

Summary of integrative structure determination of Predicted model of tissue transglutaminase 2 (TG2) in complex with plasma fibronectin type I modules 7, 8 and 9 (FNI7-9) (PDB ID: 9A3Y, PDB-Dev ID: PDBDEV_00000219)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Fibronectin: Chain B (140 residues) - Protein-glutamine gamma-glutamyltransferase 2: Chain A (687 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: DSS, 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	<ul style="list-style-type: none"> - A: 1-687 - B: 1-140
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 1 cross-links - 1 unique CrossLinkRestraint: DMTMM, 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 = 10.68, Number of Ramachandran outliers = 10, Number of sidechain outliers = 97
Model quality: assessment of excluded volume	Not applicable

<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Method</i>	Refinement
<i>Name</i>	Iterative Threading ASSEmbly Refinement
<i>Description</i>	structural refinement of starting models guided by experimental crosslinks
2. <i>Method</i>	structure prediction
<i>Name</i>	AI prediction of protein 3D structure from its amino acid sequence
<i>Description</i>	structure prediction of FN type I modules 7-9
3. <i>Method</i>	satisfied/violated crosslinks identification
<i>Name</i>	Validate measured chemical cross-links on a protein 3D structure
<i>Description</i>	calculation of Euclidean distances between crosslinked residues
4. <i>Method</i>	calculation of accessible area
<i>Name</i>	calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule
<i>Description</i>	calculation of accessible area
5. <i>Method</i>	structure evaluation
<i>Name</i>	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. <i>Method</i>	accessible interaction space
<i>Name</i>	None
<i>Description</i>	determine the number of complexes consistent with the restraints
7. <i>Method</i>	docking
<i>Name</i>	data-driven biomolecular docking

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)