

Protein Modeling

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What is Protein Modeling?

- Developed by the Milwaukee School of Engineering Center for BioMolecular Modeling
- Understand basic features of protein structure
- Explore and manipulate protein structures using the online protein visualization webpages
- Create physical models using a foam covered wire called a Mini-Toober

The Competition (3 parts)

- Pre-build model
 - Students will bring their pre-built models to the assigned impound
- On-site build model
 - Students will use a computer to build a specific region of a protein with the toober provided, guided by visualization of 3-D coordinates from the RCSB PDB, using Jmol/JSmol program
- Exam
 - Students will answer questions on a written test

Scoring

- Pre-build (40 %)
 - Rubric gets more detailed as the competition progresses
 - Invitational
 - Regional
 - States
 - Nationals
- On-site Build (30 %)
- Written Test (30 %)

What should the team bring?

- Pre-build model, fit within 61.0 cm X 61.0 cm X 61.0 cm
- Judges will pick up and rotate your model
- ONE 4 by 6 inch note card explaining their additions to the model, in the form of a table headed: what is displayed, how it is displayed, why it is important

What each student should bring?

- a pen or pencil to write the exam
- **a (colored) sharpie marker**
- **A metric ruler to make cm marks (meterstick?)**
- ONE double-sided 8 ½ by 11 page of notes, may be in a sheet protector or laminated



<https://www.shop3dmoleculardesigns.com/Science-Olympiad-Protein-Modeling-Event-Kits-p/so.htm>

Even bacteria get infected with viruses! The 2018-2019 Science Olympiad Protein Modeling event explores one way bacteria combat viral infections. Using CRISPR (clustered regularly interspersed palindromic repeats) and Cas proteins, bacteria recognize viral DNA and chop it into pieces. Viruses counterattack using AntiCRISPR. This season's protein modeling event examines the structures of CRISPR and AntiCRISPR – the war on bugs!

What the event supervisor provides?

- For the On-site build
 - On-site build toobers
 - A computer
- The Exam

Start Here

- <http://cbm.msoe.edu/scienceOlympiad/index.php>
- [http://scioly.org/wiki/index.php/Protein Modeling](http://scioly.org/wiki/index.php/Protein_Modeling)

[Home](#)[Student Programs](#)[Teacher Workshops](#)[Teaching Resources](#)[About the CBM](#)[Lending Library](#)

Science Olympiad

Participant Resources

Section 1 - Overview of the Event

★ Section 2 - This Year's Theme

Section 3 - Building Your Models

The Pre-build Visualization Environment

The Practice Visualization Environment
(based on the 2016 Regional Onsite Model)

Supervisor Resources

Overview of the Event

★ Ordering Event Materials

Video Tips from Experienced Event Supervisors

Past Protein Modeling Events



Protein models are created at the 2011 National Tournament in Madison, WI.



Science Olympiad Protein Modeling Event

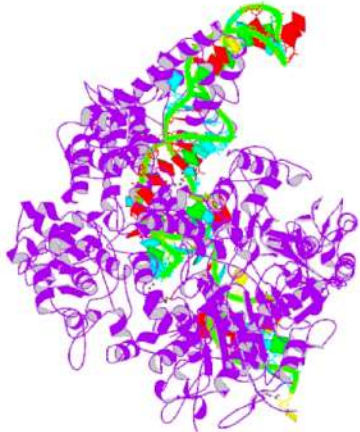
Protein Modeling is an event developed by the CBM for Science Olympiad. This event challenges students to explore protein structure/function by creating 3-dimensional models of proteins using Mini-Toobers, foam-covered wire that will hold its shape once folded.

Join the 2018-19
Protein Modeling Event
Now!

PDB for 5vw1

[Structure Summary](#) [3D View](#) [Annotations](#) [Sequence](#) [Sequence Similarity](#) [Structure Similarity](#) [Experiment](#)

Biological Assembly 1 ?



3D View: [Structure](#) | [Electron Density](#) | [Ligand Interaction](#)

Standalone Viewers
[Protein Workshop](#) | [Ligand Explorer](#)

Global Symmetry: Asymmetric - C1 ⓘ
Global Stoichiometry: Hetero 2-mer - AB ⓘ

5VW1

Crystal structure of SpyCas9-sgRNA-AcrIIA4 ternary complex
DOI: [10.2210/pdb5VW1/pdb](https://doi.org/10.2210/pdb5VW1/pdb)

Classification: [HYDROLASE](#)
Organism(s): [Streptococcus pyogenes serotype M1](#), [Listeria monocytogenes](#)
Expression System: [Escherichia coli BL21\(DE3\)](#)
Mutation(s): 2 ⓘ

Deposited: 2017-05-21 Released: 2017-06-28
Deposition Author(s): [Yang, H.](#), [Patel, D.J.](#)
Funding Organization(s): National Institutes of Health/National Institute of General Medical Sciences; Memorial Sloan Kettering Cancer Center Core Grant

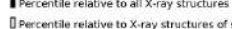
Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.598 Å
R-Value Free: 0.226
R-Value Work: 0.178

wwPDB Validation

[3D Report](#) [Full Report](#)

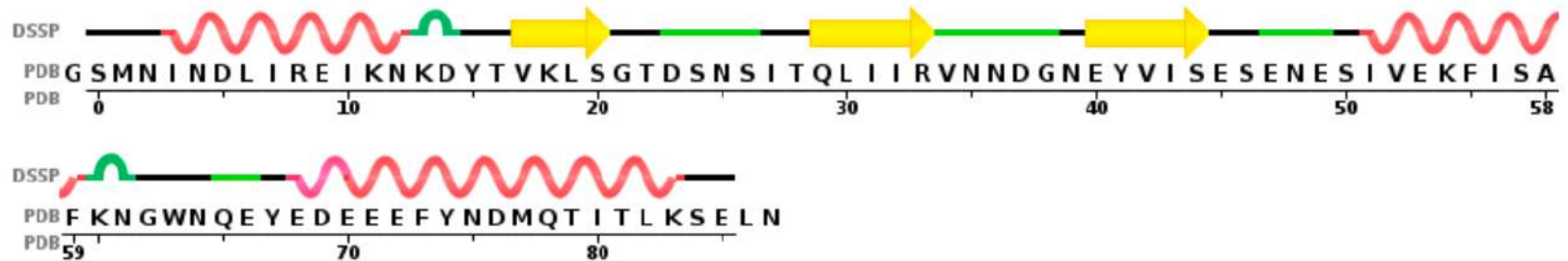
Metric	Percentile Ranks	Value
Rfree		0.227
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		5.4%
RSRZ outliers		2.1%
RNA backbone		0.50

Worse  Better
■ Percentile relative to all X-ray structures
□ Percentile relative to X-ray structures of similar resolution

Sequence

See aa 1-85

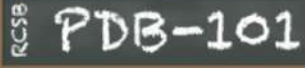
Sequence Chain View



DSSP Legend

- empty: no secondary structure assigned
- S: bend
- T: turn
- E: beta strand
- G: 3/10-helix
- H: alpha helix

<http://pdb101.rcsb.org/events/science-olympiad/overview>



Molecular explorations
through biology and medicine

Go

Educational portal of 

Protein Modeling at Science Olympiad

Overview

About

Past Events

Overview

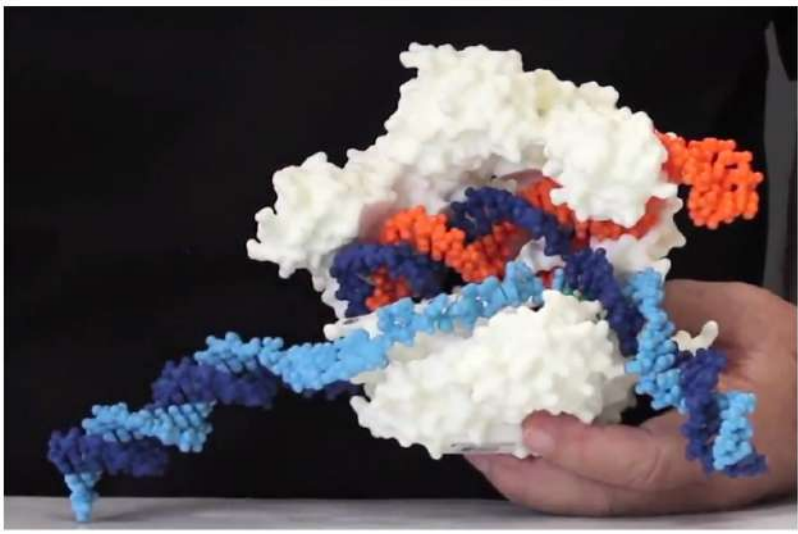
Theme for 2018-2019: CRISPR and anti-CRISPR Proteins

This year's event focuses on understanding CRISPR, a technology that has revolutionized molecular biosciences. Students will learn about identification of this adaptive immune system in nature, how it has been modified for gene editing, and identification of anti-CRISPR proteins



The Protein Modeling event is a formal collaboration between MSOE and RCSB PDB. The regional, state, and national events are sponsored by 3D Molecular Designs and Vertex.

For information on the 2019 Protein Modeling Competition please visit the [MSOE](#) site.



A model of the CRISPR Cas9 complex

There are three parts to the Protein Modeling competition:

Regional to State to National

The table below lists the proteins that will be featured as the 2018-19 pre-build as well as the various on-site builds at invitational, regional, and state competitions.

Be Sure to Click on Each Protein Listed Below to reveal additional resources that you should explore as you prepare for each level of competition. In addition to providing the pdb file for the protein that will be featured, these links also provide a copy of the original research paper (the "primary citation") that reported the protein's structure. Questions regarding the paper and the structure presented in the PDB file will be asked on the exam you will complete at each competition.

Pre-Build Model	AcrII4A Anti-CRISPR Protein	5vw1.pdb
------------------------	------------------------------------	-----------------

Invitational On-site Model	CRISPR-Cas9	5f9r.pdb
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Regional On-site Model	CRISPR-Cas9	5f9r.pdb
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State On-site Model	CRISPR-Cas9	5f9r.pdb
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National On-site Model	CRISPR-Cas9	5f9r.pdb
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Background

- Fun posters and videos
- [http://www.rcsb.org/pdb/101/static101.do?p=education discussion/educational resources /index.html](http://www.rcsb.org/pdb/101/static101.do?p=education%20discussion/educational%20resources/index.html)

Pre-Build environment

2018 Pre-Build Model Directions

Font Size:  

2018-19 Pre-Build Model

Based on [5vw1.pdb](#)

Directions:

The 2018-19 Pre-Build Model should represent **amino acids 1 - 85 of chain B** of the anti-CRISPR protein based on the PDB file 5vw1.pdb. This section is 84 amino acids long and will require a toober that is 168cm long at the scale of 1 amino acid = 2cm.

The pre-build model is worth 40% of a team's final score for the event. The pre-build model will be created using a purchased "pre-build" Mini-Toober kit from www.3dmoleculardesigns.com, or with found materials of the participant's choosing such as [KwikTwist](#) tie-down ropes. The same pre-build model will be used at each level of the competition (invitational, regional and state) and participants will take their pre-build model home after each event.

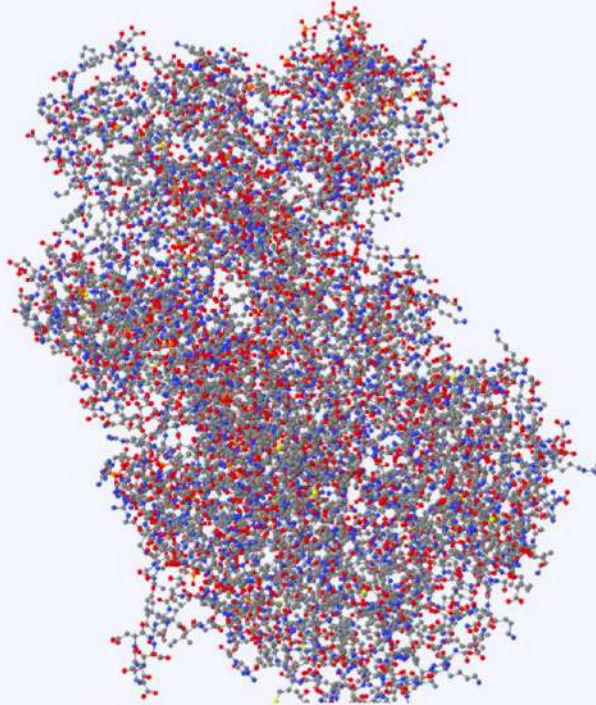
Resources:

Execute

HYDROLASE 21-MAY-17 5VW1
CRYSTAL STRUCTURE OF SPYCAS9-SGRNA-ACRIT4 TERNARY COMPLEX
found biomolecule 1: A, C, B

© Copyright 1995- 2019 - MSOE Center for BioMolecular Modeling

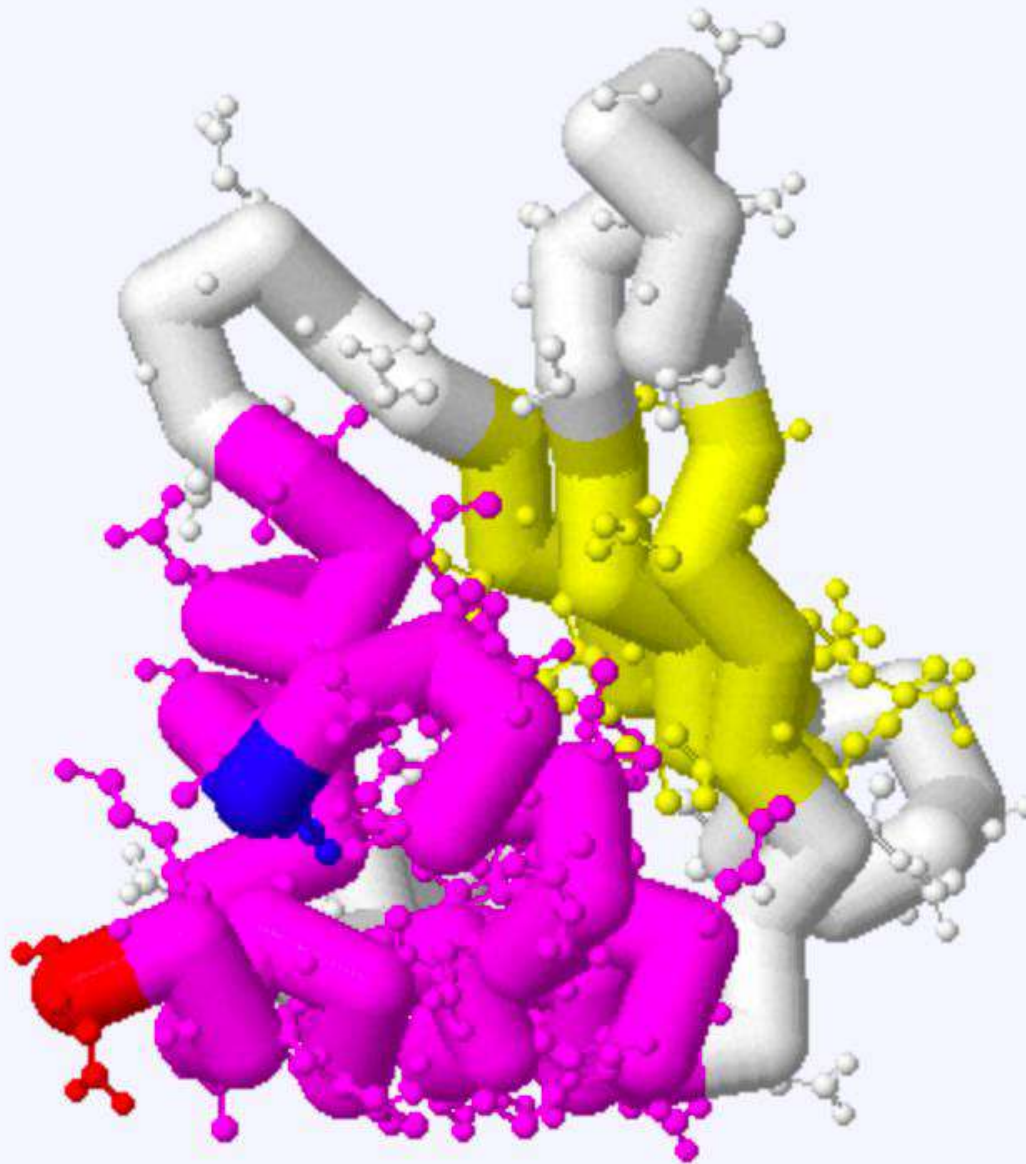
2018-19 Pre-Build Model Structure



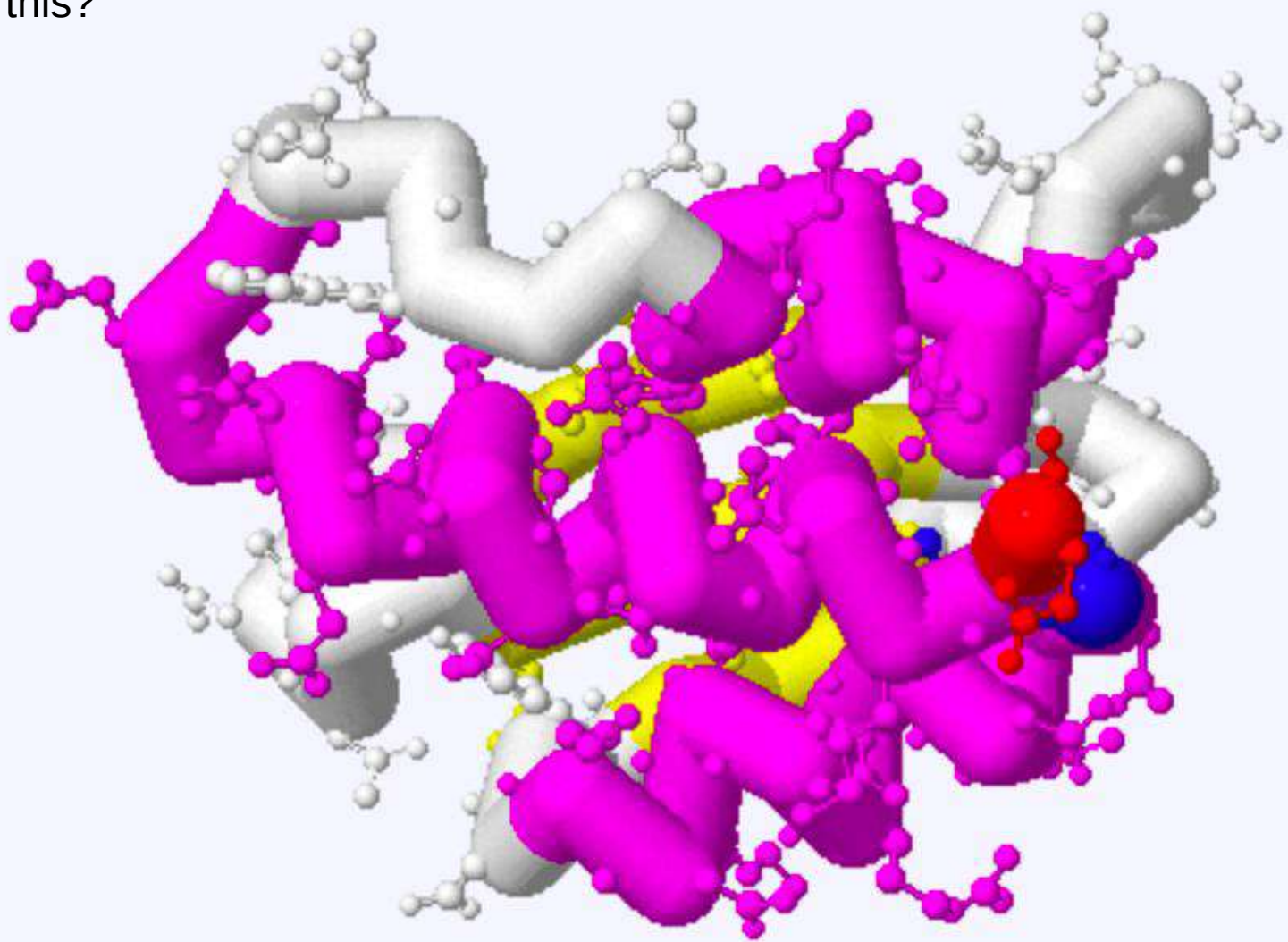
JSmol

Use amino acids 1-85 of chain B

Something like this?



Or this?



Jmol Training Guide

- <http://cbm.msoe.edu/includes/pdf/crest/jmoltrainingall.pdf>
- A free manual you can download
- Tutorial:
<http://cbm.msoe.edu/teachingResources/jmol/jmolTraining/started.html>

<http://cbm.msoe.edu/markMyweb/jmolWebsite/index.html>



**Training Guide**

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Home | Section 1 | Section 2 | Section 3 | Resources | Glossary

Home

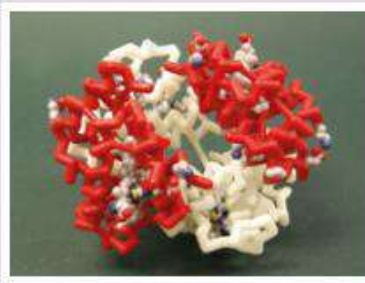
[Previous](#) | [Home](#) | [What is Jmol?](#) | [What are Physical Models?](#) | [How to Use This Site](#) | [Next](#)

Welcome to the Jmol Training Guide

Welcome to the **Jmol** Training Guide brought to you by the **MSOE Center for Biomolecular Modeling** !

This website will prepare you to design and build physical models of molecular structures using the Molecular Visualization Program Jmol and **3D Printing** technology.

The Jmol training guide is divided into three main training sections along with a home/introduction section, a glossary page and an additional resources section. To get started, explore the home/introduction pages shown below. If you are short on time, you can also dive directly into any of the three main training sections shown below.

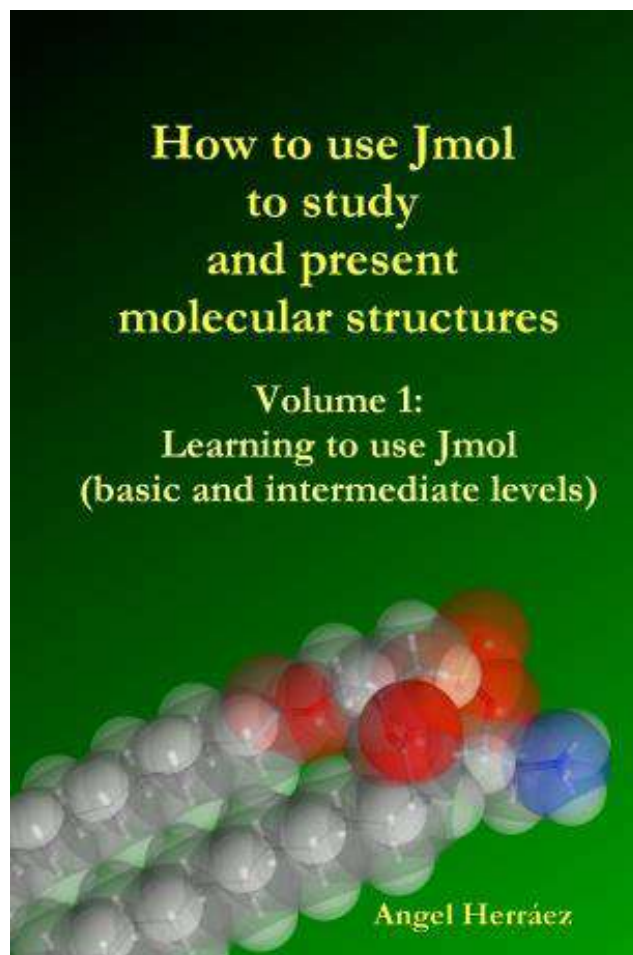


Protein model



Protein model

Jmol Book

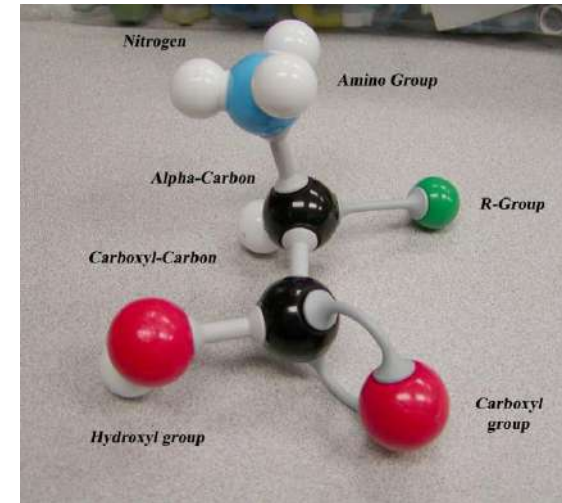


This is a Chemistry Event

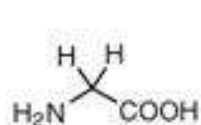
- Know the chemistry of amino acids
- Know structure
- Know how to draw amino acids
- Know the bonding involved
- Know how to make an amide (peptide) bond
- Condensation reaction with water as the by-product

Background info about 20 amino acids

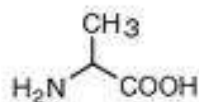
- Backbone consist of:
 - Amino group (NH_2 or NH_3^+)
 - Carbon atom, where the side chain is bound
 - Carboxyl group (COO^- or COOH)
- Side chains are:
 - Hydrophobic
 - Have only carbon and hydrogen atoms
 - Usually buried inside the protein
 - Non-polar or apolar
 - Hydrophilic
 - have hydroxyl, carboxylic acid, or amine groups
 - Are generally on the outside of the protein
 - May be acidic or basic, or polar



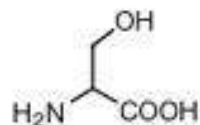
Small



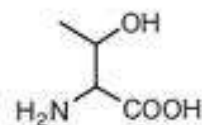
Glycine (Gly, G)
MW: 57.05



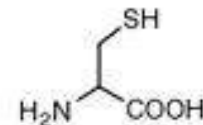
Alanine (Ala, A)
MW: 71.09



Serine (Ser, S)
MW: 87.08, pK_a ~ 16

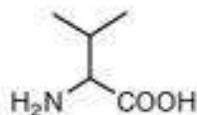


Threonine (Thr, T)
MW: 101.11, pK_a ~ 16

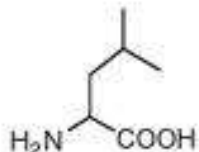


Cysteine (Cys, C)
MW: 103.15, pK_a = 8.35

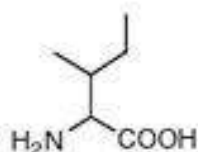
Hydrophobic



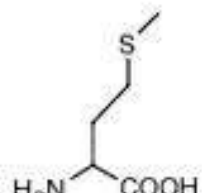
Valine (Val, V)
MW: 99.14



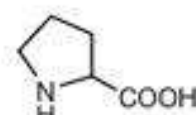
Leucine (Leu, L)
MW: 113.16



Isoleucine (Ile, I)
MW: 113.16

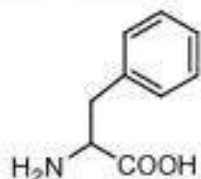


Methionine (Met, M)
MW: 131.19

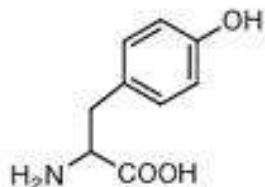


Proline (Pro, P)
MW: 97.12

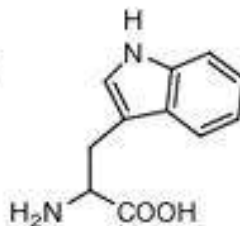
Aromatic



Phenylalanine (Phe, F)
MW: 147.18

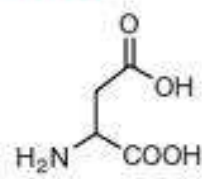


Tyrosine (Tyr, Y)
MW: 163.18

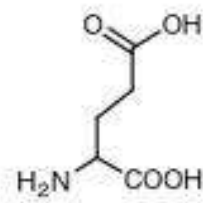


Tryptophan (Trp, W)
MW: 186.21

Acidic

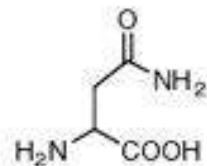


Aspartic Acid (Asp, D)
MW: 115.09, pK_a = 3.9

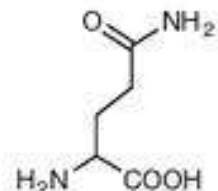


Glutamic Acid (Glu, E)
MW: 129.12, pK_a = 4.07

Amide

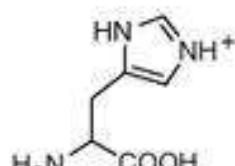


Asparagine (Asn, N)
MW: 114.11

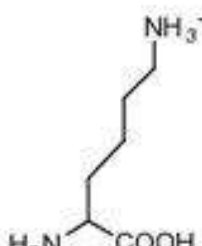


Glutamine (Gln, Q)
MW: 128.14

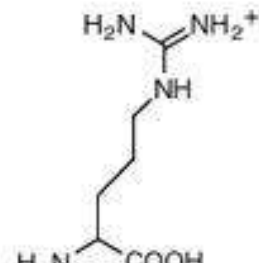
Basic



Histidine (His, H)
MW: 137.14, pK_a = 6.04



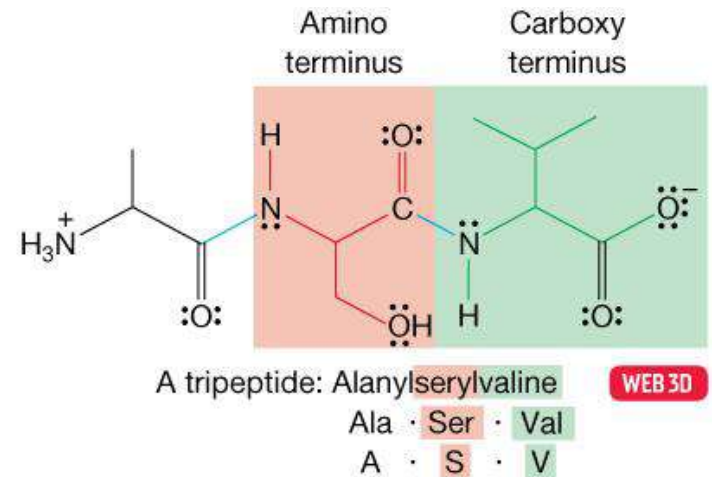
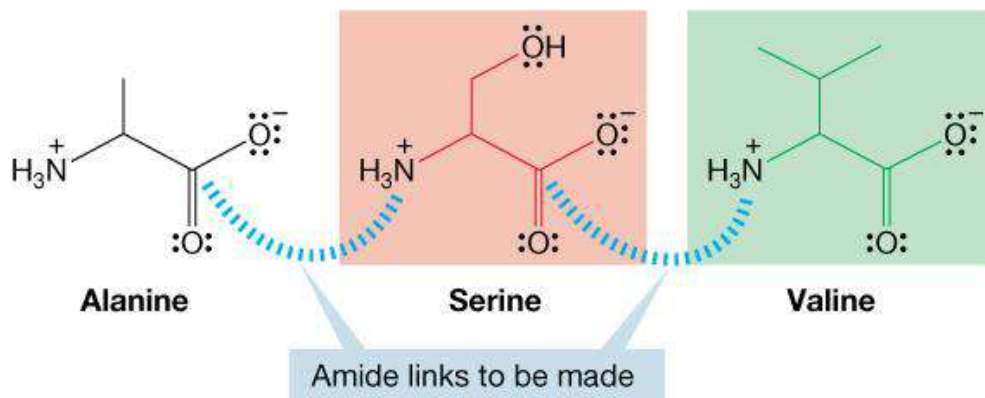
Lysine (Lys, K)
MW: 128.17, pK_a = 10.79



Arginine (Arg, R)
MW: 156.19, pK_a = 12.48

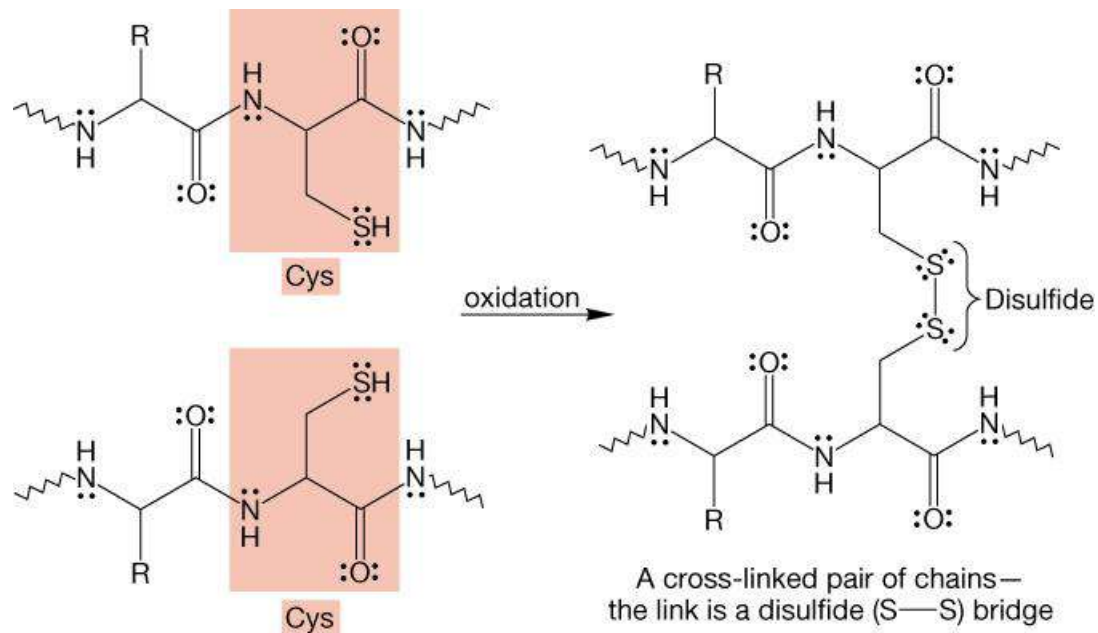
Peptide Chemistry

- Peptides usually written with the **amino terminus** on the left, proceeding toward the **carboxy terminus** on the right



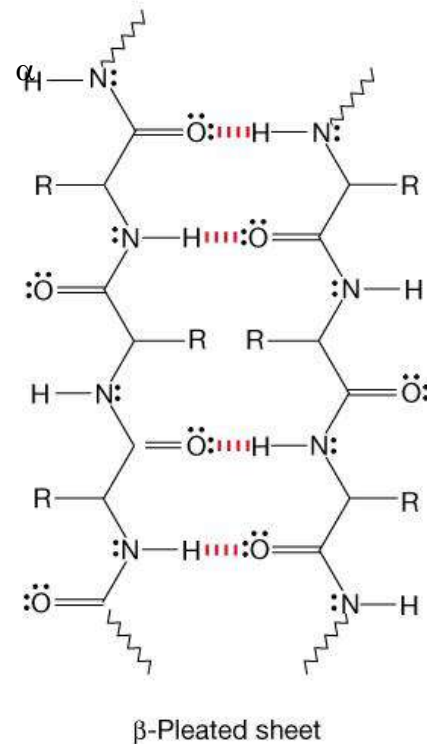
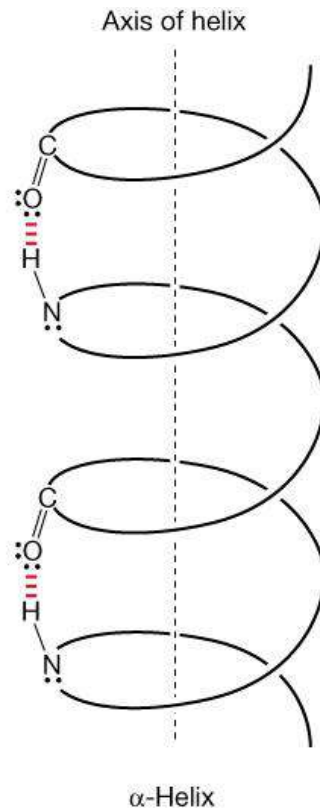
Primary Peptide Structures

- The sequence of amino acids in a peptide or protein gives the primary structure
- Connections between chains or within the same chain are often formed through disulfide bridges



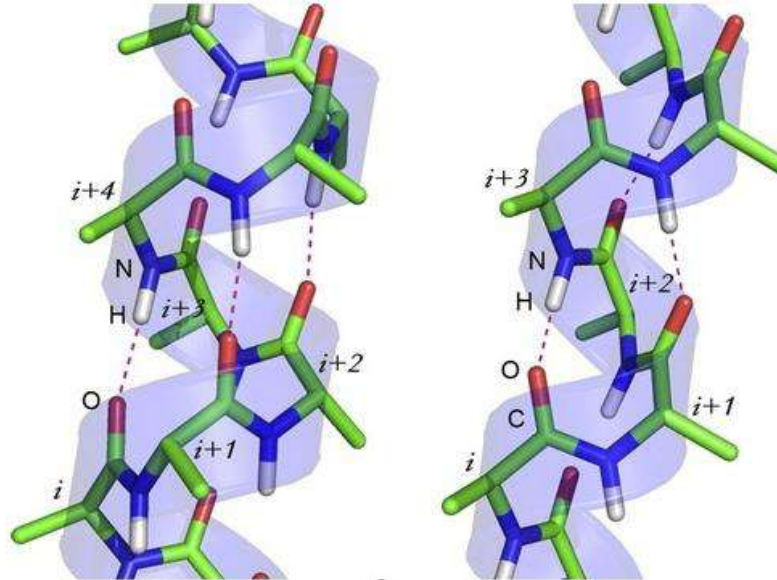
Secondary Peptide Structure

- α -helix, β -pleated sheets, or random coil of amino acids gives the secondary structure

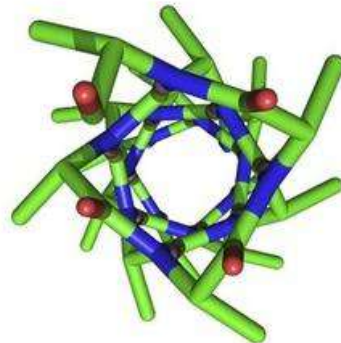


α -helix or 3_{10} helix

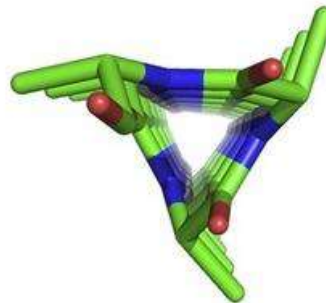
Now, what makes alpha helices more stable?



C



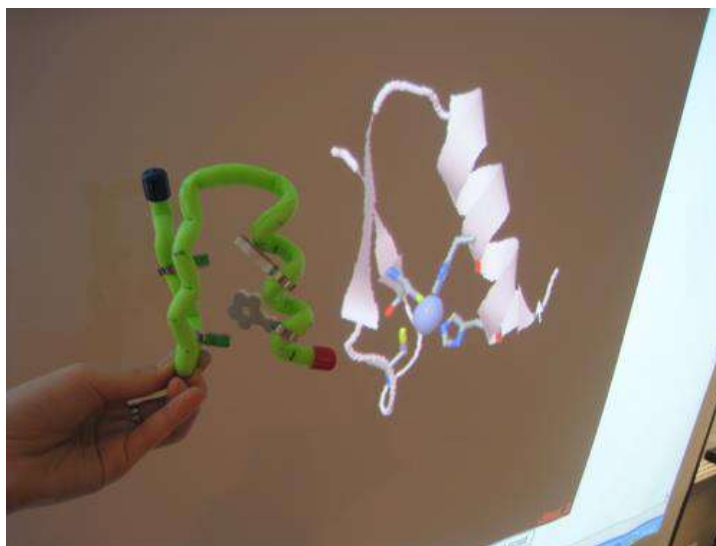
Canonical α -helix



Canonical 3_{10} helix

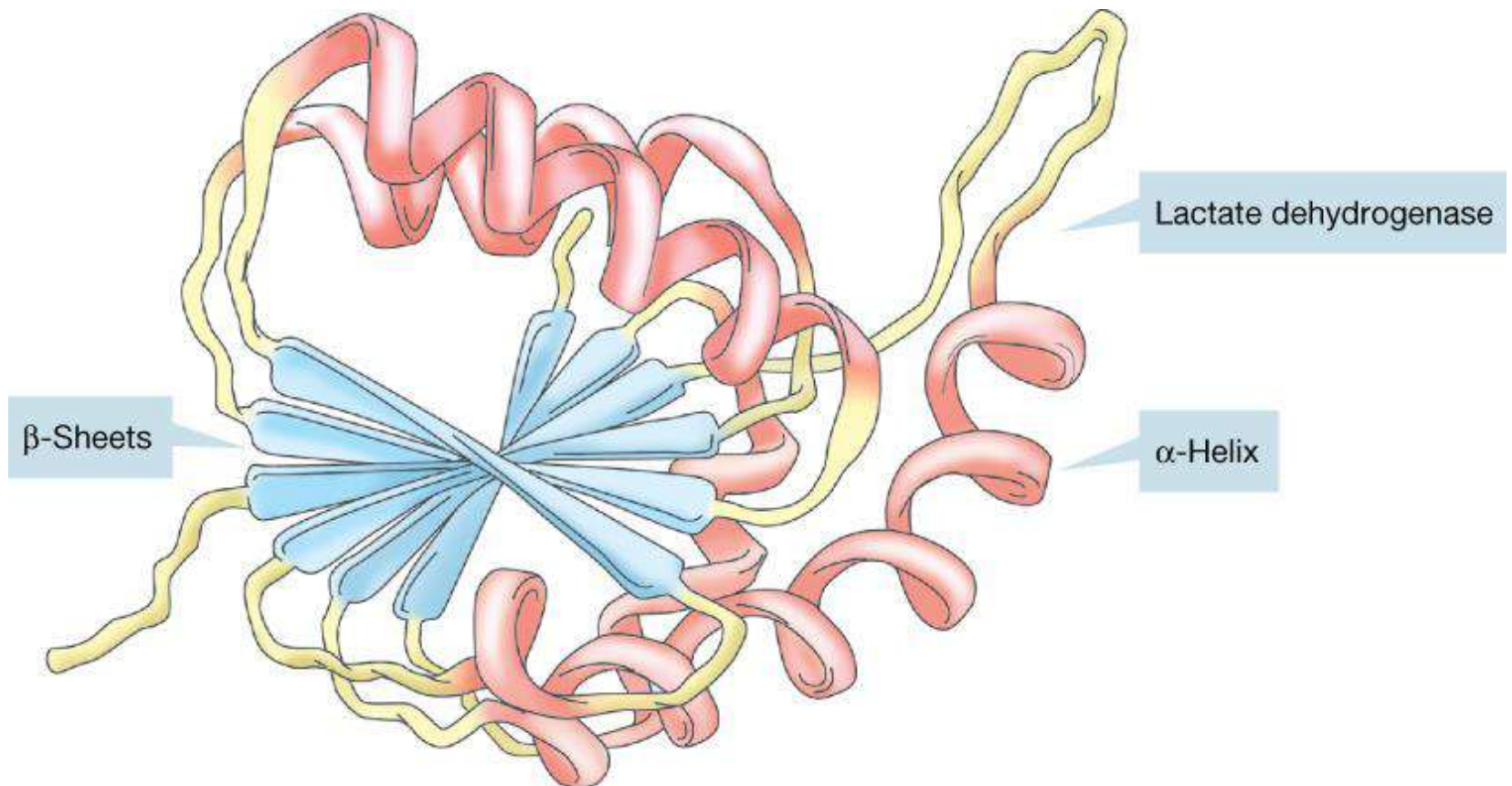
Secondary Structure of a Protein

- The 2 most common types of secondary structure are the alpha helix and beta pleat
- The alpha helix ONLY coils right-handed (if you are going up the stairs, your right hand rests on the outside banister going up)
- The beta pleat should bend back and forth in a zigzag pattern of about 20° at each start of a new amino acid



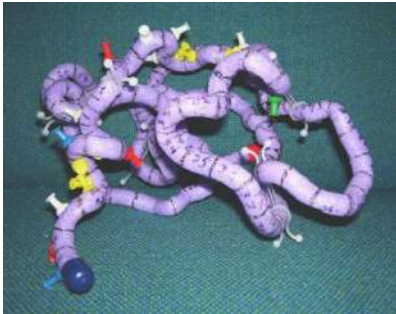
Tertiary Peptide Structure

- Peptides have three-dimensional structures



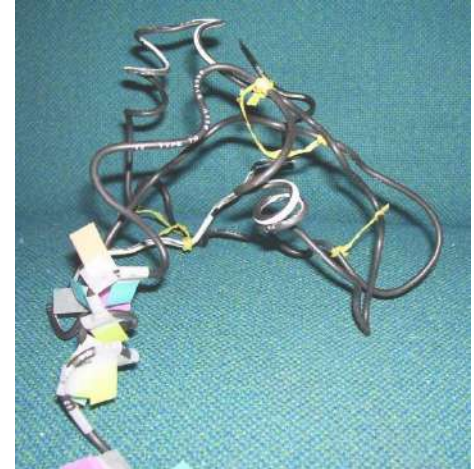
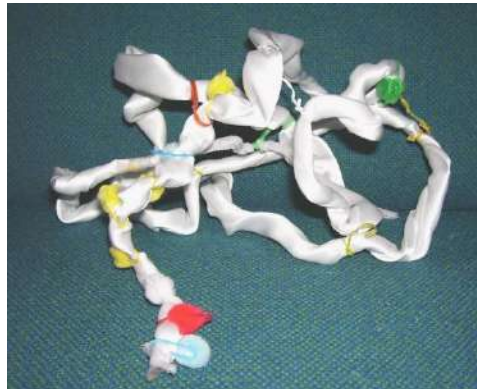
Tertiary Structure of a Protein

- The tertiary structure of the protein is the final folding that is the result of the molecular interactions formed by the primary and secondary structure.
- This is determined using the Jmol program.
- What a finished pre-build might look



Toober

Pipe Cleaner



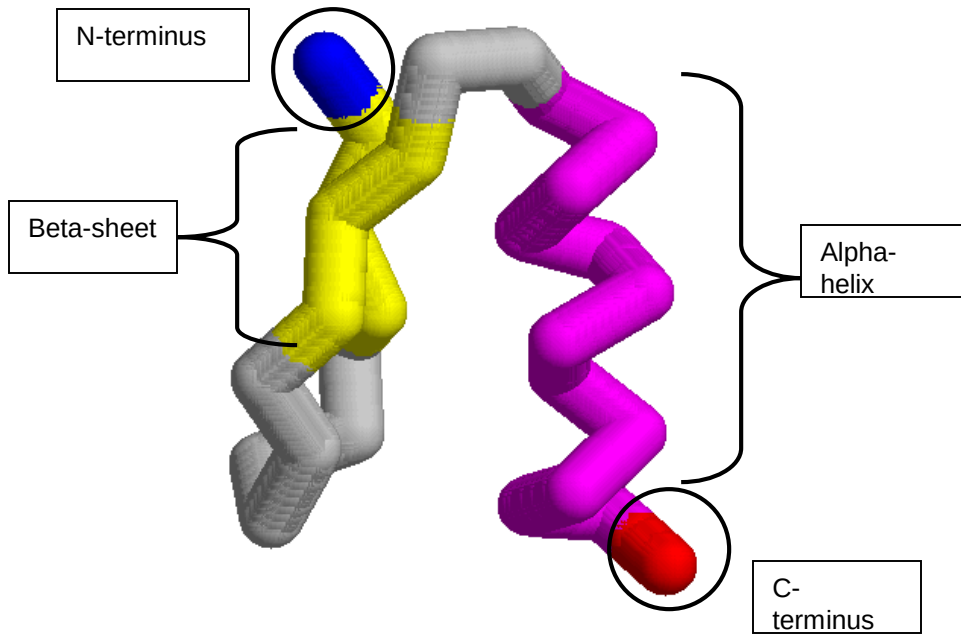
12 Gauge Wire

Past Competitions

- 2010, 2011, 2012, 2015, and 2016
- <http://cbm.msoe.edu/scienceOlympiad/scienceOlympiadPastEvents.php>

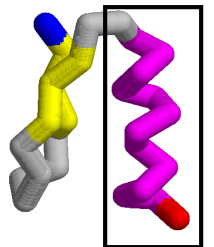
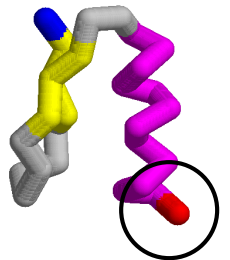
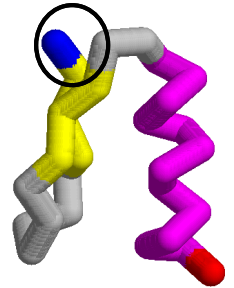
Sample Rubric Sheet

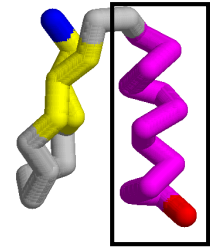
Whole Molecule Overview



Rubric Details

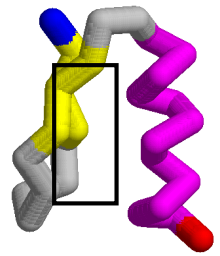
- Blue cap on N-terminal amino acid (Pro4) (1 pt)
 - To receive this point, the blue cap should be positioned on the first amino acid. This should be next to the beta-strand. See picture to the right for correct placement of the blue end cap.
- Red cap on C-terminal amino acid (Gly31) (1 pt)
 - To receive this point, the red cap should be positioned on the last amino acid. This should be next to the alpha-helix. See picture to the right for correct placement of the red end cap.
- Alpha helix (amino acids 19-31) is located at C-terminus of protein (2 pts)
 - There should be an alpha helix located at the C-terminus of the protein. See figure to right. On the model and in the figure, the alpha helix is colored magenta.





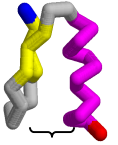
- [Alpha helix is right-handed](#) (2 pts)
 - Alpha helices are right-handed. Check the alpha helix in the model to confirm that the helix is right-handed. If the alpha helix is right-handed, the model is awarded two points.
 - To determine if the helix is right-handed, find one of the ends of the helix and imagine that the helix is a spiral staircase. Pretend that you are climbing that staircase and the helix is the hand-rail, which is always on the outside edge of the staircase. If you would put your right hand on the toober as you go up the staircase, you have a right-handed helix. If you would put your left hand on the toober, you have a left-handed helix and the model would not receive the points.
- Alpha helix is properly formed (helix resembles a telephone cord) (1 pt)
 - The helix should be formed in such a way that it resembles a telephone cord stretched out slightly. The helix should not be compacted down so that there is not any space between the turns. It should also not be so stretched out that there is a lot of space between the turns
- Alpha helix is appropriate length (13 amino acids; ~3.5 turns) (2 pts)
 - The helix is 13 amino acids, and each turn in the helix is approximately 3.6 amino acids in length. Therefore, the length of this helix should be ~3.5 turns.

Rubric Details, Continued

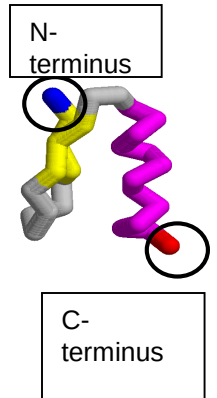


- Beta strand #1 (amino acids 5-7) (2 pts)
 - To receive these points, the model should have a beta strand from amino acids 5-7 (3 amino acids in length). The first beta strand should be located near the blue end cap. The model and the figure to the right have the beta strands colored yellow.
- . Beta strand #2 (amino acids 14-16) (2 pts)
 - To receive these points, the model should have a beta strand from amino acids 14-16 (3 amino acids in length). The second beta strand is located 6 amino acids (12 cm) away from the first. The model and the figure to the right have the beta strands colored yellow.
- Beta strand is formed properly (1 pt)
 - To receive this point, the model should have properly formed beta strands. The model can have the beta strands in a zig-zag shape (a bend every 2 cm) or it could have them be represented as straight regions to the model. There should not be any helical or coiled portions in this area

Rubric Details, Continued

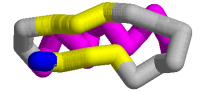


Please note that there is not much space between the two secondary structures.

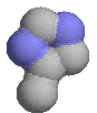
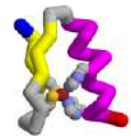


- Helix is arranged next to beta sheet (protein should be compact with a 2-stranded beta sheet lying next to an alpha helix; helix and sheet should not be too far apart) (2 pts)
 - To receive these points, the beta sheet and alpha helix should be located close to one another. There should only be enough space between the two secondary structure to allow for a zinc ion to coordinate between the 4 amino acids that bind the ion. In other words, there should not be much space between the alpha helix and the beta sheet
- 12. N-terminus (blue cap) and C-terminus (red cap) are pointed in opposite directions (2 pts)
 - To receive these points, the N-terminus and C-terminus of the protein should be facing away from each other. If you hold the model so that the beta sheet is facing the left and the helix is on the right (like the picture shown to the right), then the N-terminus should be pointing upward and the C-terminus is pointing downward.

Rubric Details, Continued



- Model should be flat in that the beta strands and alpha helix are occupying the same plane (2 pts)
 - To receive these points, the alpha helix and beta sheet should be in the same plane (please see figure to the right). The model should be “flat” in that neither the helix nor the sheet protrudes upward or downward from the main axis. You should be able to look through the beta sheet and see the alpha helix
- Creative Additions to model (2 pts each):
 - Zinc ion
 - To receive these points, the model should have a zinc ion located between the alpha helix and beta sheet closer to the C-terminus than the N-terminus. Please model and figure to the right (zinc ion is colored dark red).
 - 2 Histidines (His 25 and 29) (coordinates Zn) 2 Cysteines (Cys 7 and 12) (coordinates Zn)
 - Cysteine
 - To receive these points, the model should have 2 Cysteines at positions #7 and #12.
 - If zinc ion is present, then these Cysteines should be connected to the zinc ion.
 - Arginine 18 (attaches to DNA)
 - Arginine
 - To receive these points, the model should have an Arginine at position 18.
 - If DNA is present on model, this amino acid should interact with the DNA.
 - To receive these points, the model should have 2 Histidines at positions #25 and #29.
 - If zinc ion is present, then these Histidines should be connected to the zinc ion

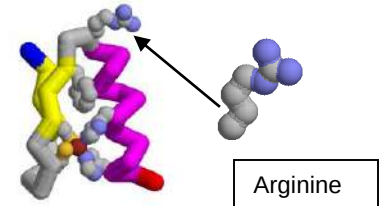


Rubric Details 6: To receive point(s) ...

○ Creative Additions to model (two points each):

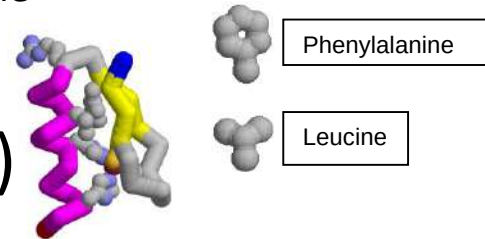
- Arginine 18 bound to DNA (2 pts)

- The model should have an Arginine at position 18.
- If DNA is present on model, this amino acid should interact with the DNA.



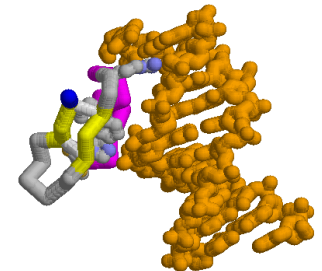
- Hydrophobic amino acids (Phe16, Leu22) (2 pts)

- These residues should face inward to create a stable hydrophobic core stabilizing protein



- DNA attached to protein (2 pts)

- The model should have DNA bound to the zinc finger.
- Zinc finger should be in the major groove of the DNA.



Rubric Details 7: To receive point(s) ...

- Creative additions are appropriate (2 pts)
 - The creative additions should be relevant to telling the functional story of the protein.
 - Any amino acid shown should play an important role in the stability (Zinc ion coordination, hydrophobic core) or function of the molecule (binding to DNA).
 - Models that have displayed all of the amino acids should not be awarded these points.
- Creative additions are accurate (2 pts)
 - The creative additions need to be accurate and reflect the scientific information that has been provided in Goodsell's Molecule of the Month, the PDB file or alternative resources.
- Students submitted a 3x5 card to explain model (2 pts)
 - A 3x5 card should be submitted along with the model, describing what additional features have been added to the model and what they represents.