

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	
<u>Entry composition</u>	<ul style="list-style-type: none"> - E6: Chain B (143 residues) - E6AP HECT Domain: Chain A (350 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: DSS, 159 cross-links - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 1C4Z - Experimental model, PDB ID: 4XR8
2. Representation	
<u>Resolution</u>	Atomic
<u>Number of rigid bodies, flexible units</u>	2, 0
<u>Rigid bodies</u>	<ul style="list-style-type: none"> - A: 497-846 - B: 1-143
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 159 cross-links
4. Validation	
<u>Number of ensembles</u>	1
<u>Number of models in ensembles</u>	500
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	None, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 10, Number of sidechain outliers = 24
<u>Model quality: assessment of excluded volume</u>	Not applicable
<u>Fit to data used for modeling</u>	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))