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Supporting Material

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Structure and dynamics of ribosomal protein L12: An ensemble model based on SAXS and NMR relaxation

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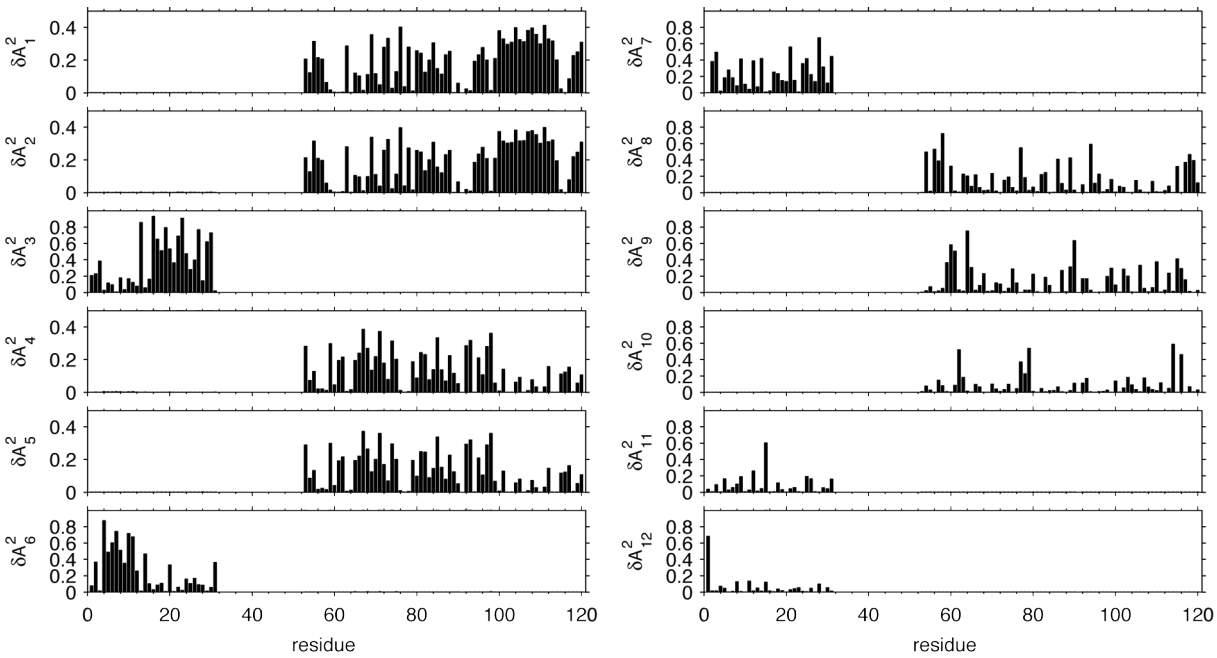

Figure S1. Backbone amide ^{15}N-^{1}H bond vector principal order parameter components, δA_m^2, obtained by rank-2 iRED analysis of the RE. Individual panels show order parameters associated with one of the 12 eigenmodes describing the domain reorientations of the RE. The order parameters are shown as averages over the two protomers. Ten reorientational eigenmodes were unique in the case of the RE, compared to 12 for the OE; 12 eigenmodes are shown here to enable direct comparison with the corresponding results for the OE in Fig. 4 of the main text. The difference between the RE and OE reflects the higher degree of NTD-CTD spatial correlation in the latter ensemble.

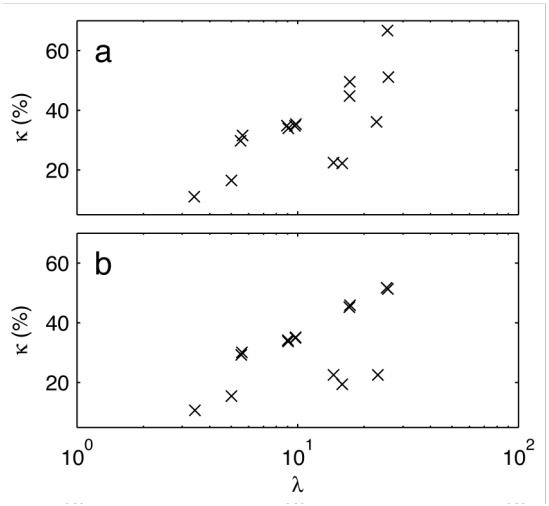

Figure S2. Collectivity (κ) plotted versus eigenvalue (λ) for each of the 15 eigenmodes. (**a**) κ for the OE. κ ranges between 11% and 67%. (**b**) κ for the RE. κ ranges between 11% and 52%. The OE yields two additional non-degenerate eigenvalues, in total 12, versus 10 non-degenerate eigenvalues for the RE. The largest value of κ is on par with those typically observed for the dominant overall modes of globular proteins (1). There is no iRED mode of the RE that affects both the NTD and CTD (see Fig. S1). These results indicate that the reorientational dynamics of L12 in solution involves a greater extent of collective motions than expected for a random ensemble. This result is in keeping with the finding that the linker region has some degree of residual order.

The eigenmode collectivity quantifies the percentage of bond vectors that are significantly affected by this mode, and is given by (1)

$$\kappa_m = \frac{1}{n}\exp\left(-\sum_{k=1}^{n}\left|\langle m|_k\right|^2 \ln\left|\langle m|_k\right|^2\right) \qquad \text{(S1)}$$

where $|m\rangle_k$ is the kth component of the normalized eigenvector. κ ranges between $1/n$ and 1, and reports the total percentage of bond vectors that are significantly affected by the eigenmode $|m\rangle$.

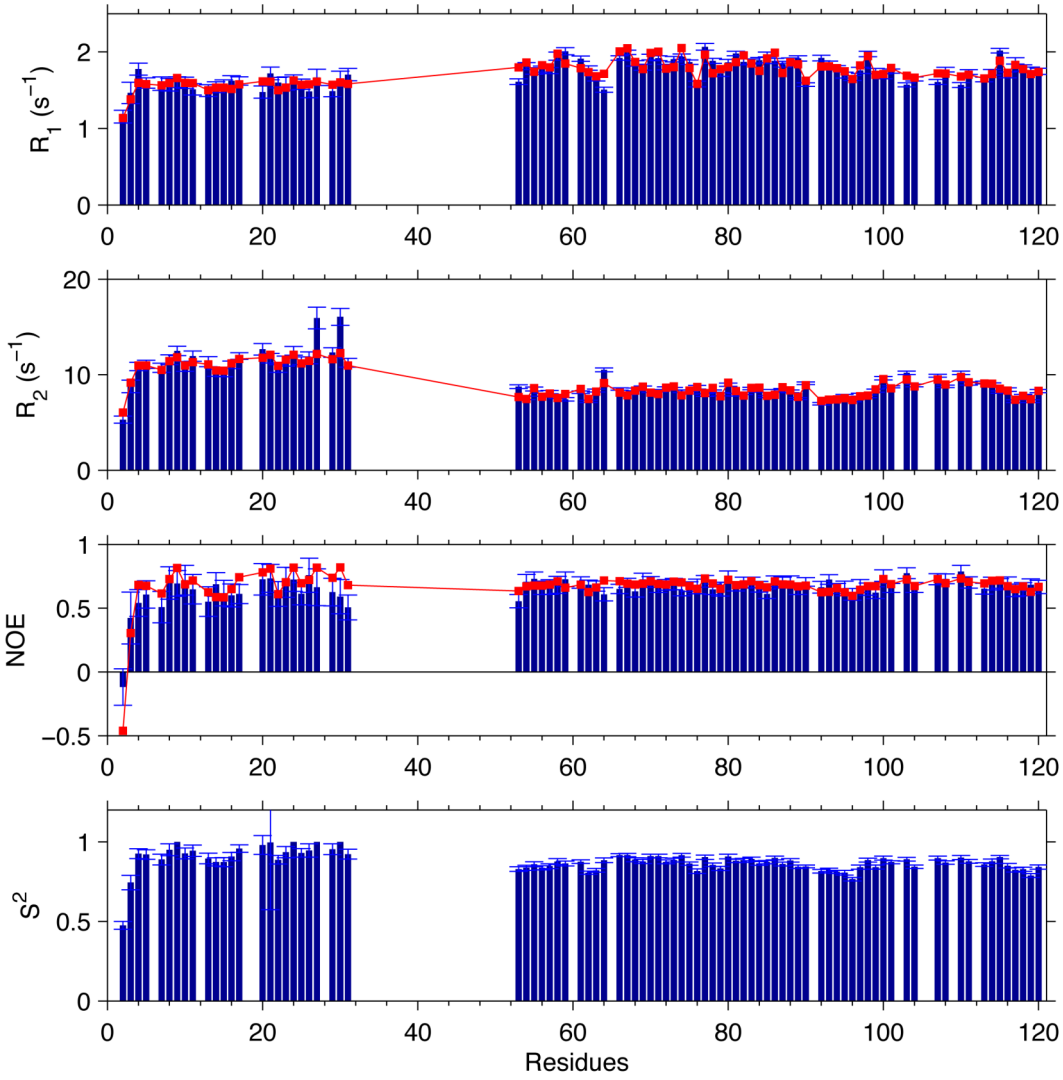

Figure S3. iRED-based model-free analysis of the experimental ^{15}N relaxation data (2). The resulting fit (red line and markers; top three panels) of the OE reorientational eigenmodes to the experimental ^{15}N relaxation data. The fit was performed as described in Methods. Note that all relaxation data were included in this fit, including R_2 values that include conformational exchange contributions; consequently, the fit is suboptimal for these cases. The resulting order parameters (S^2; bottom panel), describing the motional restriction of each N-H bond vector in the domain-specific frame. The effective correlation times (τ_e) for the internal motions were fit globally for each domain (so as to keep the number of free parameters at a minimum), yielding τ_e = 134 ps and 55 ps for the NTD and CTD, respectively.

References

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2. Mulder, F. A. A., L. Bouakaz, A. Lundell, M. Venkataramana, A. Liljas, M. Akke, and S. Sanyal. 2004. Conformation and dynamics of ribosomal stalk protein L12 in solution and on the ribosome. Biochemistry 43:5930-5936.