Supplementary Material

Enhancing ubiquitin crystallization through surface entropy reduction Patrick J. Loll, Peining J. Xu, John T. Schmidt, and Scott L. Melideo

Table S1. Details of hit rates for different ubiquitin variants.

	wt	K6S	K11S	K27S	K29S	K33S	K48S	K63S	K11S/K63S double mutant
Classics I	7	3	23	2	1	10	2	9	16
Classics II	4	1	27	1	0	11	2	9	18
PEGs I	0	0	18	0	0	4	2	0	
PEGs II	1	0	12	0	0	3	1	6	
Overall total	12	4	80	3	1	28	7	24	

Table S2. PDB entries used to calculate average wild-type ubiquitin structure

PDB entry	No. of independent chains in asymmetric unit
1UBI	1
1UBQ	1
1YIW	3
2ZCC	3
3ONS	1

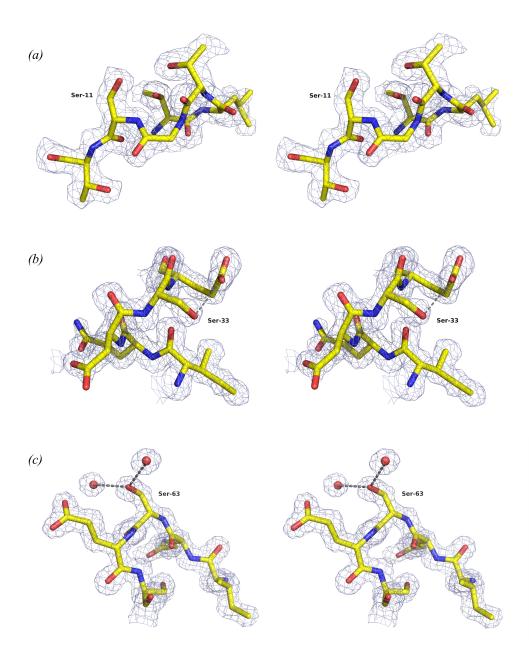


Figure S1. Representative 2Fo-Fc electron density for the structures described in this paper. Stereo views are shown for maps contoured at 1σ . Each map shows the vicinity of one of the mutant residues. (a) K11S mutant; (b) K33S mutant (B chain); a hydrogen bond is shown between the Ser-33 and Glu-34 side chains; (c) K11S/K63S double mutant; the Ser-63 side chain forms hydrogen bonds to two water molecules that bridge to an adjacent protein molecule in the lattice (adjacent molecule not shown).