

**Analysis:** This project included virtual screening as well as making a scientific research poster to display our results and analysis.

10 years

PROTEOPEDIA  
— LIFE IN 3D —

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User:Karsten Theis/Electron density

edit this page history

< User:Karsten Theis

To explore the electron density of the structure 233D (a short piece of DNA containing some sulfur-modified sugars), choose one of the two scenes below (either the entire molecule, or just a base pair. The latter will load faster and is less confusing, so maybe start with the base pair).

**DNA**

**Base pair**

**water (solvent)**

The following is the command to fetch the electron density from the [pdb.org](http://www.ebi.ac.uk/pdbe/coordinates/files/233d.ccp4.d) database and display it around the selected atoms:

```
isosurface s_one sigma 1.0 color blue within 1.5 (selected)
*http://www.ebi.ac.uk/pdbe/coordinates/files/233d.ccp4.d* mesh notl
```

**Contents** [\[hide\]](#)

- 1 Electron density
- 2 A technical note
- 3 Ferredoxin: Ultra-high resolution
- 4 Pre-calculated density

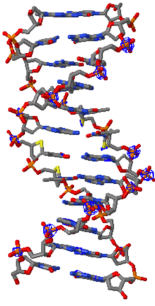
**Electron density**

Click on the following buttons to display electron density at different contour levels. One sigma means to show the area (within the chicken wire) that has values higher than one standard deviation over the mean. The higher the sigma, the less density you see (but you get to see the highest peaks in the density).

4 sigma

The peaks are mostly around the phosphorous atoms. P has about twice as many electrons as C, N and O, so it is expected to have roughly twice the electron density (and, even more roughly, twice the maximum electron density at the center of the atom).

3 sigma



JSmol

• spin • quality • labels • popup • + • -

Caption for this structure

[Export Animated Image](#)

Proteopedia Page Contributors and Editors ([what is this?](#))

Figure 16: Image shows the proteopedia page with information about electron density on it. Analysis: By selecting the number of sigmas, the diagram on the right changes to see all the various interactions in the structure.

RCSB PDB-101 Molecular explorations through biology and medicine

Educational portal of PDB

Search Molecule of the Month articles and more Go

Celebrating 20 YEARS OF Molecule of the Month

Molecule of the Month

By Category By Date By Title

**Twenty Years of Molecules**

*Celebrating the structural biology revolution*

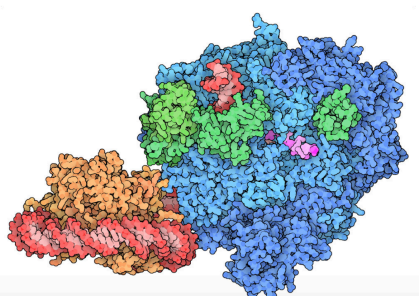
Every month, I feel lucky to be a scientist (and a scientific artist) at this point in history. Structural biology is in the middle of a revolution that is revealing the atom-level workings of living cells. It all started with the structure of myoglobin, and today, you can find structures for everything from *actin* to *zika*. I'm happy to report that as of this month, I've been exploring the PDB archive for 20 years and sharing some of what I find in these Molecule of the Month columns. Here are a few thoughts as I look back over my 20 years of molecules.

**The Structural Biology Revolution**

Structural biology has come a long way since the pioneering work of Kendrew, Perutz, Watson and Crick. Methods are more efficient and successful in a wider variety of systems, so scientists are increasingly empowered to explore all aspects of cellular life. The structural genomics effort streamlined crystallographic structure determination, and methods like XFEL are opening new doors on the time dimension. NMR spectroscopy provides orthogonal views of biological systems and their dynamics that are inaccessible to other techniques. CryoEM microscopy is revealing the structures of enormous assemblies that were completely intractable before, and is promising to be the go-to technique for the next decade of structural biology.

**Molecular Stories**

Every structure has a story to tell, giving us a new look at the inner workings of life. Some



Connect Us

Figure 17: Image shows the website on PDB about twenty years of molecules and various diagrams to show different molecules and structures. Analysis: Structures in biology are very different and unique. Some can be symmetrical while some can contain many various elements. Overall, as time continues, our understanding of these biological structures expands.

Week 4

Good work Jared. Dr. B

6/23/2020

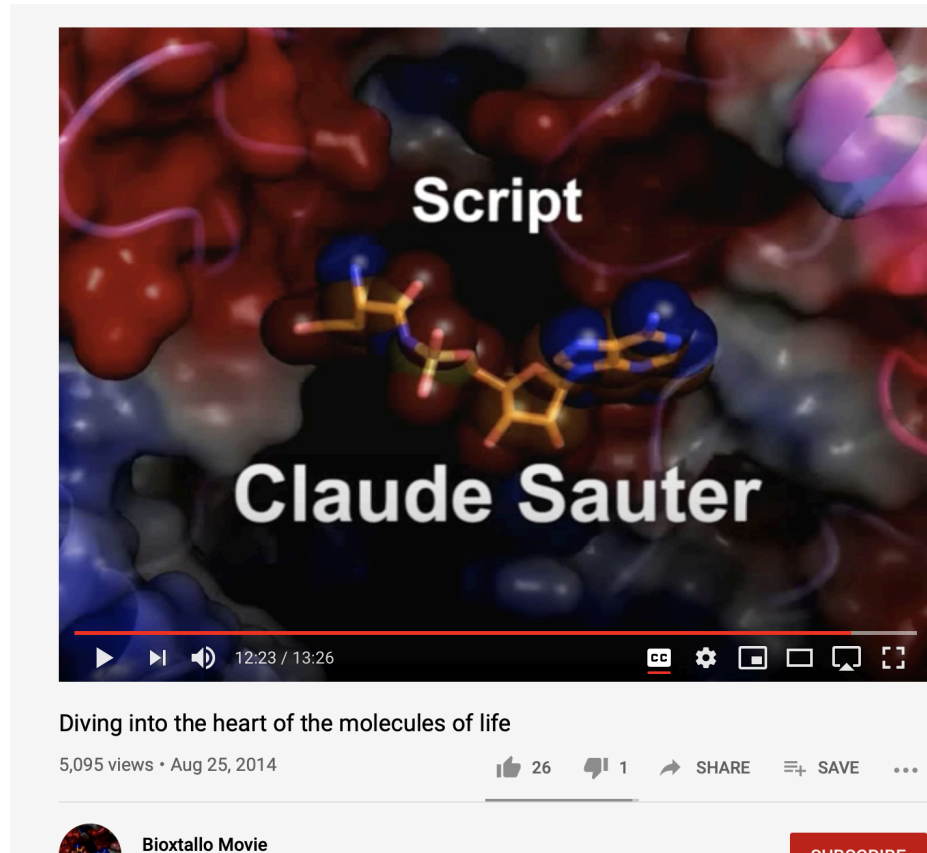


Figure 11: Image shows the video on determining protein structures.

Analysis: This video highlighted the importance of X-ray crystallography in order to photograph molecules at an atomic level.

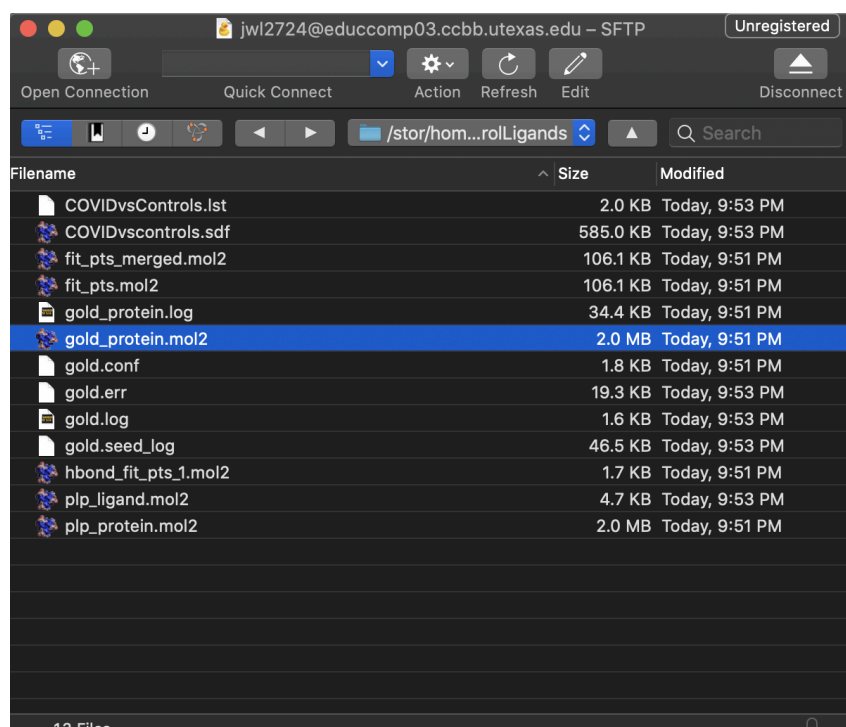


Figure 12: Image shows the run in Cyberduck from GOLD for the COVID-19 screening project.

Analysis: The virtual screening of the target for COVID-19 was done and the poster is being worked on. The result gave me a list of scores.

```

| # Download 1DLJ to your computer and open with the file menu or fetch
it.
fetch 1DLJ, type=pdb

# Color the background white
bg white

# Hide the water molecules in the structure
hide non

# Display the structure sequence ligand
set seq_view, 1

# Create a separate object for each (NAI & UGA)
sele NAI, resn NAI
sele UGA, resn UGA

# color ligands, NAI by element as magenta, UGA by element as cyan
util.cbac UGA
util.cbam NAI

# Make a selection of all of the ligands to represent the active site

```

Figure 13: Image shows the pymol script for the target UDP glucose 6 dehydrogenase. Analysis: The pymol script for the target UDP glucose 6 dehydrogenase was written. The file was then converted to .pml and can show the various angles and scenes of the structure in Pymol.

## Week 3

Excellent work Jared. - Thx, Dr. B

6/17/2020

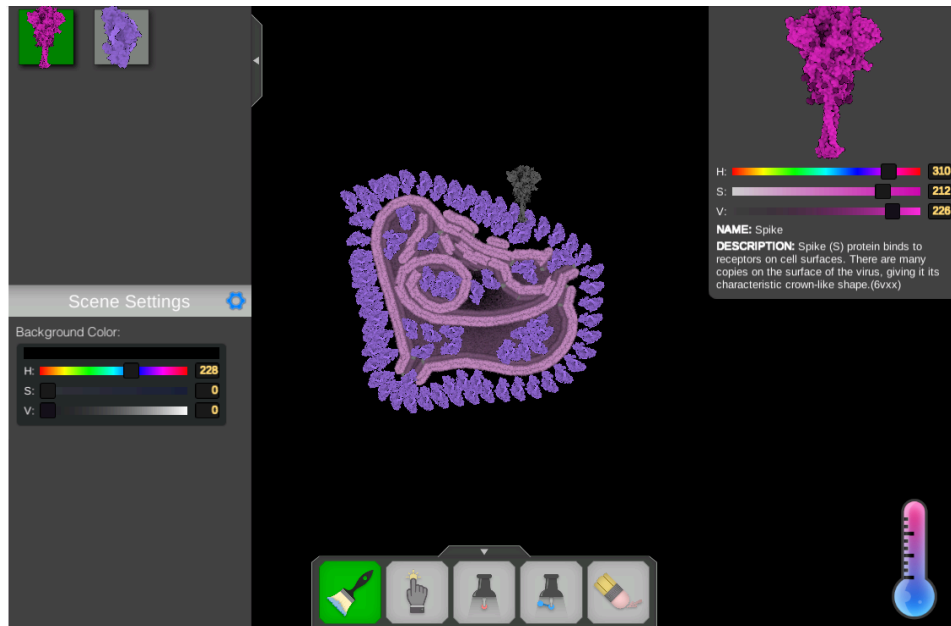


Figure 6: Image shows Cell Paint website showing viruses in blood plasma along with human cells

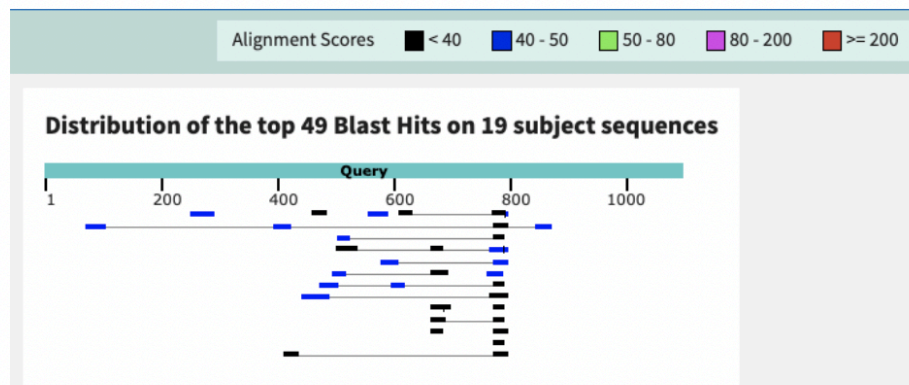
Analysis: Cell Paint was explored for about 10 minutes to see how the application can display different varieties of viruses in blood plasma along with simple human cells.





**Figure 7:** Image shows the presentation watched from the ASBMB virtual meeting website. This presentation and poster is about bacteria populations and plastic in Southern California waters.

**Analysis:** This virtual presentation of a poster describes how microbial populations such as antibiotic production affect potential plastic degradation. More specifically, the genus *Vibrio* is prevalent in these Southern California waters. Bacteria were placed on two different types of Agar in order to observe growth. At first, there was no clear pattern of colonization; however, with longer incubation times, there was an increase in unknown/uncultured bacteria. In conclusion, this poster shows that there are differences in the microbial communities growing on coastal marine plastic debris. This could then have a negative effect on humans affecting our health and environment.



Graphic Summary of BLAST of Sequence compared to Human Genome

Do another BLAST to see if your sequence is found in other genomes.  
 Under 'Database' choose 'Nucleotide collection (nr/nt)'  
 Select 'Somewhat similar sequences (blastn)'  
 Begin Search.

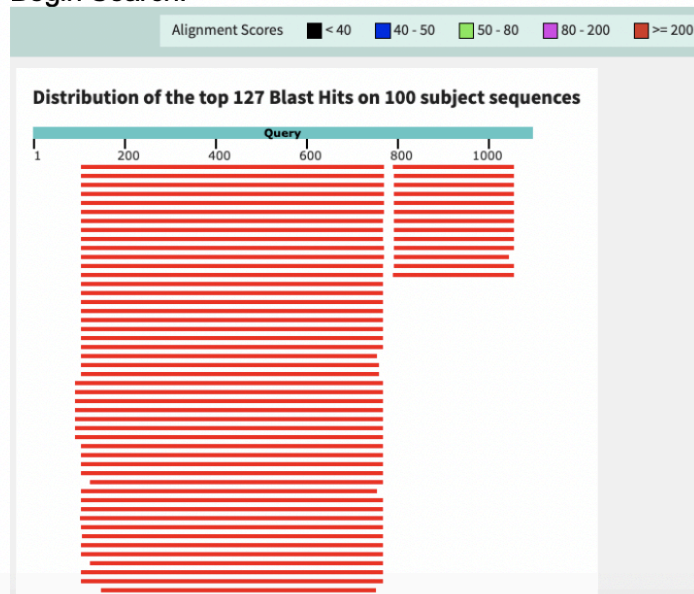
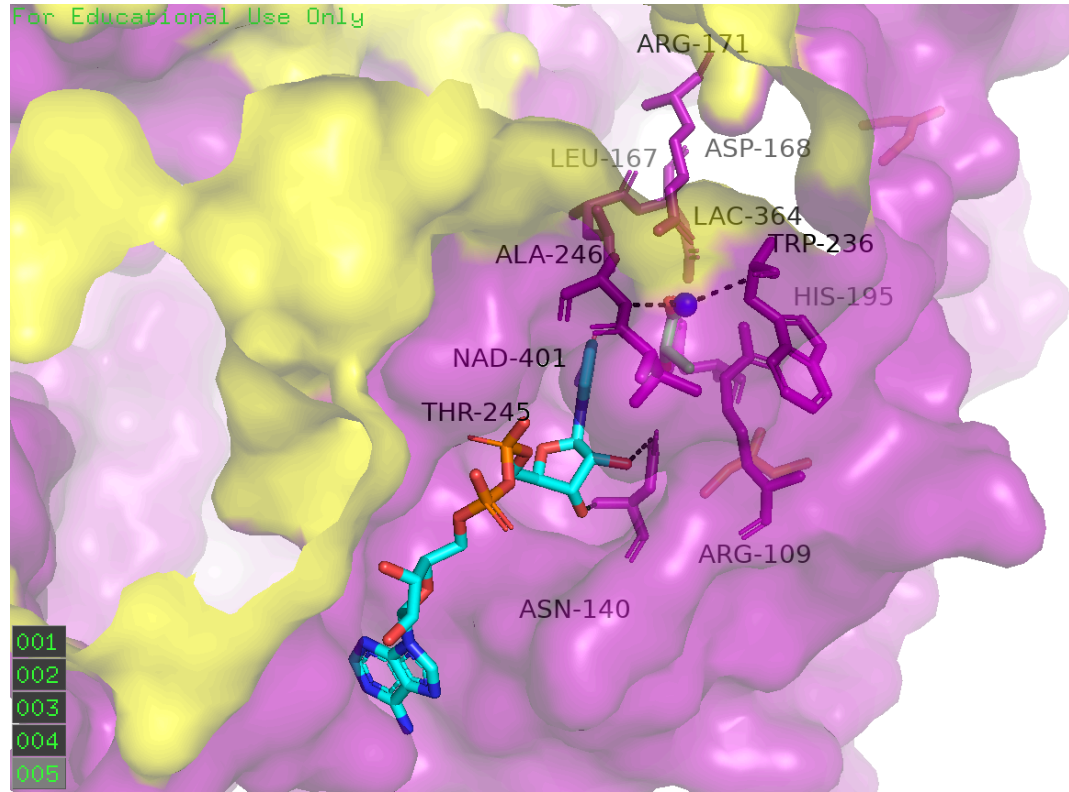


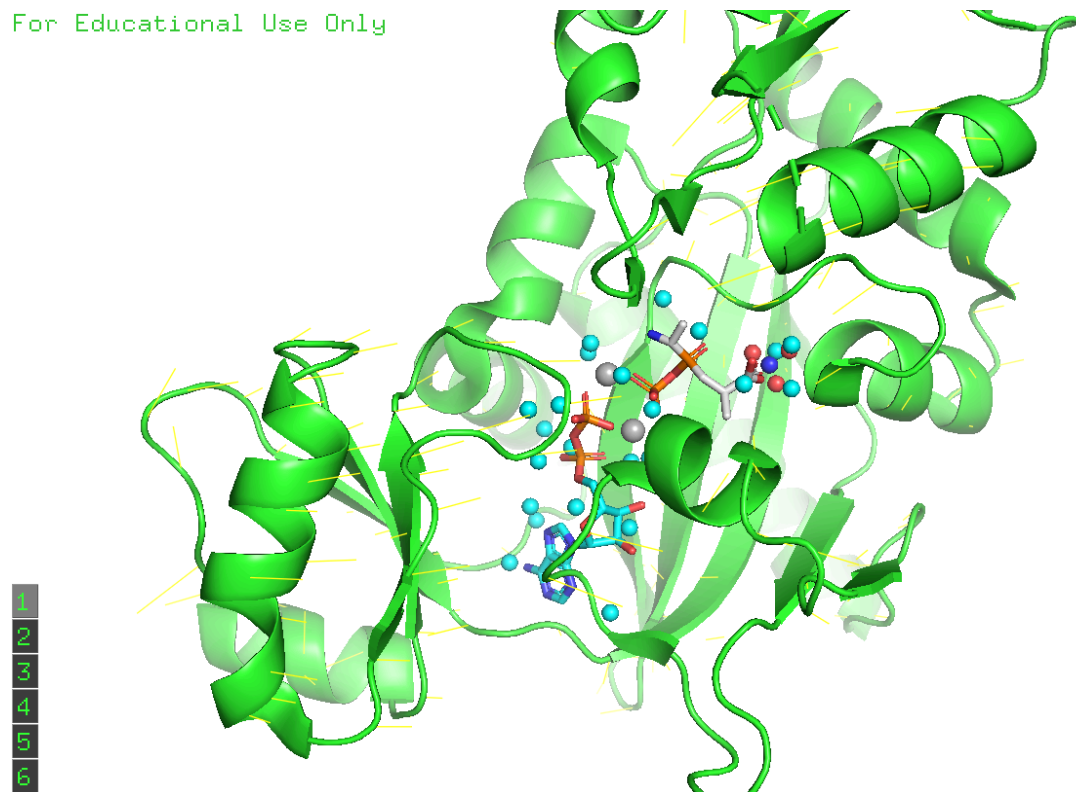
Figure 8: Image shows the alignment scores of two different sequences.

**Analysis:** This image was gathered for the assignment, Analyze DNA Sequencing. This assignment included editing DNA sequences and identifying the start and stop codons. This assignment will be useful in the future because it allows us to learn about DNA sequences.



**Figure 9:** Pymol representation shows the 5th scene in the LDF Pymol scripting assignment. The image shows the polar contacts and residues labeled. There is a pocket in the active site and the rest of the protein is shown as a surface.

**Analysis:** This assignment was done using only the medium steps. This made it more difficult than when we had the granular steps. The assignment was done to improve on Pymol skills and analyze further how active sites and proteins interact.



**Figure 10:** Pymol representation shows chain A as a cartoon and the ligand as sticks with some NO<sub>3</sub>, magnesium, and others as spheres.

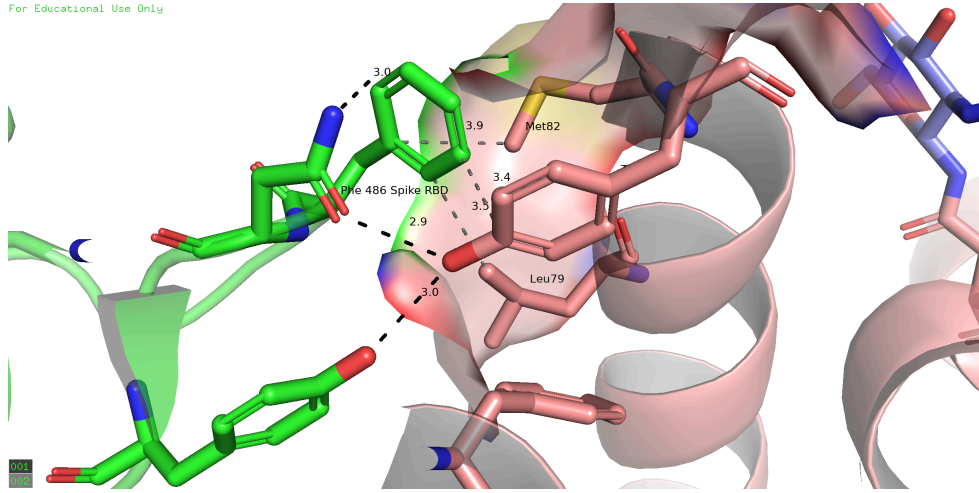
**Analysis:** This assignment was done using only the medium steps. This made it more difficult than when we had the granular steps. The assignment was done to improve on Pymol skills and analyze further how active sites and proteins interact.

## Week 2

### Week 2 - great work Jared- Dr. B

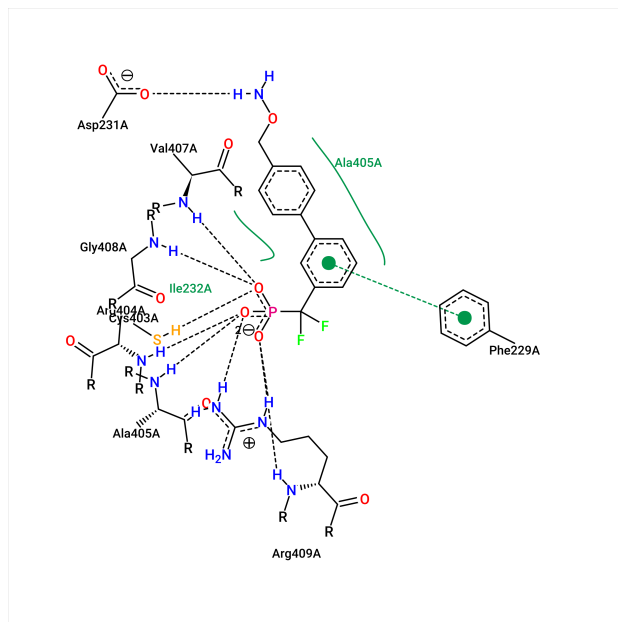
6/11/20

For Educational Use Only



**Figure 2:** Pymol representation shows a scene of 6VW1 and the polar interactions between molecules in the structure. The structure was colored by element and some amino acids were labeled.

**Analysis:** Pymol scripting was done in this activity. A set of detailed instructions were followed in order to get the correct pictures and scenes. Only line commands were used instead of using the mouse to influence and change the structure in Pymol. This activity was done to learn new line commands for future use.



**Figure 3:** Diagram shows poseview of YopH generated from the PDB file and ZBH University Hamburg website.


**Analysis:** A poseview diagram of YopH was generated. This was done to visualize how YopH looks in two dimensions.

### Summary statistics

|                         |   |              |   |
|-------------------------|---|--------------|---|
| All-Atom Contacts       | Clashscore, all atoms:  | 8.7          | 97 <sup>th</sup> percentile* (N=97, 2.90Å ± 0.25Å)    |
|                         | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. |              |   |
| Protein Geometry        | Poor rotamers   | 1            | 0.11% Goal: <0.3%                                     |
|                         | Favored rotamers  | 906          | 95.87% Goal: >98%                                     |
|                         | Ramachandran outliers   | 0            | 0.00% Goal: <0.05%                                    |
|                         | Ramachandran favored  | 1020         | 95.77% Goal: >98%                                     |
|                         | Rama distribution Z-score   | -3.06 ± 0.22 | Goal: abs(Z score) < 2                                |
|                         | MolProbity score <sup>^</sup>   | 1.76         | 100 <sup>th</sup> percentile* (N=3760, 2.90Å ± 0.25Å) |
|                         | Cβ deviations >0.25Å  | 0            | 0.00% Goal: 0   |
|                         | Bad bonds:  | 0 / 8805     | 0.00% Goal: 0%  |
| Peptide Omegas          | Bad angles:   | 1 / 11956    | 0.01% Goal: <0.1%                                     |
|                         | Cis Prolines:   | 2 / 35       | 5.71% Expected: ≤1 per chain, or ≤5%                  |
| Low-resolution Criteria | CaBLAM outliers   | 21           | 2.0% Goal: <1.0%                                      |
|                         | CA Geometry outliers  | 7            | 0.67% Goal: <0.5%                                     |
| Additional validations  | Chiral volume outliers  | 0/1354       |   |
|                         | Waters with clashes   | 0/0          | 0.00% See UnDowser table for details                  |

**Figure 4:** Image shows traffic light table generated in Molprobity of 6M71.

**Analysis:** The target 6M71 was put through Molprobity and this traffic light table was generated. Asn/Gln/His flips and hydrogens were added. In addition, Flips were made. In the picture, the summary statistics were overall very good. The only red line in the summary statistics was the Rama distribution Z-score.



**UDP Glucose 6 Dehydrogenase's Importance in the Function of Streptococcus Pyogenes**

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**ABSTRACT**  
BioRxiv

DailyScheduleSumm20 - Google Docs

**INTRODUCTION**  
BioRxiv

**MATERIALS & METHODS**  
Complete lab info (Molecular visualization: PyMol, Compound Libraries, GOLD, etc.)  
Web lab info (cloning, expression, purification, enzyme assays)

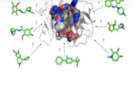
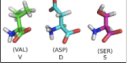
**RESULTS**  
BioRxiv

**DISCUSSION & CONCLUSIONS**  
BioRxiv

**FUTURE DIRECTIONS**  
BioRxiv

**REFERENCES**  
BioRxiv

Note: - to be deleted before printing  
put a 1 or 2 superscripts after your name depending on what school your major is in  
only put the names of those who did the research or who helped on the poster or who will be there to present the poster (should also put mentors, RE and PI)  
Change the title to match your work  
You can use the figures included here - or not  
Rearrange the orange boxes to where you need them. Change their size or whatever. They are a text box and an orange box that are "Grouped" together. So, you can "Ungroup" them if they aren't working how you want them to. (use right click to get to Ungroup)  
If you have questions, let me know.

This work is funded in part by the National Science Foundation and the Howard Hughes Medical Institute through the Frederman Research Initiative

**Figure 5:** Image shows edited template for poster with my name and title for my target and organism.

**Analysis:** The template for the poster was edited with my name and title for my target and organism. This poster will be edited throughout the summer and fall until it is completely filled out and is ready for a presentation.

Week 1

Jared- good work - put in Reverse Chronological order (newest stuff at top) - Thx, Dr. B

6/5/2020



**Analysis:** A specific disease was chosen and from that, an enzyme or target was chosen to do a target discovery page on. The target that was chosen was UDP-glucose 6-dehydrogenase in *Streptococcus pyogenes*. Most of the information found for this target was found from the Brenda website shown in Figure 1. The target met most of the criteria. For example, the target had a resolution less than 3. Also, another example is that the target is crucial for the survival of the infectious organism. The target is essential for formation of the antiphagocytic capsule that protects many virulent bacteria from the host's immune system.