Supplemental Data

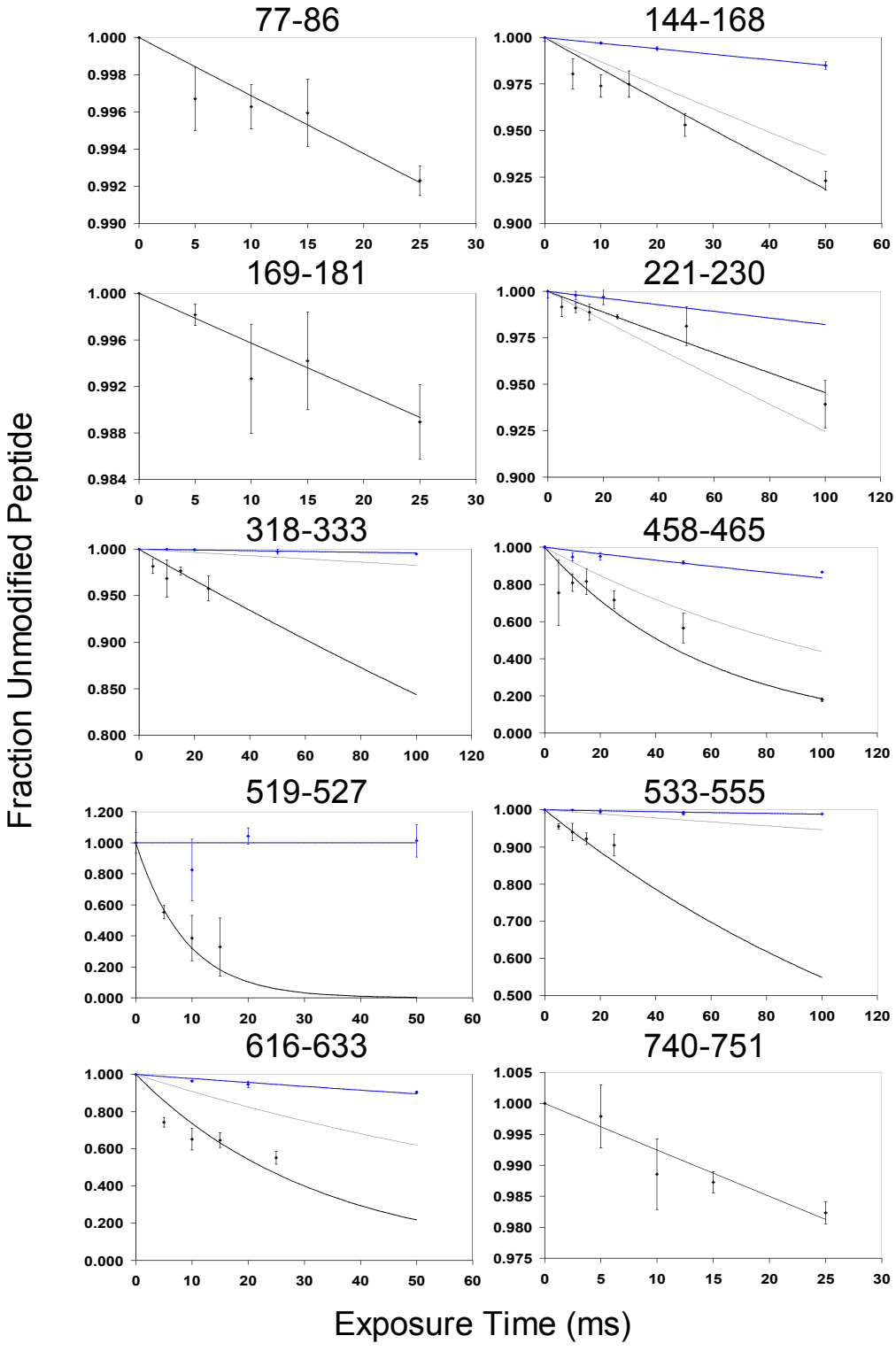

Figure S1. Dose-response curves for labeled ClpA monomer (black) and hexamer (blue) peptide modification as a function of x-ray exposure time. Grey lines indicate hexamer values normalized for the presence of ATPγS.

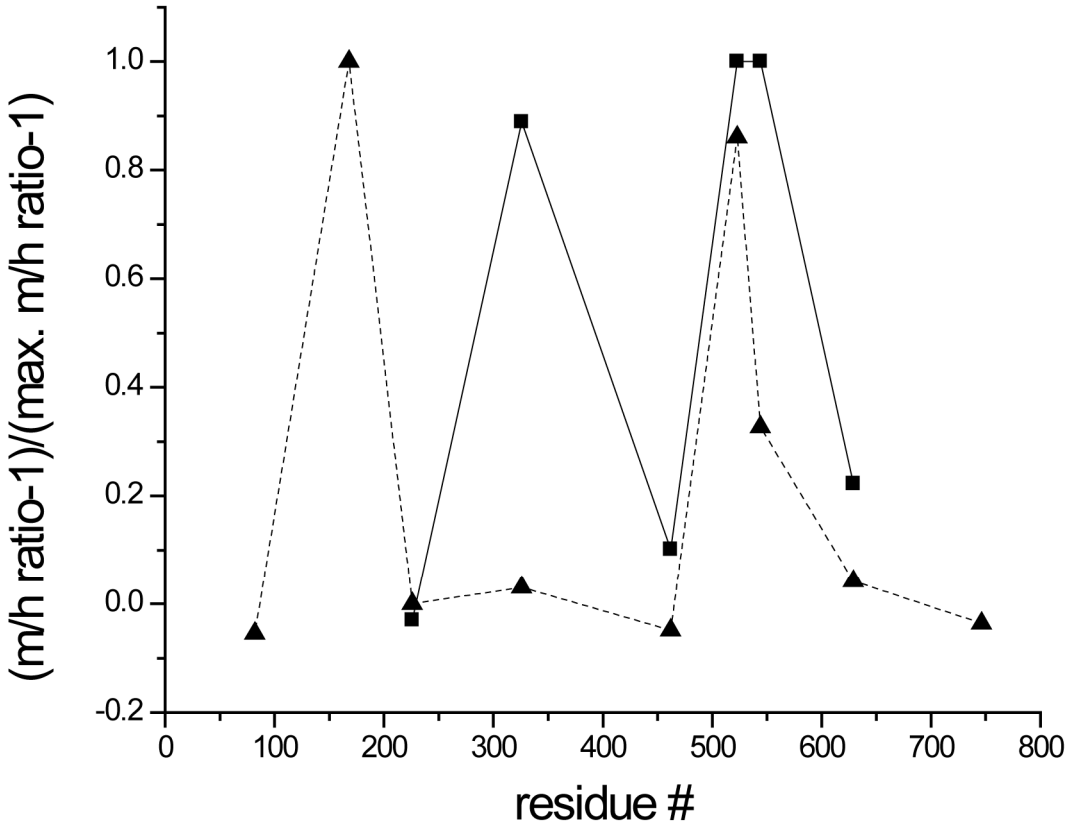

Figure S2. Relative solvent accessibilities in the monomer and hexamer states. For a given set of data, relative solvent accessibilities for the monomeric (m) and hexameric (h) states were parameterized as $[(m/h)-1]/[(m/h)_{max}-1]$, where $(m/h)_{max}$ is the maximum monomer/hexamer ratio in the set of data. This parameterization normalizes the largest increase in protection on hexamer formation to a value of 1 and the smallest to a value of 0. For peptide 519-527, where the hexamer accessibility is too low to be measured, the parameter was set to 1. Solid line: experimental modification rates, dashed line: predicted solvent accessibilities from the monomer and hexamer structural models.

Table S1. Calculated probe amino acid solvent accessibility values for structural models of ClpA

Amino Acid	Domain	Solvent Accessibility (Å^2) Monomer[a]	MonoΔN[b]	Hexamer1[c]	Hexamer2[d]	FP[e]	Monomer/ Hexamer1 Ratio	Monomer/ Hexamer2 Ratio	Monomer/ FP Model Ratio
P80	N	35.7	n/a	44.3	n/a	n/a	0.81	n/a	n/a
F84	N	4.9	n/a	9.3	n/a	n/a	0.53	n/a	n/a
P147, 153,157	N-D1 loop	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
F172	D1	152.6	152.6	40.8	67.1	67.1	3.74	2.27	2.27
L179	D1	55.4	55.4	36.8	55.9	55.9	1.51	0.99	0.99
W229	D1 near Walker A	93.1	120.0	85.0	120.3	120.3	1.10	1.00	1.00
Y324	D1 sensor 1	88.0	88	64.8	26.8	26.8	1.36	0.66	3.29
M458	D2 nucleotide int.	133.7	133.7	136.9	56.8	56.8	0.98	1.35	2.35
M521	D2	2.1	2.1	23.9	2.3	3.1	0.09	0.08	0.68
Y524	D2	16.1	16.1	18.0	14.4	12.9	0.90	0.46	1.25
M525	D2	41.3	41.3	16.2	34.6	48.9	2.55	1.95	0.84
P537	D2 loop	65.9	65.9	103.2	66.9	61.4	0.64	0.50	1.07
P538	D2 loop	131.1	131.1	32.7	132.6	62.2	4.01	12.53	2.11
Y540	D2 loop	26.9	26.9	19.4	20.1	41.8	1.39	1.82	0.64
F543	D2 loop	97.4	97.4	107.3	97.7	25.4	0.91	23.19	3.83
H621	D2 near ClpP loop	n/a	n/a	n/a	n/a	106.9	n/a	n/a	n/a
M629	D2	119.0	119.0	138.5	118.7	118.8	0.86	1.28	1.00
Y744	D2 C-term	68.1	68.1	102.6	68.4	68.4	0.66	2.22	1.00
F746	D2 C-term	67.1	67.1	73.3	64.8	64.9	0.92	1.09	1.03

[a]1KSF(Guo et al., 2002); [b]1KSF without N-domain; [c](Guo et al., 2002); [d](Hinnerwisch et al., 2005); [e]footprinting model. Due to the lack of N-domain in Hexamer2 and the footprinting model, the values are calculated for these models and the respective ratios without this portion of the structure for both monomer and hexamer. Amino acids P147, P153, P157 and H621 are missing from all models as they do not appear in the monomeric crystal structure (Guo et al., 2002).