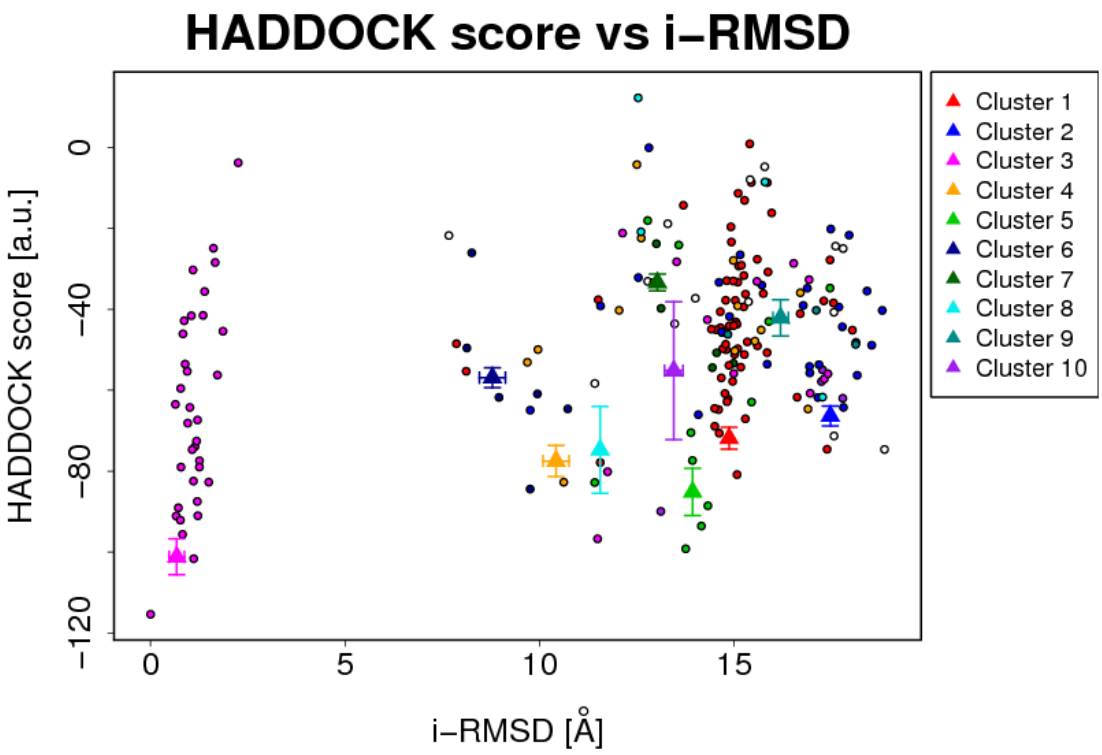
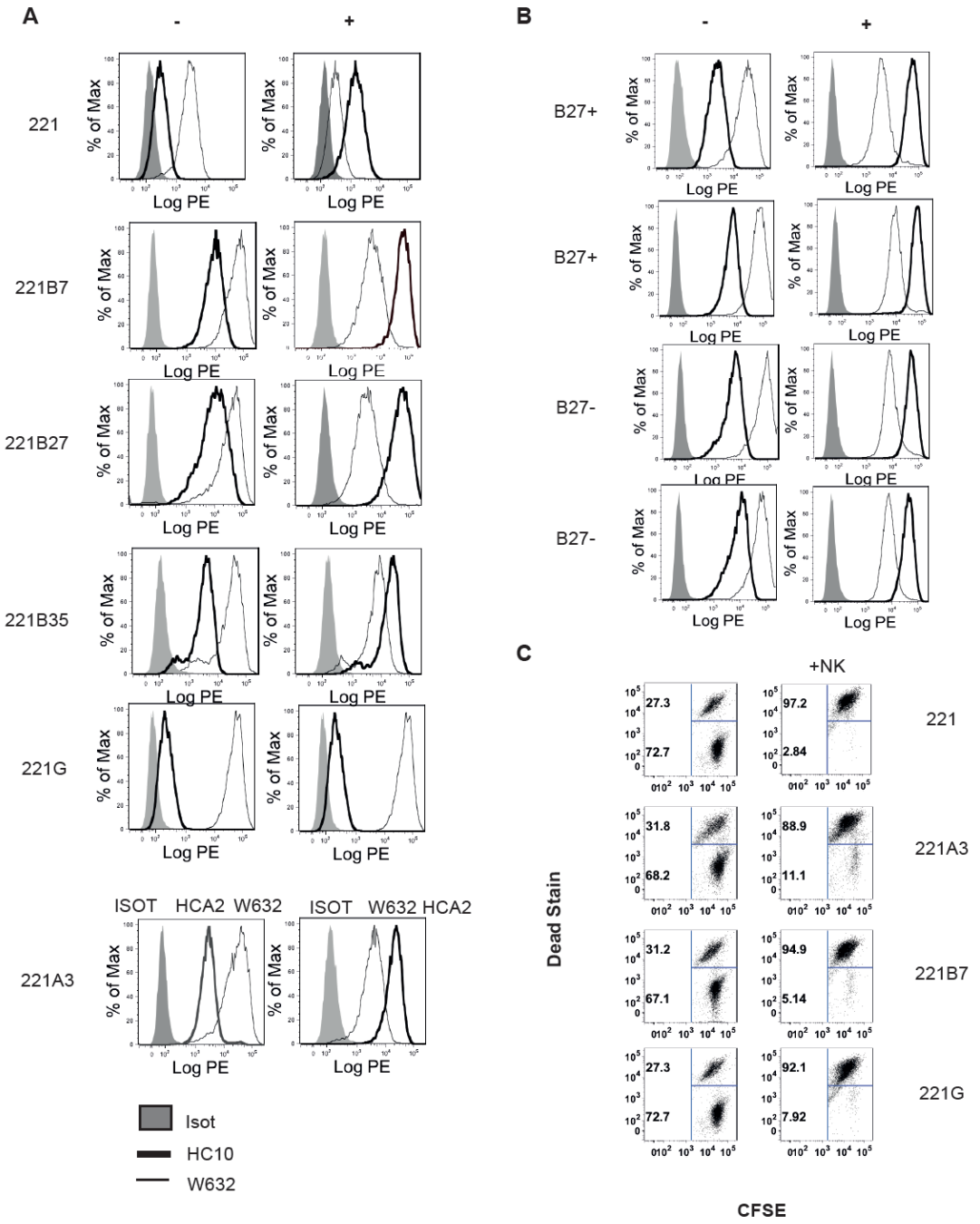


Suppl. Figure 1: The image shows plots interface RMSD against scores for complexes predicted by HADDOCK for the B27 dimer and KIR3DL2. The interface RMSD calculations are taken against a structure generated by alignment of B27 dimer and KIR3DL2 to the structure in PDB 3vh8. The best scoring cluster (Cluster 3) from HADDOCK contains structures with less than 2.5 Å interface RMSD with the structure generated via structural alignment.

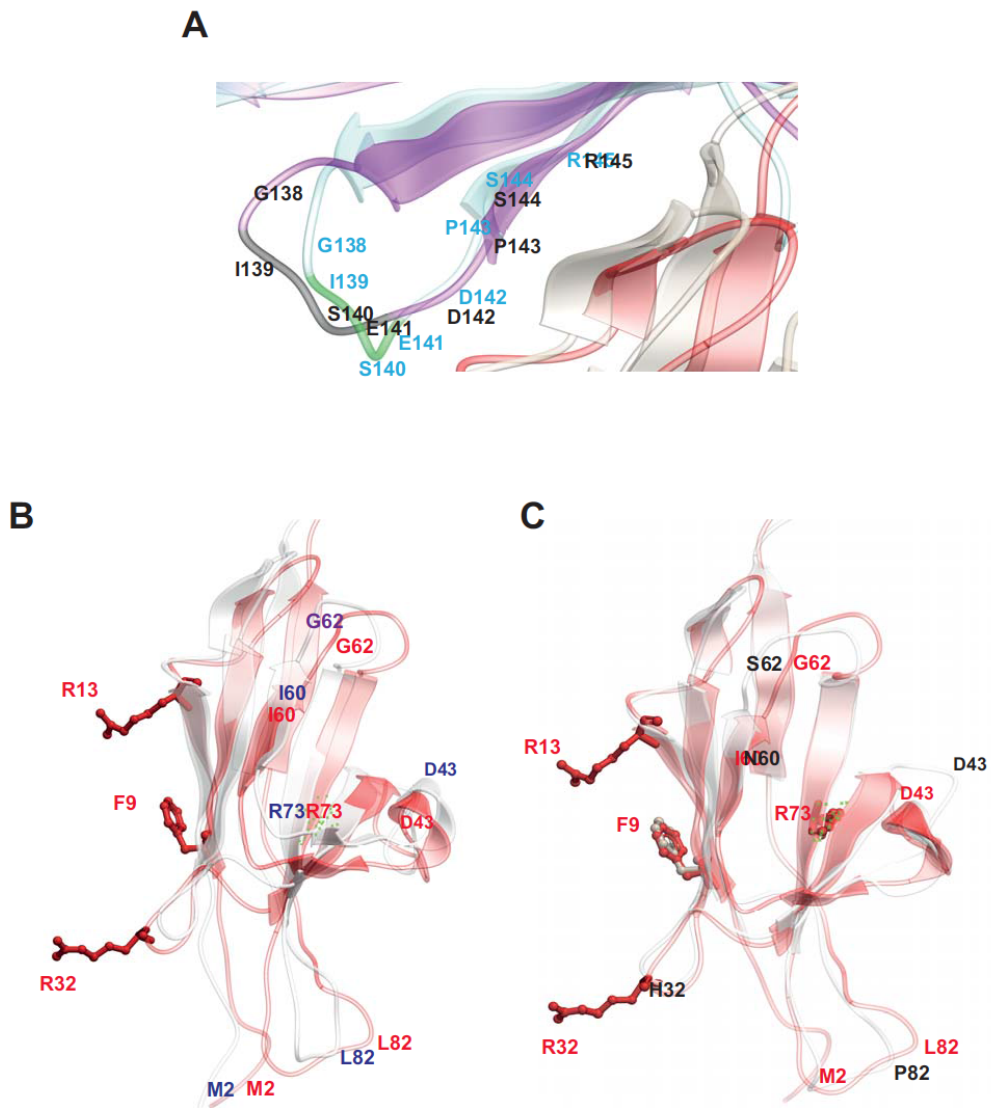


Suppl. Fig. 2A. Representative FACS stain of HLA-class I transfected LCL.721.221 cells before (-) and after (+) acid treatment with the class I antibody W632 and class I heavy chain antibodies HC10 and HCA2. **B** Representative FACS stains of EBV-transformed B cell lines from B27+ and B27-donors before (-) and after (-) acid treatment stained with W632 and HC10 antibodies. Representative stains from 1 of 3 independent experiments. **C** Representative FACS stain of CFSE-labelled parental or transfected LCL.721.221 cells with Dead Stain after 6 hour incubation with or without KIR3DL2+NK cells. Representative stains from 1 of 3 independent experiments.

Table I. Predicted contact residues between HLA-B27 free heavy chain dimers and KIR3DL2. Residues in bold form potential H-bonds.

B27 Chain	HLA-B27 Residue Number	KIR3DL2 Residue Number	HLA-B27 interface	HLA-B27 Hot Spot	KIR3DL2 Interface	KIR3DL2 Hotspot
A	GLN54	ARG73	180	123	180	53
A	GLN54	ARG73	180	123	180	53
A	GLN54	PRO91	180	123	180	0
A	**ARG62**	**GLU141**	**180**	**84**	**180**	**58**
A	**ARG62**	**ASP142**	**180**	**84**	**180**	**0**
A	**ARG62**	**PRO143**	**180**	**84**	**180**	**0**
A	**ARG62**	**SER144**	**180**	**84**	**180**	**95**
A	**ARG108**	**PHE129**	**180**	**175**	**171**	**1**
A	**ARG108**	**GLU130**	**180**	**175**	**180**	**111**
A	ARG108	VAL147	180	175	180	180
A	**ARG108**	**GLY148**	**180**	**175**	**180**	**0**
A	ARG108	VAL147	180	175	180	123
A	GLU163	LEU146	180	0	180	180
A	GLU166	VAL147	180	180	180	180
A	**ARG169**	**GLU130**	**180**	**127**	**180**	**111**
A	**ARG169**	**HIS131**	**180**	**127**	**180**	**41**
A	ARG169	VAL147	180	127	180	180
A	**ARG170**	**ARG145**	**180**	**1**	**180**	**180**
AB	GLU177	ARG44	180	32	180	9
A	**THR178**	**ASP43**	**180**	**32**	**180**	**48**
A	GLN180	ARG44	180	0	180	9
A	LYS186	MET2	180	0	180	1
A	LYS186	GLY3	180	0	179	0
A	LYS268	LEU82	180	0	180	17
A	**LYS 268**	**LEU82**	**180**	**0**	**180**	**17**
A	LYS268	THR83	180	0	180	0
B	GLY16	PHE9	180	0	180	6
B	**GLY16**	**HIS29**	**180**	**0**	**180**	**0**
B	GLY16	PHE34	180	0	180	0
B	ARG17	PHE9	178	0	180	6
B	GLY18	PHE9	180	0	180	6
B	GLN72	MET165	177	0	180	0
B	ASP77	VAL167	180	0	180	50
B	THR80	ILE139	180	0	180	101
B	THR80	VAL167	180	0	180	50
B	**ARG83**	**GLY138**	**180**	**0**	**180**	**0**
B	ARG83	ILE139	180	0	180	101
B	**SER88**	**ARG13**	**180**	**0**	**180**	**0**
B	SER88	GLN27	180	0	158	0
B	GLU89	ARG13	180	0	180	0
B	ALA90	ARG13	180	2	180	0
B	**ARG145**	**SER228**	**180**	**42**	**180**	**1**
B	ARG145	ASP230	180	42	180	0
B	LYS146	PHE276	180	33	180	174
B	ALA149	SER227	180	177	180	2
B	**ALA150**	**LEU199**	**180**	**0**	**180**	**0**
B	ALA150	TYR200	180	0	180	169
B	ALA150	GLU201	180	0	180	0
B	**ARG151**	**GLU201**	**180**	**0**	**180**	**0**

The number of interface and hot spots indicates the number of times the residue was predicted in 180 snapshots from the tail end of the molecular dynamics simulation.



Suppl Figure 3. Predicted conformational changes in KIR3DL2 upon binding to B27 FHC dimer. A. Molecular model of the D1 domain of KIR3DL2 bound to B27 FHC dimer (purple) overlaid on unbound KIR3DL2 (light blue). The positions of key residues in KIR3DL2 for binding to B27 FHC dimer and their relative orientations in the bound and unbound molecules are also indicated in black and blue respectively. **B.** Molecular model of the D0 domain of KIR3DL2 bound to B27 FHC dimer (red) overlaid on unbound KIR3DL2 (white). The positions of key residues in KIR3DL2 for binding to B27 FHC dimer and their relative orientations in the bound and unbound molecules are indicated in red and dark blue respectively. C. Molecular model of the D0 domain of KIR3DL2 bound to B27 FHC dimer (red) overlaid on the D0 domain of KIR3DL1 bound to HLAB57 (white). The positions of key residues in KIR3DL2 for binding to B27 FHC dimer and their relative orientations to residues in the bound KIR3DL1 molecule are indicated red and black respectively.