

(A) MEL8-HLA A*02:01-EAAGIGILTV**(B)**

CDR loop	TCR residue	Peptide residue	MHC residue	Number of VdW (≤ 4 Å)	Number of H-bonds (≤ 3.4 Å)	Number of Salt Bridges
CDR1 α	Gly29		Lys66	1		
			Trp167	2		
	Gln31		Glu1	2		
			Lys66	1		
	Ser32		Tyr159	2		
			Thr163	2		
			Ala2			1
			Gly4	4		1
			Ile5	1		
	CDR2 α	Tyr51		Gly4		
Ile5				1		
Glu154				2		
Gln155				4		
FW α	Lys67		Ala158	1		
			Ile5	1		
CDR3 α	Lue94		Arg65	4		
CDR1 β	Glu30		Thr163			1
			Glu166	1		
CDR2 β	Tyr48	Val50	Arg65	7		1
			Ala69	3		
			Gln72	2		
	Ala52		Gln72	4		
			Gln72	1		1
	Asp56		Arg75			1
			Lys68	3		
CDR3 β	Tyr95	Thr98	Lys68	3		2
			Lys68	3		
	Glu99		Thr9	4		1
			Ala69	1		
			Ala3	1		
			Gly4	6		
			Ile5	5		
			Gly6	1		
			Ile7	10		2
	Ala100		Ala150	1		1
			Gln155	11		1
			Gly4	1		
			Ile5	1		
		Ile7	1			
		Gln155	3		1	

CDR loop	TCR residue
CDR1 α	Arg28
	Gly29
	Gln31
CDR2 α	Ser32
	Tyr51
FW α	Lys67
CDR3 α	Asn92
	Ala94
	Gly95
CDR1 β	Lys96
	Asn30
CDR2 β	Tyr49
	Val51
CDR3 β	Gln55
	Glu59
	Thr96
	Gly97
	Leu98

Thr101	Ala150	6	1
	Gln155	1	
Tyr102	Ala150	1	
	Lue8	2	

Gly99
Thr100

) MEL5-HLA A*02:01-LLLIGILVL

(C) MEL5-HLA A*02:01-

Peptide residue	MHC residue	Number of VdW (≤ 4 Å)	Number of H-bonds (≤ 3.4 Å)	Number of Salt Bridges
	Glu166	5	2	
	Trp167	1	1	
	Trp167	4		
Lue1		1		
	Lys66	1		
	Tyr159	2		
	Thr163	2		
Lue1		1		
Lue2			1	
Lue3		3		
Gly4		5	2	
Ile5		3		
Ile5		1		
	His151	1		
	Glu154	3		
	Gln155	5		
	Ala158	1		
	Thr163		1	
Gly4		2	1	
Ile5		1		
	Gly62	6		
	Arg65	7	2	
	Lys66	3		
	Arg65	7		
	Val76	2		
	Arg65	4		
	Lys68	1		
	Ala69	1		
	Gln72	3		
	Gln72	1		
	Arg75	1		
	Arg65	2	2	
Val9		2		
	Ala69	2		
	Thr73	2		
Ile7		2		
	Lys66	1		
	Ala69	2		
	His70	2		
Leu3		1		
Gly4		2		

CDR loop	TCR residue	Peptide residue	MHC residue
CDR1 α	Arg28		Trp167
	Gly29		Trp167
	Gln31		Tyr159
			Thr163
			Asn1
		Leu2	
		Ser3	
		Ala4	
		Leu5	
	Ser32	Leu5	
CDR2 α	Tyr51		Glu154
			Gln155
			Ala158
CDR3 α	Gln92	Ala4	
	Ala94		Gly62
			Arg65
			Lys66
	Gly95	Ala4	
	Lys96		Arg65
CDR1 β	Asn30		Val76
CDR2 β	Tyr49		Arg65
	Val51		Ala69
			Gln72
	Gln55		Gln72
	Glu59		Arg75
			Arg65
CDR3 β	Glu95	Phe8	
	Thr96	Ser9	
	Gly97		Thr73
		Ile7	
	Leu98		Lys66
			Ala69
			His70
		Ser3	
		Ala4	
		Lue5	
	Gly6		
	Ile7		
	Gly99		Gln155
	Ala4		
	Lue5		

Ile5		5	
Gly6		2	1
Ile7		7	3
	Gln155	3	
Gly4		1	
Ile5		3	
Ile7		1	
Lue8		1	
	Gln155	2	

	Ile7	
Thr100		Gln155

NLSALGIFST

(D) MEL8-HLA A*02:01-LLLIGILVL Model

Number of VdW ($\leq 4 \text{ \AA}$)	Number of H-bonds ($\leq 3.4 \text{ \AA}$)	Number of Salt Bridges
3	1	
1		
1		
5		
1		
	1	
2		
6	1	
3		
2		
<hr/>		
2		
5		
1		
<hr/>		
1	1	
3		
4	1	
5		
1		
2		
<hr/>		
4		
<hr/>		
2		
1		
5		
2	1	
2	1	
1	1	
<hr/>		
1		
3		
1		
2		
2		
2		
2		
2		
1		
6		
3		
2	1	
5	4	
3		
1	1	
2		

CDR loop	TCR residue	Peptide residue	MHC residue	Number of VdW ($\leq 4 \text{ \AA}$)	Number of H-bonds ($\leq 3.4 \text{ \AA}$)	
CDR1 α	Gln31		Tyr159	5		
		Lue2		1		
		Lue3		2		
		Gly4		2		
		Ile5		5		
CDR2 α	Tyr51	Ser32		3		
			Glu154	6		
			Ala158	1		
		Ile5		2		
FW α	Lys67		Thr163	1		
CDR3 α	Gln92	Gly4		3		
CDR1 β	Glu30		Gln72	1		
			Val76	6		
CDR2 β	Tyr48		Arg65	8	2	
		Val50	Lys68	1		
			Gln72	4		
		Gly51	Gln72	6		
		Ala52	Gln72	2	1	
		Ile54	Gln72	1		
			Arg75	1		
		Asp56	Arg65	1		
	Lys68	7				
	Gln57	Arg65		1		
CDR3 β	Tyr95		Lys146	2	1	
			Val9	2		
		Ser96	Ile7		1	
			Lue8	2		
		Thr98	Gly4	5	1	
			Ile5	5	2	
			Gly6	2	1	
			Ile7	3	1	
			Leu8	2		
			Glu99	Ala150	1	
				Gln155	11	1
				Gly4	1	
				Ile5	11	
		Gly6	5			
		Leu8	2			
	Ala100	Ile5	1			
	Thr101		Ala150	8	1	
			Gln155		1	

1

4

1

Tyr102

Lys146

8

Lue8

3

(E) MEL8-HLA-A*02:01-NLSALGIFST Model

Number of Salt Bridges	CDR loop	TCR residue	Peptide residue	MHC residue	Number of VdW ($\leq 4 \text{ \AA}$)	Number of H-bonds ($\leq 3.4 \text{ \AA}$)	Number of Salt Bridges	
	CDR1 α	Gln31		Tyr159	7			
					Thr163	6	1	
					Lue2	1		
					Ala4	4		
					Lue5	7		
	CDR2 α	Ser32	Lue5		2			
		Tyr51		Glu154	4			
				Ala158	2			
			Lue5		1			
	CDR3 α	Gln92	Ala4		2			
			Leu94		Arg65	1		
	CDR1 β	Glu30		Gln72	1			
	CDR2 β	Tyr48		Arg65	12	1		
			Val50		Gln72	1		
			Gly51		Gln72	4		
			Ala52		Gln72	1		
					Arg75	1		
		Ile54		Lys68	4			
	CDR3 β	Tyr95		Lys146		1		
				Phe8		5		
				Ser9		2		
			Thr98	Ser3		1		
				Ala4		12		
				Lue5		12		
				Gly6		3	1	
				Ile7		12	1	
			Glu99		Gln155	10	2	
				Ala4		1		
				Lue5		1		
				Gly6		1		
				Phe8		4		
			Ala100		Gln155	2	1	
				Leu5		1		
		Thr101		Ala150	5	1		
		Tyr102		Ala150	1			
				Phe8	9			

