

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

1. Model Composition	
Entry composition	Ubiquitin: chain(s) A, B (76 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - SAS data, SASBDB: SASDCG7 - Experimental model, PDB: 1UBQ - Experimental model, PDB: 2N2K - Crosslinking-MS data, Zenodo: 10.5281/zenodo.1006721 - Single molecule FRET data, Zenodo: 10.5281/zenodo.1006721
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: EGS, 1 crosslinks - 1 unique CrossLinkRestraint: BS3, 1 crosslinks - 1 unique CrossLinkRestraint: BS2G, 1 crosslinks - 1 unique CrossLinkRestraint: DST, 1 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	3
Model precision (uncertainty of models)	Not available
Data quality	SASDCG7: Rg from Guinier is 2.0nm and Rg from p(r) is 2.1nm
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00-4.07 - Ramachandran outliers: 1-1 - Sidechain outliers: 8-9
Fit to data used for modeling	Satisfaction of crosslinks: 0.00-25.00%

Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	None
Software	Software details not provided