

Summary of integrative structure determination of F1N6 fully-glycosylated model of mouse N-cadherin EC1-EC5 (PDB ID: 9A46, PDB-Dev ID: PDBDEV_00000227)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Cadherin-2: chain(s) A, B (541 residues) - 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(s) C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R
Datasets used for modeling	<ul style="list-style-type: none"> - SAS data, SASBDB: SASDT35 - Experimental model, PDB: 3Q2W
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 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)	Not available
Data quality	

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 10.03-24.70 - Ramachandran outliers: 6-6 - Sidechain outliers: 70-70
<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>Name</i>	None
<i>Method</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)