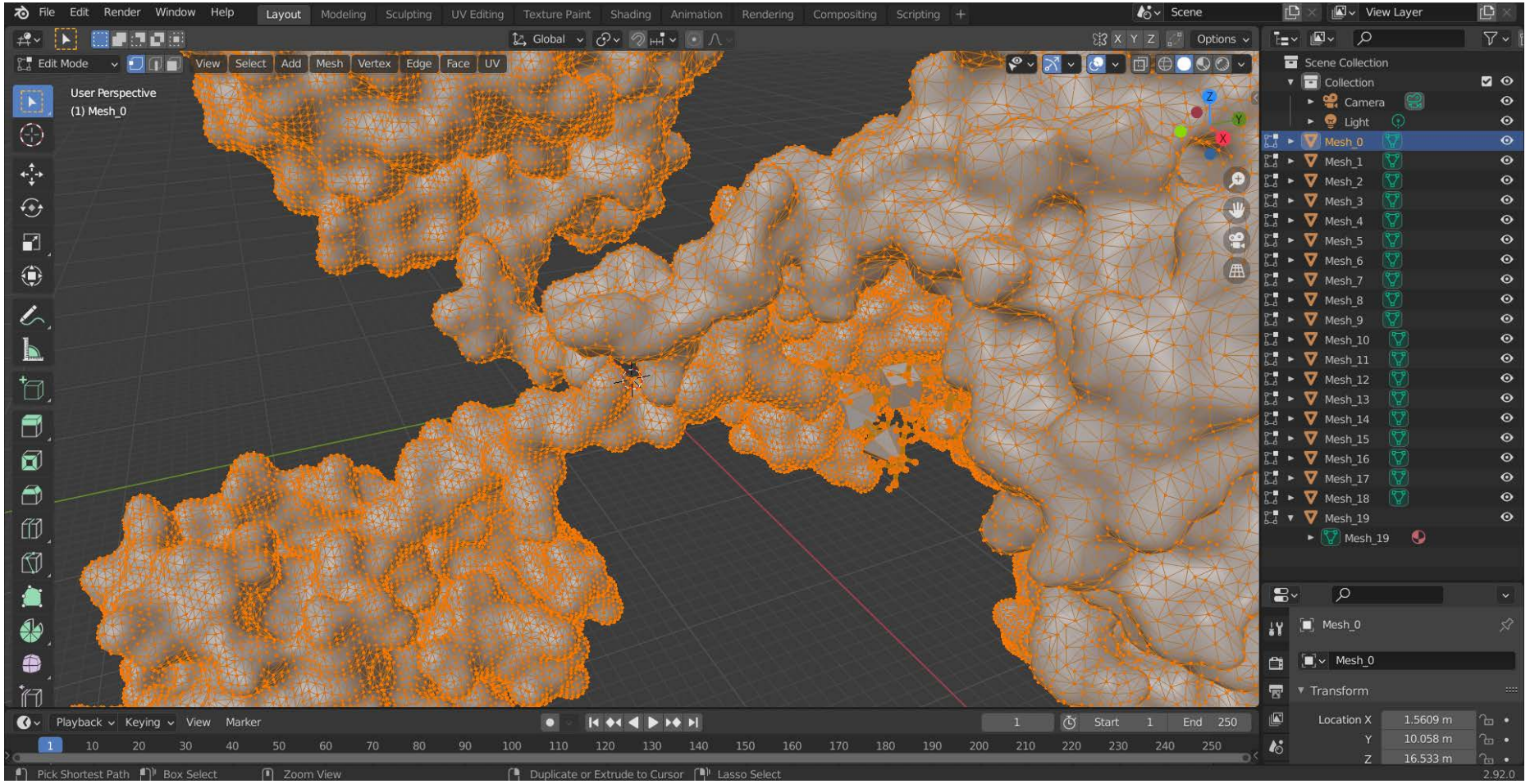




Protein ID: 1IGT (Immunoglobulin)
CC BY-SA 3.0 Blender Foundation – www.blender.org

Exporting Object

Click: File > Export > Select file type



Protein ID: 1IGT (Immunoglobulin)
CC BY-SA 3.0 Blender Foundation – www.blender.org

Pymol

An open source molecular visualization software, it uses Python-based commands to control, select, and highlight the protein in the software

https://pymol.org/2/

Downloading a PDB

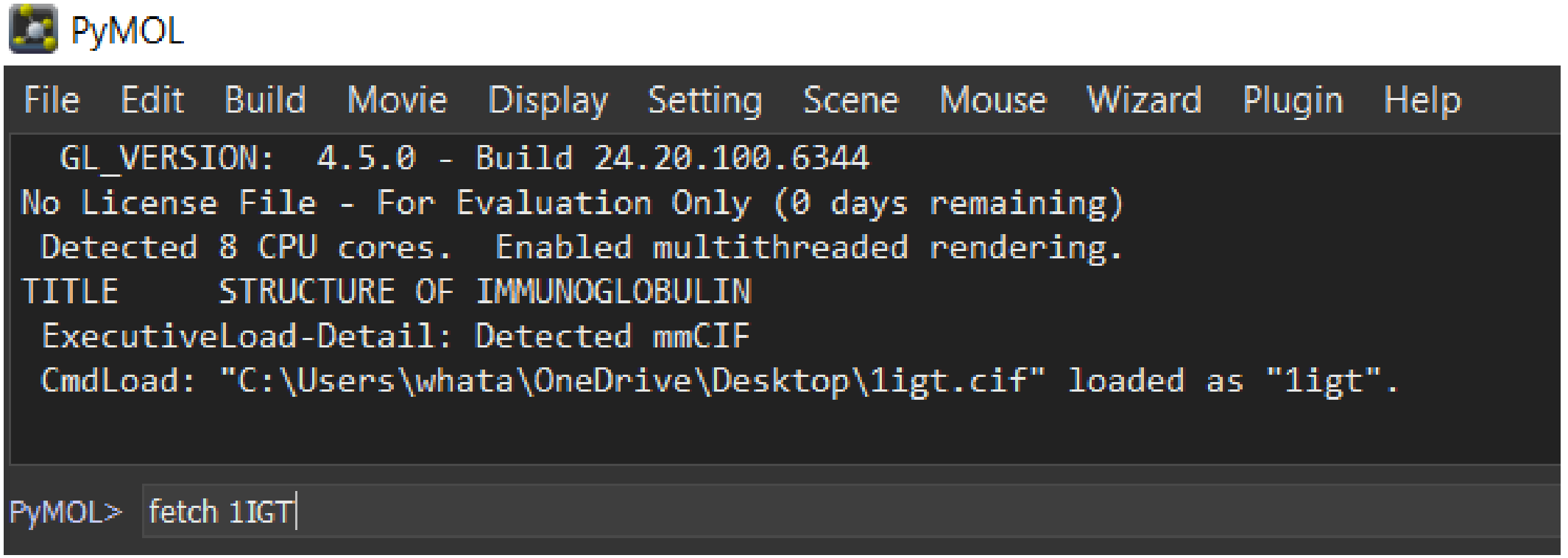
Instructions: Double-click file to open in Pymol

Protein ID: 1IGT (Immunoglobulin)

Pettersen, et al. UCSF Chimera--a visualization system for exploratory research and analysis, *J Comput Chem.* 2004 Oct;25(13):1605-12.

Fetching a PDB

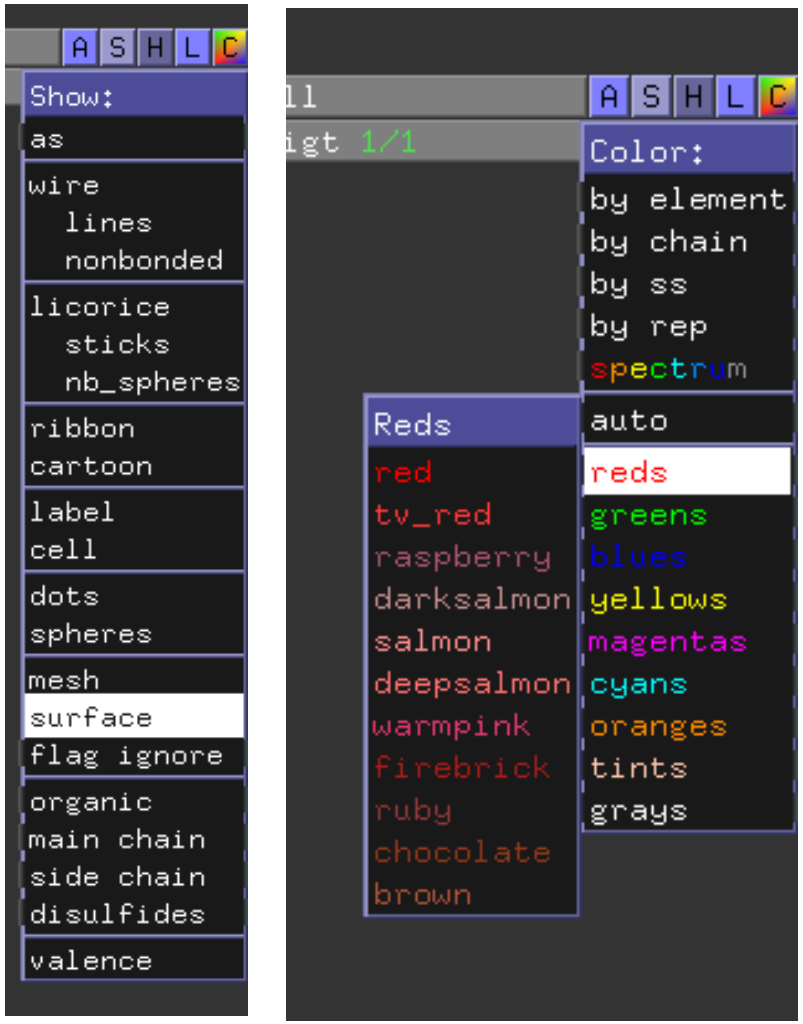
“Fetch 1IGT”



Protein ID: 1IGT (Immunoglobulin)

Show Surface

Instructions: S in the right drop down menu > C to change its color



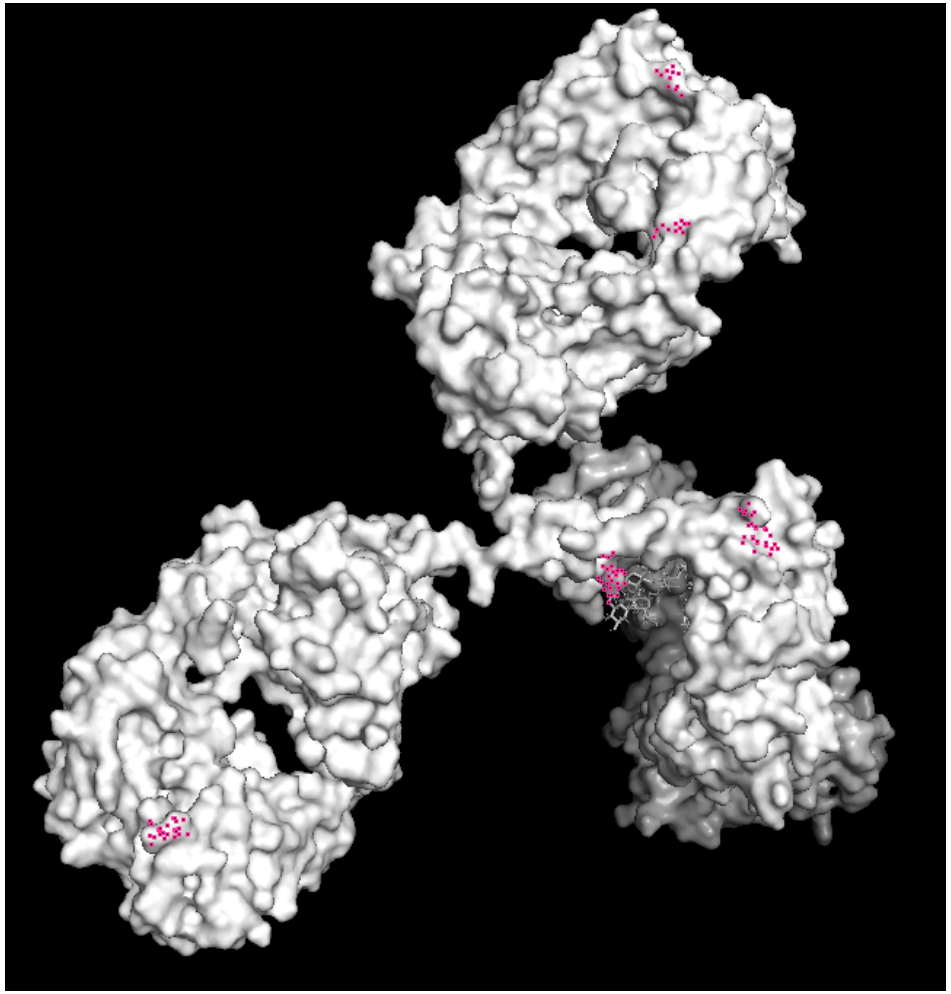
**Magnified view of drop-down bar*

Protein ID: 1IGT (Immunoglobulin)

Select Residue

Instructions: Type “Select Resi #”

```
PyMOL> select resi 1
```

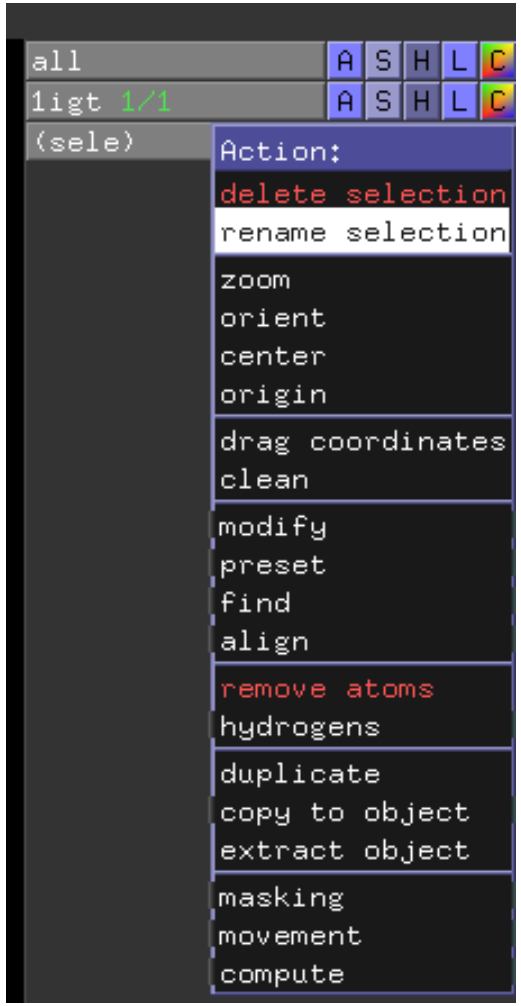


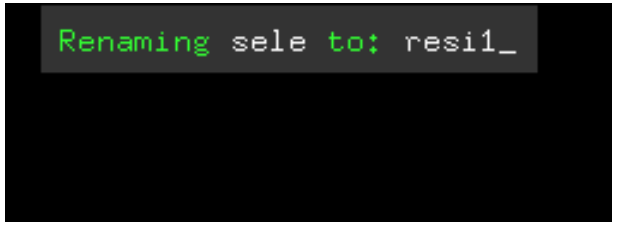
*you should see pink dots show up

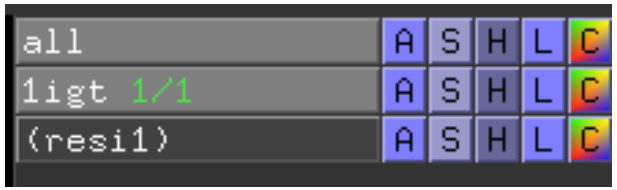
Protein ID: 1IGT (Immunoglobulin)

Rename and Recolor Selection

Instructions: Type “Select Resi #”

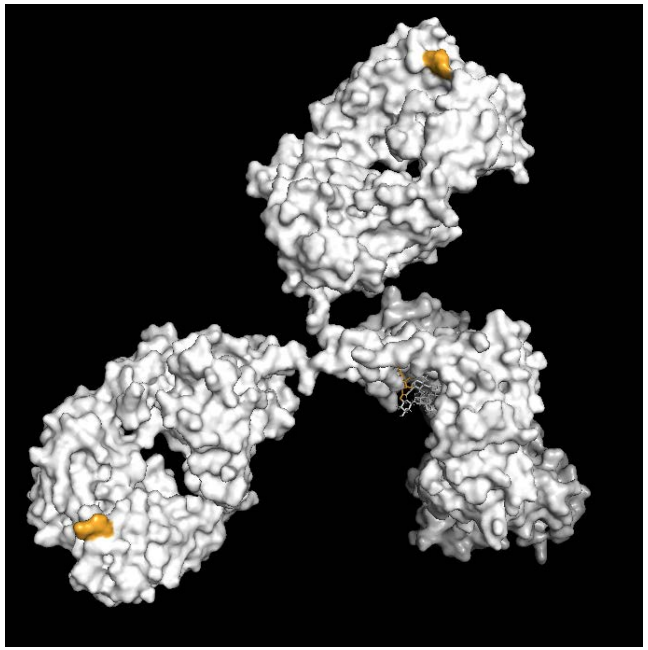






**hit enter to rename selection*

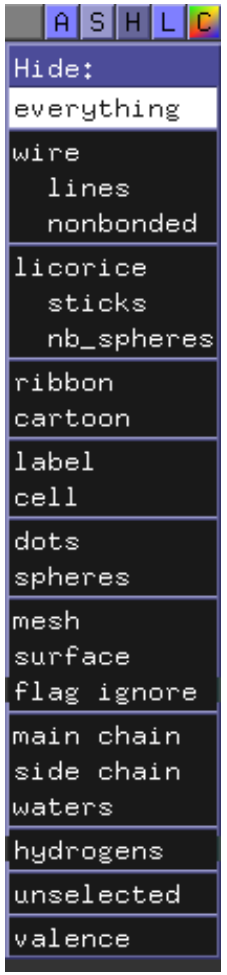
Recolor the selection the way you recolored the surface

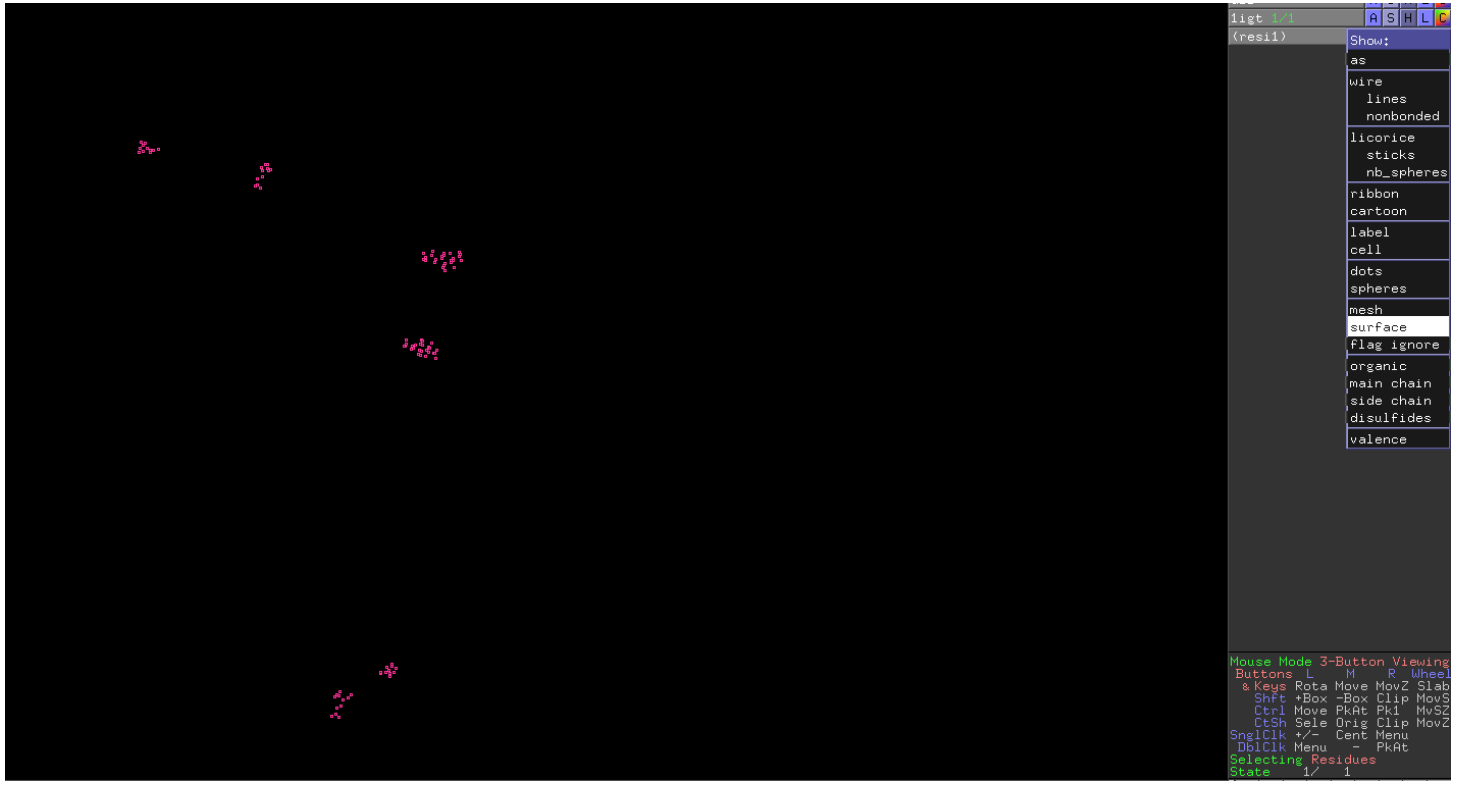


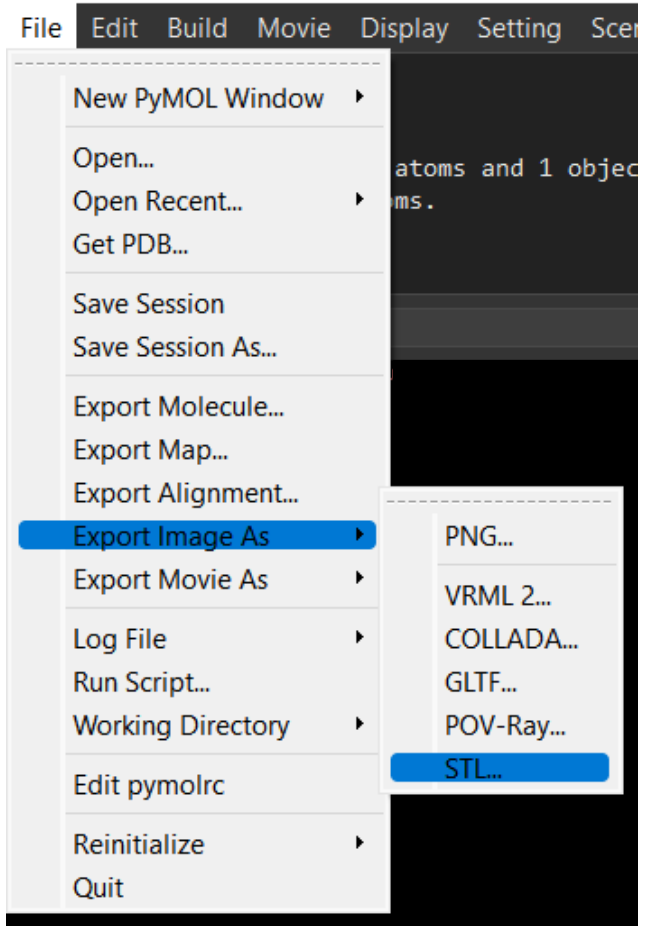
Protein ID: 1IGT (Immunoglobulin)

Make selection separate export

Instructions: Click H > Everything > Resi 1 > S > Surface > File > Export Image As





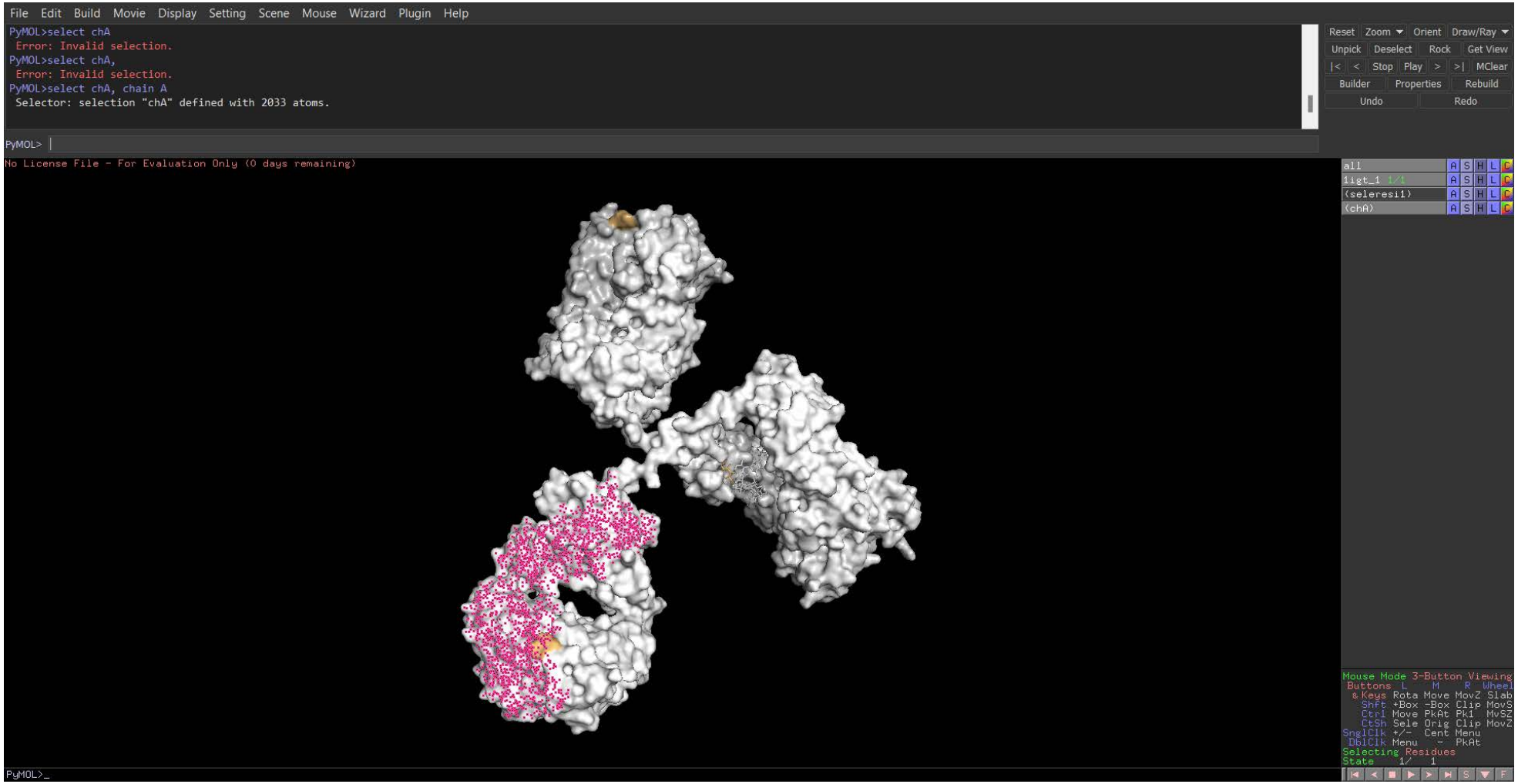


**also export the main antibody by selecting it and exporting it as an stl*

Protein ID: 1IGT (Immunoglobulin)

Selecting specific chains on your model

Instructions: Put your cursor in the command box > Type select “select chA, chain A”

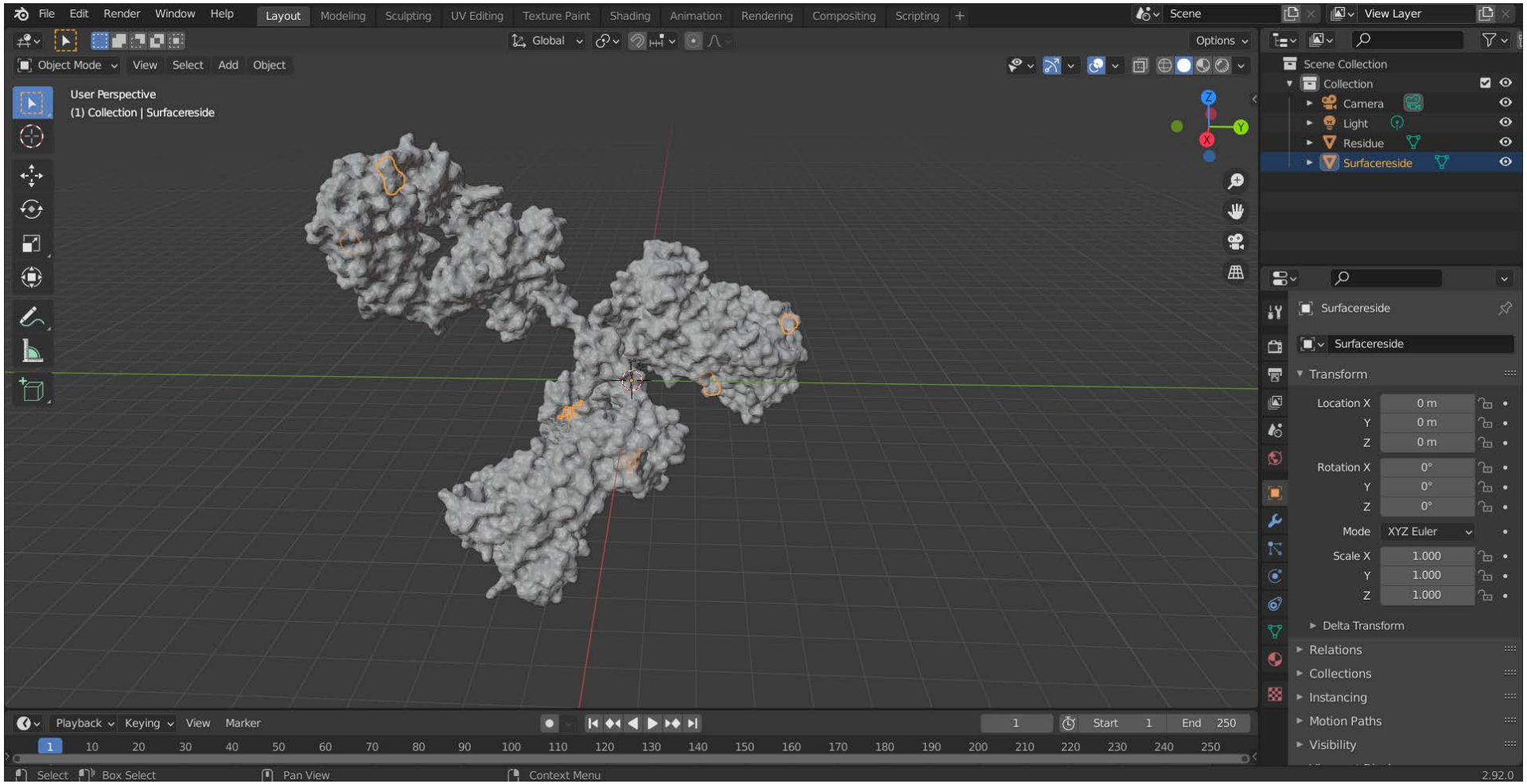


*chains can be exported using the same process to export residues, we are not going to do that as a part of this workshop

Protein ID: 1IGT (Immunoglobulin)

Overlay Residue on Blender File

Instructions: Open Blender > File > Import > STL > Select both the antibody and residue



*should come in overlapping as separate objects

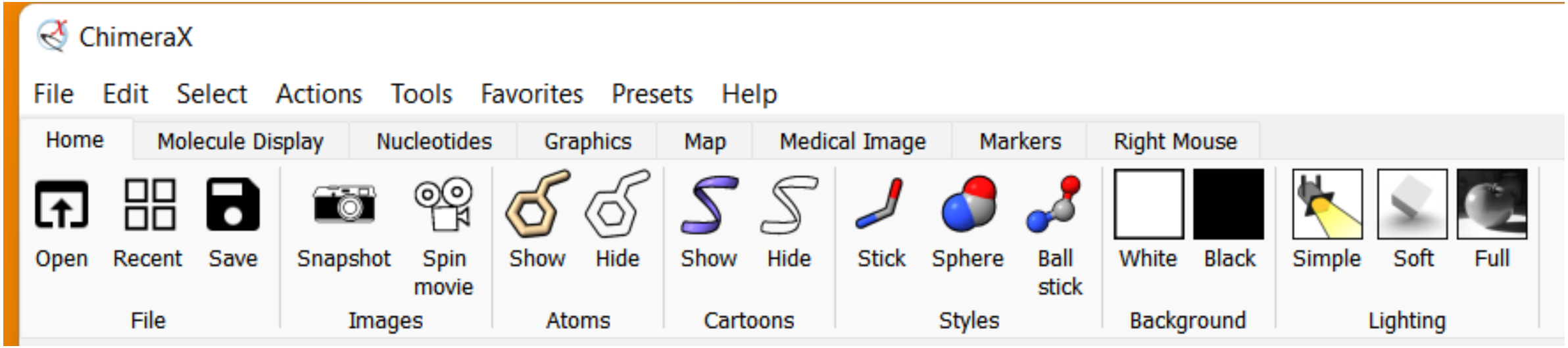
Chimera

Open-source molecular visualization software

https://www.cgl.ucsf.edu/chimera/download.html

Opening a File

Instructions: Open > Select PDB



Protein ID: 1IGT (Immunoglobulin)
Pettersen, et al. UCSF Chimera--a visualization system for exploratory research and analysis, *J Comput Chem.* 2004 Oct;25(13):1605-12.

Select Chains, Create Surface

Instructions: Select Chains in right hand menu > Go to top menu > Molecule Display > Surface

1igt.cif title:
Structure of immunoglobulin [more info...]

Chain information for 1igt.cif #1	
Chain	**Description**
A C	IGG2A intact antibody - MAB231
B D	IGG2A intact antibody - MAB231

Non-standard residues in 1igt.cif #1
BMA — beta-D-mannopyranose
FUC — alpha-L-fucopyranose
FUL — beta-L-fucopyranose (6-deoxy-β-L-galactose)
GAL — beta-D-galactopyranose
MAN — alpha-D-mannopyranose
NAG — 2-acetamido-2-deoxy-beta-D-glucopyranose

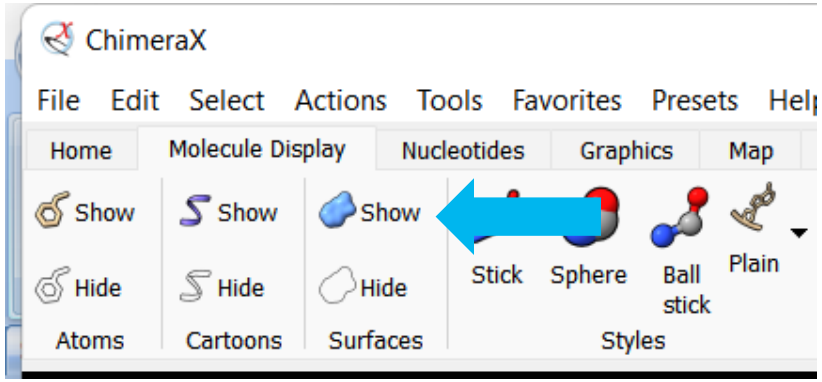
select /A:1-214
2033 atoms, 2073 bonds, 214 residues, 1 model selected

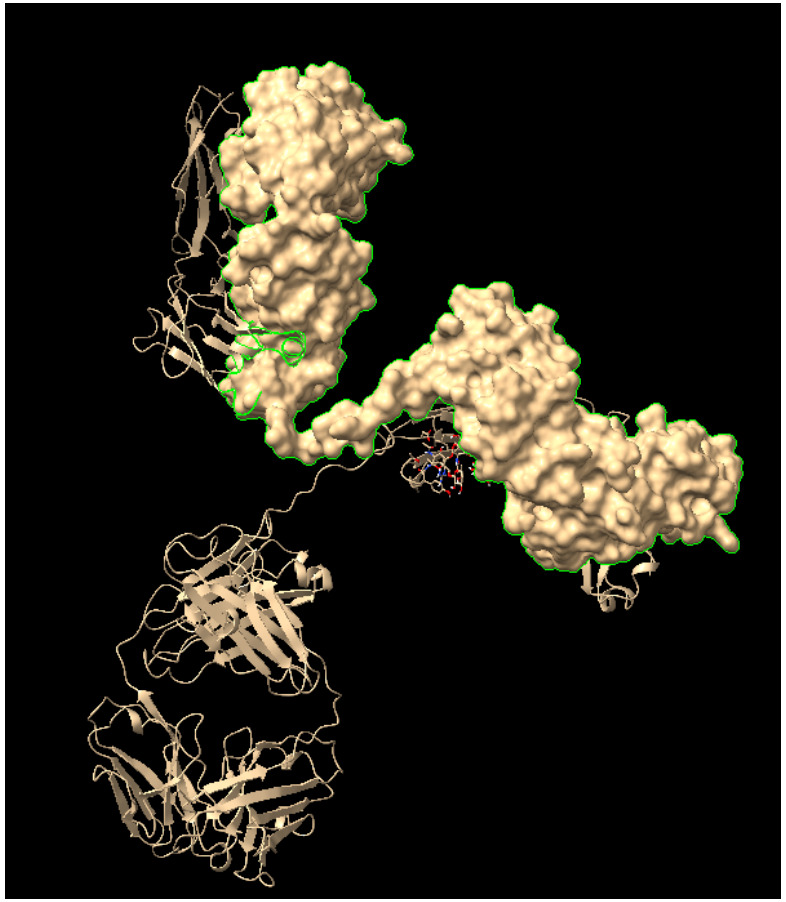
select /C:1-214
2033 atoms, 2073 bonds, 214 residues, 1 model selected

select /D:1-474
4232 atoms, 4330 bonds, 444 residues, 1 model selected

show sel surfaces

Models

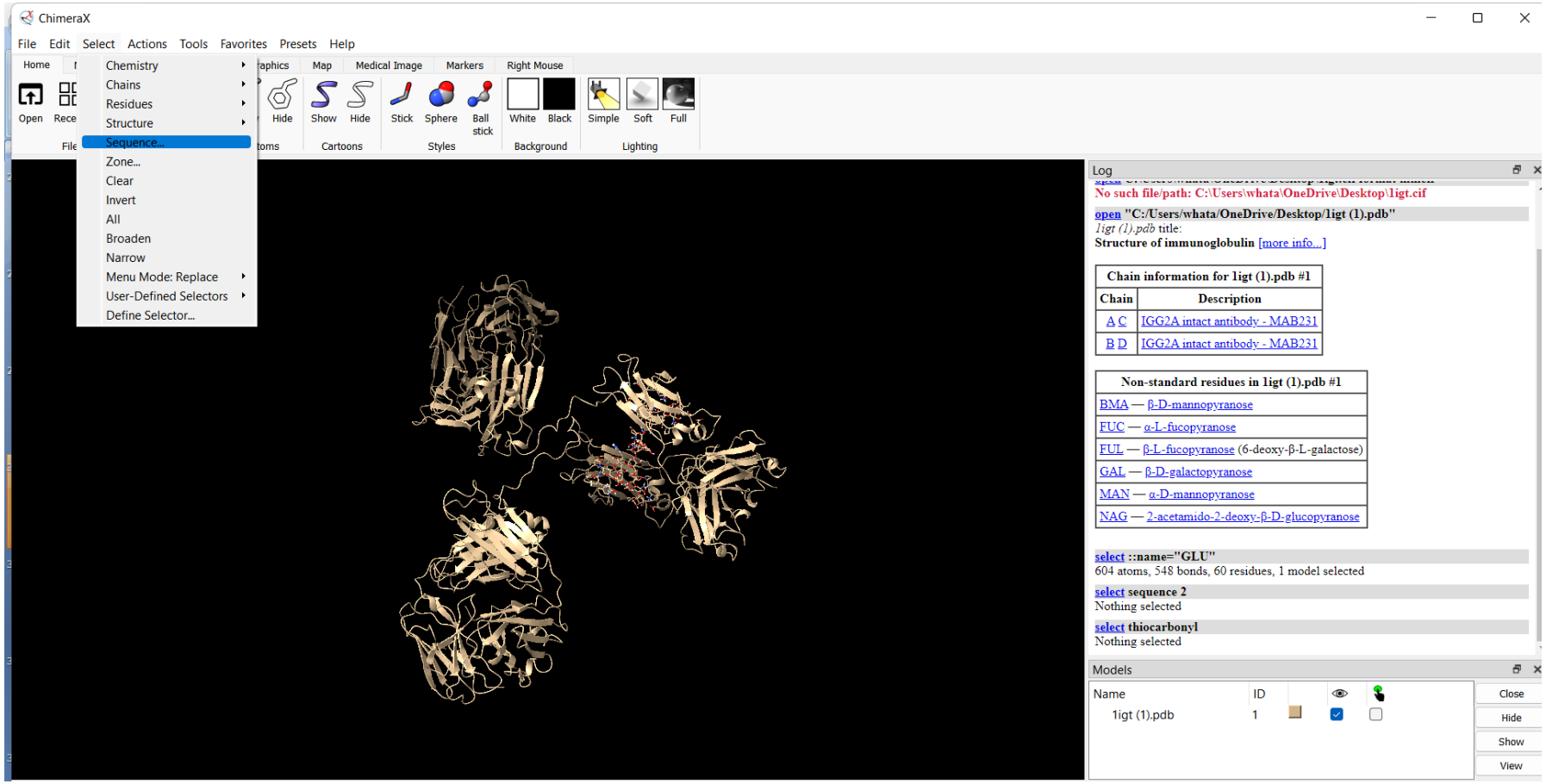




Protein ID: 1IGT (Immunoglobulin)
Pettersen, et al. UCSF Chimera--a visualization system for exploratory research and analysis, *J Comput Chem.* 2004 Oct;25(13):1605-12.

Other types of selections in chimera

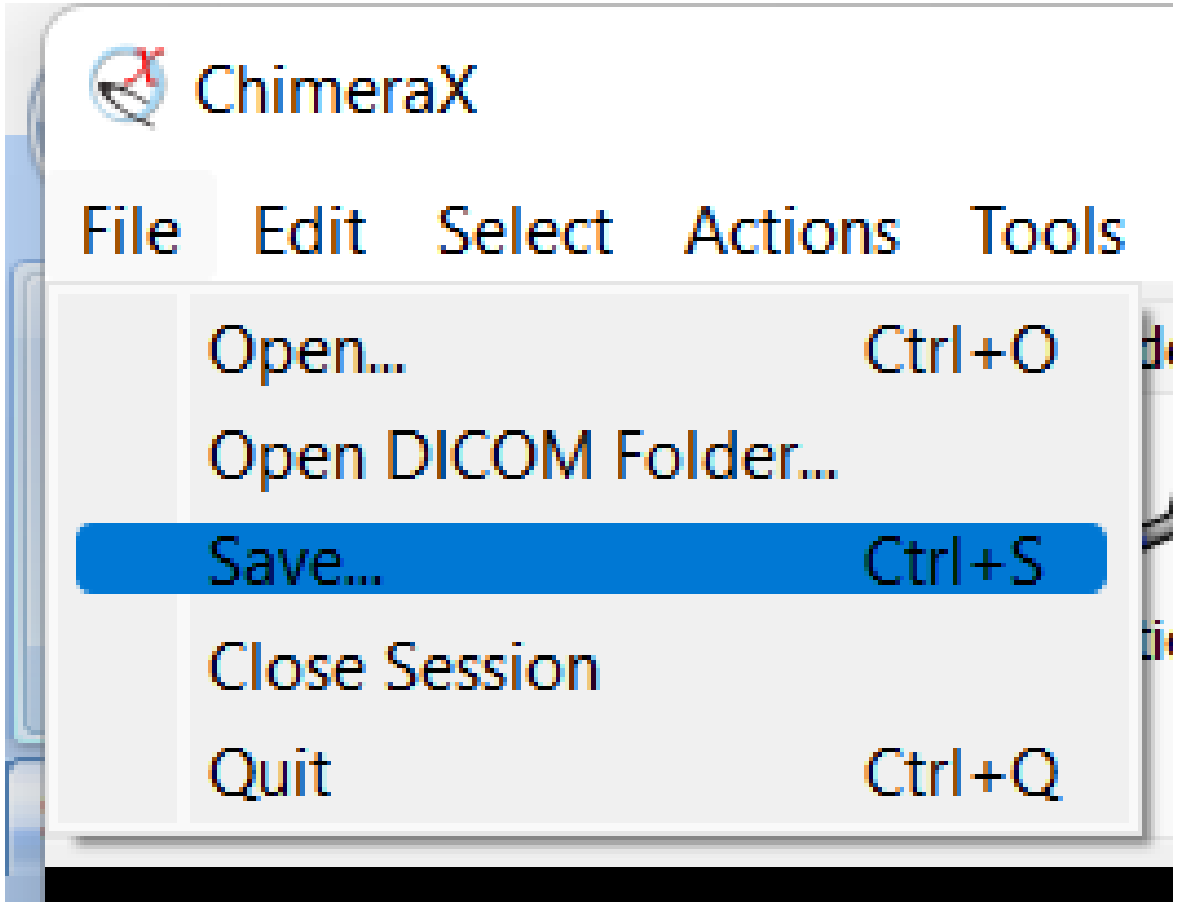
Instructions: Select > you will see a list of potential things you can select and highlight on the model



Protein ID: 1IGT (Immunoglobulin)
Pettersen, et al. UCSF Chimera--a visualization system for exploratory research and analysis, *J Comput Chem.* 2004 Oct;25(13):1605-12.

Export a File

Instructions: File > Save



Protein ID: 1IGT (Immunoglobulin)
Pettersen, et al. UCSF Chimera--a visualization system for exploratory research and analysis, *J Comput Chem.* 2004 Oct;25(13):1605-12.

Useful resources to help you get started

- **PyMol Command References:** https://pymol.org/pymol-command-ref.html
- **Additional Proteins:** https://charmm-gui.org/?doc=archive&lib=covid19
- **Visualizing Mutations:** https://pcur.princeton.edu/2021/05/visualizing-covid-19-mutations-using-pymol-a-university-provided-resource/
- **Blender for Scientists CG Figures YouTube Chanel:** https://www.youtube.com/c/CGFigures/featured
- **Blender for Biochemists YouTube Chanel:** https://www.youtube.com/c/BradyJohnston
- **Luminous Labs Blender for Scientists Youtube Channel:** https://www.youtube.com/c/LuminousLab
- **Animation in Chimera:** https://www.youtube.com/watch?v=SpfVA45oAuA

Thank you!

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