

Table S1. Test parameters of the modelled structures

Modelled structure	Test parameters		
	Alpha Chain	Beta Chain	Heterodimer
HLA-A*11:02	Template:5WJL	Template:5WJL	Ligand RMSD:0.977
	Template Resolution:3.15 Å		Clashscore:2.31
	Template Allele: HLA-A*11:01		Poor rotamers:3.37%
	Identity:0.99		Ramachandran
	Verify Score:0.9891		avored:97.30%
	Verify Score:87.0079		Molprobit score:1.54
	Core:0.92		Total RMSD:0.005
	Allow:0.076		
	Gener:0		
	Disall:0.004		
HLA-A*26:01	Template:6AT9	Template:6AT9	Ligand RMSD:0.796
	Template Resolution:2.95 Å		Clashscore:4.86
	Template Allele: HLA-A*01:01		Poor rotamers:1.22%
	Identity:0.91		Ramachandran
	Verify Score:0.9891		avored:96.76%
	Verify Score:80.8765		Molprobit score:1.52
	Core:0.88		Total RMSD:0.113
	Allow:0.116		
	Gener:0.004		
	Disall:0		
HLA-A*33:03	Template:5WJL	Template:5WJL	Ligand RMSD:0.981
	Template Resolution:3.15 Å		Clashscore:2.55
	Template Allele: HLA-A*11:01		Poor rotamers:3.67%
	Identity:0.93		Ramachandran
	Verify Score:0.9635		avored:97.30%
	Verify Score:92.8571		Molprobit score:1.6
	Core:0.917		Total RMSD:0.047
	Allow:0.079		
	Gener:0		
	Disall:0.004		
HLA-A*31:01	Template:5WJL	Template:5WJL	Ligand RMSD:0.397
	Template Resolution:3.15 Å		Clashscore:2.78
	Template Allele: HLA-A*11:01		Poor rotamers:3.66%
	Identity:0.93		Ramachandran
	Verify Score:0.9599		avored:97.30%
	Verify Score:92.4603		Molprobit score:1.63
	Core:0.917		Total RMSD:0.413
	Allow:0.079		
	Gener:0		
	Disall:0.004		