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Supporting information for article:

New conformations of linear polyubiquitin chains by crystallographic and solution-scattering studies expand the conformational space of polyubiquitin

Trung Thanh Thach, Donghyuk Shin, Seungsu Han and Sangho Lee
Figure S1  Interfacial interactions between two ubiquitin moieties in the previously known crystal structure of compact linear Ub₂. (A) There is no obvious hydrogen bonds formed in linear Ub₂ structure (PDB ID: 3AXC). (B) Two ubiquitin moieties contact each other through hydrogen bonds observed in linear Ub₂ structure (PDB ID: 3U30).

Figure S2  Distribution of hydrodynamic radii of linear Ub₂, Ub₃ and Ub₄ in solution. Hydrodynamic radii (R_h) measured by DLS are shown along with the polydispersity of each linear Ub chain. Colors are denoted as follows: linear Ub₂, red; Ub₃, blue; and Ub₄, black.
Figure S3  Guinier plots. Scattering curves were generated at 1.15, 2.3, and 4.6 mg/ml for Ub$_2$ (A); 1.05, 2.1 and 4.2 mg/ml for Ub$_3$ (B); 0.45, 0.9 and 1.8 mg/ml for Ub$_4$ (C). At low q values, the Guinier plot, ln(I(q)) as a function of $q^2$, is linear and independent of protein concentration that indicates the homologous sample. The mass distribution of the scattering particle to its centroid, radius of gyration ($R_g$), can be estimated from the slope of Guinier plot.
**Figure S4** *Sc* Åtter analyses of linear polyubiquitin chains. (A) Linear Ub$_2$, (B) Ub$_3$ and (C) Ub$_4$. Kratky-Debye plot demonstrates the plateau signal, while Porod–Debye plot illustrates loss of Porod plateau. These suggest conformational flexibility in linear polyubiquitin chains.
Figure S5  Pair distribution function derived from SAXS data of the linear Ub₂, Ub₃, and Ub₄.