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# Supplementary Information for Dipole Orientation of Hydrated Gas-phase Proteins

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### Resolution limit calculation from Fourier Ring Correlation

We assumed a Fourier Ring Correlation (FRC) of 0.5 as the threshold for when structure determination from the underlying set of diffraction images would be possible. From this the best possible resolution of the structure determination was estimated. Assuming the FRC follows a model function of the form

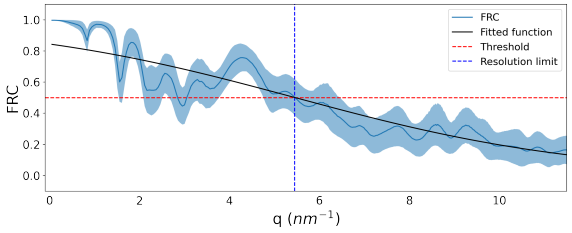
$$FRC(q) = \frac{1}{1+e^{bq+c}}, \tag{1}$$

a curve was fitted to the data, giving us a threshold value of $q$. Given this, the corresponding resolution for structure determination was calculated as $\frac{1}{q_{cutoff}}$, as illustrated in Figure 1a.

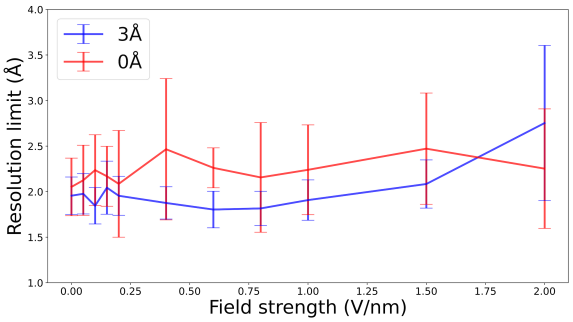
A complete presentation of the resolution limits for both hydration levels and for every electric field amplitude is shown in Figure 1b.

### Time of orientation

The external field amplitude used in the simulation influences the time needed to induce a high degree of orientation ($\cos\alpha$). Figure 2 illustrates this with three examples. In addition to orientation time, we also see in Figure 2 that a strong external electric field tends to enhance the dipole-orientation, allowing for smaller fluctuations from a completely oriented state ($\cos\alpha = 1$).




(a) Example of how resolution was calculated from an FRC-curve.




(b) Resolution limits calculated from the simulated diffraction patterns.

Fig. 1 Calculations of the resolution limit for structure determination from a single-particle diffraction pattern.

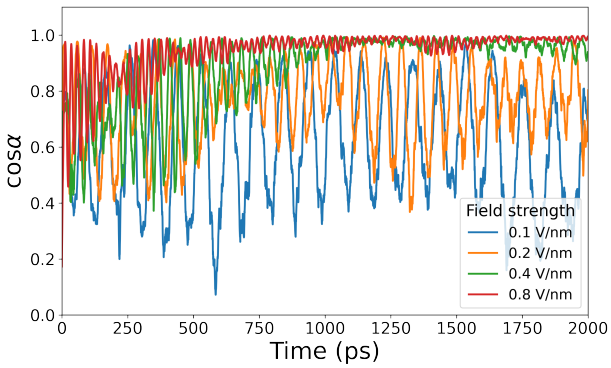



Fig. 2 Examples from simulations of 0 Å molecules with different field amplitudes. Larger field amplitude means a more rapidly increasing $\cos\alpha$, where $\alpha$ is the angle between the field and the dipole of the gas-phase protein.

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