

Summary of integrative structure determination of F1N4 fully-glycosylated model of mouse N-cadherin EC4-EC5 (PDB ID: 9A41, PDB-Dev ID: PDBDEV_00000222)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Cadherin-2: chain(s) A (211 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(s) B, C, D, E
Datasets used for modeling	<ul style="list-style-type: none"> - SAS data, SASBDB: SASDT45 - Experimental model, PDB: 3Q2W
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique SASRestraint: Assembly name: F1N4 fully-glycosylated model of mouse N-cadherin EC4-EC 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	
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 16.47-59.26 - Ramachandran outliers: 3-3 - Sidechain outliers: 10-10
Fit to data used for modeling	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 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)