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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

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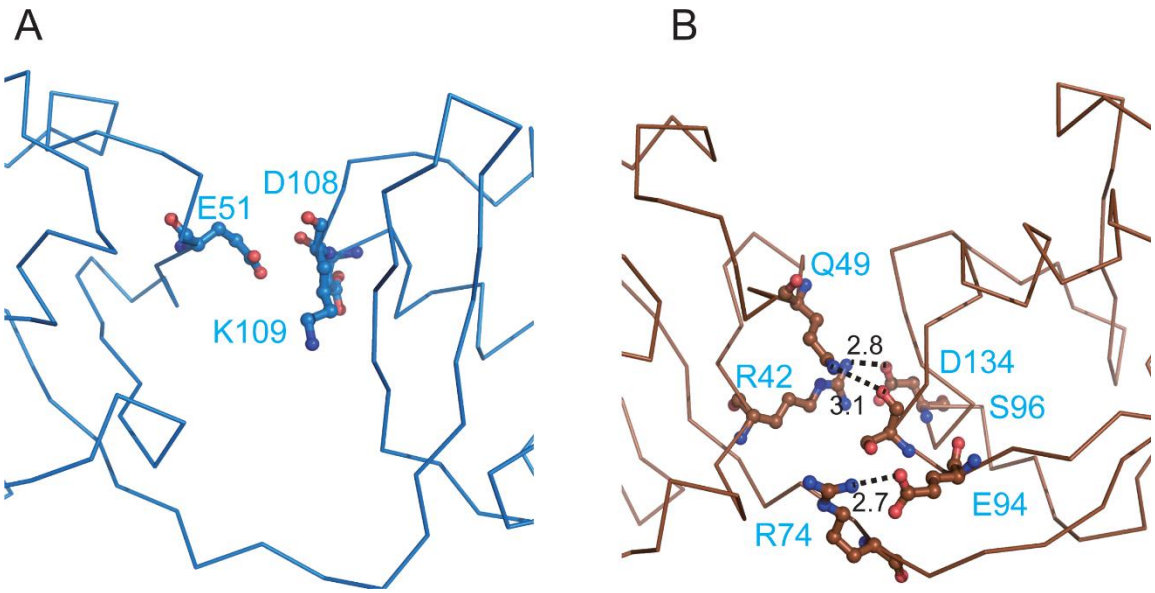

Figure S1 Interfacial interactions between two ubiquitin moieties in the previously known crystal structure of compact linear Ub_2. **(A)** There is no obvious hydrogen bonds formed in linear Ub_2 structure (PDB ID: 3AXC). **(B)** Two ubiquitin moieties contact each other through hydrogen bonds observed in linear Ub_2 structure (PDB ID: 3U30).

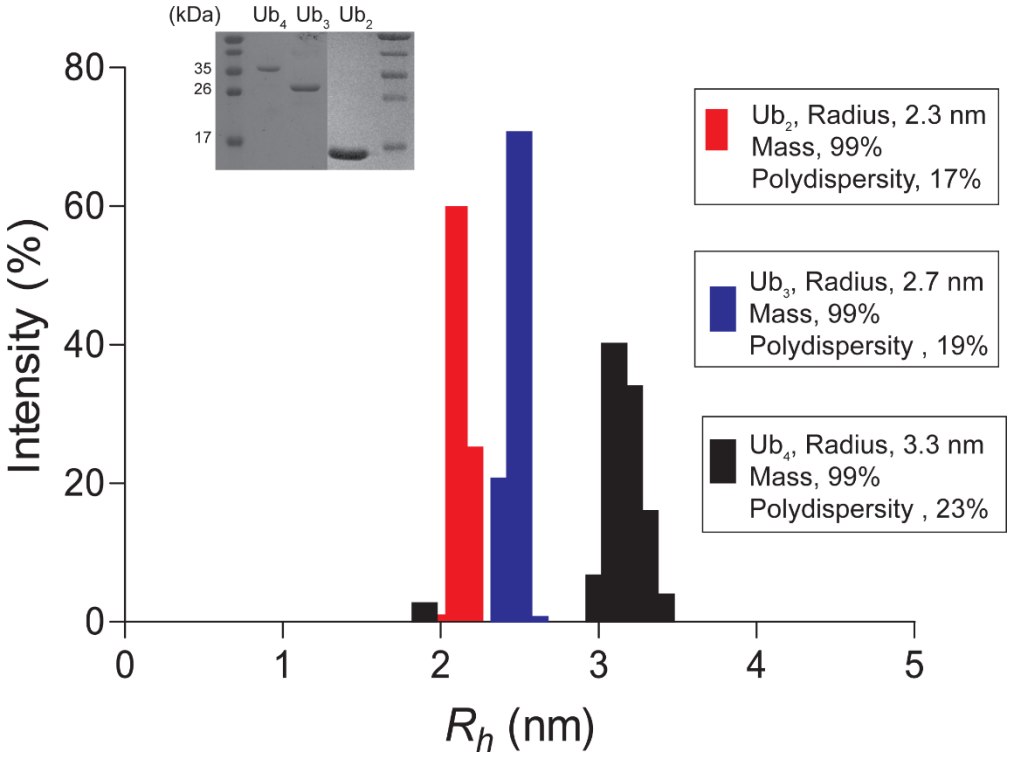

Figure S2 Distribution of hydrodynamic radii of linear Ub_2, Ub_3 and Ub_4 in solution. Hydrodynamic radii (R_h) measured by DLS are shown along with the polydispersity of each linear Ub chain. Colors are denoted as follows: linear Ub_2, red; Ub_3, blue; and Ub_4, black.

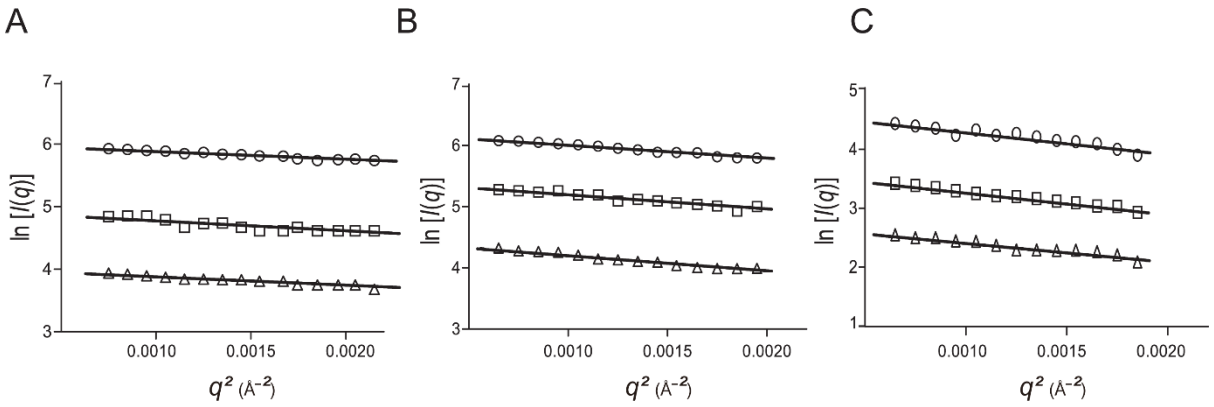

Figure S3 Guinier plots. Scattering curves were generated at 1.15, 2.3, and 4.6 mg/ml for Ub_2 (**A**); 1.05, 2.1 and 4.2 mg/ml for Ub_3 (**B**); 0.45, 0.9 and 1.8 mg/ml for Ub_4 (**C**). At low q values, the Guinier plot, ln($I(q)$) as a function of q^2, is linear and independent of protein concentration 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.

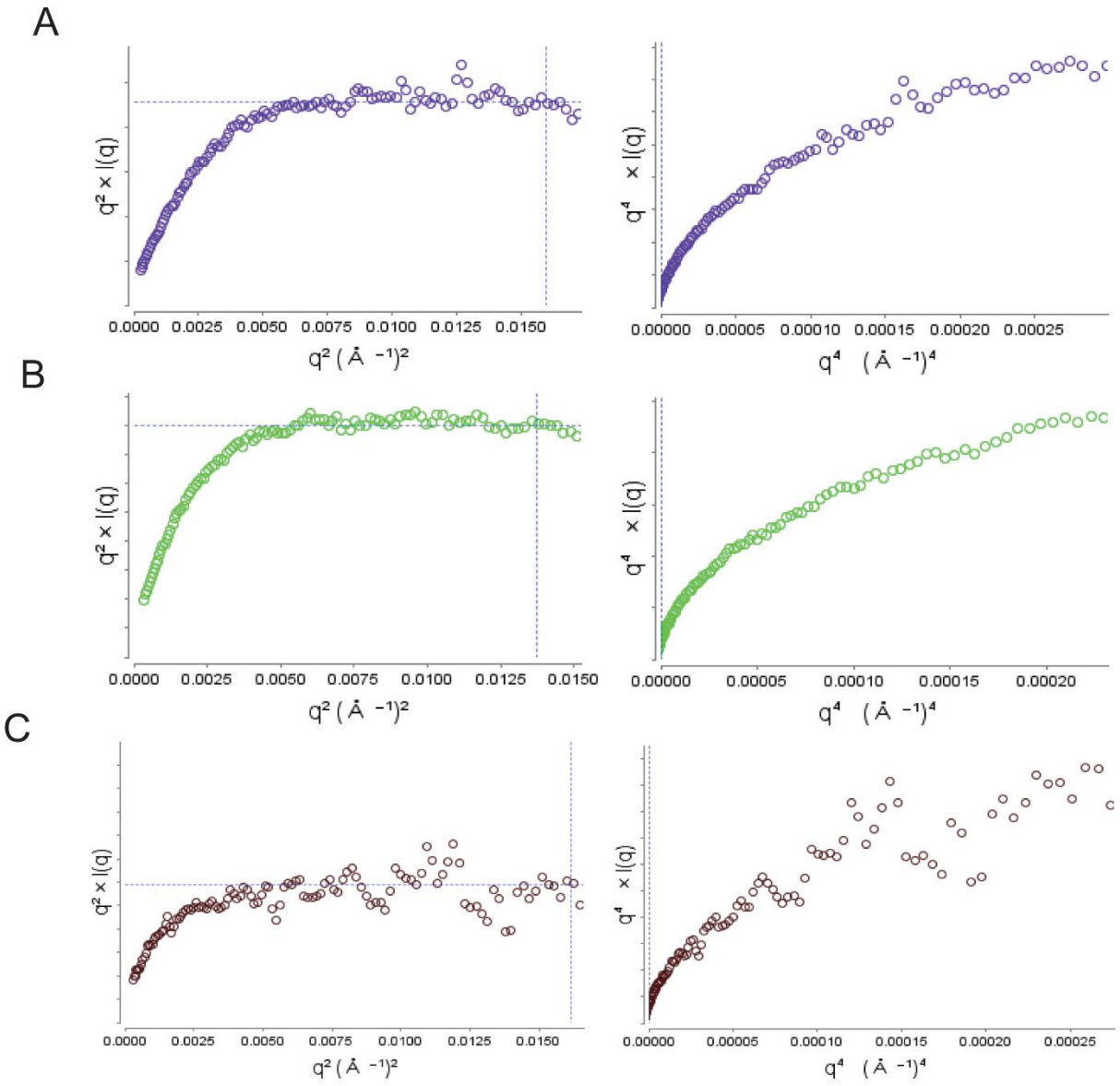

Figure S4 *Sc Åtter* analyses of linear polyubiquitin chains. **(A)** Linear Ub_2, **(B)** Ub_3 and **(C)** Ub_4. Kratky-Debye plot demonstrates the plateau signal, while Porod–Debye plot illustrates loss of Porod plateau. These suggest conformational flexibility in linear polyubiquitin chains.

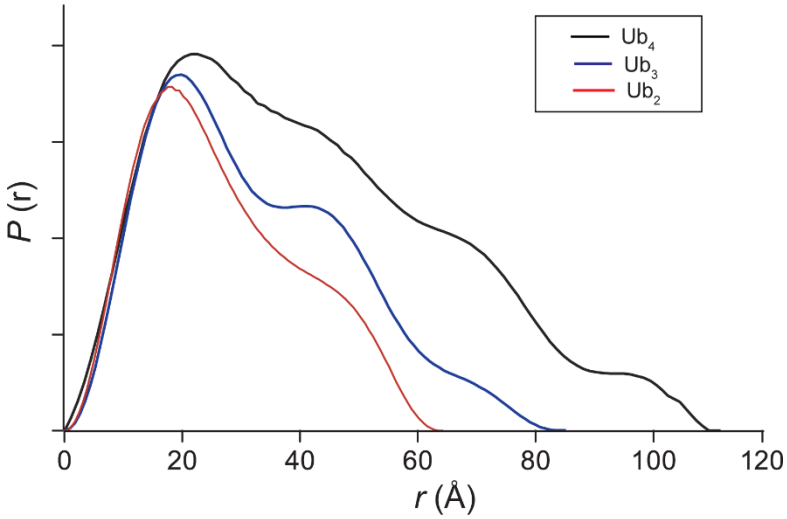

Figure S5 Pair distribution function derived from SAXS data of the linear Ub_2, Ub_3, and Ub_4.