

Summary of integrative structure determination of Insight into the structure of the unstructured tau protein (PDB ID: 8ZZX, PDB-Dev ID: PDBDEV_0000033)

1. Model Composition	
Entry composition	tau protein: chain(s) A (441 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, PRIDE: PXD015044 - Other, PRIDE: PXD015044 - Other, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: SDA, 26 crosslinks - 1 unique CrossLinkRestraint: DSA, 60 crosslinks - 1 unique CrossLinkRestraint: DSG, 16 crosslinks - 1 unique CrossLinkRestraint: DSG, 1 crosslinks
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 18.53 - Ramachandran outliers: 11 - Sidechain outliers: 58
Fit to data used for modeling	Satisfaction of crosslinks: 0.00%
Fit to data used for validation	Fit of model to information not used to compute it has not been determined

5. Methodology and Software	
1. <i>Name</i>	Discrete Molecular Dynamics
<i>Method</i>	Protein folding
<i>Number of computed models</i>	?
<i>Software</i>	<ul style="list-style-type: none">- piDMD (version Not available)- GROMACS (version 2018)