**Fig. S1** DEER profiles before background subtraction: (a) N53C-T110C cyan, (b) N53C-A103C green, (c) T34C-T117C magenta, and background subtractions used (black) superimposed.
**Fig. S2** Correlation between calculated and observed PCS (a) and RDC (b) values obtained with NMR and SAXS data (green) and with NMR, SAXS and DEER data (magenta).

Calculated with NMR and SAXS data (green) and with NMR, SAXS and DEER data (magenta).

**Fig. S3** Experimental SAXS profile (black) and fit calculated with NMR and SAXS data (green) and with NMR, SAXS and DEER data (magenta).
Fig. S4  (a) MaxOcc_D values for 1000 conformations, sorted by ascending MaxOcc_A values; (b) representation of the 1000 MaxOcc_D values of the selected conformations. Each conformation is color coded according to MaxOcc_D from low (< 5%, blue) to high (> 60%, red).
Fig. S5 (a) MaxOcc\textsubscript{E} values for 1000 conformations, sorted by ascending MaxOcc\textsubscript{A} values; (b) representation of the 1000 MaxOcc\textsubscript{E} values of the selected conformations. Each conformation is color coded according to MaxOcc\textsubscript{E} from low (< 5%, blue) to high (> 60%, red).
Fig. S6 (a) MaxOcc\textsubscript{F} values for 1000 conformations, sorted by ascending MaxOcc\textsubscript{A} values; (b) representation of the 1000 MaxOcc\textsubscript{F} values of the selected conformations. Each conformation is color coded according to MaxOcc\textsubscript{F} from low (< 5%, blue) to high (> 60%, red).
Fig. S7 (a) MaxOcc\textsubscript{G} values for 1000 conformations, sorted by ascending MaxOcc\textsubscript{A} values; (b) representation of the 1000 MaxOcc\textsubscript{G} values of the selected conformations. Each conformation is color coded according to MaxOcc\textsubscript{G} from low (< 5%, blue) to high (> 34%, red).
Fig. S8 (a) MaxOcc\textsubscript{H} values for 1000 conformations, sorted by ascending MaxOcc\textsubscript{A} values; (b) representation of the 1000 MaxOcc\textsubscript{H} values of the selected conformations. Each conformation is color coded according to MaxOcc\textsubscript{H} from low (< 5%, blue) to high (> 34%, red).
Fig. S9 (a) MaxOcc$_i$ values for 1000 conformations, sorted by ascending MaxOcc$_A$ values; (b) representation of the 1000 MaxOcc$_i$ values of the selected conformations. Each conformation is color coded according to MaxOcc$_i$ from low (< 5%, blue) to high (> 34%, red).
Fig. S10 (a) MaxOcc₇ values for 1000 conformations, sorted by ascending MaxOcc₅ values; (b) representation of the 1000 MaxOcc₇ values of the selected conformations. Each conformation is color coded according to MaxOcc₇ from low (< 5%, blue) to high (> 34%, red).
Fig. S11 MaxOcc\textsubscript{M} values for 1000 conformations, sorted by ascending MaxOcc\textsubscript{A} values.
Fig. S12 Graphical representation of \( r \) and \( \rho \) distances.
\[ r_{12} = \|cm_1 - cm_2\|_2 \]

\[ \rho_{12} = 1 - \frac{\sqrt{x_1 \cdot x_2 + y_1 \cdot y_2 + z_1 \cdot z_2 + 1}}{2} \]