Electronic Supplementary Material (ESI) for Molecular BioSystems.

Figure S1: RMSDs of glycosylated and deglycosylated Fc with respect to the starting structures for all-atoms (blue), and for Cα (red) during the 70 ns production simulations. Superimposition of one X-ray structure and two snapshots extracted at 50ns and 70ns.

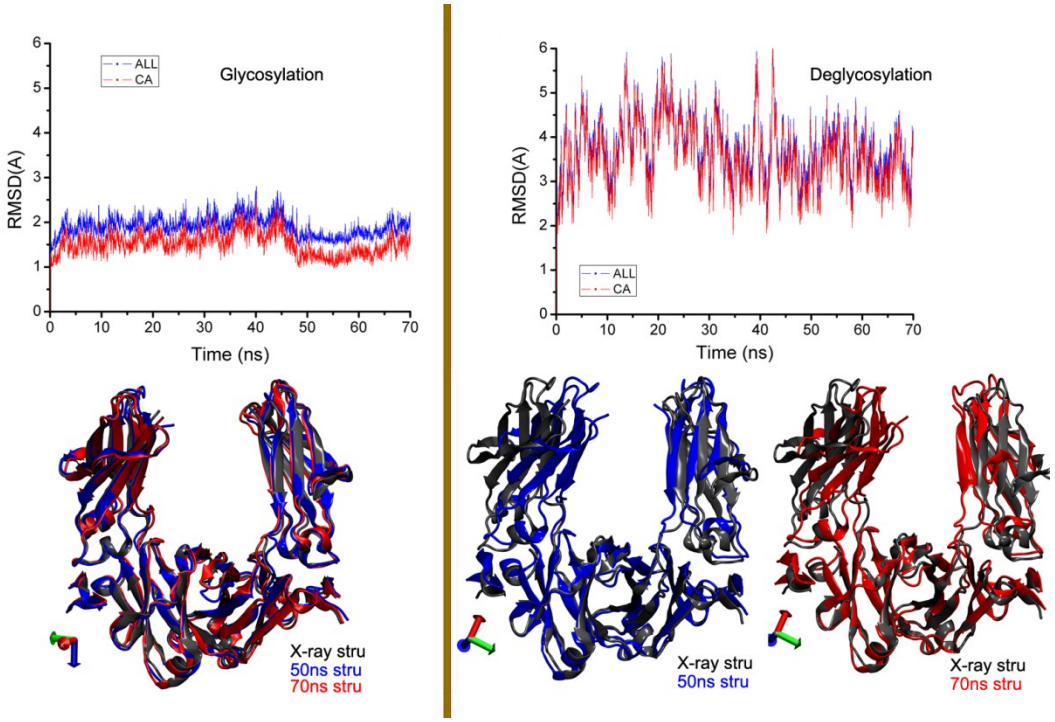

Figure S2: Time scale between 10.8ns and 18.7ns is extracted. Three snapshots representing open (10.8ns), closed (13.8ns) and open (18.7ns) states are in surface representations.

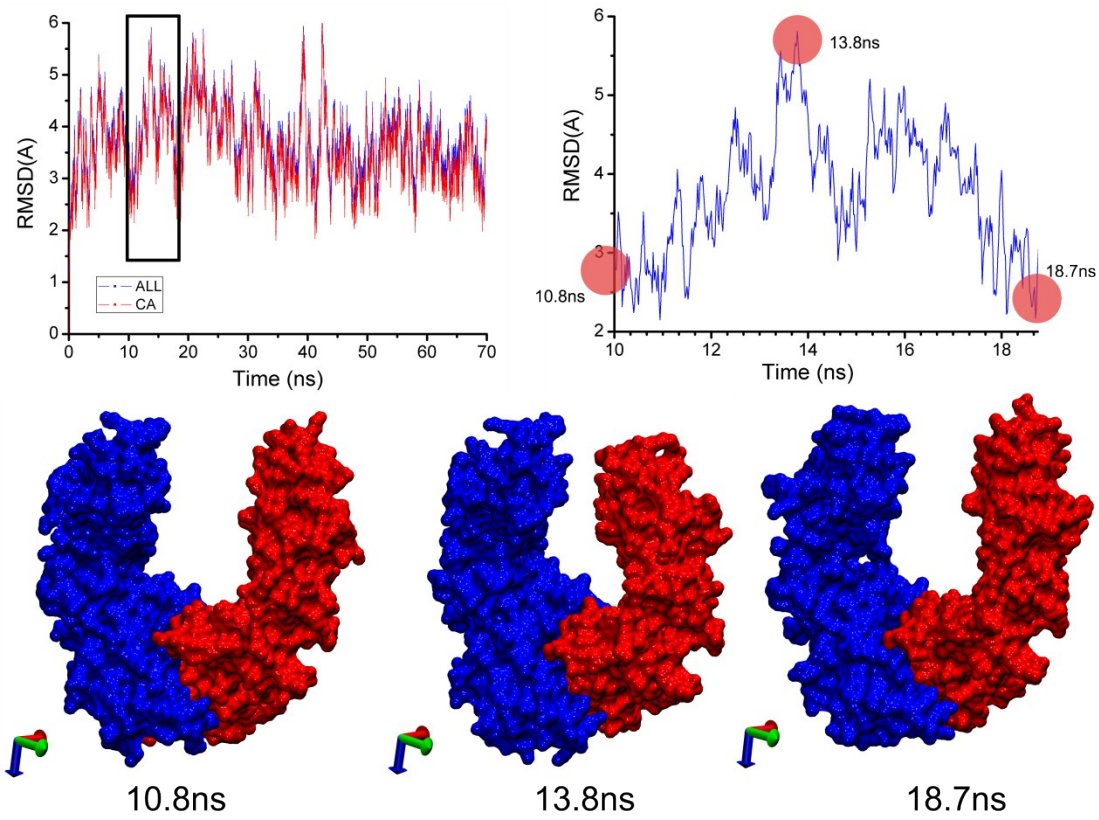

Table S1. The free energies calculated by the MM-GBSA methods for the binding of Fc to its partners P13 (PDB id: 1nd2) and P34 (PDB id: 1l6x).

Contribution[a]	1dn2	1l6x
ΔE_{ele}	-289.61 ± 21.94	-191.81 ± 27.02
ΔE_{vdW}	-104.68 ± 7.65	-120.94 ± 7.06
ΔE_{gas}[b]	-394.29 ± 21.97	-312.75 ± 29.58
ΔG_{GB}	321.30 ± 19.78	236.37 ± 24.49
$\Delta G_{sol\text{-}np,GB}$	-17.06 ± 0.82	-19.38 ± 0.75
$\Delta G_{sol,GB}$[c]	304.24 ± 19.62	216.99 ± 24.12
$\Delta G_{ele,GB}$[d]	31.69 ± 6.72	44.56 ± 6.99
$\Delta G_{bind,GB}$[e]	-90.06 ± 7.31	-95.76 ± 7.92

[a]All energies are in kcal/mol.
[b]$\Delta E_{gas} = \Delta E_{ele} + \Delta E_{vdW}$
[c]$\Delta G_{sol,GB} = \Delta G_{sol\text{-}np,GB} + \Delta G_{GB}$
[d]$\Delta G_{ele\text{-}GB} = \Delta G_{GB} + \Delta E_{ele}$
[e]$\Delta G_{bind,GB} = \Delta E_{ele} + \Delta E_{vdW} + \Delta G_{sol,GB}$