Summary of integrative structure determination of Man5 fully-glycosylated model of mouse N-cadherin EC1-EC5 (PDB ID: 9A44, PDB-Dev ID: PDBDEV_00000225)

1. Model Composition	
Entry composition	- 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 G (7 residues) - 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 N (7 residues) - 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 P (7 residues) - Cadherin-2: Chain B (541 residues) - 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 J (7 residues) - Cadherin-2: Chain A (541 residues) - 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 C (7 residues) - 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 K (7 residues) - 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 O (7 residues) - 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 H (7 residues) - 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 R (7 residues)

	- 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 M (7 residues) - 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 L (7 residues) - 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 E (7 residues) - 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 Q (7 residues) - 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 D (7 residues) - 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 I (7 residues) - 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 F (7 residues)
Datasets used for modeling	- SAS data, SASBDB: SASDT35 - Other, PDB: 3Q2W
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 18

Flexible units	- A: 1-541 - B: 1-541 - C: 1-7 - D: 1-7 - E: 1-7 - F: 1-7 - G: 1-7 - H: 1-7 - I: 1-7 - J: 1-7 - K: 1-7 - L: 1-7 - M: 1-7 - N: 1-7 - O: 1-7 - P: 1-7 - Q: 1-7 - R: 1-7
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique SASRestraint: Assembly name: Man5 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 = 11.66, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-2: Clashscore = 31.23, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-3: Clashscore = 19.4, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-4: Clashscore = 20.5, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-5: Clashscore = 11.86, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-6: Clashscore = 10.87, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-7: Clashscore = 14.61, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-8: Clashscore = 19.31, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-9: Clashscore = 23.42, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-10: Clashscore = 19.45, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-11: Clashscore = 20.38, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-12: Clashscore = 17.86, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-13: Clashscore = 17.19, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-14: Clashscore = 13.54, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-15: Clashscore = 17.06, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-16: Clashscore = 16.86, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-17: Clashscore = 18.54, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-18: Clashscore = 17.67, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-19: Clashscore = 18.15, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70 - Model-20: Clashscore = 14.99, Number of Ramachandran outliers = 6, Number of sidechain outliers = 70
Model quality: assessment of excluded volume	Not applicable

Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	None
Name	Use GlycoSHIELD, the tool we have developed, to graft MD-simulated glycan ensemble onto the x-ray protein structure (PDB ID: 3Q2W).
Number of computed models	20
Software	- GlycoSHIELD (version Not available) - GASBOR (version Not available) - FoXSDock (version Not available)