Table S1: Summary of Integrative Structure Determination of Structure of K63-linked Diubiquitin (PDBDEV00000004)

1. Model Composition	
Entry composition	- Ubiquitin: Chain A (76 residues) - Ubiquitin: Chain B (76 residues) - Ubiquitin: Chain A (76 residues) - Ubiquitin: Chain B (76 residues) - Ubiquitin: Chain A (76 residues) - Ubiquitin: Chain B (76 residues)
Datasets used for modeling	- SAS data, SASDCG7 - Experimental model, PDB ID: 1UBQ - Experimental model, PDB ID: 2N2K - CX-MS data, Linker name: E, Number of cross-links: G - Single molecule FRET data, Not listed
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	0, 2
Rigid regions	- A: - - B: -
Flexible units	- A: 1-76. - B: 1-76.
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: 50 residues per bead.
3. Restraints	
Physical principles	Excluded volume and Sequence connectivity.
Experimental data	- 1 unique CrossLinkRestraint: EGS, 1 cross-links - 1 unique CrossLinkRestraint: BS3, 1 cross-links - 1 unique CrossLinkRestraint: BS2G, 1 cross-links - 1 unique CrossLinkRestraint: DST, 1 cross-links
4. Validation	
Sampling validation	1. Information related to sampling validation has not been provided
Clustering algorithm ,clustering feature	distance threshold-based clustering, Not applicable
Number of ensembles	0
Number of models in ensembles	Not applicable
Model precision (uncertainty of models)	Model precision can not be calculated with one structure

Quality of data	1. Quality of input data has not be assessed
Assessment of atomic regions	Clashscore: 4.07, Ramachandran outliers: 0.68, Sidechain outliers: 6.13
Assessment of excluded volume	1. Not applicable
Fit of the model to information used to compute it	1. Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	1. Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	None
Name	None
Details	- Method details unspecified
Software	- Software details not provided - No location specified