

Crystal Structure of the Human 4-1BB/4-1BBL Complex

Ryan N. Gilbreth, Vaheh Oganessian, Hamza Amdouni, Shabazz Novarra, Luba

Grinberg, Arnita Barnes and Manuel Baca

Supporting Information Contents

Table S1

Figures S1-S2

Table S1. TNF Superfamily Ligand/Receptor Interface Properties
BSA = Buried surface area. Data generated using the PISA web server.

Complex	PDB ID	“Left” Monomer Interface BSA (Å²)	“Right” Monomer Interface BSA (Å²)	Total Interface BSA (Å²)	% Interface BSA Contributed by “Left” Monomer	% Interface BSA Contributed by “Right” Monomer
4-1BB/4-1BBL	6BWV	837.9	77.9	915.8	91.8	8.2
Fas/FasL	4MSV	460.1	471.8	931.9	49.4	50.6
LIGHT/DcR3	4J6G	611.5	480.9	1092.4	56.0	44.0
RANKL/OPG	3URF	589.7	520.1	1109.8	53.1	46.9
TNF α /TNFR2	3ALQ	618.8	689.0	1307.8	47.3	52.7
CD40/CD40L	3QD6	645.2	592.1	1237.3	52.1	47.9
TL1 α /DcR3	3K51	654.5	420.9	1075.4	60.9	39.1
LIGHT/HVEM	4RSU	707.1	389.3	1096.4	64.5	35.5
OX40L/OX40	2HEV	583.3	447.3	1030.6	56.6	43.4
LT α /TNFR1	1TNR	518.0	599.1	1117.1	46.4	53.6

THD

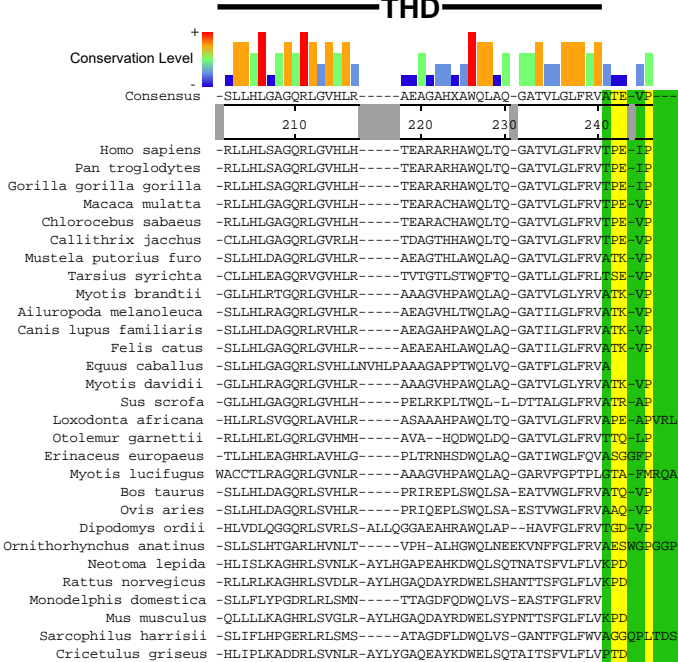
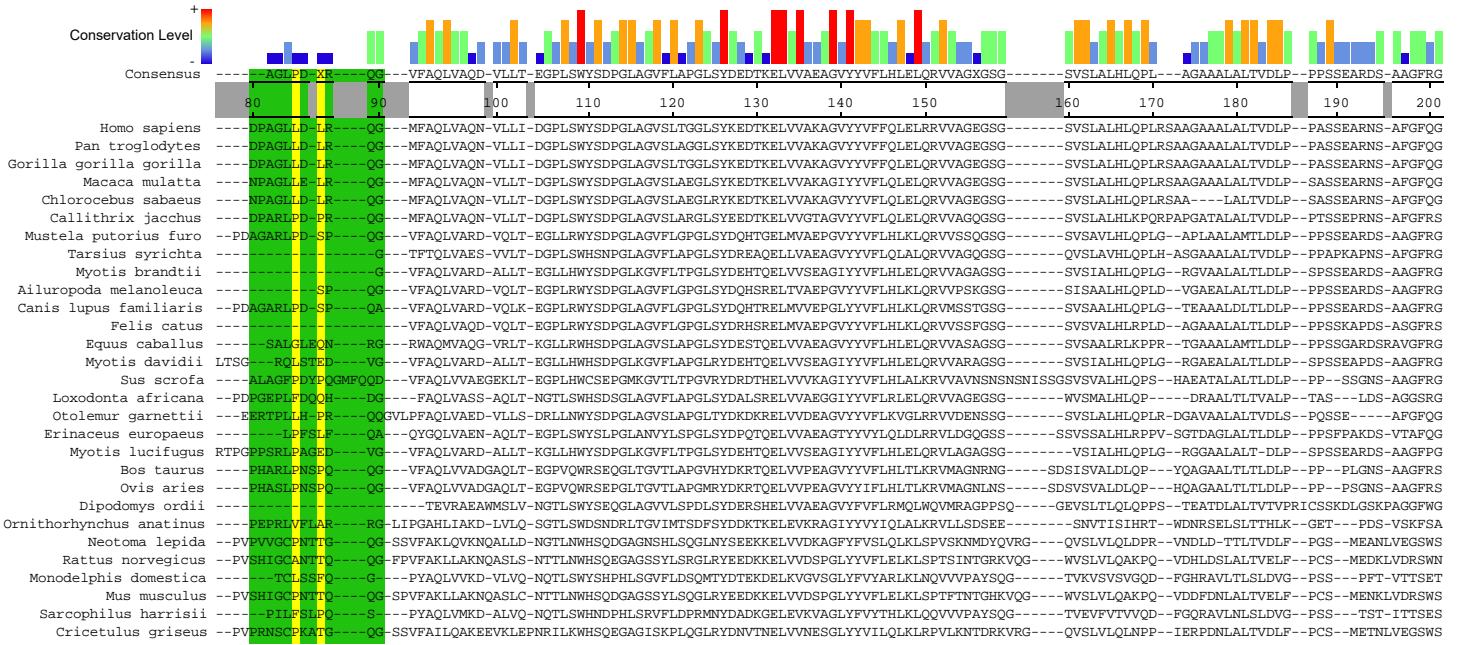


Figure S1, Gilbreth et al.

Figure S1. Sequence Conservation in 4-1BBL. Sequence alignment of the 4-1BBL extracellular region from human and other species. Sequences have been trimmed to include only those residues that were ordered in the e4-1BBL crystal structure reported by Won et al. The region corresponding the TNF homology domain (THD) is indicated. Residues outside the THD that contribute to either folded monomer structure or trimer assembly in the e4-1BBL structure are highlighted (green). Residues at the C-terminus that bury more than 80% of their accessible surface area in the trimer interface and residues at the N-terminus that are inward facing and appear to contribute to the monomer hydrophobic core are also highlighted (yellow).

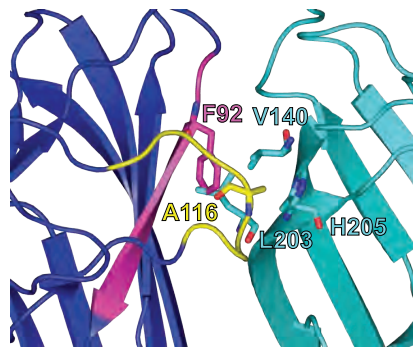


Figure S2. Gilbreth et al.

Figure S2. Steric clashes prevent e4-1BBL monomer superposition on THD-only 4-1BBL trimer. Structural detail showing some of the most pronounced steric clashes arising from superposition of the e4-1BBL monomer onto the THD-only 4-1BBL trimer reported here. Neighboring monomers are colored (blue and cyan). A-strand (magenta) and AA' loop residues (yellow) near the site of close contacts and clashes are highlighted. Sticks are shown for residues directly involved in clashes/close contacts.