Supplementary Material for

X-ray vs. NMR structures as templates for computational protein design

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Table S1: Re-evaluation of the Rosetta designs with a CHARMM-based energy function or FoldEF.

	Mean energy difference (lowest-energy-NMR – X-ray)[1]		Number of NMR designs better than or within 2 kcal/mol of X-ray design	
Method	CHARMM	FoldEF	CHARMM	FoldEF
C-RELAX	-22.9 ± 33.7	3.26 ± 6.9	23	13
R-RELAX	-16.6 ± 37.7	3.07 ± 8.22	21	14
R-ITER	-26.0 ± 31.9	3.66 ± 7.93	23	12

[1] Average of energy differences between the lowest-NMR design and the respective X-ray derived design over all structure pairs.

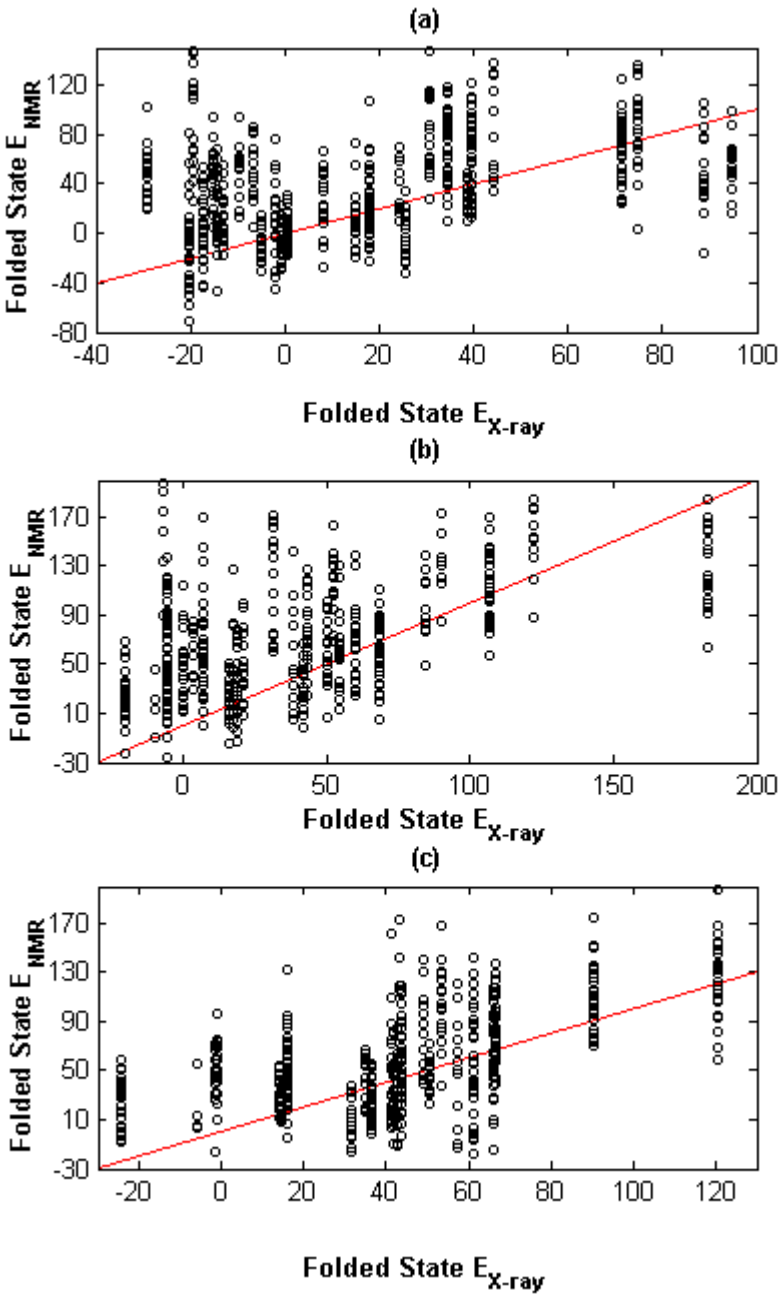

Figure S1: Re-evaluation of designed structures with a CHARMM-based energy function. Templates were prepared using three different methods and sequences were designed on each structure, as described in the text. (a) C-RELAX, (b) R-RELAX, (c) R-ITER.

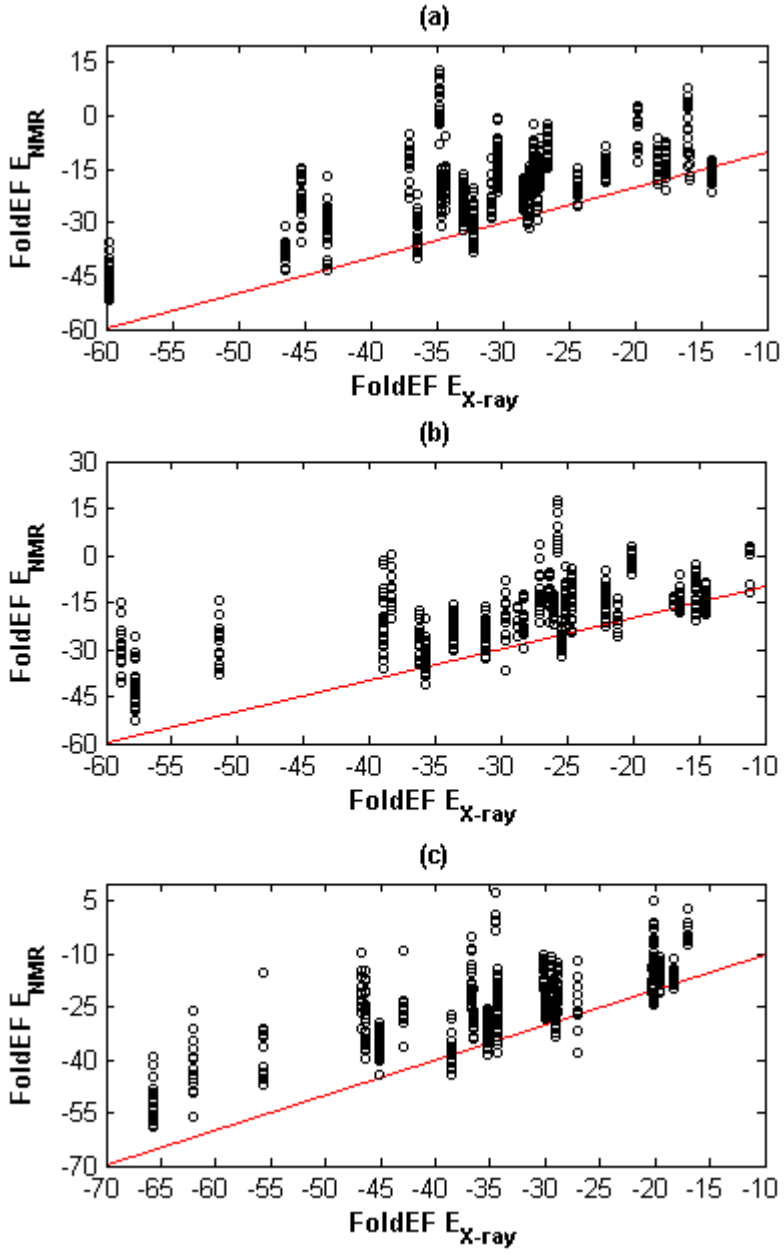

Figure S2: Re-evaluation of designed structures with the FOLDEF potential. Templates were prepared using three different methods and sequences were designed on each structure, as described in the text. (a) C-RELAX, (b) R-RELAX, (c) R-ITER.

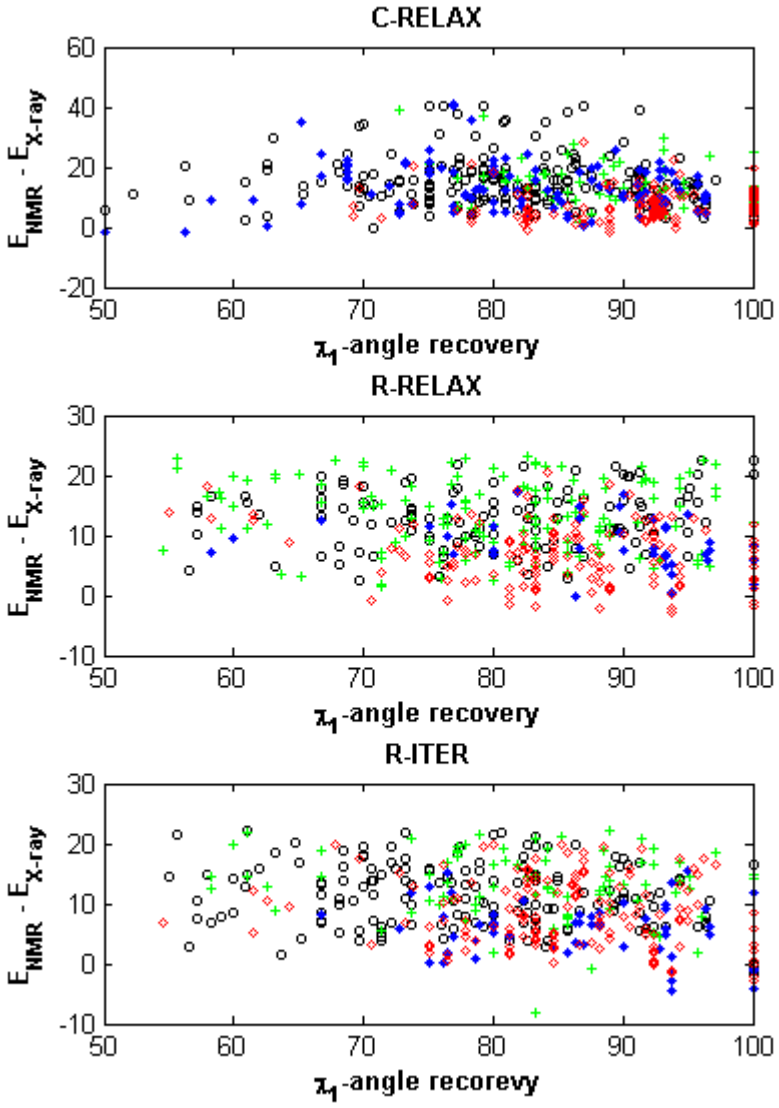

Figure S3: The energy difference ($E_{NMR} - E_{X\text{-}ray}$) plotted vs. NMR template χ_1-angle recovery for all NMR templates used in design calculations. Different symbols highlight properties of the designed structures and sequences as in Table III: Green "+" symbols show structures with native sequence recoveries similar to the X-ray design; blue diamonds are used for designs with SASApack values similar to the X-ray design; red diamonds are used for designs that satisfy both criteria; black circles are for designs that satisfy neither criterion.

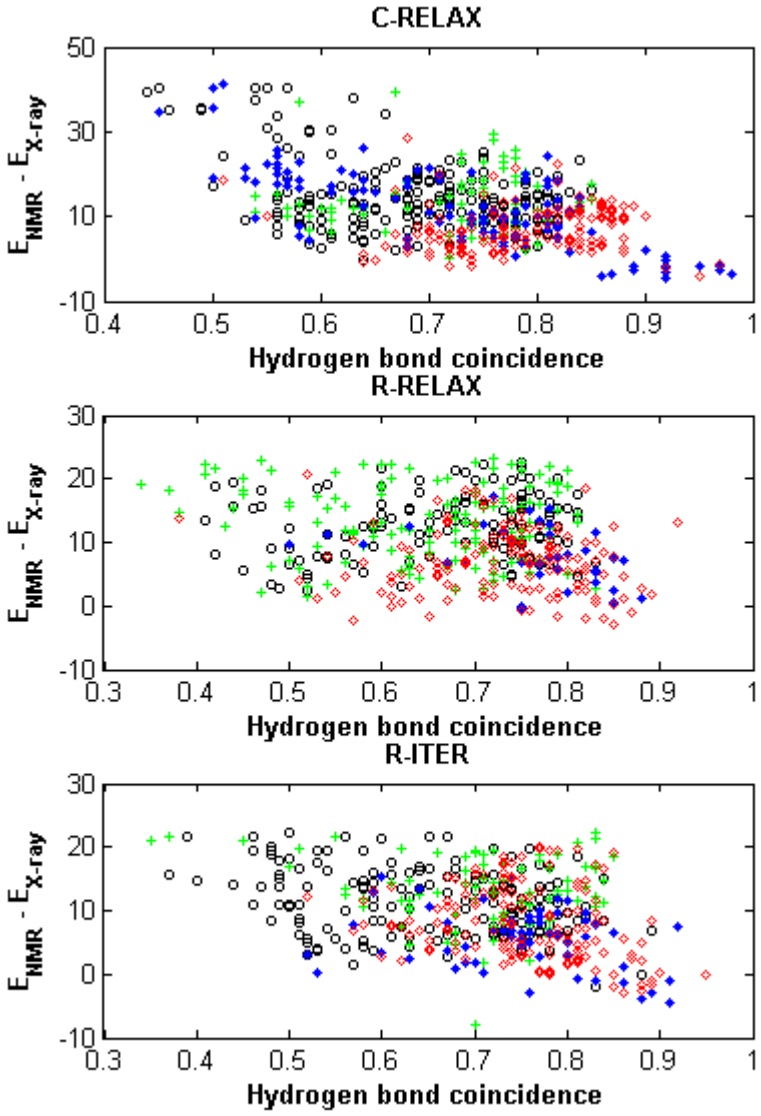

Figure S4: The energy difference ($E_{NMR} - E_{X\text{-}ray}$) plotted vs. hydrogen-bond coincidence with the X-ray template for all NMR templates used in design calculations. Different symbols highlight properties of the designed structures and sequences as in Table III: Green "+" symbols show structures with native sequence recoveries similar to the X-ray design; blue diamonds are used for designs with SASApack values similar to the X-ray design; red diamonds are used for designs that satisfy both criteria; black circles are for designs that satisfy neither criterion.