

Table S1: Summary of Integrative Structure Determination of Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex (PDBDEV00000023)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - E6AP HECT Domain: Chain A (350 residues) - E6: Chain B (143 residues) - p53: Chain C (199 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - CX-MS data, Linker name: D, Number of cross-links: S - Comparative model, template PDB ID: Not listed - Experimental model, PDB ID: 1C4Z - Experimental model, PDB ID: 4XR8
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies , flexible units	3, 0
<i>Rigid regions</i>	<ul style="list-style-type: none"> - A: 497-846:Comparative model/None. - B: 1-143:Comparative model/None. - C: 94-292:Comparative model/None.
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: - - B: - - C: -
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: 50 residues per bead.
3. Restraints	
Physical principles	Excluded volume and Sequence connectivity.
Experimental data	- 1 unique CrossLinkRestraint: DSS, 127 cross-links
4. Validation	
Sampling validation	1. Information related to sampling validation has not been provided
Clustering algorithm ,clustering feature	distance threshold-based clustering, RMSD
Number of ensembles	1
Number of models in ensembles	500
Model precision (uncertainty of models)	NoneÅ
Quality of data	1. Quality of input data has not be assessed
Assessment of atomic regions	

<i>Assessment of excluded volume</i>	
<i>Fit of the model to information used to compute it</i>	1. Fit of model to information used to compute it has not been determined
<i>Fit of the model to information not used to compute it</i>	1. Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>Method</i>	MC based Bayesian sampling using crosslinks
<i>Name</i>	IMP
<i>Details</i>	- Method details unspecified
<i>Software</i>	- Integrative Modeling Platform (IMP) (version git checkout 2018/01/08 (commit 5eb8151c651256d50bbcd847932bc913df94090c)) - No location specified