

Summary of integrative structure determination of Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex (PDB ID: 8ZZN, PDB-Dev ID: PDBDEV_0000023)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - E6: Chain B (143 residues) - p53: Chain C (199 residues) - E6AP HECT Domain: Chain A (350 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: DSS, 127 cross-links - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 1C4Z - Experimental model, PDB ID: 4XR8
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	3, 0
Rigid bodies	<ul style="list-style-type: none"> - A: 497-846 - B: 1-143 - C: 94-292
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSS, 127 cross-links
4. Validation	
Number of ensembles	1
Number of models in ensembles	500
Number of deposited models	1
Model precision (uncertainty of models)	None, Å
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashescore = 0.0, Number of Ramachandran outliers = 11, Number of sidechain outliers = 27
Model quality: assessment of excluded volume	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	
1. <i>Method</i>	MC based Bayesian sampling using crosslinks
<i>Name</i>	IMP
<i>Number of computed models</i>	720000
<i>Software</i>	Integrative Modeling Platform (IMP) (version git checkout 2018/01/08 (commit 5eb8151c651256d50bbcd847932bc913df94090c))
