SUPPORTING MATERIAL

Molecular dynamics simulation of Autotaxin: Roles of the nuclease-like domain and the glycan modification

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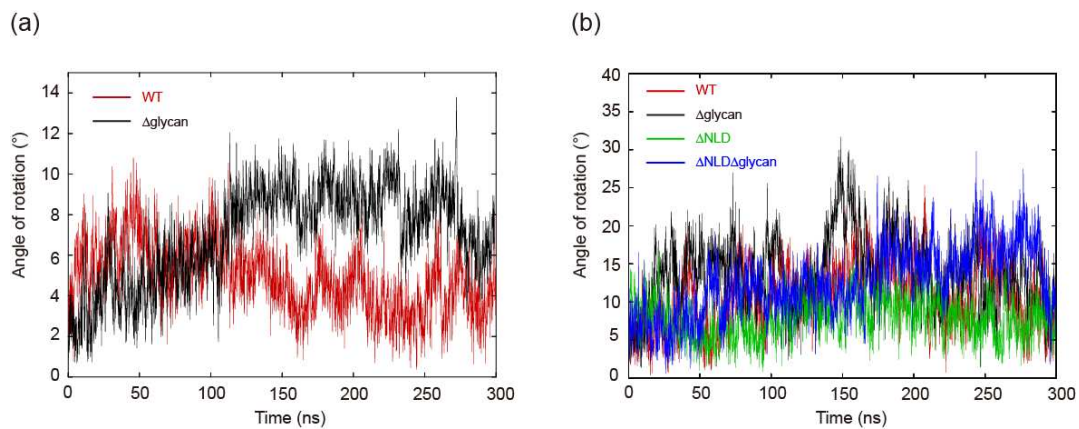
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Figure S1

Domain rotation between (a) the CAT and NLD domains and (b) SMB-like

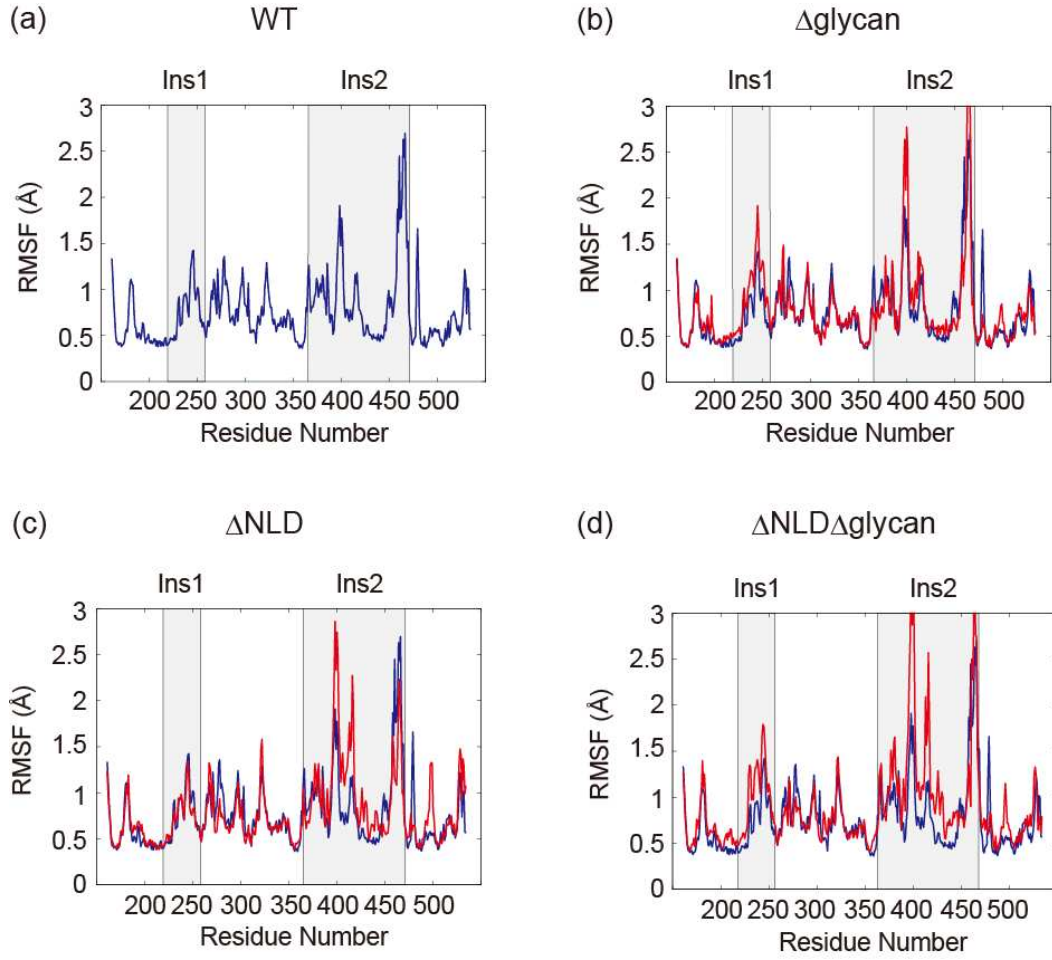domain 1 and the CAT domain in each simulation.

Figure S2

RMSF values for each simulation. The blue lines show the RMSF values of the WT simulation (a-d), and the red lines show the RMSF values of the (b) Δglycan, (c) ΔNLD, and (d) ΔNLDΔglycan simulations.
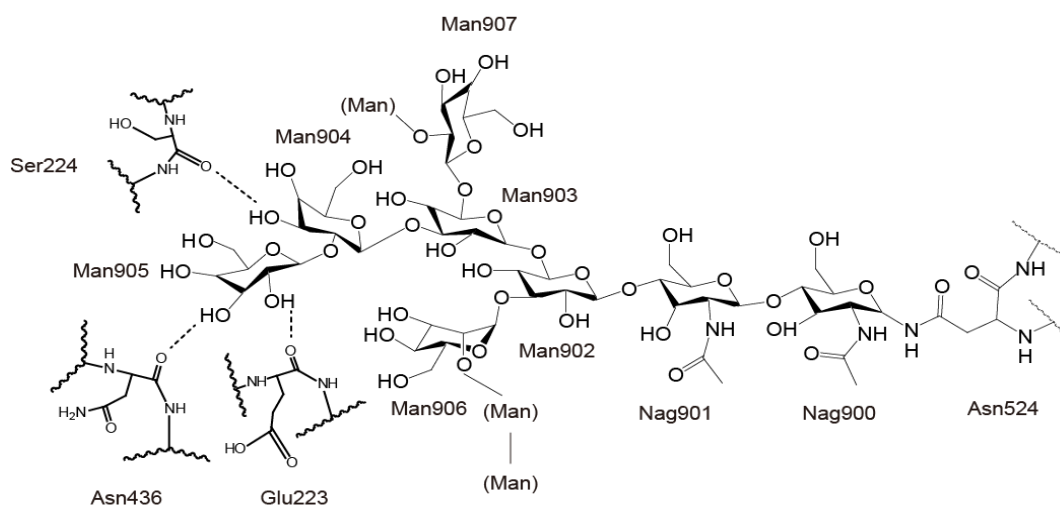
Figure S3

The structure of the glycan on Asn-524. Mannoses with undefined electron

densities in the crystal structure are shown in parentheses. Hydrogen bonds

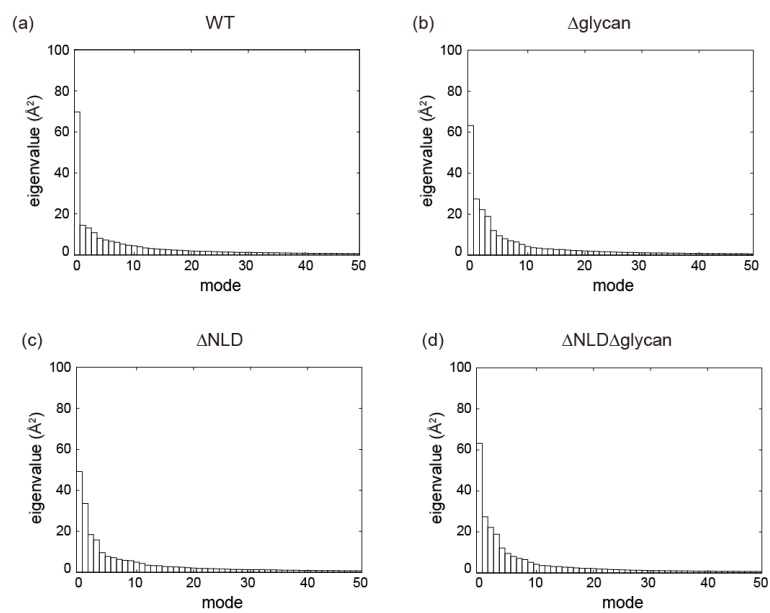between the glycan on Asn-524 and ATX are shown as dashed lines.

Figure S4

The eigenvalues of PCA for each simulation.