Supplementary Table 1. Crystallographic Statistics

Crystallographic data	
Source	4A (HFMX)
Wavelength, Å	0.9797
Resolution limits (Å)	50.0-2.3
Space group	P321
Unit cell *a, c,* (Å)	121.85, 33.58
Total Reflections	556,694
Unique reflections	13,136
Completeness	100 (100)
R_{sym} (%)	8.3 (15.0)
Average I/σ (I)	31.3 (8.1)
FOM after density modification With CNS	0.78
Refinement statistics	
Resolution range (Å)	50.0-2.3
R_{factor} (%)[b]	23.5
R_{free} (%)[c]	24.9
Number of protein atoms	1,233
Number of water molecules	57
r.m.s.d. from ideality	
Bond length (Å)	0.006
Bond angles (°)	1.374
Ramachandran plot (%)	
Most favored	92.9
Additionally allowed	7.1
Generously allowed	0

[a] $R_{sym}=\Sigma|I_{obs}-I_{avg}|/ I_{obs}$, where I_{obs} is the observed intensity of individual reflection and I_{avg} is average over symmetry equivalents.

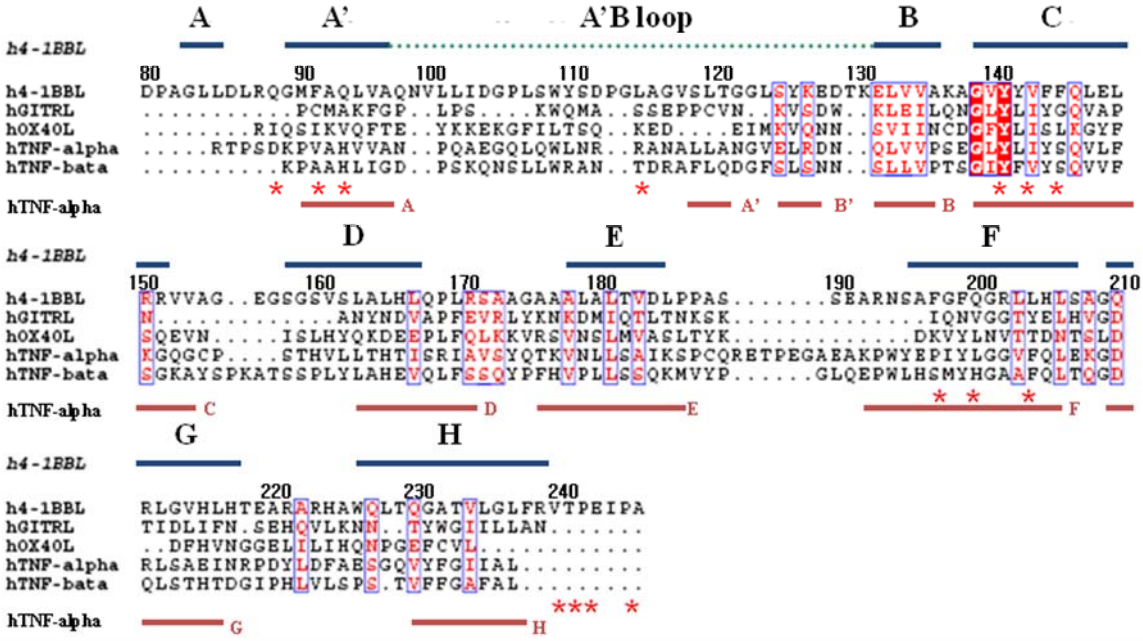
[b] $R_{cyst} = \Sigma||F_{obs}|-|F_{calc}||/ \Sigma|F_{obs}| \times 100$ for 95% of recorded data

[c] R_{free} is the *R*-factor calculated by using 5% of the reflection data chosen randomly and omitted from the start of refinement.

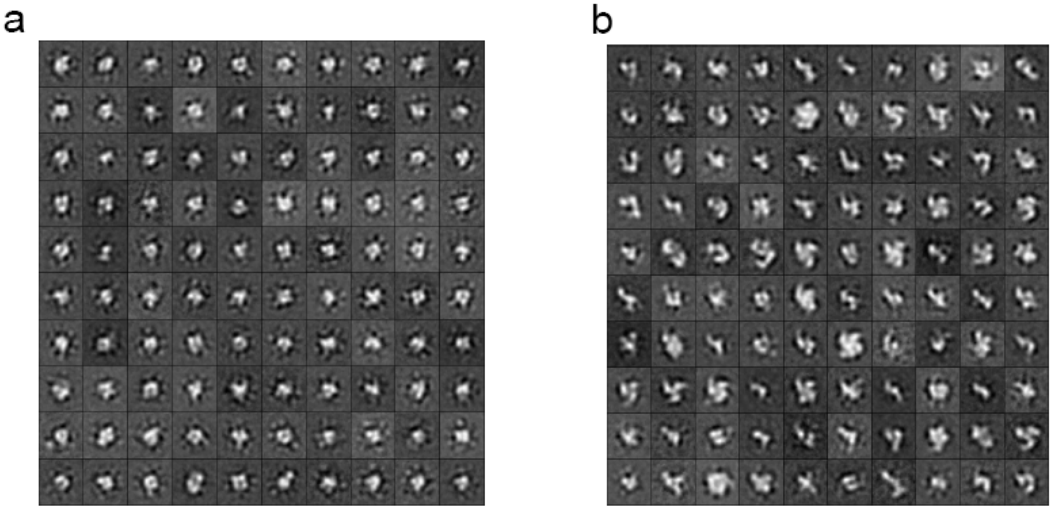
Supplementary Table 2. The Mutations of 4-1BBL residues predicted to mediate trimeric interactions and receptor binding

Trimer interface		
Residue number	Binding portion with 4-1BB	Oligomeric state
Q89A	55.2 %	Trimer
L115G	15.4 %	Trimer
V140A	89.7 %	Dimer
F199A	85.5 %	Trimer/Dimer
H205A	89.0 %	Trimer
V240A	63.4 %	Trimer
P242K	86.9 %	Trimer
P242E	88.3 %	Trimer
P245D	88.8 %	Trimer
Δ240-254	Insoluble	Insoluble

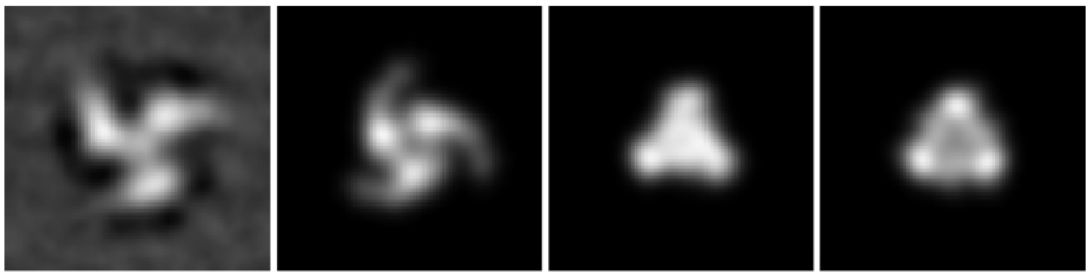
Receptor binding sites from modeling		
Residue number	Binding portion with 4-1BB	Oligomeric state
K127A	0.5 %	N/A
Q227A	4.3 %	Trimer
Q230A	Insoluble	Insoluble
Receptor binding sites from comparision with other complex structures		
R171G	82.3 %	Trimer
S172G	90.7 %	Trimer
H205A	89.0 %	Trimer



Supplementary Figure 1.



Supplementary Figure 2.



Supplementary Figure 3.