Supplemental Information

for

H-bonds in Crambin:
Coherence in an α-helix

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Error Estimates

**Stochastic errors** can be evaluated from the estimation procedures described in some detail in the text. These are nearly summarized in the Table below, reworked from Bendat and Piersol.

### Random Error Formulas

| Name                        | Function (symbol) | Random error |
|-----------------------------|-------------------|--------------|
| Coherence                   | $\hat{\gamma}_{xy}(f)$ | $\frac{\sqrt{2}[1 - \hat{\gamma}_{xy}(f)]}{\hat{\gamma}_{xy}(f) \sqrt{n_d}}$ |
| Power                       | $\hat{G}_{xx}(f) = \hat{\gamma}_{xy}(f) \hat{G}_{yy}(f)$ | $\frac{[2 - \hat{\gamma}_{xy}(f)]^{\frac{1}{2}}}{\hat{\gamma}_{xy}(f) \sqrt{n_d}}$ |
| Magnitude of Frequency Function | $|\hat{H}_{xy}(f)|$ | $\frac{[1 - \hat{\gamma}_{xy}(f)]^{\frac{1}{2}}}{\hat{\gamma}_{xy}(f) \sqrt{2n_d}}$ |
| Phase of Frequency Function | $\hat{\phi}_{xy}(f)$ | $SD[\hat{\phi}_{xy}(f)] = \frac{[1 - \hat{\gamma}_{xy}(f)]^{\frac{1}{2}}}{|\hat{\gamma}_{xy}(f)| \sqrt{2n_d}}$ |

$n_d = number of data points; SD = standard deviation

Modified version of Bendat & Piersol, Table 9.6, p. 312

**Systematic Error**

Most systematic errors of concern arise from details in the computations of molecular dynamics and estimation of the parameters of Table S1. These are discussed in the main text.

The comparison (see Figures 3-6 of text) of analytical expressions and stochastic estimation of the model system defined in Figure 2 suggest that systematic errors are not present in large amounts. The finding that non-interacting atoms have very low coherence (Figure 9) gives comfort that whatever errors remain do not create coherence out of nothing.

Further checks were made to show that displacement of the structure did not change estimates of coherence.

First (Figure S1) the coherence of the crambin protein was estimated after 100 uniformly sampled displacements. That is, we translated every atom in the protein by displacement uniformly sampled between $-200$ and $+200$ Angstroms.
The results shown are the coherences of a particular H-bond (PHE13N and ALA9O) in the main alpha helix but every atom examined showed similar results. We see slight deviations in coherence for mostly higher frequencies, where the mean coherence itself is less reliable. Coherence at lower frequencies are $> 0.9$ despite displacements.

Figure S1

![Figure S1](image.png)

Figure S1: The black line is the coherence calculated from the native trajectory and the average of all the translated coherences is shown in blue. We see there is not much discrepancy between the averaged (blue) coherence and the coherence calculated from the native trajectory, especially in the low frequency range.
Figure S2: Histogram of the averaged coherence between 0.39 GHz and 5.09 GHz (the main range of interest) of all the translated trajectories. Each trajectory was separately translated by different amounts, as specified above. The standard deviation of $4.69 \times 10^{-3}$ in the mean coherence suggests that our coherence estimation is not sensitive to translation.
Figure S3: Rotating the protein does not change the coherence.