Supporting materials

The analysis of ^{15}N relaxation of free L11

The dipole-dipole coupling and chemical shift anisotropy are dominant relaxation mechanisms for an amide ^{15}N spin at high field. Therefore, rate constants for spin-lattice relaxation (R_1), spin-spin relaxation ($R_{1\rho}$), and dipolar cross-relaxation ^{15}N-[^{1}H] NOE are given by[22,23,38,68]:

$$R_1 = \frac{d^2}{4}[J(\omega_H - \omega_N) + 3J(\omega_N) + 6J(\omega_H + \omega_N)] + c^2 J(\omega_N) \quad (1)$$

$$R_2 = \frac{d^2}{8}(4J(0) + J(\omega_H - \omega_N) + 3J(\omega_N) + 6J(\omega_H) + 6J(\omega_H + \omega_N)) + \frac{c^2}{6}(4J(0) + 3J(\omega_N)) + R_{ex} \quad (2)$$

$$^{15}N - \{^1H\} NOE = 1 + \frac{d^2}{4R_1}\frac{\gamma_H}{\gamma_N}(6J(\omega_H + \omega_N) - J(\omega_H - \omega_N)), \quad (3)$$

in which $d = (\mu_0 h \gamma_N \gamma_H / 8\pi^2) < r_{NH}{}^{-3} >$, $c = \omega_N \Delta\sigma_N / \sqrt{3}$, μ_0 is the permeability in vaccum; h is Planck's constant; γ_H and γ_N are the magnetic gy-ratios of ^{1}H and ^{15}N, respectively; r_{NH}=1.02 Å is the nitrogen-proton bond length; ω_N and ω_H are the Larmor frequencies of ^{1}H and ^{15}N, respectively; $\Delta\sigma_N$=-160 ppm is the chemical shift anisotropy for ^{15}N; and R_{ex} is the chemical exchange rate. Since we have used the 1 ms delay between the refocusing pulses in CPMG sequence, the significant dephasing of the signal may be possible only if the exchange rate exceeds approximately 1000 s^{-1}. Using the results from the rotational diffusion tensor calculation ($D_{:}$=1.97 10^{-7} s^{-1}, D_{f}=1.27 10^{-7} s^{-1}, and θ =0.63 °; Table 2), we have analyzed the data of ^{15}N relaxation using the spectral density function given by:[22]

$$J(\omega) = \frac{2}{5}\left(\sum_{k=1}^{3} A_k \left(\frac{S^2 \tau_k}{1+(\omega\tau_k)^2} \right) + \frac{(1-S^2)\tau}{1+(\omega\tau)^2} \right), \qquad (4)$$

where $A_1=(3/2\ \cos^2\theta-1/2)^2$; $A_2=3\ \sin^2\theta\ \cos^2\theta$; and $A_3=3/4\ \sin^4\theta$. θ is the angle the nitrogen-proton bond vector makes with the unique diffusion tensor axis, $\tau_1=(6\ D_f)^{-1}$; $\tau_2=(D_: + 5\ D_f\ )^{-1}$; $\tau_3=(4\ D_: + 2\ D_f)^{-1}$; $1/\tau = 1/\ \tau_c + 1/\ \tau_e$ $\tau_c=(D_: + 2\ D_f\ )/3$ τ_e is the effective correlation time of the internal motion; and S is the generalized order parameter, which contains information about the spatial extent of nitrogen-proton bond motion. Since a maximum of three free parameters (two [S^2, τ_e] from equation (4) and one [R_{ex}] from equation (2)) are required to fit experimental data, we have used the model using S^2, τ_e and R_{ex} to fit the experimental data.

Figure S1. The structure of L11 based on the NOE and dihedral angle constraints. The L11-NTD (a) and the L11-CTD (b) are superimposed for the best fit using residues 5–66 and 75–140, excluding the RBL, respectively.

Figure S2. Relaxation parameters for free L11. The (a) R_1, (b) R_2, and (c) ^{15}N-[^{1}H] NOE were measured at pH 6.5 and 30 °C using Bruker Avance 600. The error was estimated by duplicated the measurement separated by several days. The concentrations of ^{15}N,^{2}H-labeled L11 were 0.7 mM.

Figure S3. Model-free parameters for free L11. (a) Generalized order parameters (*S^2*); (b) the effective internal correlation time of the internal motion (τ_e); and (c) the chemical exchange contributions (R_{ex}) were determined from ^{15}N relaxation measurements.

Figure S4. Comparison of the relative orientation between the L11-NTD and -CTD. (a) The solution structure of L11 is shown in ribbon drawing. (b) The L11-CTD and (c) the L11-NTD structures placed onto the rotational diffusion tensor frame were obtained by using R_2/R_1 ratios in each domain separately for the calculation of the rotational diffusion tensor.

Figure S5. Comparison of the solution structure of L11 (blue) and the polypeptide chain of L11-rRNA complex in the crystal form (gold). (a) The L11-NTD and (b) the L11-CTD are superimposed for the best fit using residues 8–66 and 75–139, excluding the RBL.

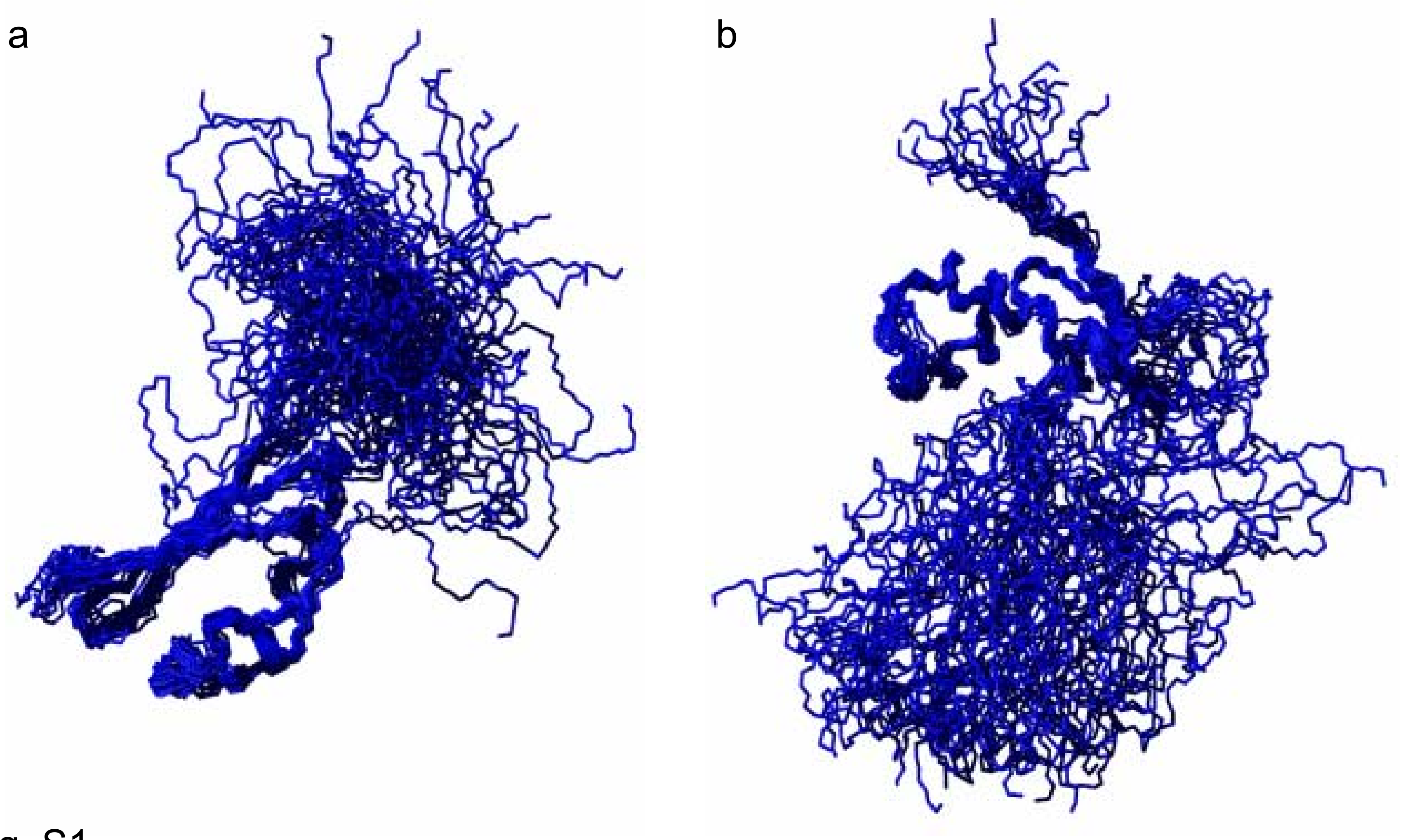
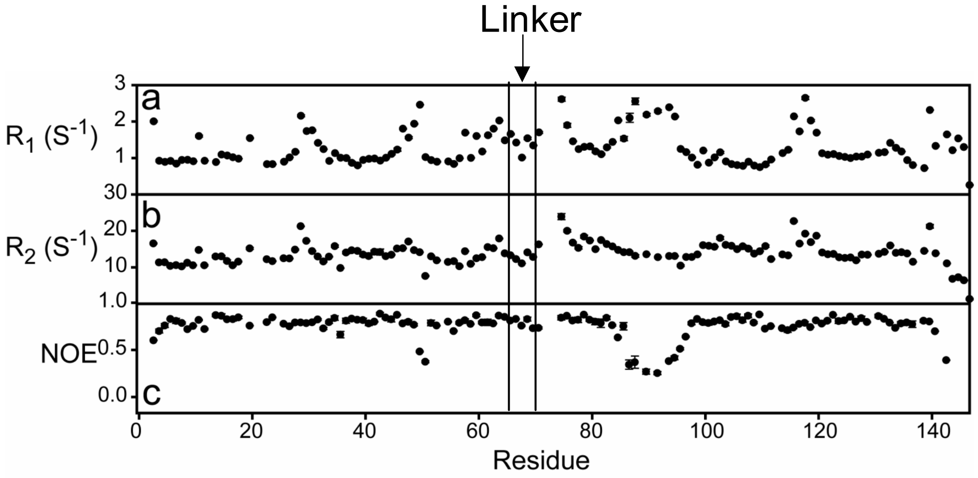
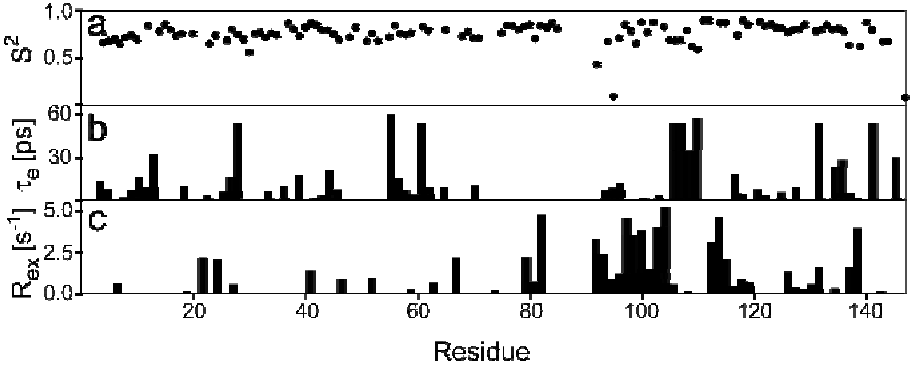


Fig. S1



Linker
a
b
c
R$_1$ (S^{-1})
R$_2$ (S^{-1})
NOE
3
2
1
30
20
10
1.0
0.5
0.0
0
20
40
60
80
100
120
140
Residue

Fig. S2



a
b
c
1.0
0.5
S^2
60
30
τ_e [ps]
5.0
2.5
0.0
R_{ex} [s^{-1}]
20
40
60
80
100
120
140
Residue

Fig. S3

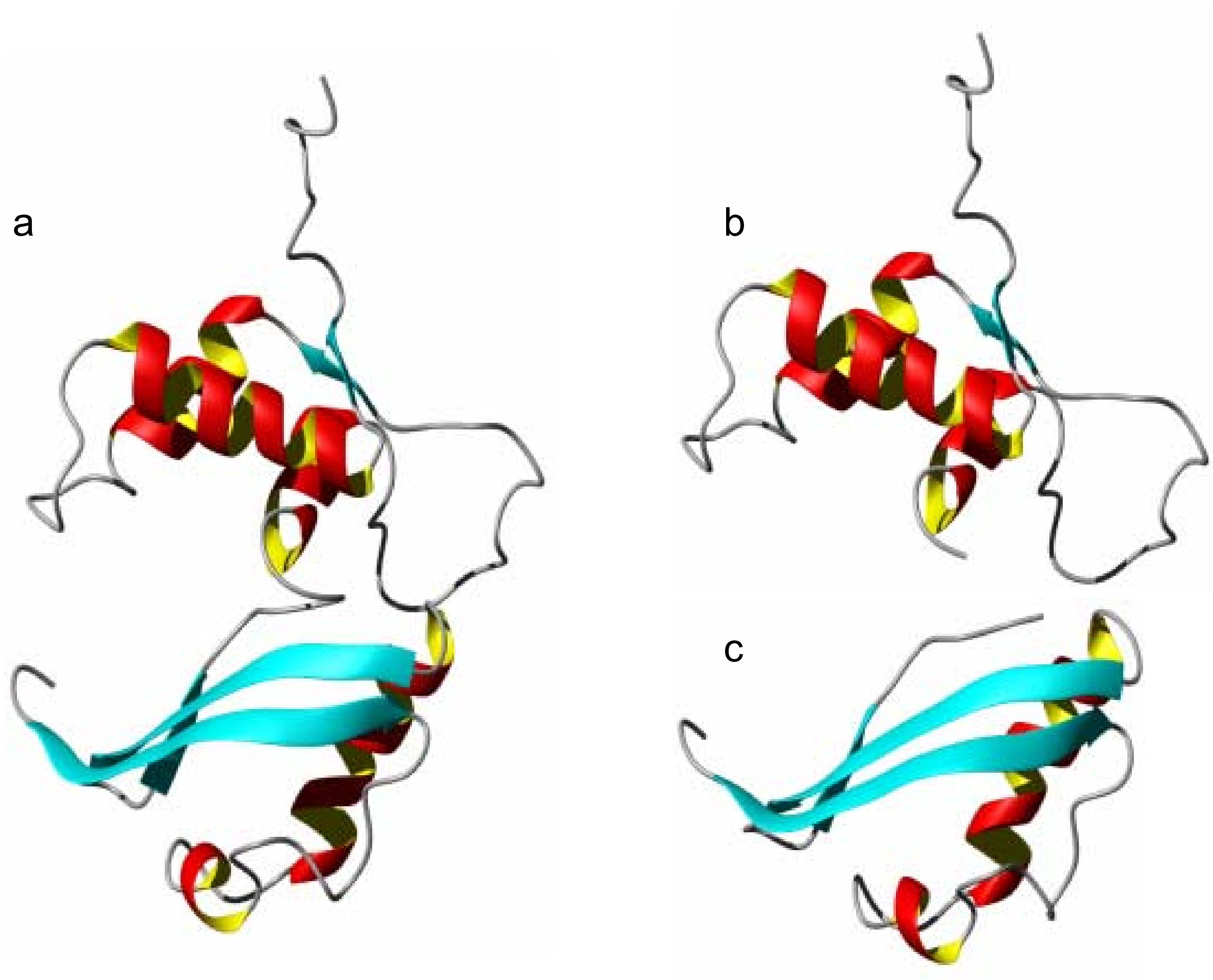


Fig. S4

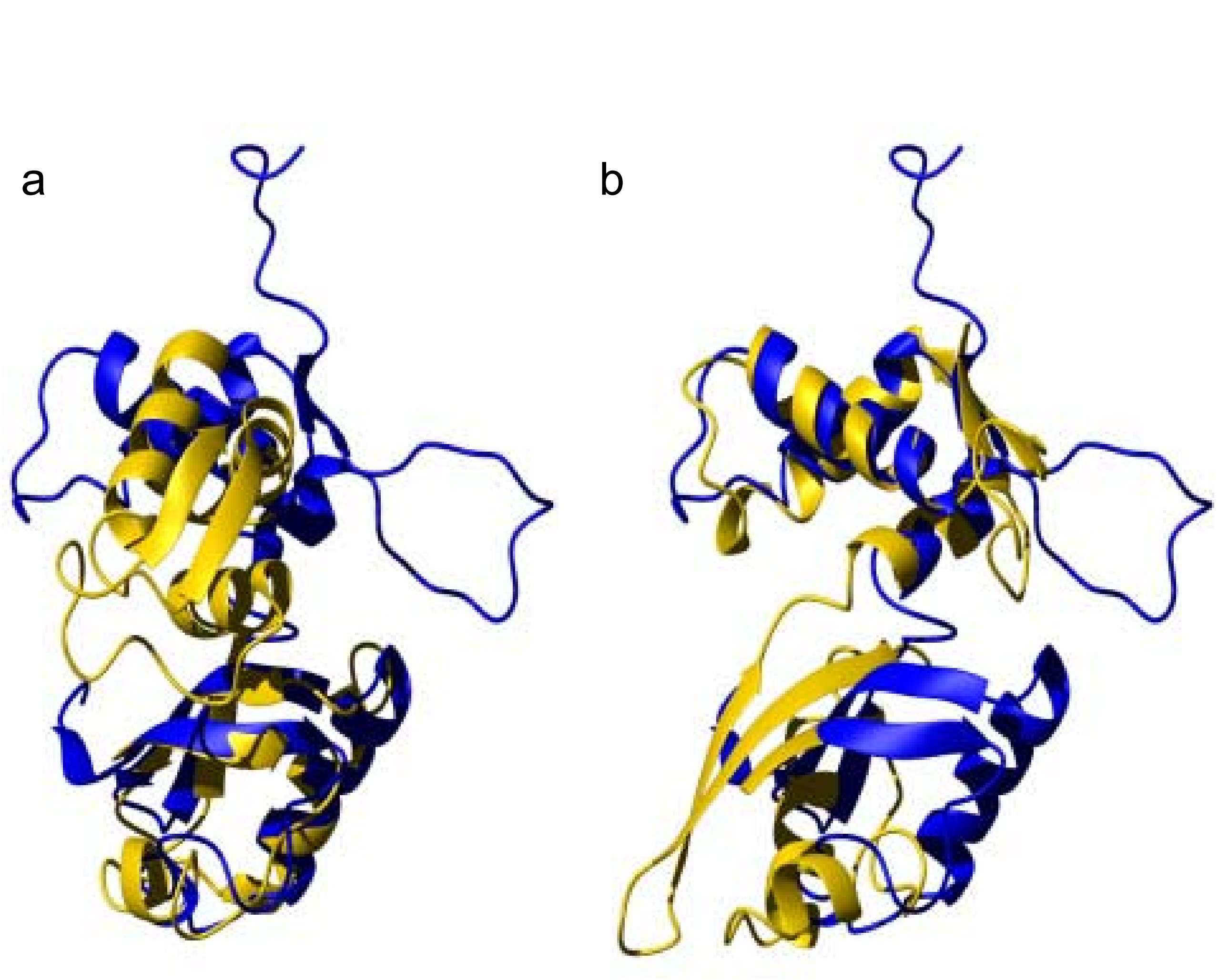


Fig. S5