

SUPPLEMENTARY ONLINE DATA

Differential conformational dynamics in the closely homologous FK506-binding domains of FKBP51 and FKBP52

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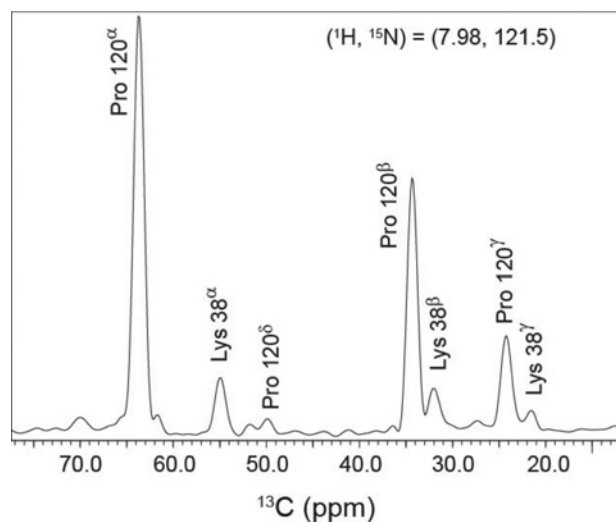


Figure S1 1D slice from a 3D HCCCONH NMR experiment on the U-¹³C, ¹⁵N-enriched FK1 domain of FKBP52

Correlations to the amide ¹H and ¹⁵N frequencies for Lys¹²¹ were observed for the side-chain ¹³C resonances of Pro¹²⁰, indicating a 10.0 p.p.m. separation for the C^β and C^γ resonances. Partial overlap was also observed for the ¹³C correlations of Lys³⁸ to the nearby ¹H and ¹⁵N frequencies for the amide of Arg³⁹.

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Backbone resonance assignments for FKBP51 and FKBP52 have been deposited in the BMRB under accession numbers 19787 and 19788 respectively.

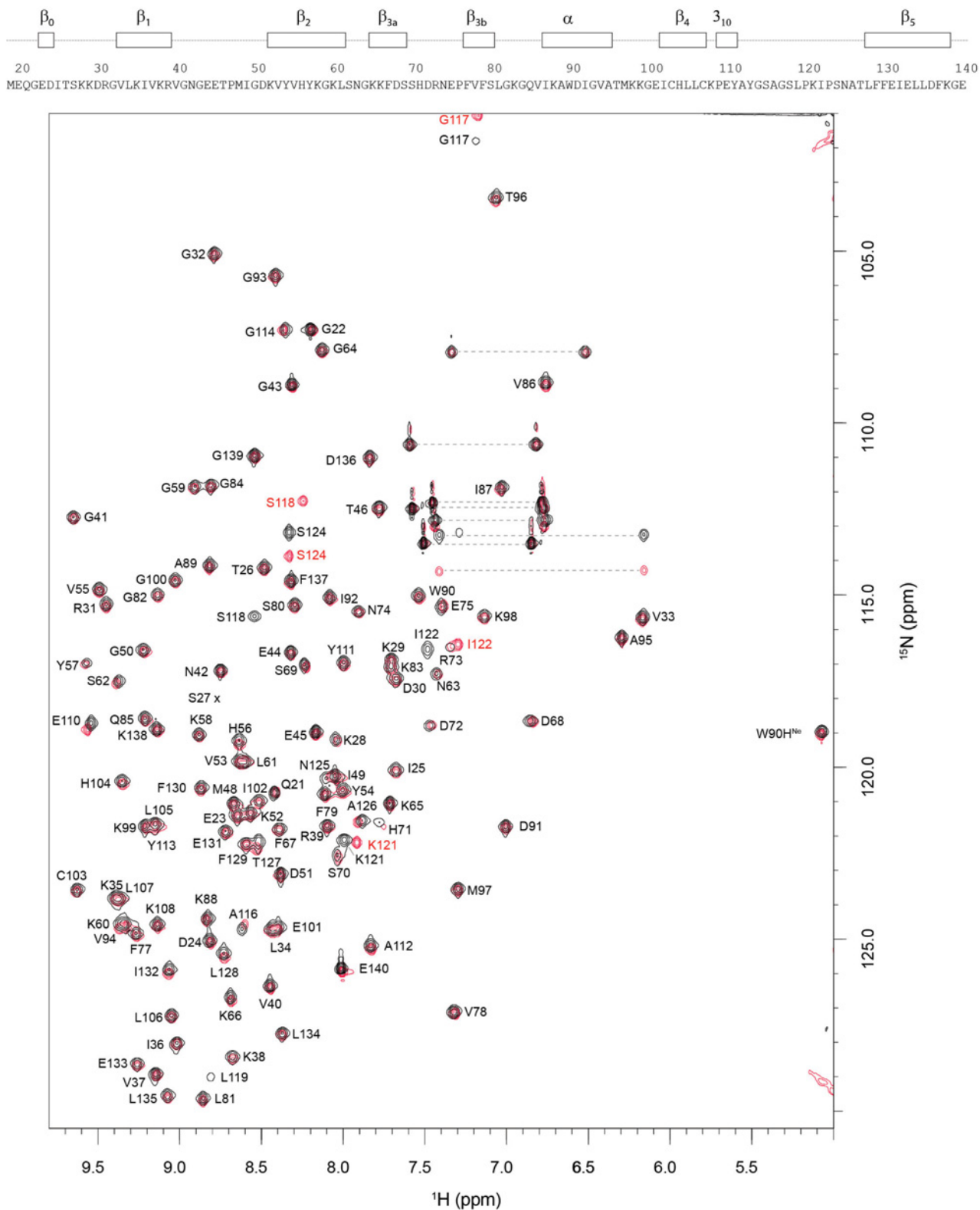


Figure S2 2D ^1H - ^{15}N -NMR correlation spectra for ^{15}N enriched the wild-type (black) and the L119P variant (red) of FKBP51

Resonances for side-chain amides are connected by broken lines.

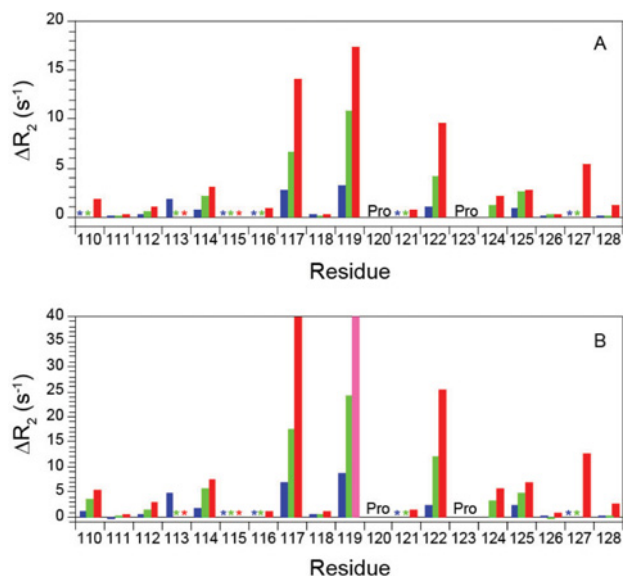


Figure S3 Differential transverse relaxation rates in the β_4 - β_5 loop for the P119L (blue) and P119L/P124S (green) variants of FKBP52 and the L119P variant (red) of FKBP51 compared with the wild-type proteins at 600 MHz (A) and higher field (B)

Asterisks denote residues for which well-resolved decay profiles were not obtained. For residue 119 of FKBP51, the attenuated peak intensities at 900 MHz precluded a reliable rate determination, although the value is $>50 s^{-1}$ (pink). The higher field data for the two variants of FKBP52 were collected at 800 MHz, whereas 900 MHz was used for the other samples. Following normalization to the mean R_2 value for the wild-type FKBP52 data, for residues exhibiting a differential larger than $1.0 s^{-1}$ that difference was scaled by the square of the magnetic field $(9/8)^2$, consistent with motion near the fast exchange limit.

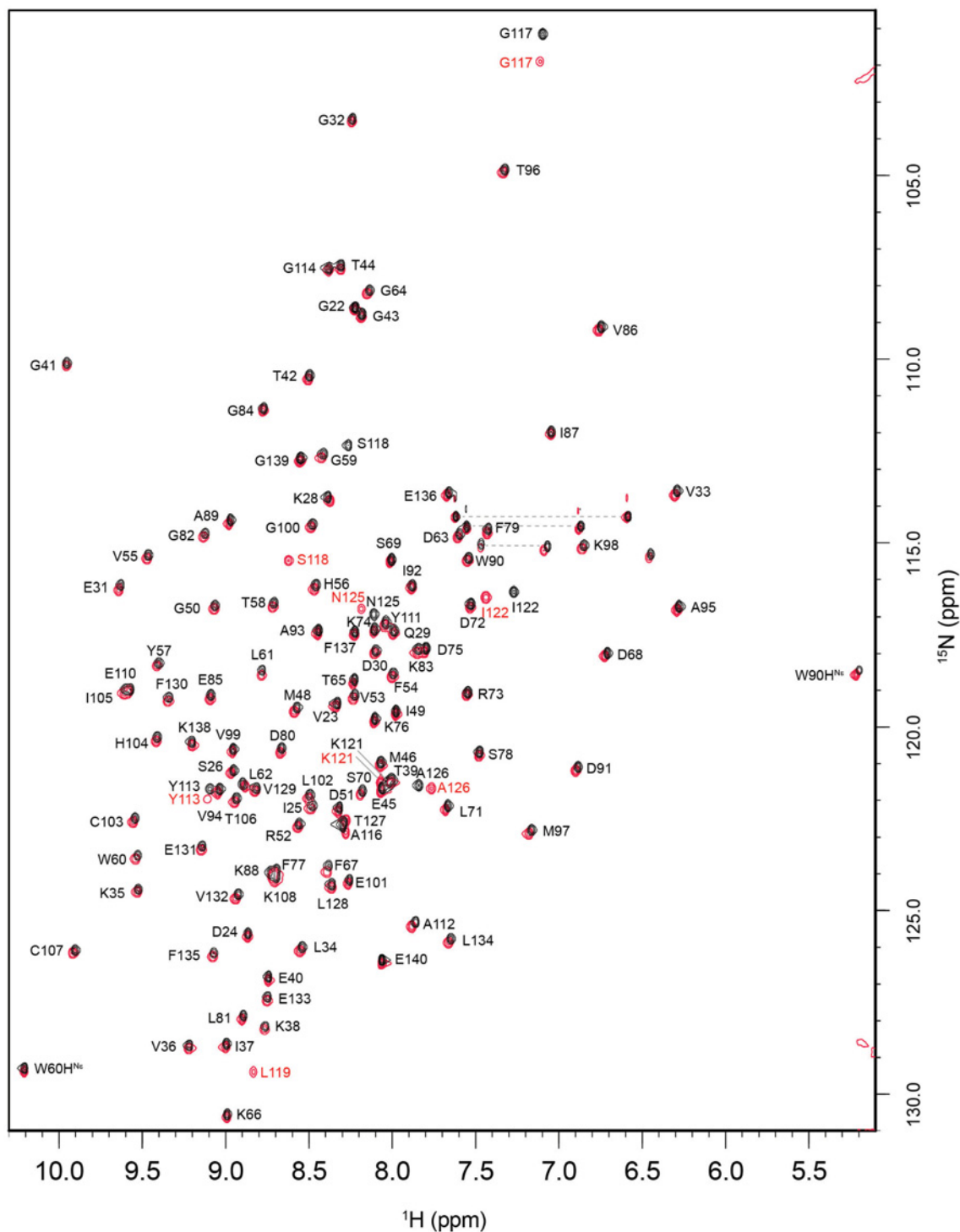
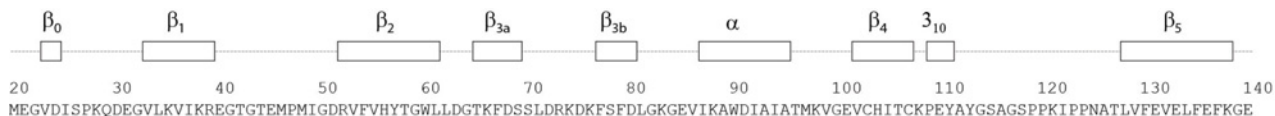


Figure S4 2D ^1H - ^{15}N -NMR correlation spectra for ^{15}N enriched the wild-type (black) and the P119L variant (red) of FKBP52

Resonances for side-chain amides are connected by broken lines.

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