Problem 1 (Transformations between peptide unit poses). Compute $M(b, A)$ such that $\text{pose}(C_i^\alpha, C'_i, N_{i+1}) = \text{pose}(C_{i-1}^\alpha, C'_{i-1}, N_i) M(b, A)$. You may leave $A$ in the form of a product of rotation matrices. Give a geometric interpretation of the vector $b$. Do not make any simplifying assumptions concerning bond lengths, bond angles, or wedge angles.

Problem 2 (Peptide helix parameters). Assume an ideal peptide unit (i.e. $\omega = \pi$, $l(\{C_i^\alpha, C'_{i-1}\}) = l(\{N_i, C_i^\alpha\}) = l$, 120° angles at $C_{i-1}$ and $N_i$, and 109.47° angle at $C_i^\alpha$) and compute $(e^{i\theta}, u)$ such that $A = R(e^{i\theta}, u)$, where $A$ is the rotation matrix from problem 1. (Hint: Use quaternions.) Express your answer in terms of the angles $\phi_i + \psi_i$ and $\phi_i - \psi_i$. The angle $\theta$ is called the twist angle of the helix. Evaluate $(e^{i\theta}, u)$ in the example of the ideal $\beta$ sheet: $\phi = -\psi = -144.7^\circ = -\cos^{-1}(-\sqrt{2}/3)$. Compute a vector $r$ from $C'_{i-1}$ to the nearest point on the axis of the helix for this example, the radius $\|r\|$ of the helix, and the rise $|b \cdot u|$. Draw a diagram illustrating these quantities in this example.

Problem 3 (3_{10} helix). Consider a chain of three ideal peptide units spanning residues numbered 1 through 4. Assume $\phi_2 = \phi_3 = \phi$ and $\psi_2 = \psi_3 = \psi$ are the unknown independent variables. Write down two equations in the two unknowns expressing the geometric relation that the three atoms $O_1$, $N_4$, and $HN_4$ are collinear. Solve these two equations (numerically if necessary) for $\phi$ and $\psi$. For this particular (idealized) $3_{10}$ helix compute the $\{O_1, HN_4\}$ hydrogen bond length, the helix axis vector $u$, the twist angle, the rise, and the helix radius (as in problem 2). Make a Z-system of your $3_{10}$ helix in IMIMOL and print out a labelled stereo picture of it using RASMOL.

Problem 4 (Endocyclic torsion angles for the chair conformation). Consider an ideal chair conformation of an equilateral hexagon with equal endocyclic bond angles of 109.47°. Recall that from our discussion in class this conformation had $\phi = -\phi' = 60^\circ$ and $\psi = 180^\circ$. Compute all the other endocyclic torsion angles for this conformation.