

**Summary of integrative structure determination of Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex (PDB ID: 8ZZN, PDB-Dev ID: PDBDEV\_00000023)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- E6AP HECT Domain: chain(s) A (852 residues)</li> <li>- E6: chain(s) B (151 residues)</li> <li>- p53: chain(s) C (393 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, Zenodo: <a href="https://zenodo.org/record/10.5281/zenodo.1346675">10.5281/zenodo.1346675</a></li> <li>- Comparative model, Zenodo: <a href="https://zenodo.org/record/10.5281/zenodo.1346675">10.5281/zenodo.1346675</a></li> <li>- Experimental model, PDB: <a href="#">1C4Z</a></li> <li>- Experimental model, PDB: <a href="#">4XR8</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	3, 0
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: DSS, 127 crosslinks
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	500
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 0.00</li> <li>- Ramachandran outliers: 11</li> <li>- Sidechain outliers: 27</li> </ul>
<a href="#">Fit to data used for modeling</a>	Satisfaction of crosslinks: 89.66%
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	

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1. <a href="#"><i>Name</i></a>	MC based Bayesian sampling using crosslinks
<a href="#"><i>Method</i></a>	IMP
<a href="#"><i>Number of computed models</i></a>	720000
<a href="#"><i>Software</i></a>	<a href="#">Integrative Modeling Platform (IMP)</a> (version git checkout 2018/01/08 (commit 5eb8151c651256d50bbcd847932bc913df94090c))