

Summary of integrative structure determination of Man5 fully-glycosylated model of mouse N-cadherin EC4-EC5 (PDB ID: 9A43, PDB-Dev ID: PDBDEV_00000224)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Cadherin-2: chain(s) A (211 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(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 rigid and flexible 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: Man5 fully-glycosylated model of mouse N-cadherin EC4-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	
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 10.93-42.43 - 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
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. <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)