

Summary of integrative structure determination of Docking model of HLA class I with HLA class II (PDB ID: 9A0U, PDB-Dev ID: PDBDEV_00000066)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN): chain(s) A (275 residues) - BETA 2-MICROGLOBULIN: chain(s) B (100 residues) - INFLUENZA A MATRIX PROTEIN M1 (RESIDUES 58-66): chain(s) C (9 residues) - GLY residue: chain(s) D, H (1 residues) - HLA class II histocompatibility antigen, DR alpha chain: chain(s) E (179 residues) - HLA class II histocompatibility antigen, DRB1-4 beta chain: chain(s) F (193 residues) - Alpha-enolase: chain(s) G (14 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 1HHI - Experimental model, PDB: 5NI9 - Crosslinking-MS data, PRIDE: PXD022675 - Other, Not available - Other, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	8, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 13 crosslinks - 1 unique DerivedDistanceRestraint: Upper Bound Distance: 73.0 - 14107 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	2
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 9.80-10.53 - Ramachandran outliers: 2-3 - Sidechain outliers: 45-50
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 61.54-69.23%
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Rigid-body minimization
<i>Method</i>	Rigid-body minimization in HADDOCK (it0)
<i>Number of computed models</i>	1000
2. <i>Name</i>	Simulated annealing
<i>Method</i>	Semi-flexible SA in HADDOCK (it1)
<i>Number of computed models</i>	200
3. <i>Name</i>	Refinement
<i>Method</i>	Water refinement in HADDOCK (itw)
<i>Number of computed models</i>	200
<i>Software</i>	Haddock (version 2.2)