

Supporting Information

MOLECULAR DYNAMICS SIMULATION OF HLA-CW4- B2M- KIR2DL1 PROTEIN AND HOMOLGY MODELING OF A COMPLEX ASSOCIATED WITH PSORIASIS DISEASE (HLA- CW6-B2M-KIR2DS1)

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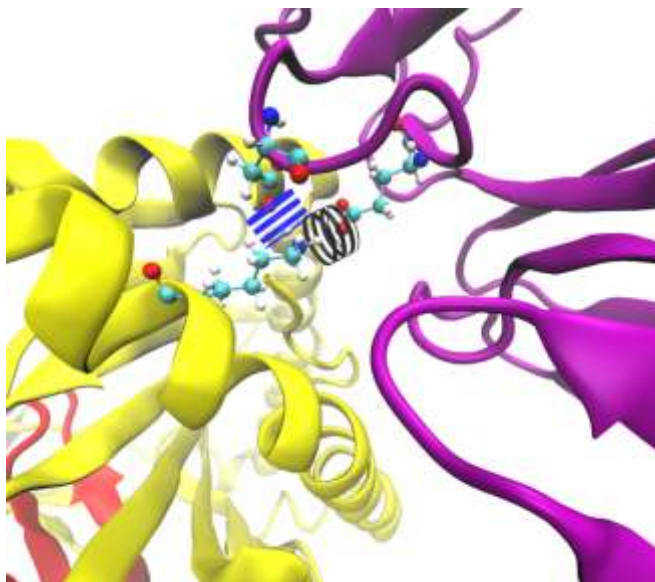


Fig. S1. Snapshot illustrating inter-molecular H-bonds between Lys80 from chain A with Asp183 from chain D (the H-bond is indicated by a dashed blue line) and Lys80 from chain A with Glu187 from chain D (the H-bond is indicated by a dashed black line).

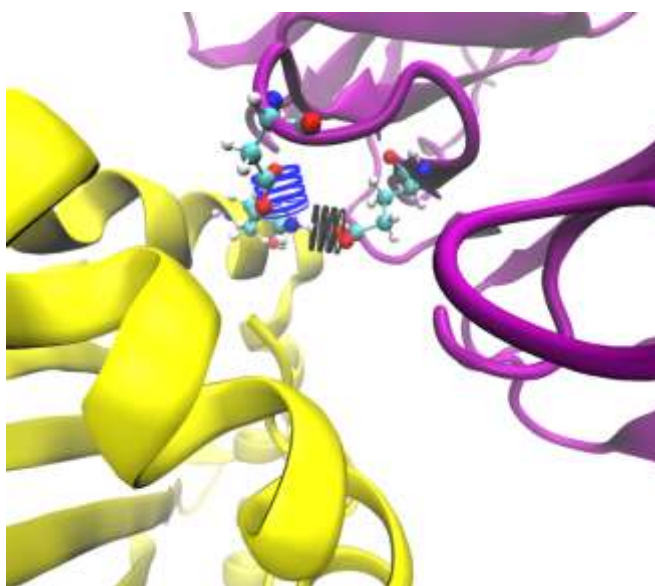


Fig. S2. Snapshot illustrating inter-molecular H-bonds between Lys146 from chain A with Asp183 from chain D (the H-bond is indicated by a dashed blue line) and Lys146 from chain A with Glu187 from chain D (the H-bond is indicated by a dashed black line).

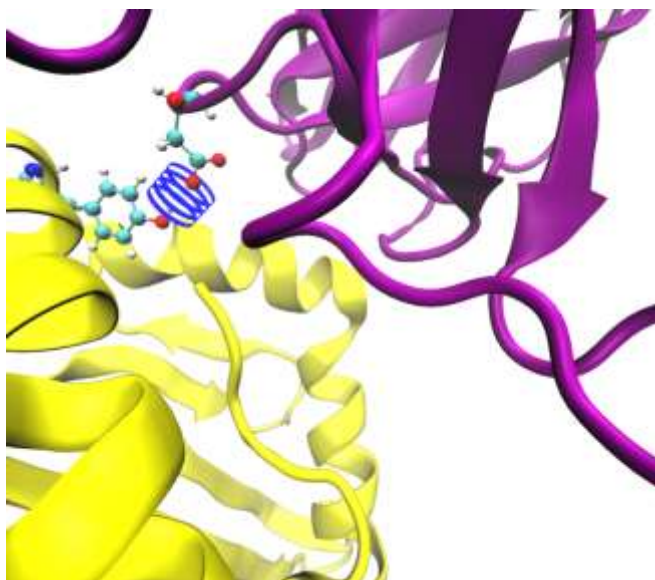


Fig. S3. Snapshot illustrating inter-molecular H-bonds between Tyr84 from chain A with Asp183 from chain D (the H-bond is indicated by a dashed blue line).

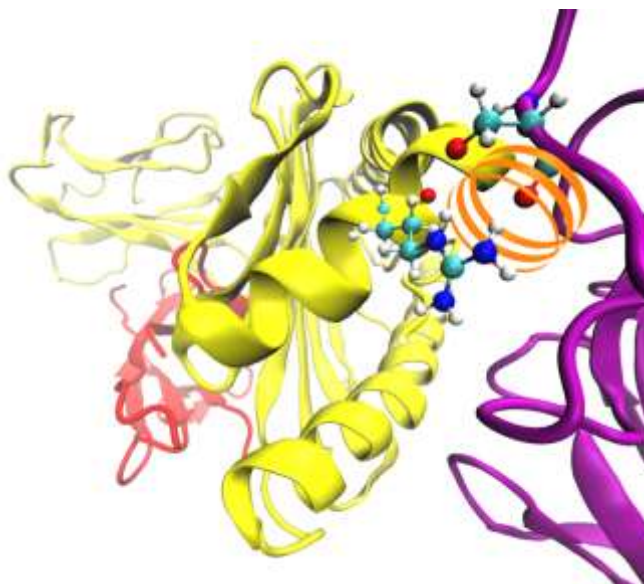


Fig. S4. Snapshot illustrating inter-molecular H-bonds between Arg145 from chain A with Ser133 from chain D (the H-bond is indicated by a dashed orange line).

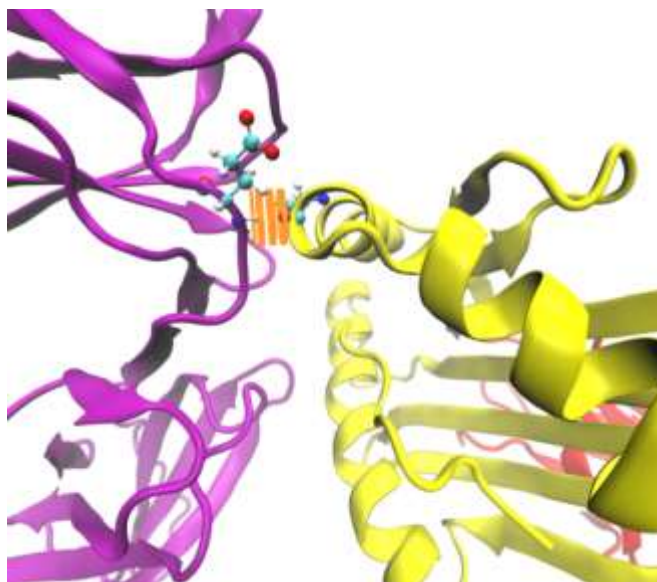


Fig. S5. Snapshot illustrating inter-molecular H-bonds between Ala149 from chain A with Glu106 from chain D (the H-bond is indicated by a dashed orange line).

Table S1

Hydrogen bonds between the ligand HLA-Cw4 and its specific peptide.

HLA-Cw4 Specific Peptide	HLA- Cw4	Occupancy
PAla ⁵ -Main-O	Arg ¹⁵⁶ -Side-NH1	58.00%
PLys ⁸ -Main-O	Trp ¹⁴⁷ -Side-NE1	56.00%
PLeu ⁹ -Main-N	Asn ⁷⁷ -Side-OD1	50.00%
PTyr ⁷ -Side-OH	Asp ⁷⁴ -Side-OD1	46.00%
PAsp ³ -Side-OD1	Arg ⁹⁷ -Side-NH1	42.00%
PAsp ⁴ -Side-OD1	Lys ⁶⁶ -Side-NZ	42.00%
PLeu ⁹ -Side-OT2	Lys ¹⁴⁶ -Side-NZ	38.00%
PAsp ³ -Side-OD2	Arg ⁹⁷ -Side-NH1	32.00%
PTyr ² -Main-O	Lys ⁶⁶ -Side-NZ	32.00%
PGln ¹ -Main-O	Tyr ¹⁵⁹ -Side-OH	30.00%
PAsp ³ -Side-OD2	Arg ⁹⁷ -Side-NH1	30.00%
PAsp ³ -Side-OD1	Arg ⁹⁷ -Side-NH2	26.00%
PTyr ⁷ -Main-O	Asn ⁷⁷ -Side-ND2	22.00%
PLeu ⁹ -Side-OT1	Lys ⁸⁰ -Side-NZ	22.00%
PGln ¹ -Side-NE2	Glu ⁶³ -Side-OE2	18.00%
PAsp ⁴ -Side-OD2	Lys ⁶⁶ -Side-NZ	18.00%
PTyr ⁷ -Main-O	Gln ⁷⁰ -Side-NE2	16.00%
PTyr ⁷ -Side-OH	PGln ¹ -Main-N	16.00%
PGln ¹ -Main-N	Glu ⁶³ -Side-OE1	14.00%
PTyr ² -Side-OH	Gln ⁷⁰ -Side-OE1	14.00%
PLys ⁸ -Side-NZ	Glu ¹⁵² -Side-OE1	14.00%

PTyr ⁷ -Main-N	Gln ⁷⁰ -Side-OE1	14.00%
PVal ⁶ -Main-O	Arg ¹⁵⁶ -Side-NH2	12.00%
PAsp ³ -Side-OD1	Arg ¹⁵⁶ -Side-NH1	10.00%
PTyr ⁷ -Side-OH	Asp ⁷⁴ -Side-OD2	10.00%
PLeu ⁹ -Side-OT1	Lys ¹⁴⁶ -Side-NZ	8.00%
PGln ¹ -Side-NE2	Tyr ¹⁵⁹ -Side-OH	8.00%
PGln ¹ -Main-N	Glu ⁶³ -Side-OE2	6.00%
PTyr ² -Side-OH	PSer ⁹ -Side-OG	6.00%
PTyr ² -Side-OH	Arg ⁹⁷ -Side-NH1	6.00%
PLeu ⁹ -Side-OT2	Lys ⁸⁰ -Side-NZ	6.00%
PAsp ⁴ -Side-OD2	Tyr ¹⁵⁹ -Side-OH	4.00%
PAsp ⁴ -Side-OD1	Tyr ¹⁵⁹ -Side-OH	4.00%
PTyr ⁷ -Side-OH	Asn ⁷⁷ -Side-ND2	4.00%
PGln ¹ -Side-OE1	Lys ⁶⁶ -Side-NZ	2.00%
PGln ¹ -Side-NE2	Trp ¹⁶⁷ -Side-NE1	2.00%
PGln ¹ -Side-NE2	Tyr ¹⁷¹ -Side-OH	2.00%
PGln ¹ -Side-OE1	Tyr ¹⁵⁹ -Side-OH	2.00%
PAsp ³ -Side-OD2	Arg ¹⁵⁶ -Side-NH1	2.00%
PAsp ³ -Main-O	Lys ⁶⁶ -Side-NZ	2.00%
PLys ⁸ -Side-NZ	Glu ¹⁵² -Side-OE2	2.00%

Table S2**Nonbonded Interactions between KIR2DL1 and HLA-Cw4.**

KIR2DL1	HLA-Cw4	Nonbonded	Elec	vdW
Asp ¹⁸³	Lys ¹⁴⁶	-105.681	-107.447	1.7658
Glu ¹⁰⁶	Arg ¹⁵¹	-91.406	-92.3041	0.8981
Asp ¹³⁵	Arg ¹⁴⁵	-91.0549	-91.7595	0.7056
Glu ¹⁸⁷	Lys ⁸⁰	-80.0464	-81.0005	0.9542
Ser ¹³³	Arg ¹⁴⁵	-27.4284	-27.1864	0.2421
Asp ¹⁸³	Tyr ⁸⁴	-15.6974	-16.064	0.3666
Met ⁴⁴	Arg ⁷⁹	-8.08945	-5.3702	-2.7193
Tyr ¹⁰⁵	Lys ¹⁴⁶	-5.5869	-3.3145	-2.2724
Phe ⁴⁵	Arg ⁷⁵	-4.2565	0.8282	-4.2565
Tyr ¹⁰⁵	Ala ¹⁴⁹	-4.2084	-2.0087	-2.1997
Asp ⁷²	Val ⁷⁶	-4.1351	-3.0198	-1.1153
Phe ¹⁸¹	Lys ¹⁴⁶	-1.6768	1.3306	-3.0074
Phe ⁴⁵	Val ⁷⁶	-1.2849	-0.0905	-1.944
Ser ¹³²	Ala ¹⁴⁹	-1.1198	-0.3506	0.7692
Phe ⁴⁵	Arg ⁷⁹	-0.5779	0.009	-0.587
Met ⁴⁴	Lys ⁸⁰	-0.567	2.1283	-2.6953
Ser ¹⁸⁴	Lys ¹⁴⁶	1.98008	2.2654	-0.2854