

**Summary of integrative structure determination of Man9 fully-glycosylated model of mouse N-cadherin EC1-EC5 (PDB ID: 9A48, PDB-Dev ID: PDBDEV\_0000229)**

1. Model Composition	
	<ul style="list-style-type: none"> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain O (11 residues)</li> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain E (11 residues)</li> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain R (11 residues)</li> <li>- Cadherin-2: Chain A (541 residues)</li> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain G (11 residues)</li> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain I (11 residues)</li> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain D (11 residues)</li> <li>- alpha-D-mannopyranose-(1-2)-alpha-D-</li> </ul>



	<p>mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain K (11 residues)</p> <p>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain Q (11 residues)</p> <p>- alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose: Chain C (11 residues)</p>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- SAS data, SASBDB: SASDT35</li> <li>- Other, PDB: 3Q2W</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of rigid bodies, flexible units</a>	0, 18
<i>Flexible units</i>	<ul style="list-style-type: none"> <li>- A: 1-541</li> <li>- B: 1-541</li> <li>- C: 1-11</li> <li>- D: 1-11</li> <li>- E: 1-11</li> <li>- F: 1-11</li> <li>- G: 1-11</li> <li>- H: 1-11</li> <li>- I: 1-11</li> <li>- J: 1-11</li> <li>- K: 1-11</li> <li>- L: 1-11</li> <li>- M: 1-11</li> <li>- N: 1-11</li> <li>- O: 1-11</li> <li>- P: 1-11</li> <li>- Q: 1-11</li> <li>- R: 1-11</li> </ul>
<a href="#">Structural coverage (rigid bodies)</a>	100%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided

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<a href="#">Experimental data</a>	- 1 unique SASRestraint: Assembly name: Man9 fully-glycosylated model of mouse N-cadherin EC1-EC5 Fitting method: GASBOR Multi-state: True
<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>	None, Å
<a href="#">Data quality</a>	

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<p><a href="#"><i>Model quality: assessment of atomic segments</i></a></p>	<ul style="list-style-type: none"> <li>- Model-1: Clashscore = 8.62, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-2: Clashscore = 12.46, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-3: Clashscore = 12.97, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-4: Clashscore = 15.25, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-5: Clashscore = 17.02, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-6: Clashscore = 22.51, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-7: Clashscore = 21.19, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-8: Clashscore = 20.01, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-9: Clashscore = 28.51, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-10: Clashscore = 21.93, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-11: Clashscore = 18.03, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-12: Clashscore = 11.85, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-13: Clashscore = 17.94, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-14: Clashscore = 25.12, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-15: Clashscore = 14.3, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-16: Clashscore = 23.67, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-17: Clashscore = 17.62, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-18: Clashscore = 19.2, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-19: Clashscore = 29.39, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> <li>- Model-20: Clashscore = 29.64, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70</li> </ul>
<p><a href="#"><i>Model quality: assessment of excluded volume</i></a></p>	<p>Not applicable</p>

<a href="#"><i>Fit to data used for modeling</i></a>	Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit to data used for validation</i></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>Method</i></a>	None
<a href="#"><i>Name</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>Description</i></a>	The starting model is the same x-ray diffraction data mentioned in the input datasets. 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>