Hydrogen Bond Practice

The following is text from the kinemage file HbondPractice.kin. The student is asked to recognize hydrogen bonding in increasingly less apparent situations (less clues). Five kinemages are in this file:
Kin 1: H-bonding in beta with polar H's, pointID's, and balls
Kin 2: Repeat of Kin 1 without H's and balls
Kin 3: H-bonding in alpha with polar H's, pointID's, and balls
Kin 4: H-bonding in a small loop and beta piece
Kin 5: H-bonding in Protein/DNA complex

KINEMAGE 1 - A beta hairpin, with polar H's, pointID's, and balls:

This kinemage shows the backbone (in white), sidechains (cyan), and polar hydrogens (gray) for a small piece out of a protein structure, with red balls on the O atoms and skyblue balls on the N atoms. The ends are truncated at Calphas for clarity. Move the image around to see the arrangement in 3D. Occasionally return to View1, or find a view you like and choose "Set Reader's View" on the Views pulldown menu so you can get back to it.

The object of the exercise is to find the hydrogen bonds and draw them in, starting on a simple example with clear, unambiguous H-bonds and lots of clues included.

This kinemage has the drawline function already turned on. Click on two atoms to draw a green line between them, which is shortened at each end for less confusion with the covalent bonds. In this exercise, you should work with the H atoms turned on, and draw the H-bond between the H and the O (either direction is always fine); the scoring function in kins 1 & 2 will think you did it wrong if you draw between N and O (in later exercises you will practice finding H-bonds without the help of seeing the H's). [Tip: If you uncheck the drawline button temporarily, you can take advantage of the atom-identity and distance displays at the bottom of the screen, without producing any new lines.]

Turn off the sidechains and start looking for possible donor-acceptor pairs on the backbone, with suitable geometry. The H-bond donor should be a peptide NH and the acceptor a backbone CO. They should approximately point at each other, with an H-O distance less than 2.5Å (1.7-2.0Å is best). The N-H-O angle is best at 180° and should be above about 135 degrees. [For the NH, both the electrostatic dipole interaction and the bonding contribution in an H-bond are optimal at 180°.] The C-O-H angle is less critical, but should be above 100 degrees. [For the CO, the electrostatic effect is optimal at 180°, but the bonding contribution is best at the lone-pair positions, at an angle near 120°.] H-bond energy decreases with each factor that is non-ideal, but of course setting specific limits is arbitrary. In this kinemage, however, all the possible H-bonds are close to ideal.

When you find a pair with suitable geometry, draw in the H-bond. (If you don't like it, once you move it around and look from all angles, then remove it with the "eraselast" button.)

Once you have drawn lines for all the backbone H-bonds, turn the sidechains back on and see if you can find any sidechain-to-backbone or sidechain-sidechain H-bonds and draw them in also, again checking for suitable geometry. There are many more potential H-bond donors (e.g., any OH, Lys NH3, Asn/Gln NH2) and acceptors (e.g., the exposed side of an OH O, Asp/Glu carboxyl O, Asn/Gln CO) on the sidechains.

When you are done, choose "Score & Stay" on the Kinemage pulldown menu, and the program will both give you an overall score and show what you got right and wrong: correct H-bonds will stay

green, incorrect ones will be hotpink, and ones you didn't find will be shown in gray. Study the ones you got wrong, to figure out what makes them unacceptable.

If you want to try again, turn off "score" and "answer". You can then either edit and add to your previous H-bonds (the "new group"), or you can erase them all and start over. When done, you can get a new score. Then choose "Next" on the Kinemage menu to move on to the next exercise. [If it's grayed out, there are no more exercises and you should quit Mage.]

KINEMAGE 2 - Retrial on beta hairpin, without H's and balls

This is the same beta hairpin you last worked on, but this time the task is to draw all the H-bonds without the help of seeing the N and O balls and the polar H atoms in the display. Again, first draw in the backbone H-bonds, this time clicking on an O and an N atom. You may want to keep on the sidechains, to mark where the Calphas are. Then find and draw the sidechain H-bonds.

When done, use the "Score & Stay" function and study any you got wrong. Cycle thru the exercise again if you want, or choose Next to move on.

KINEMAGE 3 - A small helix, with polar H's, pointID's, and balls:

This exercise is set up the same way as the first one, but for an alpha-helix plus a bit extra on each end. First, turn off the sidechains and identify and draw in the alpha-helical H-bonds in the regular central part of the helix (keep on the H atoms and the N and O balls, and draw between H and O, checking for suitable geometry as described above).

Most of the helical H-bonds have nearly ideal geometry and the classic alpha-helix pattern of CO(i)-NH(i+4). At the C-terminus, however, that pattern is distorted, with some of the H-bonds weak or marginal (with bad angles and/or longer distances), and sometimes bifurcated. Although the cutoff is fairly arbitrary, O(36)-NH(40) and O(38)-NH(41) are acceptable, O(37)-NH(40) is very marginal (both angles are bad), and O(37)-NH(41) is clearly unacceptable (the N-H-O angle is 110°). You may need to use measures to check out marginal cases, but for good H-bonds you should learn to spot them by eye. Make your analysis, and draw in the H-bonds for the C-terminal end of the helix.

Once you have drawn lines for all the backbone H-bonds, turn the sidechains back on and see if you can find any sidechain-to-backbone H-bonds and draw them in also, again checking for suitable geometry. There are many more potential H-bond donors (e.g., any OH, Lys NH3) and acceptors (e.g., Asp Od, Glu Oe, His N) on the sidechains. In this case, there are no sidechain-sidechain H-bonds.

When you are done, choose "Score & Stay" and study any you got wrong. Turn off "score" and "answer", erase your previous H-bonds, and try the task again with the N/O atom balls turned off (leave on the H atoms, and draw from them). Score again, and choose "Next" to move on.

KINEMAGE 4 - A small loop and beta piece, without H's and balls

In this exercise, you see the structure with just the heavier atoms for backbone and sidechains, the way it would usually be shown in a published figure or in most graphics programs.

First identify the backbone H-bonds, and draw them in by clicking on the N and the O atoms. (In this kinemage, the score will not work if you draw from the H.) [The balls and H atoms can be turned on temporarily, if you get confused or to check your assignments, but try to do without

them .]

This example includes good H-bonds with quite non-linear C-O-H angles.

Turn sidechains back on, look for sidechain-to-mainchain H-bonds, and draw them in. [Turn on H's temporarily to remind you of where they should be, but don't draw from them.]

When you are done, choose "Score & Stay" and study any you got wrong. To try again, turn off "score" and "answer", erase your previous H-bonds, and start over. Score again, and choose "Next" to move on.

KINEMAGE 5 - Protein/DNA complex (partial)

This time you will identify H-bonds that make up one part of the functional binding site for the complex of lambda repressor with its DNA operator site. The protein is in shades of yellow, and the DNA has white backbone and lilac bases. Polar H atoms (gray) and atom balls on N, O, & P are included. The second, more distant, DNA strand has its backbone simplified.

First look for and draw H-bonds between protein sidechains and DNA bases, which provide sequence-specific interactions (mostly on the top half of the interface, in View1). Draw between the hydrogen and the acceptor atom.

Then draw lines to show the H-bonds between protein and the DNA backbone; at least one should involve an atom on the protein backbone.

Turn off the DNA but leave on the protein and your "new group" of drawn H-bonds. Look for two places where sidechains that contact DNA are also held in place by H-bonds between two of the sidechains; draw in those H-bonds.

Use "Score & Stay", study any wrong or missing H-bonds, and cycle thru the exercise again if you want.

Several features not used in the scoring are visible for study. As in many protein/DNA interactions, here there are indirect H-bonds that join lambda to the DNA through well-ordered water molecules; two such interfacial waters can be turned on for examination.

Turn on the "Hb dots" button to visualize directly the favorable atomic overlaps that constitute these protein/DNA H-bonds, shown as lens shapes of pale green dots (including the ones thru the waters).

Also, you may want to practice drawing the base-pair H-bonds in the DNA (3 for GC, 2 for AT). Remember that they are not included in the scoring function, so you must evaluate their appearance for yourself.

This is the last H-bond practice example. When done, quit out of Mage.