

**Summary of integrative structure determination of Man5 fully-glycosylated model of mouse N-cadherin EC1-EC5 (PDB ID: 9A44, PDB-Dev ID: PDBDEV\_00000225)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Cadherin-2: chain(s) A, B (541 residues)</li> <li>- alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: chain(s) C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- SAS data, SASBDB: <a href="#">SASDT35</a></li> <li>- Experimental model, PDB: <a href="#">3Q2W</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
<a href="#">Number of <i>rigid</i> and <i>flexible</i> segments</a>	0, 2
<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 SASRestraint: Assembly name: Man5 fully-glycosylated model of mouse N-cadherin EC1-EC5 Fitting method: GASBOR Multi-state: True</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	20
<a href="#">Number of deposited models</a>	20
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	
<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 10.87-31.23</li> <li>- Ramachandran outliers: 6-6</li> <li>- Sidechain outliers: 70-70</li> </ul>
<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="#"><i>Name</i></a>	None
<a href="#"><i>Method</i></a>	Use GlycoSHIELD, the tool we have developed, to graft MD-simulated glycan ensemble onto the x-ray protein structure (PDB ID: 3Q2W).
<a href="#"><i>Number of computed models</i></a>	20
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"><li>- <a href="#">GlycoSHIELD</a> (version Not available)</li><li>- <a href="#">GASBOR</a> (version Not available)</li><li>- <a href="#">FoXSDock</a> (version Not available)</li></ul>