
Supplementary information

**LAG3 ectodomain structure reveals
functional interfaces for ligand and
antibody recognition**

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authors and unedited

Supplementary Table 1. X-ray data collection and refinement statistics

	hLAG3*:F7	hLAG3 ^{D34} :F7	mLAG3 ^{D12}	FGL1 ^{FD}
Data Collection				
Wavelength (Å)	1.0332	1.033	1.0000	0.97918
Space group	P 21 21 21	C 1 2 1	P 1 21 1	P 2 21 21
Unique reflections	19409 (1894)	34601 (3383)	29753 (2954)	25188 (2424)
a, b, c (Å)	78.44, 142.93, 158.17	119.16 78.52 107.17	35.73 92.53 81.77	45.28, 110.89, 148.89
α , β , γ (°)	90.00, 90.00, 90.00	90.00, 111.44, 90.00	90.00, 90.78, 90.00	90.00, 90.00, 90.00
Resolution (Å)	45.62-3.71	36.53 - 2.43	40.27-2.12	45.3 - 2.55
R _{merge}	0.196 (1.127)	0.068 (0.822)	0.0816 (1.205)	0.337 (1.311)
I/ σ (I)	7.55 (1.56)	11.35 (1.64)	9.01 (1.09)	7.52 (1.83)
Completeness (%)	99.78 (99.58)	99.55 (98.25)	98.45 (99.19)	99.51 (98.29)
Multiplicity	5.1 (5.0)	3.4 (3.5)	3.8 (4.0)	5.8 (4.6)
CC1/2	0.994 (0.529)	0.997 (0.707)	0.997 (0.605)	0.929 (0.404)
Refinement				
Resolution (Å)	45.62-3.71	36.53 - 2.43	40.27 - 2.12	45.3 - 2.55
R _{work} / R _{free}	0.236/0.283	0.211/0.253	0.212/0.237	0.188/0.233
No. of Atoms				
Protein	8618	5904	3227	5625
Ligand	98	28	64	0
Water	0	169	81	129
B-Factors (Å ²)				
Protein	147.5	73.3	76.16	42.19
Ligand	194.06	120.36	81.9	N/A
Water	N/A	55.54	83.57	35.55
RMSDs				
Bond length (Å)	0.006	0.005	0.006	0.009
Bond angles (°)	1.10	0.81	1.06	1.14
Ramachandran Plot (%)				
Favored region	93.8	96.45	98.28	97.03
Allowed region	6.2	3.56	1.23	2.97
Outlier region	0	0	0.49	0
PDB ID	7TZG	7TZH	7TZE	7TZ2

Values in parentheses represent outer shell. RMSD: root mean-square deviation.

Supplementary Table 2. Yeast-display mutant library primers

Yeast library	Primer	Sequence 5' → 3'
hLAG3 ^{D12} EP-PCR	Forward	GTTTTTCAATATTTTCTGTTATTGCTAGCGTTTTAGCAGCTC CAGTGAAGCCTCTCCAG
	Reverse	CCAAGTCTTCTTCGGAGATAAGCTTTTGTTCAGAACAGT GAGGTTATACAT
hLAG3 ^{D12} amplification	Forward	CGGTTTGTATTACTTCTTATTCAAATG
	Reverse	GGGATTTGCTCGCATATAGTTG
FGL1 ^{FD} EP- PCR	Forward	TTTCAATATTTTCTGTTATTGCTAGCGTTTTAGCATTGCAG GAGAATGAAGTCCAGTTCCTTG
	Reverse	CCCAAGTCTTCTTCGGAGATAAGCTTTTGTTC AATTACATT TGGAATAAAATCATT
FGL1 ^{FD} amplification	Forward	CGGTTTGTATTACTTCTTATTCAAATG
	Reverse	GGGATTTGCTCGCATATAGTTG