

**Summary of integrative structure determination of Structure of K63-linked Diubiquitin
(PDB ID: 8ZZ4, PDB-Dev ID: PDBDEV_00000004)**

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Ubiquitin: Chain B (76 residues) - Ubiquitin: Chain A (76 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - SAS data, SASBDB: SASDCG7 - Experimental model, PDB ID: 1UBQ - Experimental model, PDB ID: 2N2K - Crosslinking-MS data, Linker name and number of cross-links: EGS, 1 cross-links - Single molecule FRET data, File: 10.5281/zenodo.1006721
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 2
Flexible units	<ul style="list-style-type: none"> - A: 1-76 - B: 1-76
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
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	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	3
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	SASDCG7: Rg from Guinier is 2.0nm and Rg from p(r) is 2.1nm

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Model-1: Clashscore = 4.07, Number of Ramachandran outliers = 1, Number of sidechain outliers = 8 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 1, Number of sidechain outliers = 8 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 1, Number of sidechain outliers = 9
<i>Model quality: assessment of excluded volume</i>	Not applicable
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>1. Method</i>	None
<i>Name</i>	None
<i>Software</i>	Software details not provided