

Summary of integrative structure determination of F1N6 fully-glycosylated model of mouse N-cadherin EC1-EC5 (PDB ID: 9A46, PDB-Dev ID: PDBDEV_0000227)

1. Model Composition	
	<p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 (18 residues)</p> <p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 (18 residues)</p> <p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 (18 residues)</p> <p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-</p>

	<p>acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 J (18 residues)</p> <p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 K (18 residues)</p> <p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 (18 residues)</p> <p>- Cadherin-2: Chain B (541 residues)</p> <p>- Cadherin-2: Chain A (541 residues)</p> <p>- N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]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 (18 residues)</p>
<p>Datasets used for modeling</p>	<p>- SAS data, SASBDB: SASDT35</p> <p>- Other, PDB: 3Q2W</p>
<p>2. Representation</p>	

Resolution	Atomic
Number of rigid bodies, flexible units	0, 18
Flexible units	<ul style="list-style-type: none"> - A: 1-541 - B: 1-541 - C: 1-18 - D: 1-18 - E: 1-18 - F: 1-18 - G: 1-18 - H: 1-18 - I: 1-18 - J: 1-18 - K: 1-18 - L: 1-18 - M: 1-18 - N: 1-18 - O: 1-18 - P: 1-18 - Q: 1-18 - R: 1-18
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique SASRestraint: Assembly name: F1N6 fully-glycosylated model of mouse N-cadherin EC1-EC5 Fitting method: GASBOR Multi-state: True
4. Validation	
Number of ensembles	1
Number of models in ensembles	20
Number of deposited models	20
Model precision (uncertainty of models)	None, Å
Data quality	

[*Model quality: assessment of atomic segments*](#)

- Model-1: Clashscore = 24.7, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-2: Clashscore = 14.6, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-3: Clashscore = 11.75, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-4: Clashscore = 22.66, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-5: Clashscore = 14.31, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-6: Clashscore = 21.53, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-7: Clashscore = 18.52, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-8: Clashscore = 21.89, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-9: Clashscore = 10.03, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-10: Clashscore = 14.47, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-11: Clashscore = 13.68, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-12: Clashscore = 14.54, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-13: Clashscore = 15.86, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-14: Clashscore = 14.94, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-15: Clashscore = 10.44, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-16: Clashscore = 17.88, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-17: Clashscore = 10.99, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-18: Clashscore = 15.43, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-19: Clashscore = 11.92, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
- Model-20: Clashscore = 14.66, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70

<i>Model quality: assessment of excluded volume</i>	Not applicable
<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	
<i>1. 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)