Summary of integrative structure determination of Insight into the structure of the unstructured tau protein (PDB ID: 8ZZX, PDB-Dev ID: PDBDEV_00000033)

1. Model Composition	
Entry composition	tau protein: Chain A (441 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: SDA, 26 cross-links - Other, PRIDE: PXD015044 - Other, Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 1
Flexible units	A: 1-441
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: SDA, 26 cross-links - 1 unique CrossLinkRestraint: DSA, 60 cross-links - 1 unique CrossLinkRestraint: DSG, 16 cross-links - 1 unique CrossLinkRestraint: DSG, 1 cross-links
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 18.53, Number of Ramachandran outliers = 11, Number of sidechain outliers = 58
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined

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. Method	Discrete Molecular Dynamics
Name	Protein folding
Number of computed models	?
Software	- piDMD (version Not available) - GROMACS (version 2018)