Supporting Information

Numbat: an interactive software tool for fitting Δχ-tensors to molecular coordinates using pseudocontact shifts

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Table S1 Experimentally determined $^{1}H^{N}$ PCS for θ in complex with ε186 at pH 7.0 and 25°C[a]

Residue		PCS Dy^{3+} (ppm)	PCS Er^{3+} (ppm)
ASP	9	-1.28	0.31
GLN	10	-1.19	0.3
THR	11	-1.11	0.25
GLU	12	-1.24	0.27
MET	13	-1.84	0.38
ASP	14	-2	0.32
LYS	15	-1.5	
VAL	16	-1.97	0.13
VAL	18	-1.91	0.14
ASP	19	-1.32	-0.03
LEU	20	-1.29	-0.03
ALA	21	-1.37	-0.14
ALA	22	-0.57	-0.18
ALA	23	0.15	-0.38
GLY	24	0.37	-0.46
VAL	25	0.29	-0.26
ALA	26	0.54	-0.3
PHE	27	1.21	
LYS	28	0.85	-0.31
GLU	29	0.68	-0.19
ARG	30	0.81	-0.23
ASN	32	0.72	
MET	33	0.6	
VAL	35	0.02	
ILE	36	-0.29	0.08
ALA	37	-0.12	0
GLU	38	-0.22	0.04
ALA	39	-0.4	
VAL	40	-0.55	
GLU	41	-0.51	-0.06
ARG	42	-0.56	0.09
GLU	43	-0.84	0.12
GLU	46	-0.66	0.11
LEU	48	-0.71	-0.01
ARG	49	-0.58	0.08
SER	50	-0.45	0.05
TRP	51	-0.5	
PHE	52	-0.58	
ARG	53	-0.38	

GLU	54	-0.26	-0.01
ARG	55	-0.23	-0.07
LEU	56	-0.15	-0.09
ILE	57	0.02	-0.09
ALA	58	0.14	-0.11
HIS	59	0.3	-0.18
ARG	60	0.39	-0.17
LEU	61	0.42	-0.15
SER	63	0.8	-0.27
VAL	64	0.71	-0.19
ASN	65	0.8	-0.21
LEU	66		-0.26

[a] Experimental conditions as described in Pintacuda et al. (2006) *J. Am. Chem. Soc.* **128**, 3696-3702

Table S2 Comparison of the $\Delta\chi$-tensor parameters determined from PCS data of θ when using only conformer 10 [a] or all conformers [b] of the NMR structure of θ.

	Fixed[a]		Fixed(Family)[b]	
	Dy^{3+}	Er^{3+}	Dy^{3+}	Er^{3+}
$\Delta\chi_{ax}$[c]	42.3	-10.7	42.3	-10.7
$\Delta\chi_{rh}$[c]	5.3	-5.1	5.3	-5.1
α[d]	42.2	34.9	40.5	34.5
β[d]	119.2	121.5	118.9	121.2
γ[d]	44.7	177.4	38.1	174.8
m_x[e]	4.3	4.3	4.7	4.7
m_y[e]	-5.5	-5.5	-5.8	-5.8
m_z[e]	-19.8	-19.8	-19.7	-19.7

[a] $\Delta\chi$-tensor determined using the optimization scheme with $\Delta\chi_{ax}$ and $\Delta\chi_{rh}$ fixed to the values determined for ε186 and using conformer 10 of the NMR structure of θ (PDB accession code 2AXD)

[b] $\Delta\chi$-tensor determined as in footnote a, but with the back-calculated PCS averaged over all 12 conformers of the NMR structure

[c] In units of 10^{-32} m^3

[d] Euler rotations in the ZYZ convention (degrees)

[e] Metal ion coordinate (Å) in the protein frame (PDB data set 2AXD)