

**Summary of integrative structure determination of Structural model of UDP-glucose:glycoprotein glucosyl-transferase bound to Fab (PDB ID: 9A0I, PDB-Dev ID: PDBDEV\_00000054)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Fab Light Chain: Chain C (214 residues)</li> <li>- Fab Heavy Chain: Chain B (214 residues)</li> <li>- TdUGGT: Chain A (1368 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- 3DEM volume, EMDB: EMD-30386</li> <li>- Other, File: 10.1038/s41598-017-12283-w</li> <li>- Experimental model, PDB ID: 5Y7O</li> <li>- Experimental model, PDB ID: 5MU1</li> <li>- Experimental model, PDB ID: 5H18</li> <li>- Experimental model, PDB ID: 1FGN</li> <li>- Other, Not available</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Atomic
<a href="#">Number of rigid bodies, flexible units</a>	16, 0
<a href="#">Rigid bodies</a>	<ul style="list-style-type: none"> <li>- A: 1-129, 130-137, 138-222, 223-342, 343-354, 355-623, 624-633, 634-677, 678-681, 682-695, 696-699, 700-977, 978-1091, 1092-1368</li> <li>- B: 1-214</li> <li>- C: 1-214</li> </ul>
<a href="#">Structural coverage (rigid bodies)</a>	100%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	<ul style="list-style-type: none"> <li>- 2 unique DerivedDistanceRestraint: restraint type DistanceRestraintOther</li> <li>- 1 unique EM3DRestraint: None</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	2
<a href="#">Model precision (uncertainty of models)</a>	Model precision can not be calculated with one structure
<a href="#">Data quality</a>	Data quality has not been assessed

<a href="#">Model quality: assessment of atomic segments</a>	- Model-1: Clashscore = 712.54, Number of Ramachandran outliers = 21, Number of sidechain outliers = 47 - Model-2: Clashscore = 635.26, Number of Ramachandran outliers = 21, Number of sidechain outliers = 47
<a href="#">Model quality: assessment of excluded volume</a>	Not applicable
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">Method</a>	Fitting the TdUGGT and Fab models in the negative stain EM map
<a href="#">Name</a>	None
<a href="#">Software</a>	- <a href="#">Coot</a> (version Not available) - <a href="#">Modeller</a> (version Not available) - <a href="#">Chimera</a> (version Not available)