

Summary of integrative structure determination of Man9 fully-glycosylated model of mouse N-cadherin EC4-EC5 (PDB ID: 9A47, PDB-Dev ID: PDBDEV_0000228)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - 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) - 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 B (11 residues) - 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) - 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) - Cadherin-2: Chain A (211 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - SAS data, SASBDB: SASDT45 - Other, PDB: 3Q2W
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 5
Flexible units	<ul style="list-style-type: none"> - A: 1-211 - B: 1-11 - C: 1-11 - D: 1-11 - E: 1-11

<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	- 1 unique SASRestraint: Assembly name: Man9 fully-glycosylated model of mouse N-cadherin EC4-EC5 Fitting method: GASBOR Multi-state: True
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	20
<i>Number of deposited models</i>	20
<i>Model precision (uncertainty of models)</i>	None, Å
<i>Data quality</i>	

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 13.02, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-2: Clashscore = 10.39, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-3: Clashscore = 22.66, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-4: Clashscore = 14.88, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-5: Clashscore = 13.42, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-6: Clashscore = 20.82, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-7: Clashscore = 17.09, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-8: Clashscore = 15.22, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-9: Clashscore = 49.2, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-10: Clashscore = 31.26, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-11: Clashscore = 19.67, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-12: Clashscore = 22.66, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-13: Clashscore = 27.92, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-14: Clashscore = 42.96, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-15: Clashscore = 19.67, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-16: Clashscore = 21.9, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-17: Clashscore = 23.44, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-18: Clashscore = 30.94, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-19: Clashscore = 29.42, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10 - Model-20: Clashscore = 28.95, Number of Ramachandran outliers = 3, Number of sidechain outliers = 10
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>

<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>	None
<i>Name</i>	Use GlycoSHIELD, the tool we have developed, to graft MD-simulated glycan ensemble onto the ectodomains 4 to 5 of x-ray protein structure (PDB ID: 3Q2W).
<i>Number of computed models</i>	20
<i>Software</i>	<ul style="list-style-type: none"> - GlycoSHIELD (version Not available) - GASBOR (version Not available) - FoXSDock (version Not available)