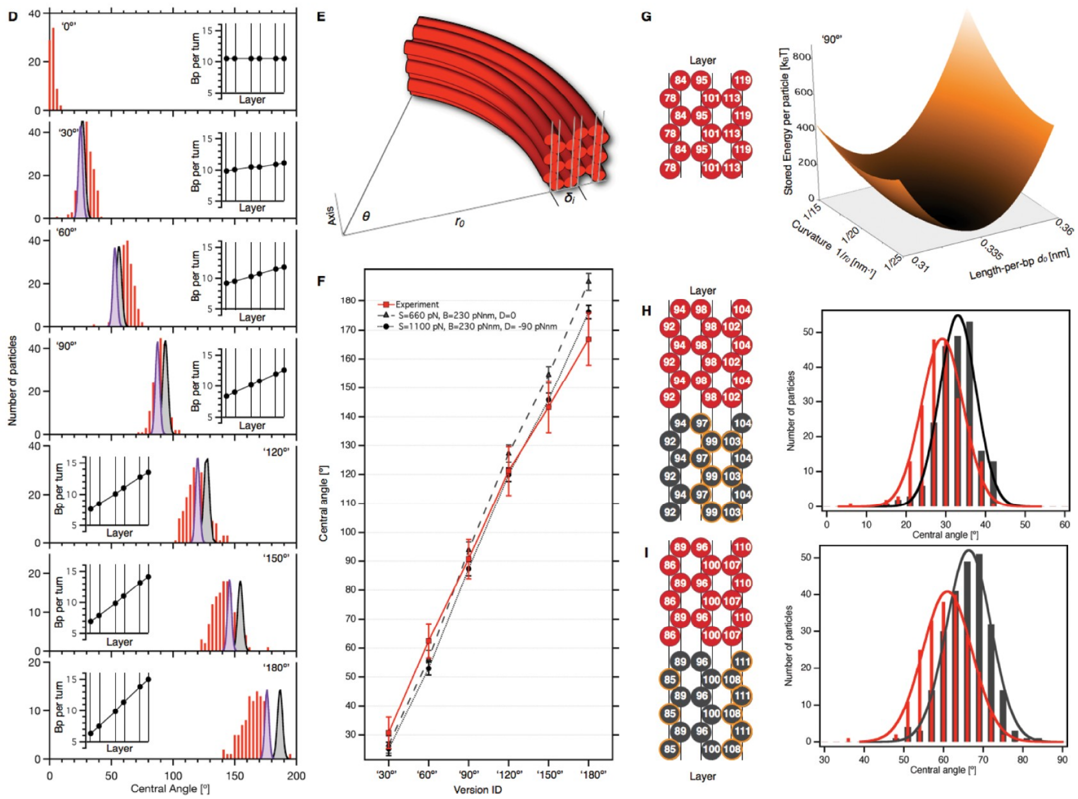
Supporting Figure 1



Approximation of Energy for bending DNA bundle

(stretch-compression and bend terms only)
(no twist, twist-stretch coupling yet)

$$E_{total} = E_{stretch/compression} + E_{bend}$$

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}} \sum_i n_i (d_i - d_{eq})^2$$

$$E_{bend} = \frac{1}{2} B d_{eq} \sum_i \frac{n_i}{r_i^2}$$

$$where\ r_i = r_{ref}\left(\frac{delta_i}{r_{ref}} + 1\right)$$

$$q_i = \frac{n_i d_{eq}}{r_i}$$

$$E_{bend} = \frac{1}{2}\frac{B}{d_{eq}} \sum_i q_i^2 \frac{1}{n_i}$$

$$but \quad \sum_i q_i^2 \frac{1}{n_i} \approx q^2 \sum_i \frac{1}{n_i}$$

$$\therefore\ E_{bend} \approx \frac{1}{2}\frac{B}{d_{eq}} q^2 \sum_i \frac{1}{n_i}$$

The rationale for the above approximation is based on the idea that the underestimate in bending energy for the convex-face helices will be mostly offset by the overestimate in bending energy for the concave-face helices.

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}} \sum_i n_i (d_i - d_{eq})^2 + \frac{1}{2}\frac{B}{d_{eq}} q^2 \sum_i \frac{1}{n_i}$$

Please note that for this approximation of energy, the following relations hold:

At fixed values of d_i

$$\frac{\partial E_{stretch/compression}}{\partial q} = 0$$

At fixed values of θ

$$\frac{\partial E_{bend}}{\partial d_i} = 0$$

Step 0: Obtain an expression for the length $n_{ref}d_{ref}$ of a reference double helix in the curved bundle as a function of angle, assuming the bundle is at the equilibrium length for that angle. Do this by letting $\partial E_{stretch/compression}/\partial n_{ref}d_{ref} = 0$ and solving for $n_{ref}d_{ref}$ (recall from the previous page that $\partial E_{bend}/\partial d_{ref} = 0$). The position in the bundle of the reference double helix is encoded in the $delta_i$ offset values. The reference helix could be imaginary, the position within the bundle is arbitrary, and the value of n_{ref} never has to be specified (it cancels out during Step 1).

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}} \sum_i n_i (d_i - d_{eq})^2$$

$$d_i = \frac{n_{ref} d_{ref}}{n_i} \left(\frac{delta_i}{r_{ref}} + 1 \right)$$

$$r_{ref} = n_{ref} d_{ref} / q$$

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}} \sum_i n_i \left[\frac{n_{ref} d_{ref}}{n_i} \left(\frac{delta_i}{n_{ref} d_{ref} / q} + 1 \right) - d_{eq} \right]^2$$

$$E_{stretch/compression} = \frac{1}{2}\frac{S}{d_{eq}} \sum_i n_i \left[\frac{1}{n_i} (n_{ref} d_{ref} + q \, delta_i) - d_{eq} \right]^2$$

$$\frac{\partial E_{stretch/compression}}{\partial (n_{ref} d_{ref})} = \frac{S}{d_{eq}} \sum_i n_i \left[\frac{1}{n_i} (n_{ref} d_{ref} + q \, delta_i) - d_{eq} \right] \frac{1}{n_i}$$

$$= \frac{S}{d_{eq}} \sum_i \left[\frac{1}{n_i} (n_{ref} d_{ref} + q \, delta_i) - d_{eq} \right]$$

$$0 = \frac{S}{d_{eq}} \sum_i \left[\frac{1}{n_i} (n_{ref} d_{ref} + q \, delta_i) - d_{eq} \right]$$

$$= n_{ref} d_{ref} \sum_i \frac{1}{n_i} + q \sum_i \frac{delta_i}{n_i} - d_{eq} \sum_i 1$$

$$n_{ref} d_{ref} = \frac{1}{\sum_i \frac{1}{n_i}} \left(d_{eq} \sum_i 1 - q \sum_i \frac{delta_i}{n_i} \right)$$

Step 1: Use the expression for the length $n_{ref}d_{ref}$ from Step 0 to obtain an expression for the length d_i of double helix$_i$ in the curved bundle as a function of angle, assuming the bundle is at its equilibrium length for that angle.

$$n_{ref}d_{ref} = \frac{1}{{}_i\,\frac{1}{n_i}}\; d_{eq} \quad {}_i 1 - q \quad {}_i \frac{delta_i}{n_i}$$

$$d_i = \frac{n_{ref}d_{ref}}{n_i} \; \frac{delta_i}{r_{ref}} + 1$$

$$q = \frac{n_{ref}d_{ref}}{r_{ref}}$$

$$d_i = \frac{1}{n_i}(q \;\; delta_i + n_{ref}d_{ref})$$

$$= \frac{1}{n_i \quad {}_i\,\frac{1}{n_i}} \; q \;\; delta_i \quad {}_i\frac{1}{n_i} + d_{eq} \quad {}_i 1 - q \quad {}_i \frac{delta_i}{n_i}$$

$$d_i = \frac{1}{n_i \quad {}_i\,\frac{1}{n_i}} \; q \;\; delta_i \quad {}_i\frac{1}{n_i} - \quad {}_i \frac{delta_i}{n_i} + d_{eq} \quad {}_i 1$$

Step 2: Use the expression for the length d_i from Step 1 to obtain an expression for the total (= stretch/compression + bending) of the bundle as a function of angle. Since we are concerning ourselves here with only the equilibrium length of the bundle at every angle, therefore length is a dependent variable, and angle is the only independent variable.

$$d_i = \frac{1}{n_i \quad {}_i\frac{1}{n_i}} \; q \;\; delta_i \quad {}_i\frac{1}{n_i} - \quad {}_i\frac{delta_i}{n_i} + d_{eq} \quad \underset{i}{1}$$

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}} \quad {}_i n_i(d_i - d_{eq})^2 + \frac{1}{2}\frac{B}{d_{eq}} q^2 \quad {}_i\frac{1}{n_i}$$

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$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}} \quad {}_i n_i \; \frac{1}{n_i \quad {}_i\frac{1}{n_i}} \; q \;\; delta_i \quad {}_i\frac{1}{n_i} - \quad {}_i\frac{delta_i}{n_i} + d_{eq} \quad \underset{i}{1} - d_{eq} \quad + \frac{1}{2}\frac{B}{d_{eq}} q^2 \quad {}_i\frac{1}{n_i}$$

Step 3: Use the expression for total energy from Step 2 to obtain an expression for the angle of curvature that gives the minimum stretch-compression plus bending energy for the bundle. Do this by setting to zero the derivative of the combined energy with respect to angle, and solving for angle.

$$E_{total} = \frac{1}{2}\frac{S}{d_{eq}} \sum_i n_i \left[\frac{1}{n_i \sum_i \frac{1}{n_i}} \left(q \left(delta_i \sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i} \right) + d_{eq} \sum_i 1 \right) - d_{eq} \right]^2 + \frac{1}{2}\frac{B}{d_{eq}} q^2 \sum_i \frac{1}{n_i}$$

$$\frac{E_{total}}{q} = \frac{S}{d_{eq}} \sum_i n_i \left[\frac{1}{n_i \sum_i \frac{1}{n_i}} \left(q \left(delta_i \sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i} \right) + d_{eq} \sum_i 1 \right) - d_{eq} \right] \frac{1}{n_i \sum_i \frac{1}{n_i}} \left(delta_i \sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i} \right)$$
$$+ q \frac{B}{d_{eq}} \sum_i \frac{1}{n_i}$$

$$\textit{for convenience, let} \quad b_i = \frac{1}{n_i \sum_j \frac{1}{n_j}} \left(delta_i \sum_j \frac{1}{n_j} - \sum_j \frac{delta_j}{n_j} \right)$$

$$0 = \frac{S}{d_{eq}} \sum_i b_i n_i \left[\frac{1}{n_i \sum_i \frac{1}{n_i}} \left(q \left(delta_i \sum_i \frac{1}{n_i} - \sum_i \frac{delta_i}{n_i} \right) + d_{eq} \sum_i 1 \right) - d_{eq} \right] + q \frac{B}{d_{eq}} \sum_i \frac{1}{n_i}$$

$$= q \left(\sum_i b_i delta_i \sum_i \frac{1}{n_i} - \sum_i b_i \sum_i \frac{delta_i}{n_i} + \frac{B}{S} \left(\sum_i \frac{1}{n_i} \right)^2 \right) + d_{eq} \left(\sum_i b_i \sum_i 1 - \sum_i b_i n_i \sum_i \frac{1}{n_i} \right)$$

$$\theta = d_{eq} \frac{\sum_i b_i n_i \sum_i \frac{1}{n_i} - \sum_i b_i \sum_i 1}{\sum_i b_i delta_i \sum_i \frac{1}{n_i} - \sum_i b_i \sum_i \frac{delta_i}{n_i} + \frac{B}{S} \left(\sum_i \frac{1}{n_i} \right)^2}$$

$$\textit{where } b_i = \frac{1}{n_i \sum_j \frac{1}{n_j}} \left(delta_i \sum_j \frac{1}{n_j} - \sum_j \frac{delta_j}{n_j} \right)$$

Note that ${}_{i}\beta_i = 0$

Therefore

$$\theta = \frac{d_{eq} \quad {}_{i} b_i n_i}{{}_{i} b_i delta_i + \frac{B}{S} \quad {}_{i} \frac{1}{n_i}}$$

$$where\ b_i = \frac{1}{n_i \quad {}_{j} \frac{1}{n_j}} \ delta_i \quad {}_{j} \frac{1}{n_j} - \quad {}_{j} \frac{delta_j}{n_j}$$

and from before

$$d_i = \frac{1}{n_i \quad {}_{i} \frac{1}{n_i}} \ q \ delta_i \quad {}_{i} \frac{1}{n_i} - \quad {}_{i} \frac{delta_i}{n_i} + d_{eq} \quad \underset{i}{1}$$