

Table S1. HLA-B/KIR3LD1 Contact Map Analysis. Complexes were analyzed with different bound peptides respect to the original crystal structures.

KIR	Contact Residues													
	HLA-B*07:02		HLA-B*14:02		HLA-B*35:01		HLA-B*27:05		HLA-B*51:01		HLA-B*57:01		HLA-B*58:01	
	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA
KIR3DL1*001	F9	G16	F9	G16	F9	G16	F9	P15	F9	G16	F9	G16	F9	G16
	S11	R17	S11	R17	S11	R17	S11	G16	S11	R17	W13	R17	S11	R17
	W13	G18	W13	E19	W13	E19	W13	R17	H29	E19	R27	E19	W13	E19
	H29	E19	H29	E76	H29	E76	R27	G18	K141	E76	H29	Q72	H29	E76
	S140	E76	K141	Y84	S140	N80	H29	E19	L166	R83	S140	E76	K141	I80
	L166	N80	L166	E89	L166	Y84	S140	E76	P199	Y84	M165	R79	L166	R83
	P167	G83	P167	R145	P199	E89	L166	R83	Y200	I142	L166	R83	P199	Y84
	P199	Y84	P199	K146	Y200	I142	A167	Y84	E201	R145	A167	Y84	Y200	A90
	Y200	E89	Y200	A149	S227	R145	Y200	N86	S227	K146	Y200	E89	S228	I142
	S227	I142	E201	A150	S228	K146	E201	E89	S228	A149	E201	R145	D230	R145
	S228	R145	S227	R151	D230	A149	S227	I142	D230	A150	S227	K146	F276	K146
	D230	K146	S228		F276		S228	R145	F276		S228	A149	R277	A149
	F276	A149	D230		R277		D230	K146	R277		D230	R151	H278	A150
	R277	A150	F276		H278		F276	A149	H278		F276		S279	
	H278		R277		S279		H278	R151	S279		H278			
	S279		S279				S279		E282		S279			
E282		E282				E282				E282				
KIR3DL1*005	F9	G16	F9	G16	F9	G16	F9	G16	F9	G16	F9	R17	F9	G16
	S11	R17	S11	R17	S11	R17	S11	R17	S11	R17	W13	E19	S11	R17
	W13	G18	W13	G18	W13	E19	W13	E19	W13	E19	H29	Q72	H29	E19
	H29	E19	S140	E19	H29	E76	S140	E76	H29	E76	G138	E76	S140	E76
	G138	E76	L166	E76	S140	N80	L166	R83	K141	R83	S140	R79	L166	I80
	S140	R79	P167	Y84	L166	G83	A167	Y84	P199	Y84	M165	R83	Y200	R83
	L166	N80	P199	E89	P199	Y84	P199	E89	Y200	E89	L166	Y84	E201	Y84
	P167	G83	Y200	A90	Y200	E89	Y200	R145	E201	I142	A167	E89	S228	I142
	P199	Y84	S228	I142	S228	I142	S228	K146	S227	R145	Y200	R145	D230	R145
	Y200	E89	D230	R145	D230	R145	D230	A150	S228	K146	E201	K146	F276	K146
	S228	R145	F276	K146	F276	K146	F276		D230	A149	S227	A149	R277	A149
	D230	K146	R277	A150	R277	A150	H278		F276	A150	S228	A150	H278	A150
	F276	A150	H278		H278		S279		R277		D230	R151	E282	
	H278		S279		S279		E282		H278		F276			
	S279		E282		E282				E282		R277			
	E282										H278			
										S279				
										E282				
KIR3DL1*007/015	F9	G16	F9	G16	F9	G16	F9	G16	F9	G16	F9	R17	F9	G16
	S11	R17	S11	R17	S11	R17	S11	R17	S11	R17	W13	E19	S11	R17
	W13	G18	W13	G18	W13	E19	W13	G18	W13	E19	H29	Q72	H29	E19
	H29	E19	H29	E76	H29	E76	H29	E19	H29	E76	S140	E76	S140	E76
	S140	E76	L166	Y84	S140	N80	S140	E76	K141	I80	M165	R79	L166	I80
	L166	N80	A167	E89	L166	G83	L166	R83	L166	R83	L166	R83	P199	R83
	P167	G83	P199	I142	A167	Y84	A167	Y84	P199	Y84	A167	Y84	Y200	Y84
	P199	Y84	Y200	R145	P199	E89	S228	E89	Y200	E89	P199	E89	S227	I142
	Y200	E89	S228	K146	Y200	I142	D230	I142	E201	I142	E201	R145	S228	R145
	S228	I142	D230	A150	S228	R145	F276	R145	S227	R145	S227	K146	D230	K146
	D230	R145	F276		D230	K146	R277	K146	S228	K146	S228	A149	F276	A149
	F276	K146	R277		F276	A150	H278		D230	A149	D230	A150	R277	A150
	R277	A150	H278		R277		E282		F276	A150	F276	R151	H278	
	H278		S279		H278				R277		H278			
	S279		E282		E282				H278		S279			
	E282								E282		E282			
KIR3DL1*009	F9	G16	F9	G16	F9	G16	F9	G16	F9	G16	F9	G16	F9	G16
	S11	R17	S11	R17	S11	R17	S11	R17	S11	R17	W13	R17	S11	R17
	W13	G18	W13	G18	W13	E19	W13	E19	H29	E19	R27	E19	W13	E19
	H29	E19	H29	E76	H29	E76	H29	E76	K141	E76	H29	Q72	H29	E76
	S140	E76	L166	Y84	S140	N80	S140	R83	L166	R83	S140	E76	S140	I80
	L166	N80	A167	E89	L166	Y84	A167	Y84	P199	Y84	M165	R79	L166	R83
	P167	G83	P199	I142	A167	E89	Y200	N86	Y200	E89	L166	R83	P199	Y84
	P199	Y84	Y200	R145	P199	I142	S228	E89	E201	I142	A167	Y84	Y200	E89
	Y200	E89	S228	K146	S227	R145	D230	R145	S227	R145	E201	E89	S227	A90
	S228	I142	D230	A150	S228	K146	F276	K146	S228	K146	S227	A90	S228	I142
	D230	R145	F276		D230	A149	R277		D230	A149	S228	R145	D230	R145
	F276	K146	R277		F276	A150	H278		F276	A150	D230	K146	F276	K146
	R277	A150	H278		R277		S279		R277		F276	A149	R277	A149
	H278		S279		H278		E282		H278		H278	R151	H278	A150
	S279		E282		E282				E282		S279			

Table S2. HLA-B/KIR3DL1 H-bond Analysis

KIR	H-Bond Residues													
	<i>Bw6 epitope</i>							<i>Bw4 epitope</i>						
	HLA-B*07:02		HLA-B*14:02		HLA-B*35:01		HLA-B*27:05		HLA-B*51:01		HLA-B*57:01		HLA-B*58:01	
	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA	KIR	HLA
KIR3DL1*001	S11	G16	K141	E19	K141	E19	K141	E19	K141	E19	H29	R17	K141	E19
	K141	E19	D230	R145	A167	E76	H278	R83	H278	R83	G138	R79	D230	R145
	A167	E76	S279	K146	D230	R145	D230	R145	S279	R145	S140	R79	S279	K146
	D230	R145	E282	K146	D230	R145	S279	K146	D230	R145	H278	R83		
	S279	K146		A149	S279	K146	E282	K146	S279	K146	S279	R83		
	E201	A149	E201	R151	E282	K146	E201	A149	E282	K146	S228	R145		
					E201	A149	E201	R151	E201	A149	D230	R145		
											E282	K146		
											E201	A149		
											R151			
KIR3DL1*005	S11	G16	S11	G16	S11	G16	S11	G16	S11	G16	H29	R17	S11	G16
	S140	E19	S140	E19	K141	E19	S140	E19	K141	E19	G138	R79	S140	E19
	A167	E76	R277	Y84	D230	R145	H278	R83	H278	R83	S140	R79	H278	R83
	G138	R79	D230	R145	E282	K146			S228	R145	H278	R83	S279	Y84
	D230	R145	S279	K146			D230	R145	D230	R145	S279	R83	D230	R145
	S279	K146	E282	K146			S279	K146	S279	K146	S228	R145	E282	K146
	E282	K146	E201	A149			E282	K146	E282	K146	D230	R145		
	E201	A149					E201	A149	E201	A149	E282	K146		
											E201	A149		
											R151			
KIR3DL1*007/015	S11	G16	S11	G16	S11	G16	S11	G16	S11	G16	H29	R17	S11	G16
	K141	E19	S140	E19	S140	E19	S140	E19	K141	E19	G138	R79	S140	E19
	A167	E76	H278	N80	K141	E19	H278	R83	H278	R83	S140	R79	H278	R83
	D230	R145	R277	Y84	E282	K146			S228	R145	H278	R83	S279	Y84
	S279	K146	S279	K146			S279	Y84	D230	R145	S279	R83	D230	R145
	E201	A149	D230	R145			S279	K146	E282	K146	S228	R145		
			S279	K146			D230	R145	E201	A149	D230	R145		
			E282	K146			S279	K146			E282	K146		
			E201	A149			E282	K146			E201	A149		
							E201	A149			R151			
KIR3DL1*009	S11	G16	S11	G16	S11	G16	S11	G16	S11	G16	H29	R17	S11	G16
	A167	E76	S140	E19	S140	E19	S140	E19	K141	E19	G138	R79	S140	E19
	D230	R145	H278	N80	K141	E19	H278	R83	H278	R83	S140	R79	S279	Y84
	S279	K146	R277	Y84	E282	K146			S228	R145	H278	R83	D230	R145
	E201	A149	S279	K146			D230	R145	E282	K146	S279	R83		
			D230	R145			S279	K146	E201	A149	S228	R145		
			S279	K146			E282	K146			D230	R145		
			E201	A149			E201	A149			E282	K146		
											E201	A149		
											R151			

Table S3. H-bound between amino acid residues belonging to HLA-B and LILRB1 molecules.

LILRB1s Haplotypes	H-Bond Ile 194								H-Bond Val 194					
	HLA-B*07:02		HLA-B*14:02		HLA-B*27:05		HLA-B*57:01		HLA-B*35:01		HLA-B*51:01		HLA-B*58:01	
	LIR	HLA	LIR	HLA	LIR	HLA	LIR	HLA	LIR	HLA	LIR	HLA	LIR	HLA
LILRB1.01	Arg36	Asp196	Arg36	Asp196	Tyr76	Asp196	Arg36	Asp196	Tyr76	Asp196	Lys41	Glu198	Arg36	Asp196
	Tyr76		Tyr76		Arg36		Tyr76		Arg84	Lys41			Glu198	Arg84
	Tyr38	His197	Lys41	Glu198	Lys41	Glu198	Lys41	Glu198					Lys41	Glu198
	Lys41	Glu198		Thr200										
			Thr200											
	LILRB1.02	Tyr76	Asp196	Tyr76	Asp196	Tyr76	Asp196	Arg36	Asp196	Arg36	Asp196	Tyr76	Asp196	Tyr76
Tyr38		His197	Lys41	Glu198	Arg36			Arg84		Tyr38	His197	Arg84		Asp196
Lys41		Glu198		Thr200	Tyr38	His197	Lys41	Glu198	Lys41	Glu198	Lys41	Glu198	Lys41	Glu198
					Lys41	Glu198		Lys41						
						Thr200								
LILRB1.03	Tyr76	Asp196	Tyr76	Asp196	Tyr76	Asp196	Arg36	Asp196	Arg36	Asp196	Arg36	Asp196	Tyr76	Asp196
	Lys41	Glu198	Lys41	Glu198			Arg36		Tyr76	Lys41	Glu198	Lys41	Glu198	
		Thr200		Thr200	Tyr38	His197	Lys41	Glu198					Lys41	Glu198
					Lys41	Glu198		Thr200						
							Thr200							

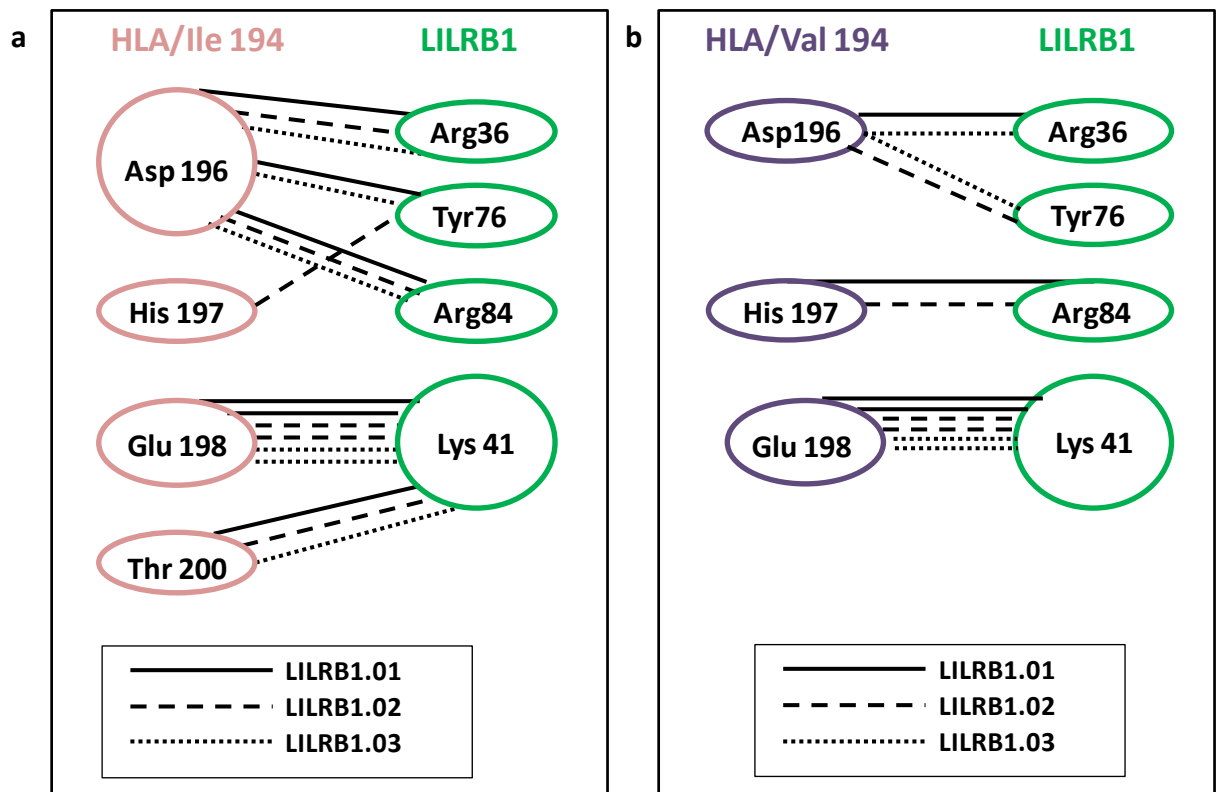


Figure S1. Scheme of amino acid residues involved in H-bond between LILRB1 residues (Green) and HLA-B alleles carrying Ile 194 (a) or Val 194 (b). Continuous line, segmented line and dotted line represents H-bond respectively in LILRB1.01, LILRB1.02 and LILRB1.03 haplotypes.

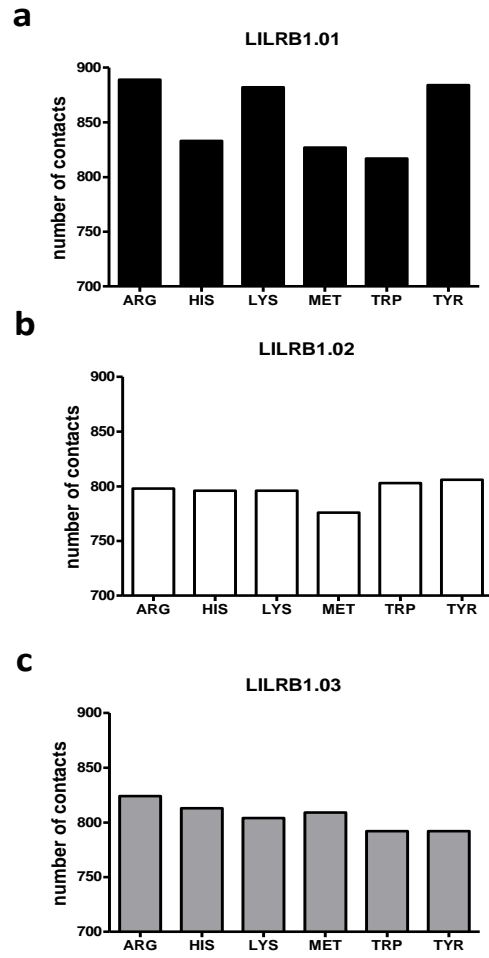


Figure S2. Number of contacts between HLA.B*27:05 and LILRB1.01 (a), LILRB1.02 (b) and LILRB1.03 (c) haplotypes in presence of peptide position 1 amino acid residues.