Summary of integrative structure determination of A predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin's gelatin binding domain (FNI6FNII1-2FNI7-9). (PDB ID: 9A3Z, PDB-Dev ID: PDBDEV_00000220)

1. Model Composition	
Entry composition	- Protein-glutamine gamma-glutamyltransferase 2: Chain A (687 residues) - Fibronectin: Chain B (297 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: DMTMM, 1 cross-links - Experimental model, PDB ID: 4PYG - De Novo model, Not available - Experimental model, PDB ID: 3EJH
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 2
Flexible units	- B: 1-297 - A: 1-687
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DMTMM, 1 cross-links - 1 unique CrossLinkRestraint: DSS, 0 cross-links - 1 unique CrossLinkRestraint: PDH, 0 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 = 10.24, Number of Ramachandran outliers = 3, Number of sidechain outliers = 109
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	Refinement
Name	Iterative Threading ASSEmbly Refinement
Description	structural refinement of starting models guided by experimental crosslinks
2. Method	structure prediction
Name	AI prediction of protein 3D structure from its amino acid sequence
Description	structure prediction of fibronectin's gelatin binding domain
3. Method	satisfied/violated crosslinks identification
Name	Validate measured chemical cross-links on a protein 3D structure
Description	calculation of Euclidean distances between crosslinked residues
4. Method	calculation of accessible area
Name	calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule
Description	calculation of accessible area
5. Method	quality assessment
Name	composite scoring function which is able to derive both global (i.e. for the entire structure) and local (i.e. per residue) absolute quality estimates on the basis of one single model
6. Method	accessible interaction space
Name	None
Description	determine the number of complexes consistent with the restraints
7. Method	docking
Name	data-driven biomolecular docking

Description	generates predicted model of a protein complex
Software	- I-TASSER (version Not available) - AlphaFold2 (version Not available) - Xwalk (version Not available) - NACCESS (version Not available) - QMEAN (version Not available) - DisVis (version Not available) - HADDOCK (version Not available)