Table S1: Summary of Integrative Structure Determination of Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex (PDBDEV00000022)

| 1. Model Composition | |
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| Entry composition | - E6AP HECT Domain: Chain A (350 residues) - E6: Chain B (143 residues) |
| Datasets used for modeling | - 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 <u>rigid bodies</u> , <u>flexible units</u> | 2, 0 |
| Rigid regions | - A: 497-846:Comparative model/None. - B: 1-143:Comparative model/None. |
| Flexible units | - A: - - B: - |
| 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, 159 cross-links |
| 4. Validation | |
| Sampling validation | Information related to sampling validation has no 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 | Quality of input data has not be assessed |
| Assessment of atomic regions | |
| Assessment of excluded volume | |
| | Fit of model to information used to compute it has |

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