

Summary of integrative structure determination of F1N4 fully-glycosylated model of mouse N-cadherin EC1-EC5 (PDB ID: 9A45, PDB-Dev ID: PDBDEV_0000226)

1. Model Composition	
	<ul style="list-style-type: none"> - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain P (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain L (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain F (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain C (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain G (12 residues) - Cadherin-2: Chain A (541 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-

	<p>glucopyranose: Chain N (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain R (12 residues) - Cadherin-2: Chain B (541 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain E (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain D (12 residues) - N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose: Chain O (12 residues)</p>
Datasets used for modeling	<ul style="list-style-type: none"> - SAS data, SASBDB: SASDT35 - Other, PDB: 3Q2W
2. Representation	
Resolution	Atomic
Number of rigid bodies , flexible units	0, 18

<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-541 - B: 1-541 - C: 1-12 - D: 1-12 - E: 1-12 - F: 1-12 - G: 1-12 - H: 1-12 - I: 1-12 - J: 1-12 - K: 1-12 - L: 1-12 - M: 1-12 - N: 1-12 - O: 1-12 - P: 1-12 - Q: 1-12 - R: 1-12
<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: F1N4 fully-glycosylated model of mouse N-cadherin EC1-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 = 21.44, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-2: Clashscore = 15.52, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-3: Clashscore = 14.84, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-4: Clashscore = 29.05, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-5: Clashscore = 13.45, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-6: Clashscore = 29.99, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-7: Clashscore = 30.76, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-8: Clashscore = 27.51, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-9: Clashscore = 22.79, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-10: Clashscore = 24.96, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-11: Clashscore = 43.28, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-12: Clashscore = 34.13, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-13: Clashscore = 31.91, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-14: Clashscore = 25.47, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-15: Clashscore = 23.58, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-16: Clashscore = 23.84, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-17: Clashscore = 24.76, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-18: Clashscore = 11.35, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-19: Clashscore = 20.74, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-20: Clashscore = 21.9, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
<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 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)