Summary of integrative structure determination of Predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin type I modules 2 and 3 (FNI2-3) (PDB ID: 9A3X, PDB-Dev ID: PDBDEV_00000218)

1. Model Composition	
Entry composition	- Protein-glutamine gamma-glutamyltransferase 2: chain(s) A (687 residues) - Fibronectin: chain(s) B (90 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD043976 - Experimental model, PDB: 4PYG - Experimental model, PDB: 2CG7
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DMTMM, 1 crosslinks - 1 unique CrossLinkRestraint: DSS, 0 crosslinks - 1 unique CrossLinkRestraint: PDH, 0 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	- Clashscore: 11.96 - Ramachandran outliers: 10 - Sidechain outliers: 86
Fit to data used for modeling	Satisfaction of crosslinks: 100.00%
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. Name	Refinement
Description	structural refinement of starting models guided by experimental crosslinks
2. Name	satisfied/violated crosslinks identification
Description	calculation of Euclidean distances between crosslinked residues
3. Name	calculation of accessible area
Description	calculation of accessible area
4. Name	accessible interaction space
Description	determine the number of complexes consistent with the restraints
5. Name	docking
Description	generates predicted model of a protein complex
Software	- I-TASSER (version Not available) - Xwalk (version Not available) - NACCESS (version Not available) - DisVis (version Not available) - HADDOCK (version Not available)