Homework 1

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Contents

1 Problem 1

- Name: SPERM WHALE MYOGLOBIN F46V N-BUTYL ISOCYANIDE AT PH 9.0
- ID: 101M

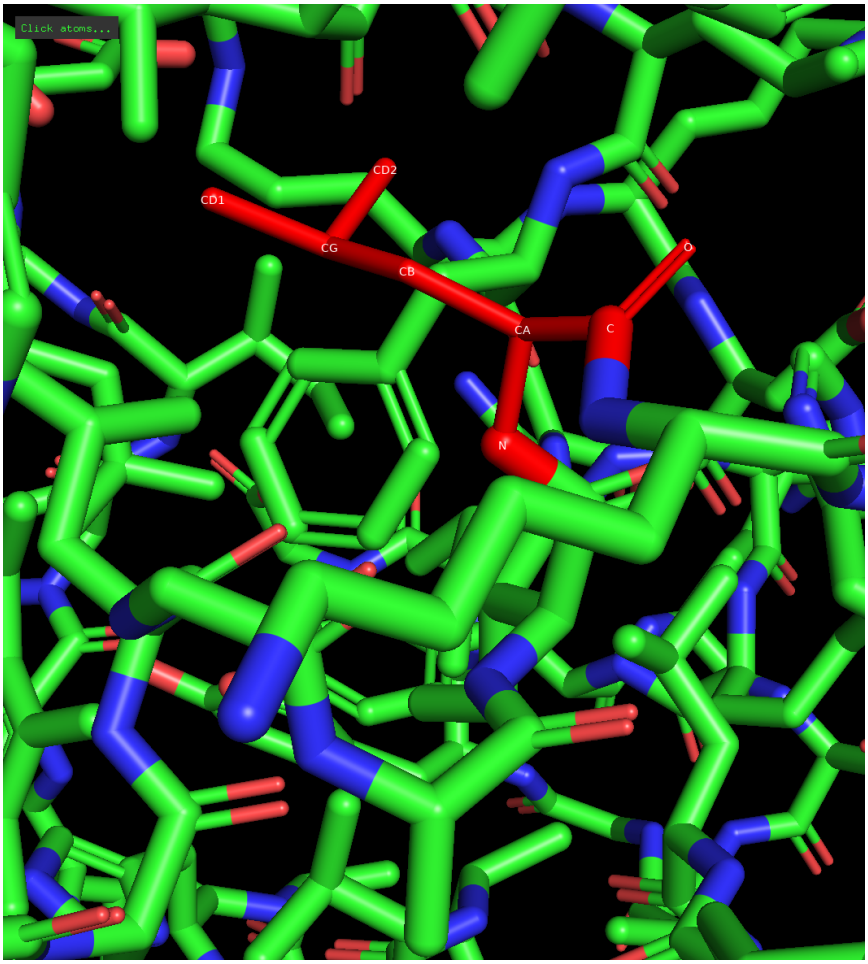

Figure 1: Illustration of molecule with sticks, atoms names of one amino acid labeled.

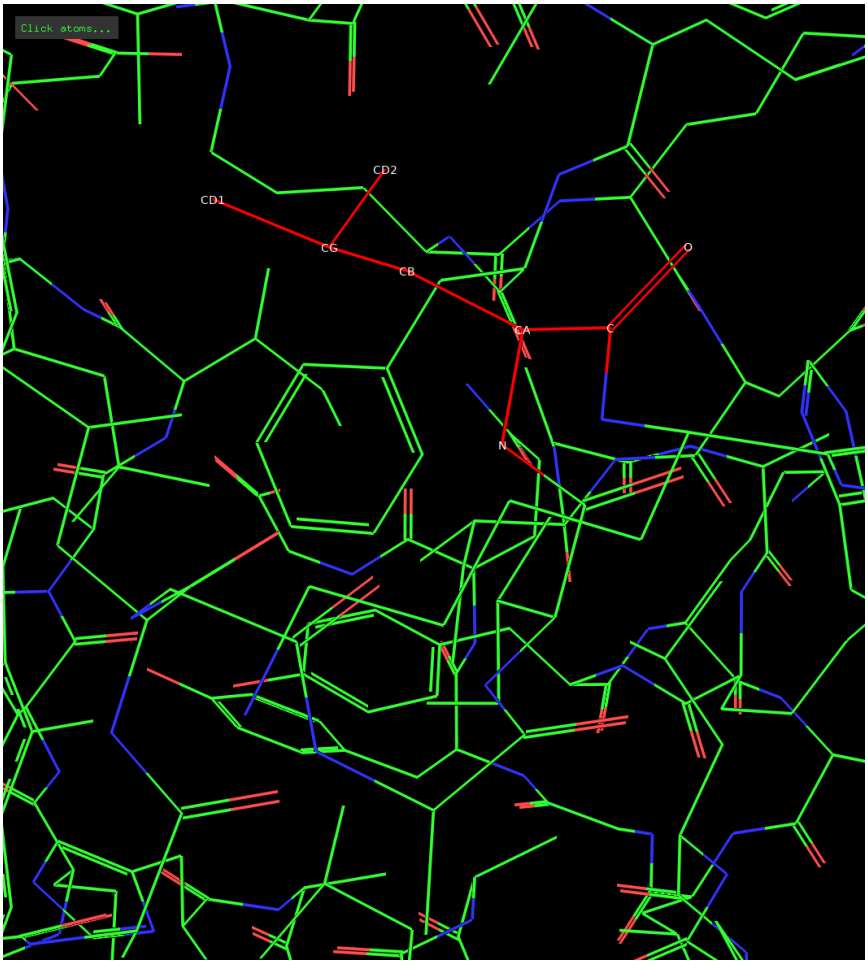

Figure 2: Illustration of molecule with lines, atoms of one amino acid labelled

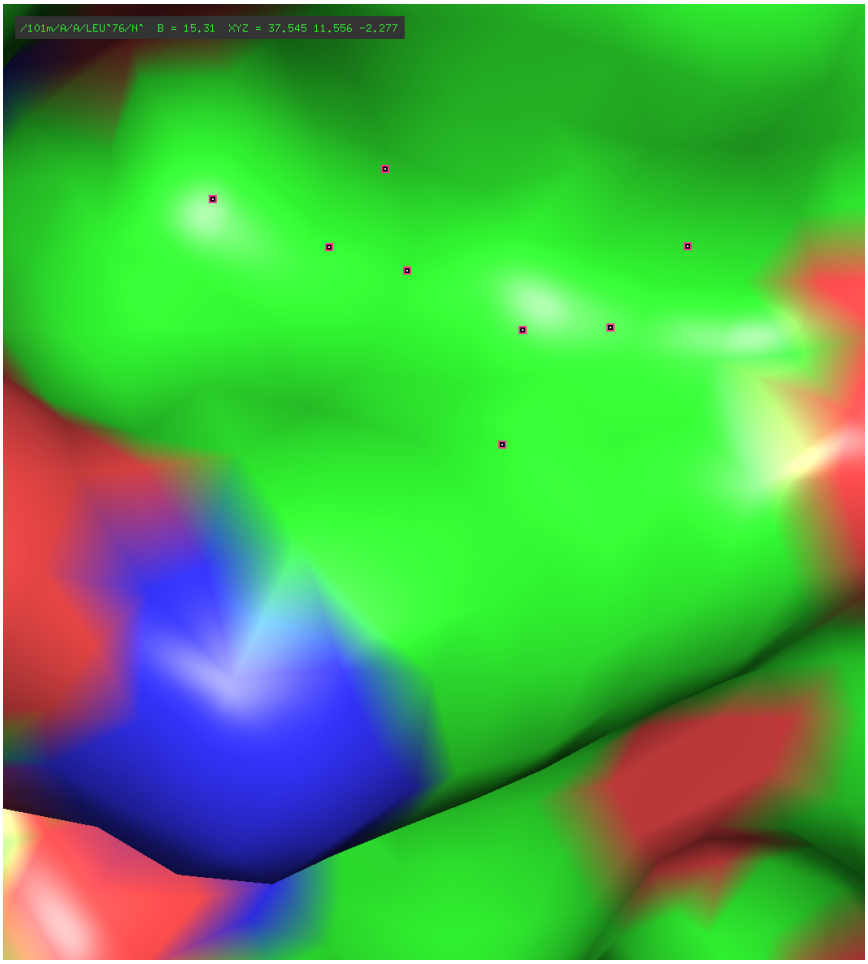

Figure 3: Illustration of molecule with surfaces, atoms and names hidden under surface

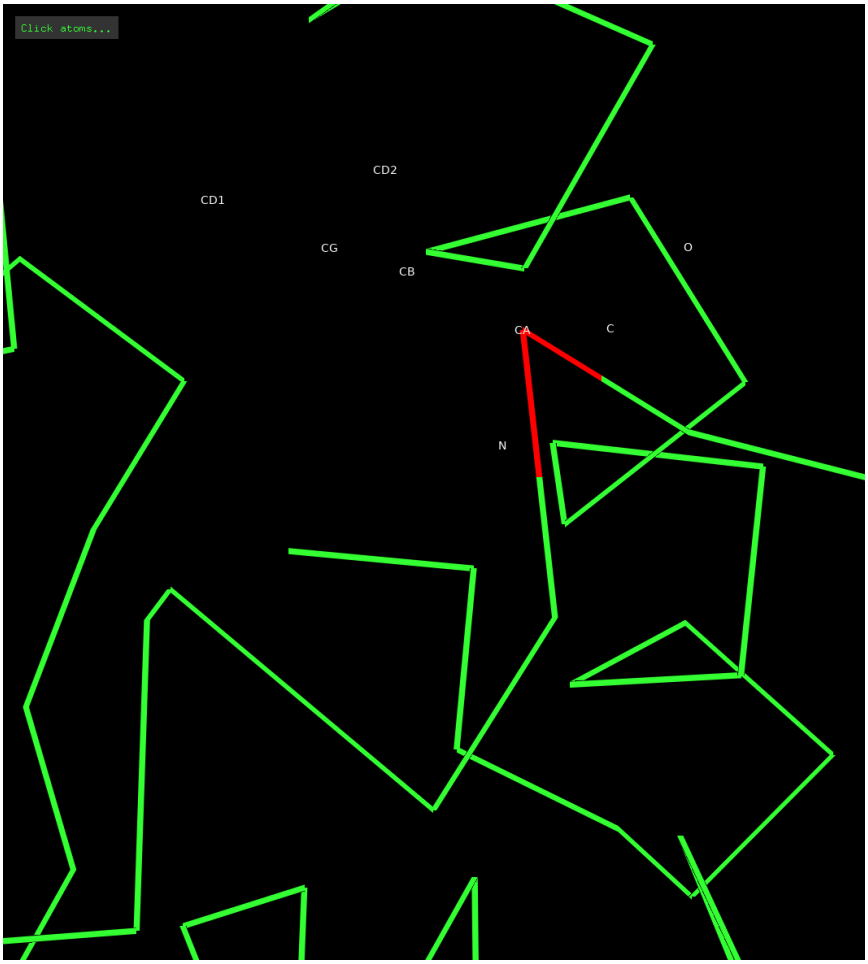

Figure 4: Illustration of molecule with ribbons, atoms hidden but labels are in view.

2 Problem 2

Since $\beta \equiv 1/(k_B T)$, $\partial\beta = -\frac{1}{k_B T^2}\partial T$.

$$
\begin{aligned}
c_v &\equiv \frac{\partial < U >}{\partial T} && (1)\\
&= -\frac{1}{k_B T^2}\frac{\partial < U >}{\partial \beta} && (2)\\
&= \frac{1}{k_B T^2}\frac{\partial}{\partial \beta}(\frac{\partial ln(Z)}{\partial \beta}) && (3)\\
&= \frac{1}{k_B T^2}\frac{\partial}{\partial \beta}(\frac{\partial Z/\partial \beta}{Z}) && (4)\\
&= \frac{1}{k_B T^2}\frac{\frac{\partial^2 Z}{\partial \beta^2}Z - (\frac{\partial Z}{\partial \beta})^2}{Z^2} && (5)\\
&= \frac{1}{k_B T^2}(\frac{\frac{\partial^2 Z}{\partial \beta^2}}{Z} - (\frac{\partial Z}{\partial \beta}/Z)^2) && (6)\\
&= \frac{1}{k_B T^2}(< U^2 > - < U >^2) && (7)
\end{aligned}
$$

For the last step, we used the fact that $Z = \sum e^{-U\beta}$, taking derivative with respect to β twice will bring down U^2.