

Biomolecular Structure**Exam #2**

This exam is to be worked on independently. You must not talk, or otherwise communicate, with *anyone* other than Professor Martin about *any* aspect of the exam. You may not communicate with your fellow students in the class, nor with any other colleagues, faculty or student.

Due in Craig Martin's office (LRGT 403D), December 17, 9:00am

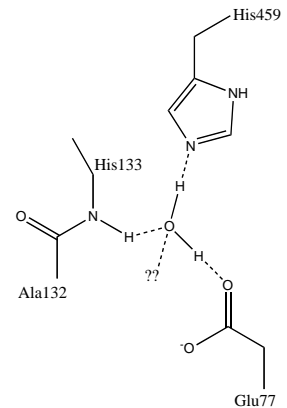
Honesty and integrity are absolute essentials for this class. In fairness to others, dishonest behavior will be dealt with to the full extent of University regulations.

1. a) (5 points, one sentence) What are crystals?

b) (10 points, 2-4 sentences) Which properties of proteins make protein crystals difficult to obtain (think of how they are different from NaCl crystals), and which properties of crystals are essential for obtaining X-ray crystallographic data and solving a structure?
2. (10 points, 4-5 sentences) What is the difference between crystal structures determined to high resolution (say, 1.5 Å) and to lower resolution (say 3.0 Å)? Please comment on the following: a) quality of the crystals; b) quality and amount of diffraction data; c) detail, accuracy and certainty of the atomic model
3. (10 points, 2-3 sentences) All of the amino acids in a particular loop of your protein have B-Factors higher than the rest of the protein. Describe two different explanations for this.

4. Bound water molecules can play important catalytic and structural roles in protein. Go to the presentation for a mutant of yeast bleomycin hydrolase (2e00) at our class WEB site.

- a) (15 points, 2-3 sentences and a drawing) The cited reference notes that **water 512** is an important “structural” water. Study the likely coordination for this water, and draw its coordination following the example shown at right (showing explicitly where the H atoms and lone pair electrons should lie). Justify this particular coordination.



- b) (15 points, 2-3 sentences and a drawing) Do the same for **water 479**. Again, please justify your coordination assignments.

5. In the synthesis of new retro-viral particles, RNA must be packaged. A specific region of HIV RNA (HIV-1 RNA) contains a number of structural features which are important in this packaging, making this segment of RNA a potential target for new types of AIDS-directed drugs. Go to the presentation for guanidino neomycin B recognition of an HIV-1 RNA helix (2JUK) at our class WEB site.
- a) (15 points, 2 sentences) In order to accommodate the bound neomycin ligand, the RNA helix is distorted. Which base pair is most disrupted in this structure? Describe the nature of the disruption.
- b) (15 points, 2 sentences) What is the nature of the interaction between the RNA helix and the bound ligand?