DockTope: a Web-based tool for automated pMHC-I modelling.

Maurício Menegatti Rigo,

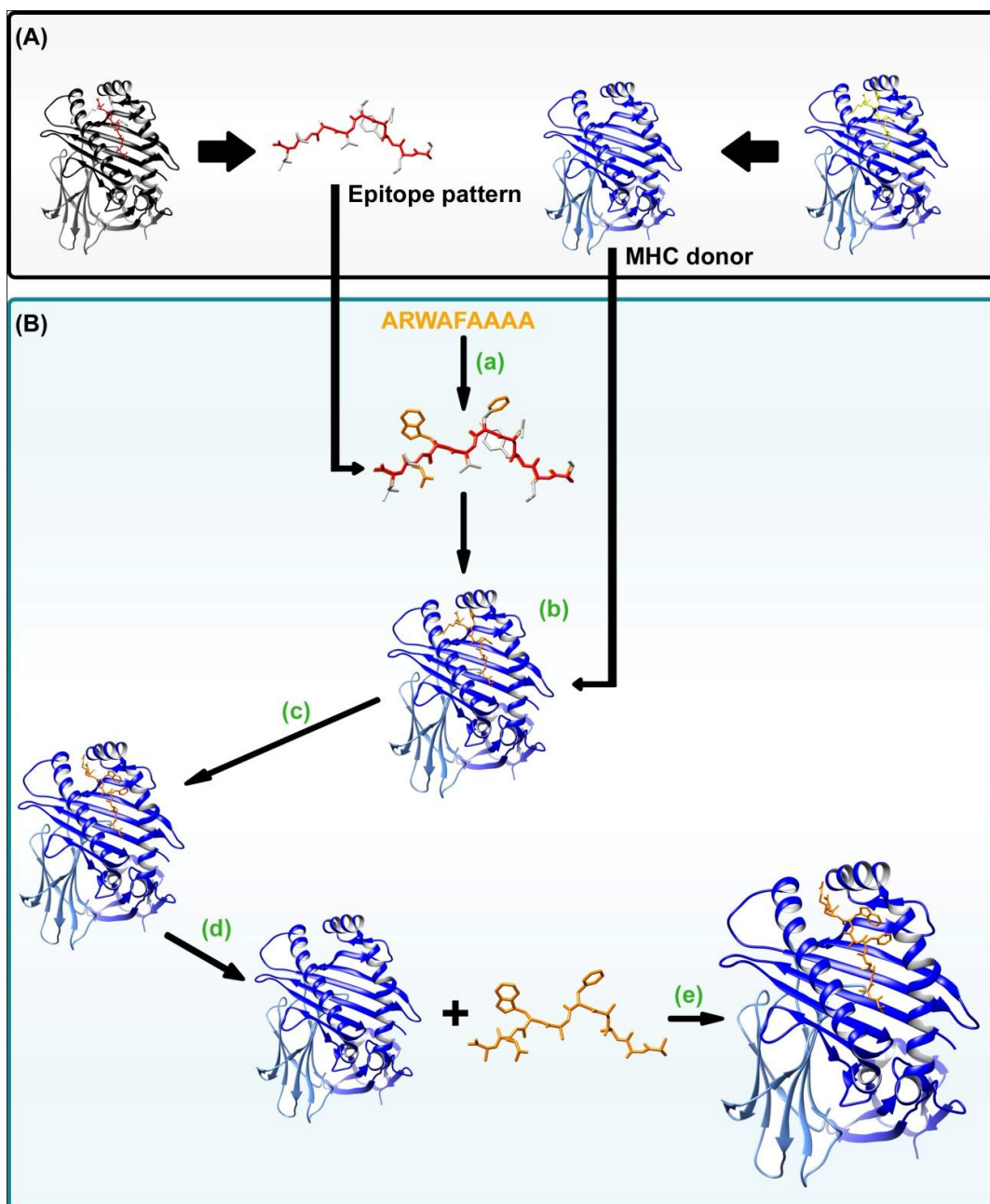Dinler Amaral Antunes,

Martiela Vaz de Freitas,

Marcus Fabiano de Almeida Mendes,

Lindolfo Meira,

Marialva Sinigaglia,

Gustavo Fioravanti Vieira.

Supplementary Figure S1. pMHC-I complex construction process employed by DockTope. In (A), the MHC donor and the epitope pattern were obtained for each allotype (Table 1 of the manuscript for details). In (B), the full automated process. The automation follows a sequence of steps: (a) structural alignment between the target and the modeled epitope, (b) first molecular docking between the MHC-I and the modeled epitope, (c) energy minimization, (d) separation of MHC-I and modeled epitope and (e) second molecular docking as a final refinement.

Supplementary Table S1. List of the 135 structures from PDB. Each structure was used to reproduce and validate DockTope, based on Cα and all atoms RMSD values for the epitope.

MHC-I Structure	PDB ID	Amino Acid Sequence	Sequence Length	RMSD (Cα)	RMSD (All atoms)
HLA-A*02:01	1B0G	ALWGFFPVL	9	1.349	2.446
HLA-A*02:01	1DUZ	LLFGYPVYV	9	0.996	2.739
HLA-A*02:01	1EEY	ILSALVGIV	9	0.557	1.053
HLA-A*02:01	1EEZ	ILSALVGIL	9	0.61	1.273
HLA-A*02:01	1HHG	TLTSCNTSV	9	1.082	2.391
HLA-A*02:01	1I1F	FLKEPVHGV	9	0.681	1.607
HLA-A*02:01	1I1Y	YLKEPVHGV	9	0.564	1.589
HLA-A*02:01	1I7R	FAPGFFPYL	9	1.532	3.575
HLA-A*02:01	1I7T	ALWGVFPVL	9	1.458	2.485
HLA-A*02:01	1I7U	ALWGFVPVL	9	0.836	1.566
HLA-A*02:01	1QEW	FLWGPRALV	9	0.907	2.038
HLA-A*02:01	1QR1	IISAVVGIL	9	1.39	2.053
HLA-A*02:01	1S8D	SLANTVATL	9	0.355	1.239
HLA-A*02:01	1S9X	SLLMWITQA	9	0.856	1.713
HLA-A*02:01	1S9y	SLLMWITQS	9	0.88	1.819
HLA-A*02:01	1T1W	SLFNTIAVL	9	0.327	1.409
HLA-A*02:01	1T1X	SLYLTVATL	9	0.417	1.239
HLA-A*02:01	1T1Y	SLYNVVATL	9	0.445	1.275
HLA-A*02:01	1T1Z	ALYNTAAAL	9	0.649	1.378
HLA-A*02:01	1T20	SLYNTIATL	9	0.453	1.395
HLA-A*02:01	1TVB	ITDQVPFSV	9	1.217	1.794
HLA-A*02:01	1TVH	IMDQVPFSV	9	1.093	1.813

HLA-A*02:02	2GIT	LLFGKPVYV	9	1.039	1.732
HLA-A*02:01	2GTW	LAGIGILTV	9	3.129	3.419
HLA-A*02:01	2GTZ	ALGIGILTV	9	1.435	1.493
HLA-A*02:01	2V2W	SLYNTVATL	9	0.605	1.253
HLA-A*02:01	2V2X	SLFNTVATL	9	1.384	2.403
HLA-A*02:01	2VLL	GILGFVFTL	9	0.788	2.475
HLA-A*02:01	2X4O	KLTPLCVTL	9	0.965	1.684
HLA-A*02:01	2X4S	AMDSNTLEL	9	1.258	2.042
HLA-A*02:01	2X4U	ILKEPVHGV	9	0.409	1.170
HLA-A*02:01	3D25	VLHDDLLEA	9	0.559	1.489
HLA-A*02:01	3FQT	GLLGSPVRA	9	1.135	1.652
HLA-A*02:01	3GSO	NLVPMVATV	9	0.603	1.337
HLA-A*02:01	3GSQ	NLVPSVATV	9	0.522	0.959
HLA-A*02:01	3GSR	NLVPVVATV	9	0.535	1.033
HLA-A*02:01	3GSU	NLVPTVATV	9	0.702	1.067
HLA-A*02:01	3GSV	NLVPQVATV	9	0.439	0.996
HLA-A*02:01	3GSW	NLVPMVAAV	9	0.883	1.694
HLA-A*02:01	3GSX	NLVPMVAVV	9	0.587	1.38
HLA-A*02:01	3H7B	MLWGYLQYV	9	0.684	2.449
HLA-A*02:01	3HPJ	RMFPNAPYL	9	1.111	1.492
HLA-A*02:01	3I6G	GLMWLSYFV	9	0.463	3.124
HLA-A*02:01	3KLA	SLLMWITQL	9	0.81	1.926
HLA-A*02:01	3MR9	NLVPAVATV	9	0.655	0.995
HLA-A*02:01	3MRB	NLVPMVHTV	9	0.681	1.497
HLA-A*02:01	3MRC	NLVPMCATV	9	1.63	2.613
HLA-A*02:01	3MRD	NLVPMGATV	9	1.608	2.537
HLA-A*02:01	3MRE	GLCPLVAML	9	1.093	2.092
HLA-A*02:01	3MRG	CINGVCWTV	9	0.978	1.623

HLA-A*02:01	3MRH	CISGVCWTV	9	0.853	2.576
HLA-A*02:01	3MRI	CINMWCWTV	9	1.481	3.778
HLA-A*02:01	3MRJ	CINGMCWTV	9	0.667	1.106
HLA-A*02:01	3MRK	PLFQVPEPV	9	0.696	1.299
HLA-A*02:01	3MRL	CINGVVWTV	9	0.606	1.9
HLA-A*02:01	3MYJ	YMFPNAPYL	9	1.659	1.858
HLA-A*02:01	3PWJ	LLYGFVNYV	9	0.804	2.492
HLA-A*02:01	3PWL	LGYGFVNYI	9	0.902	2.954
HLA-A*02:01	3PWN	LLYGFVNYI	9	0.733	2.355
HLA-A*02:01	3QFD	AAGIGILTV	9	1.377	1.421
HLA-A*02:01	3REW	CLGGLLTMV	9	1.158	2.224
HLA-A*02:01	3TO2	LACFVLAAV	9	1.006	2.79
HLA-A*02:01	3V5D	KVAELVHFL	9	1.099	2.378
HLA-A*02:01	3V5H	KVAEIVHFL	9	0.592	1.656
HLA-A*02:01	3V5K	KVAELVWFL	9	0.837	1.973
HLA-A*02:01	4I4W	ILAKFLHRL	9	1.219	3.494
HLA-A*02:01	4K7F	VCWGELMNL	9	0.971	1.713
HLA-A*02:01	4L3C	YLLMWITQV	9	1.003	2.273
HLA-B*27:05	1HSA	ARAAAAAAA	9	0.622	0.635
HLA-B*27:05	1JGE	GRFAAAIAK	9	0.557	0.894
HLA-B*27:05	1OGT	RRKWRRWHL	9	0.928	2.518
HLA-B*27:05	1UXS	RRRWRRLTV	9	1.685	4.355
HLA-B*27:05	1W0V	RRLPIFSRL	9	0.754	2.163
HLA-B*27:05	2A83	RRRWHRWRL	9	1.533	4.259
HLA-B*27:05	2BSR	RRIYDLIEL	9	0.673	1.816
HLA-B*27:05	2BST	SRYWAIRTR	9	0.686	2.637
HLA-B*27:05	3BP4	IRAAPPPLF	9	2.061	2.710
HLA-B*27:05	3LV3	SRRWRRWNR	9	0.774	2.994

H2-Db (9-mer epitope)	1BZ9	FAPGVFPYM	9	1.693	2.757
H2-Db (9-mer epitope)	1CE6	FAPGNYPAL	9	1.225	1.822
H2-Db (9-mer epitope)	1FFO	AAVYNFATM	9	0.852	1.694
H2-Db (9-mer epitope)	1FFP	SAVYNFATM	9	1.009	1.462
H2-Db (9-mer epitope)	1FG2	KAVYNFATC	9	0.379	2.034
H2-Db (9-mer epitope)	1HOC	ASNENMETM	9	0.744	1.658
H2-Db (9-mer epitope)	1INQ	SSVVGVWYL	9	1.18	2.6
H2-Db (9-mer epitope)	1JPG	FQPQNGQFI	9	0.5	1.109
H2-Db (9-mer epitope)	1JUF	SSVIGVWYL	9	1.182	2.647
H2-Db (9-mer epitope)	1S7U	KAVYNFATM	9	0.331	2.089
H2-Db (9-mer epitope)	1S7V	KAVYNLATM	9	1.135	2.339
H2-Db (9-mer epitope)	1S7W	KALYNFATM	9	0.271	2.064
H2-Db (9-mer epitope)	1S7X	KAVFNFATM	9	0.371	1.727
H2-Db (9-mer epitope)	1ZHB	KALYNYAPI	9	0.291	2.09
H2-Db (9-mer epitope)	2ZOK	ASLWNGPHL	9	0.592	1.226
H2-Db (9-mer epitope)	3CC5	KVPRNQDWL	9	0.308	1.856
H2-Db (9-mer epitope)	3CCH	EGSRNQDWL	9	0.495	2.288
H2-Db (9-mer epitope)	3CH1	EGPRNQDWL	9	0.656	2.214
H2-Db (9-mer epitope)	3CPL	ASNENAETM	9	0.845	1.769
H2-Db (9-mer epitope)	3FTG	ASAENMETM	9	0.912	1.518
H2-Db (9-mer epitope)	3QUK	KAVANFATM	9	0.454	1.742
H2-Db (9-mer epitope)	3QUL	KAVSNFATM	9	0.377	1.489
H2-Db (9-mer epitope)	3TBS	KAPANFATM	9	0.47	1.893
H2-Db (9-mer epitope)	3TBT	KAPSNFATM	9	0.336	1.536
H2-Db (9-mer epitope)	3TBV	KGPANFATM	9	0.653	1.912
H2-Db (9-mer epitope)	3TBW	KGPSNFATM	9	0.781	1.890
H2-Db (9-mer epitope)	3TBY	KAPFNFATM	9	0.436	2.288
H2-Db (9-mer epitope)	4HUU	ASNENIETM	9	0.695	2.005

H2-Db (9-mer epitope)	4HUV	ASNENWETM	9	0.64	1.792
H2-Db (9-mer epitope)	4HUW	ASNENTETM	9	0.537	1.72
H2-Db (9-mer epitope)	4L8C	ASDENMETM	9	0.639	1.517
H2-Db (9-mer epitope)	4L8D	ASNEDMETM	9	0.537	1.506
H2-Db (9-mer epitope)	4NSK	KAPYNFATM	9	0.629	2.416
H2-Db (10-mer epitope)	1N3N	SALQNAASIA	10	0.855	1.395
H2-Db (10-mer epitope)	1WBX	SQLKNNAKEI	10	0.441	1.685
H2-Db (10-mer epitope)	1YN6	SSLENFRAYV	10	0.315	2.54
H2-Db (10-mer epitope)	1YN7	SSLENFAAYV	10	0.233	0.937
H2-Db (10-mer epitope)	3L3H	SSLENARAYV	10	0.355	1.822
H2-Kb	1G7Q	SAPDTRPA	8	0.824	2.678
H2-Kb	1KJ3	KVITFIDL	8	1.322	2.298
H2-Kb	1LEG	EQYKFYSV	8	0.836	2.494
H2-Kb	1LK2	GNYSFYAL	8	0.653	1.778
H2-Kb	1RK0	SSIEFARL	8	0.692	1.601
H2-Kb	1RK1	SEIEFARL	8	0.658	1.504
H2-Kb	1VAC	SIINFEKL	8	0.416	1.455
H2-Kb	2CLV	SQYYYNSL	8	1.292	2.128
H2-Kb	2CLZ	INFDFNTI	8	1.442	1.849
H2-Kb	2FO4	SAPDFRPL	8	0.787	2.494
H2-Kb	3FOL	VNDIFERI	8	1.521	2.35
H2-Kb	3FON	VNDIFEAI	8	1.216	2.153
H2-Kb	3TID	AVYNFATM	8	1.367	2.135
H2-Kb	3TIE	AIVNYANL	8	1.25	1.438
H2-Kb	3P4M	YTVKYPNL	8	1.544	2.563
H2-Kb	3P4N	YTVKFPNM	8	1.604	2.172
H2-Kb	3P4O	YTAKYPNL	8	1.431	2.415
H2-Kb	3P9M	SIIGFEKL	8	1.341	1.559

H2-Kb	3PAB	EIINFEKL	8	1.312	2.392
Mean ± SD				**0.882 Å ± 0.437 Å**	**1.964 Å ± 0.655 Å**