

Summary of integrative structure determination of Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex (PDB ID: 8ZZM, PDB-Dev ID: PDBDEV_00000022)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - E6AP HECT Domain: chain(s) A (852 residues) - E6: chain(s) B (151 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Zenodo: 10.5281/zenodo.1346675 - Comparative model, Zenodo: 10.5281/zenodo.1346675 - Experimental model, PDB: 1C4Z - Experimental model, PDB: 4XR8
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	2, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSS, 159 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	500
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00 - Ramachandran outliers: 10 - Sidechain outliers: 24
Fit to data used for modeling	Satisfaction of crosslinks: 90.91%
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. <i>Name</i>	MC based Bayesian sampling using crosslinks
<i>Method</i>	IMP
<i>Number of computed models</i>	720000
<i>Software</i>	Integrative Modeling Platform (IMP) (version git checkout 2018/01/08 (commit 5eb8151c651256d50bbcd847932bc913df94090c))