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**Sample-size estimation**

* You should state whether an appropriate sample size was computed when the study was being designed
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* High-throughput sequence data should be uploaded before submission, with a private link for reviewers provided (these are available from both GEO and ArrayExpress)

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The error bars in the order parameters shown in Figure 2 (and Figure 2 – figure supplement 2 B/C and 3) were determined using procedures widely adopted in the NMR community. As indicated in the legend to Figure 2, Monte Carlo simulations and a bootstrap analysis were used for error estimation from the experimental and simulation data respectively. The Monte Carlo method is described in the ‘NMR Spectroscopy’ section on p. 14. The same procedure was used for the errors for e listed in Figure 2 – source data 2. The analysis of errors in the MD simulations is described in the ‘Analysis of the MD simulations’ section on p. 15/16. This bootstrap analysis was also used for the errors on the RDCs calculated from the MD simulations shown in Figure 2 – figure supplement 1 C/D and the errors on the order parameters shown in Figure 2 – figure supplement 3.

The error bars for the heteronuclear NOEs shown in Figure 2 – figure supplement 2A were estimated from 500 Monte Carlo simulations using the baseline noise as a measure of the error in the peak heights, as described in the ‘NMR Spectroscopy’ section on p. 14.

The error bars for the relaxation dispersion data analysis shown in Figure 6D/E/F, Figure 7, Figure 6 – figure supplement 1A and Figure 6 – source data 1 were determined using a bootstrap analysis and the program CATIA as described in the footnotes to Figure 6 – source data 1.

The errors shown in Figure 7 – source data 1 for the chemical shift differences measured in HSQC versus HMQC spectra were obtained as the standard deviations from the mean of 3 independent measurements of chemical shift differences in the pairs of NMR spectra.

**Statistical reporting**

* Statistical analysis methods should be described and justified
* Raw data should be presented in figures whenever informative to do so (typically when N per group is less than 10)
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(For large datasets, or papers with a very large number of statistical tests, you may upload a single table file with tests, Ns, etc., with reference to sections in the manuscript.)

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* Indicate how samples were allocated into experimental groups (in the case of clinical studies, please specify allocation to treatment method); if randomization was used, please also state if restricted randomization was applied
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