

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

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - 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	<ul style="list-style-type: none"> - SAS data, SASDCG7 - Experimental model, PDB ID: 1UBQ - Experimental model, PDB ID: 2N2K - CX-MS data, Linker name and number of cross-links: EGS, 1 cross-links - Single molecule FRET data, Not listed
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies , flexible units	0, 2
<i>Rigid regions</i>	<ul style="list-style-type: none"> - A: - - B: -
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-76. - B: 1-76.
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: N/A
3. Restraints	
Physical principles	Physical principles were not used for modeling
Experimental data	<ul style="list-style-type: none"> - 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 used if ensembles are deposited, 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

<i>Quality of data</i>	1. SASDCG7: Rg from Gunier is 2.1nm and Rg from p(r) is 2.0nm
<i>Assessment of atomic regions</i>	Clashscore: 4.07, Ramachandran outliers: 0.68% , Sidechain outliers: 6.13%
<i>Assessment of excluded volume</i>	1. Not applicable
<i>Fit of the model to information used to compute it</i>	
<i>Fit of the model to information not used to compute it</i>	1. Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>Method</i>	None
<i>Name</i>	None
<i>Details</i>	- Method details unspecified
<i>Software</i>	- Software details not provided - No location specified