

**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)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Fibronectin: Chain B (90 residues)</li> <li>- Protein-glutamine gamma-glutamyltransferase 2: Chain A (687 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, Linker name and number of cross-links: DMTMM, 1 cross-links</li> <li>- Experimental model, PDB ID: 4PYG</li> <li>- Experimental model, PDB ID: 2CG7</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of <i>rigid bodies</i>, <i>flexible units</i></a>	0, 2
<a href="#">Flexible units</a>	<ul style="list-style-type: none"> <li>- B: 1-90</li> <li>- A: 1-687</li> </ul>
<a href="#">Structural coverage (<i>rigid bodies</i>)</a>	100%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: DMTMM, 1 cross-links</li> <li>- 1 unique CrossLinkRestraint: DSS, 0 cross-links</li> <li>- 1 unique CrossLinkRestraint: PDH, 0 cross-links</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (<i>uncertainty of models</i>)</a>	Model precision can not be calculated with one structure
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: <i>assessment of atomic segments</i></a>	Model-1: Clashescore = 11.96, Number of Ramachandran outliers = 10, Number of sidechain outliers = 86
<a href="#">Model quality: <i>assessment of excluded volume</i></a>	Not applicable

<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">Method</a>	Refinement
<a href="#">Name</a>	Iterative Threading ASSEmby Refinement
<a href="#">Description</a>	structural refinement of starting models guided by experimental crosslinks
2. <a href="#">Method</a>	satisfied/violated crosslinks identification
<a href="#">Name</a>	Validate measured chemical cross-links on a protein 3D structure
<a href="#">Description</a>	calculation of Euclidean distances between crosslinked residues
3. <a href="#">Method</a>	calculation of accessible area
<a href="#">Name</a>	calculates the atomic accessible area when a probe is rolled around the Van der Waal's surface of a macromolecule
<a href="#">Description</a>	calculation of accessible area
4. <a href="#">Method</a>	accessible interaction space
<a href="#">Name</a>	None
<a href="#">Description</a>	determine the number of complexes consistent with the restraints
5. <a href="#">Method</a>	docking
<a href="#">Name</a>	data-driven biomolecular docking
<a href="#">Description</a>	generates predicted model of a protein complex
<a href="#">Software</a>	<ul style="list-style-type: none"> <li>- <a href="#">I-TASSER</a> (version Not available)</li> <li>- <a href="#">Xwalk</a> (version Not available)</li> <li>- <a href="#">NACCESS</a> (version Not available)</li> <li>- <a href="#">DisVis</a> (version Not available)</li> <li>- <a href="#">HADDOCK</a> (version Not available)</li> </ul>