Supplementary Table S7: MLG43-ectodomains interaction energies.

Protein-glycan interaction energies [Molecular Mechanics (MM) with Poisson-Boltzmann (PB) and surface area (SA) solvation MM/PBSA approach]							
PRR ECD (PDB)	ΔE_{elec} [1]	ΔE_{vdW} [1]	ΔE_{int} [2]	ΔG_{np} [3]	ΔG_{pol} [4]	ΔG_{sol} [5]	Σ [6]
CERK1 (4EBZ)	-15.9 ± 1.6	-20.5 ± 3.5	-36.45 ± 1.9	0.4 ± 0.1	33.1 ± 2.4	33.5 ± 2.5	**-2.9** ± 4.4
BAK1 (4MN8.B)	-26.45 ± 1.8	-16.2 ± 4.1	-42.75 ± 5.9	0.5 ± 0.3	45.2 ± 10	45.7 ± 9.8	**2.9** ± 4.0
SOBIR1 (6R1H)	-25.5 ± 3.8	-20.8 ± 3.8	-46.35 ± 7.7	0.2 ± 0.4	43.35 ± 13.2	43.5 ± 12.7	**-2.85** ± 4.9

[1] ΔE_{elec} and ΔE_{VdW} energies (kcal mol^{-1}) calculated at the corresponding optimized geometries with the "NAMD energy" tool implemented in VMD 1.9.3.

[2] $\Delta E_{int} = \Delta E_{elec} + \Delta E_{VdW}$

[3] ΔG_{np} free energies (kcal mol^{-1}) estimated from the empirical linear relation to the solvent-accessible surface area (SASA) $G_{np} = \gamma\,(\mathrm{SASA}) + b$, where the parameter values depend on how the polar contribution to solvation is obtained. Values were $\gamma = 0.00526$ kcal mol^{-1} Å^{-2} and $b = 0.918$ kcal mol^{-1}. SASA values were calculated with the SPDBV tool.

[4] ΔG_{pol} free energies (kcal mol^{-1}) obtained by solving the Poisson-Boltzmann equation with the PBEQ Solver tool implemented in CHARMM-GUI.

[5] $\Delta G_{sol} = \Delta G_{np} + \Delta G_{pol}$

[6] $\Sigma = \Delta E_{int} + \Delta G_{sol}$

Energy values under 1kT (k: Boltzmann constant, T: absolute temperature) are considered irrelevant. At normal thermodynamically temperature of 298 K, noisy kT values start below 0.6 kcal/mol.