Magn. Reson. Discuss.,
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Interactive comment on "Phosphoserine for the generation of lanthanide binding sites on proteins for paramagnetic NMR" *by* Sreelakshmi Mekkattu Tharayil et al.

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The revised Fig. S1 belonging to the previous author comment.

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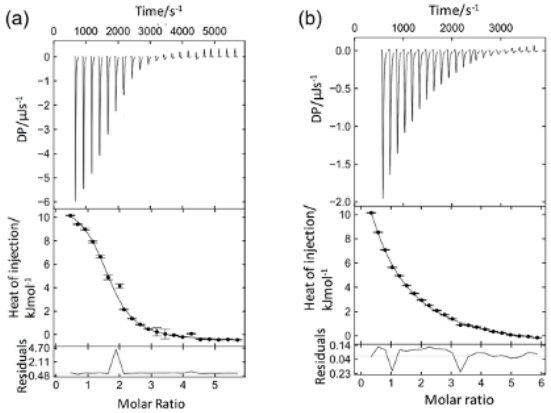

Figure S1. Representative isothermal titration calorimetry experiments of ubiquitin E18Sep titrated with $LnCl_3$. (a) Cell = 150 µM ubiquitin E18Sep; syringe = 2.7 mM $TbCl_3$. (b) Cell = 150 µM ubiquitin E18Sep; syringe = 2.7 mM $TmCl_3$. The top panel shows the baseline-corrected power traces. The middle panel displays the heat data and best fit. The bottom panel shows the residual of the fit. Error bars calculated by the program NITPIC (Keller et al., 2015) indicate the standard error in the integration of the peaks. DP denotes the power differential between the reference and sample cells to maintain a zero temperature difference between the cells.

Values for the dissociation constant K_d were derived from global fits to data from two and three different measurements with Tb^{3+} and Tm^{3+}, respectively. Fits were performed either with inclusion of the binding stoichiometry n as a fitting parameter or setting $n = 1$, with the result shown underneath.

Fitted parameters	Tb^{3+}		Tm^{3+}	
	setting $n = 1$	fitting n[a]	setting $n = 1$	fitting n[b]
ΔH (kJ mol^{-1})	15	23	20	12
ΔS (Jmol^{-1}K)	137	161	143	128
K_d (µM)	25	42	133	32

[a] The fit yielded $n = 0.7$.
[b] The fit yielded $n = 1.4$.

Fig. 1. revised Figure S1

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