
BIOLOGICAL
CRYSTALLOGRAPHY

**Volume 71 (2015)**

**Supporting information for article:**

# Structural insights into human IgG1 interaction with FcγRI: no direct role of glycans in binding

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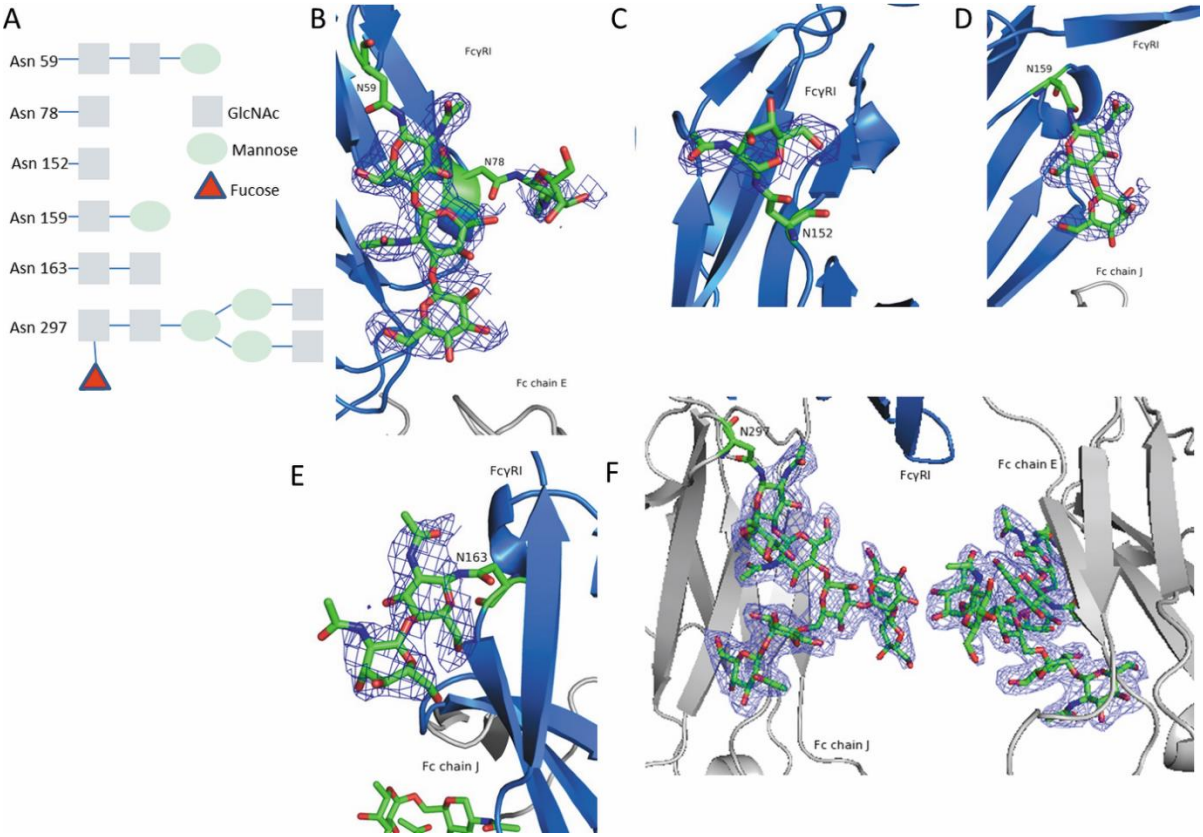


**Figure S1** (A) Schematic representation of N-linked oligosaccharides attached to FcγRI and Fc, (B) Omit map showing oligosaccharides attached to FcγRI N59 and N78 in D1. SigmaA weighted $2mF_oDF_c$ electron density map allowed the placement of GlcNAc-GlcNAc-Man near N59; however, the quality of that near N78 was considerably lower and only the first GlcNAc was placed, (C) Omit map showing one oligosaccharide attached to FcγRI N152 in D2. SigmaA weighted $2mF_oDF_c$ electron density map allowed the placement of only one GlcNAc, (D) Omit map showing two oligosaccharides attached to FcγRI N159 in D2. SigmaA weighted $2mF_oDF_c$ electron density map allowed the placement of GlcNAc-Man near N159; however, the quality of that around Man was considerably lower than for GlcNAc, (E) Omit map showing two oligosaccharides attached to FcγRI N163 in D2. SigmaA weighted $2mF_oDF_c$ electron density map allowed the placement of GlcNAc-GlcNAc, (F) Omit map showing oligosaccharides attached to both Fc N297. SigmaA weighted $2mF_oDF_c$ electron density map allowed the placement of bi-antennary glycans. Terminal galactose and sialic acid residues did not show in the electron density. All electron density maps are shown at 0.8σ.

**Table S1** Summary of hydrogen bonds and electrostatic interactions formed between FcγRI and Fc.

| FcγRI | Distance (Å) | Fc |
|---|---|---|
| A:LYS 130[Nζ][a] | 3.50 | E:GLU 233[Oε2] |
| A:LEU 131[N] | 2.74 | E:GLU 233[O] |
| A:LYS 173[N] | 2.85 | E:LEU 235[O] |
| A:HIS 174[ Nε2] | 3.50 | E:SER 239[Oγ] |
| A:LEU 131[O] | 3.07 | E:LEU 235[N] |
| A:TYR 176[Oη] | 3.47 | E:GLY 237[N] |
| A:ASN 134[Nδ2] | 2.79 | J:GLY 237[O] |
| A:LYS 145[Nζ] | 3.07 | J:GLU 269[Oε2] |
| A:HIS 148[Nε2] | 3.22 | J:ASP 265[O] |
| A:ARG 102[Nη2] | 3.46 | E:PRO 329[O] |
| A:LYS 130[Nζ] | 3.50 | E:233 GLU[Oε2] |
| A:HIS 148[Nδ1] | 3.30 | J:267 SER[Oγ] |

[a]Letters in bracket refer to the corresponding interacting atoms.

**Table S2 Hydrogen bonds between FcγR1 D1 and D2 in unliganded and ligand-bound states.**

| D1 | Hydrogen bond distance (Å) Unliganded | Hydrogen bond distance (Å) Ligand-bound | D2 |
|---|---|---|---|
| A:VAL 31[N] | 2.97 | 3.22 | A:VAL 109[O] |
| A:VAL 31[O] | 3.09 | 2.76 | A:ARG 112[Nη2] |
| A:SER 32[O] | 2.90 | 2.63 | A:GLN 108[Nε2] |
| A:GLU 37[Oε2] | 2.79 | 2.70 | A:HIS 125[Nε2] |
| A:GLN 97[O] | 2.79 | 2.68 | A:ARG 112[Nη2] |
| A:GLU 99[Oε1] | 3.37 | 2.95 | A:ARG 112[Nη] |