



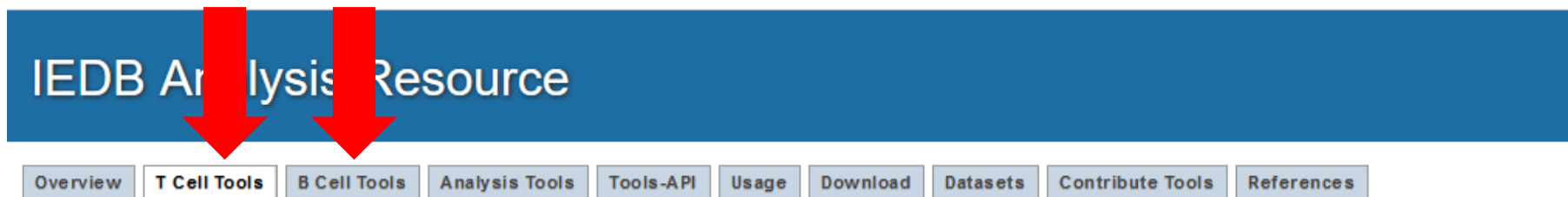
# LYRA & SCEptRe

[tools.iedb.org](https://tools.iedb.org)

Presented by: Paolo Marcatili, Associate Professor

Slides: Morten Nielsen

# Tools accessible from both T cell & B cell tabs



## Structure Tools



### [LYRA \(Lymphocyte Receptor Automated Modelling\):](#)

The LYRA server predicts structures for either T-Cell Receptors (TCR) or B-Cell Receptors (BCR) using homology modelling. Framework templates are selected based on BLOSUM score, and complementary determining regions (CDR) are then selected if needed based on a canonical structure model and grafted onto the framework templates.



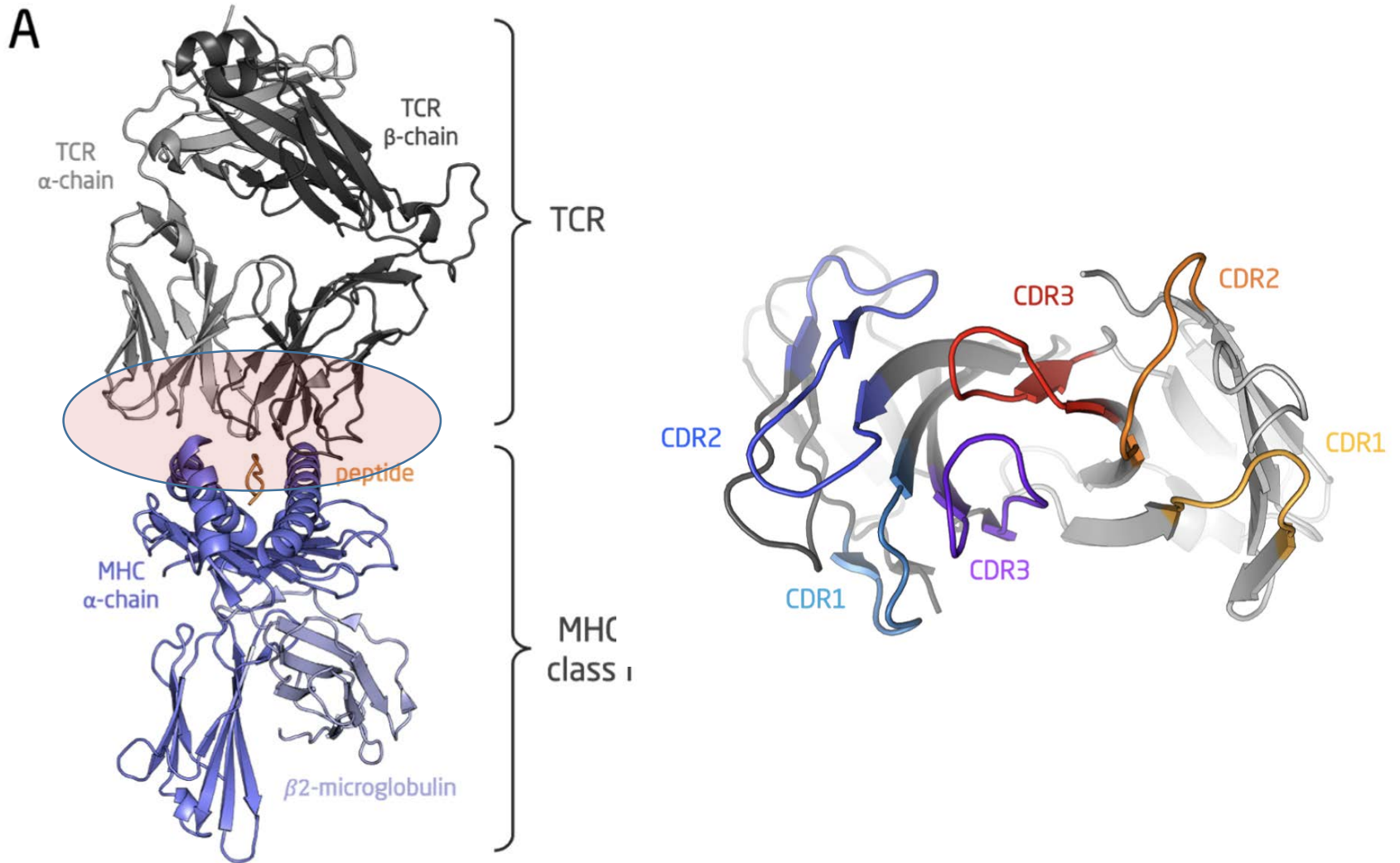
### [SCEptRe: Structural Complexes of Epitope Receptor](#)

SCEptRe provides weekly updated, non-redundant, user customized benchmark datasets with information on the immune receptor features for receptor-specific epitope predictions. This tool extracts weekly updated 3D complexes of antibody-antigen, TCR-pMHC and MHC-ligand from the Immune Epitope Database (IEDB) and clusters them based on antigens, receptors and epitopes to generate benchmark datasets. Users can customize structural quality and clustering parameters (e.g. resolution, R free factors, antigen or epitope sequence identity) to generate these datasets based on their need.

# SCEptRe: Structural Complexes of Epitope-Receptor

- Provides automatically updated benchmark datasets based on curated structural IEDB data
- User defines criteria to select set of quality and clustering parameters
- Clustering to address redundancy (and overfitting) in the resulting dataset when used for epitope predictions.
- Antibody-antigen, TCR-pMHC and MHC-ligand complexes

# What are BCR and TCR structures?



# Why is this important?

- Most current methods for epitope prediction are BCR/TCR agnostic
- Advances in T and B cell profiling by sequencing T and B cell receptors (TCR/BCR)
- Limited ability to interpret these data, since we most often do not know the cognate target of the differentially profiled TCR/BCRs
- The next major computational challenge is to develop tools to predict this
- TCR/BCR data sets are however very redundant, with multiple highly similar sequences

# Why is this important?

- Example from the IEDB. TCRb targeting GLCTLVAML

ASSQSPGGTQY

ASSQSPGGTQYS

ASSQSPGGTQYL

ASSQSPGGTQH

ASSQSPGGTQN

ASSQSPGGTQS

- Likewise do many distinct BCR/TCRs share identical CDR sequence


and often a TCR binds several very similar peptides

ASSLDQGAQDNEQF YLYDRLLRI

ASSLDQGAQDNEQF YLYDRLLRV

- If one seeks to make extrapolatable predictions/rules (and not just reproduce the measurements), one needs to deal with this redundancy

# SCEptRe: TCR-pMHC 3D complexes

IEDB Analysis Resource - Labs 

Home TCR MHC BCR Help Reference Contact

## Structural Complexes of Epitope Receptor: Dataset of TCR-pMHC 3D complexes

**Select structural quality parameters**

Resolution <=	<input type="text" value="3.0"/>
R free factor <=	<input type="text" value="optional"/>
Include TCRs with missing CDR residues	<input type="button" value="v"/> Yes No

**Select epitope features**

Epitope molecule type	<input type="button" value="v"/> Peptidic
Epitope length >=	<input type="text" value="10"/>
Epitope sequence identity >=	<input type="button" value="v"/> 90%
Clustering based on	<input type="button" value="v"/> core epitope

**Select MHC features**

Organism	<input type="button" value="v"/> All
MHC Class	<input type="button" value="v"/> All


<http://tools.iedb.org/sceptre/tcr/>

Resolution is a measure of the quality of the crystal structures

R-free factor is a measure of the quality of the atomic model obtained from the crystallographic data

Decide whether to include complexes with missing residues in the CDR regions in the final dataset

# SCEptRe: TCR-pMHC 3D complexes

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## Structural Complexes of Epitope Receptor: Dataset of TCR-pMHC 3D complexes

Select structural quality parameters	
Resolution <=	<input type="text" value="3.0"/>
R free factor <=	<input type="text" value="optional"/>
Include TCRs with missing CDR residues	<input type="text" value="No"/>
Select epitope features	
Epitope molecule type	<input type="text" value="Peptidic"/>
Epitope length >=	<input type="text" value=""/>
Epitope sequence identity >=	<input type="text" value="90%"/>
Clustering based on	<input type="text" value="core epitope"/>
Select MHC features	
Organism	<input type="text" value="All"/>
MHC Class	<input type="text" value="All"/>

<http://tools.iedb.org/sceptre/tcr/>

**Peptidic** - clustered based on epitope sequence, TCR CDR sequences and MHC G-domains

**Non-peptidic** - filtered based on specified structural quality parameters & clustered based on TCR CDR sequences and MHC G-domains


Filter out complexes below the specified epitope length threshold

### Clustering Parameters

- Specify sequence identity threshold
- Choose core-epitopes (peptide residues in direct contact) or whole epitope sequences



# SCEptRe: TCR-pMHC 3D complexes

IEDB Analysis Resource - Labs 

Home TCR MHC BCR Help Reference Contact

## Structural Complexes of Epitope Receptor: Dataset of TCR-pMHC 3D complexes

Select structural quality parameters	
Resolution <=	<input type="text" value="3.0"/>
R free factor <=	<input type="text" value="optional"/>
Include TCRs with missing CDR residues	<input type="button" value="No"/>
Select epitope features	
Epitope molecule type	<input type="button" value="Peptidic"/>
Epitope length >=	<input type="text" value="10"/>
Epitope sequence identity >=	<input type="button" value="90%"/>
Clustering based on	<input type="button" value="core epitope"/>
Select MHC features	
Organism	<input type="button" value="human (Homo sapiens)"/>
MHC Class	<input type="button" value="MHC I"/>

<http://tools.iedb.org/sceptre/tcr/>

### Filter complexes based on:

- MHC source organism

<input type="button" value="All"/>
human (Homo sapiens)
mouse (Mus musculus)
chicken (Gallus gallus)
cattle (Bos taurus)
horse (Equus caballus)
rat (Rattus norvegicus)
pig (Sus scrofa)
rhesus macaque (Macaca mulatta)
dog (Canis lupus familiaris)
duck (Anas platyrhynchos)

- MHC class

<input type="button" value="All"/>
MHC I
MHC II
Non classical

# SCEptRe: TCR-pMHC 3D complexes -results

<http://tools.iedb.org/sceptre/tcr/>

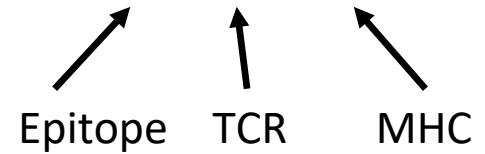
## Structural Complexes of Epitope Receptor: TCR - Results

Input Parameters

Parameter	Value
Resolution <=	3.0
Include TCRs with missing CDR residues	no
Molecule type	peptidic
Length >=	10
Identity >=	0.90
Clustering based on	core_epitope
Organism	human (Homo sapiens)
MHC Class	I

Link outs to iedb.org details pages

ClusterID: N.Ax\_By.aX(bY)



Download result

Show 10 entries

Search:

Cluster	Assay_id	Epitope_id	Receptor_id	Antigen	Structure	Structure_quality	MHC	Receptor	Chain1 CDRs	Chain2 CDRs	Chain1 VDJ genes	Chain2 VDJ genes	calc_epitope_residues	ep_lea
4.A1_B1.a1	<a href="#">1005001</a> <a href="#">View 3D Structure</a>	<a href="#">20354</a>	<a href="#">2277</a>	Epitope: GILGFVFTL Core Epitope: GILGFVFTL Antigen: Matrix protein 1 (58-66) Organism: Influenza A virus	pdb_id: <a href="#">1OGA</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C	Resolution: 1.4 R Free: 0.2 Missing residues in CDR: 0	Class: I Allele: HLA-A*02:01 Organism: human (Homo sapiens)	receptor_type: : alphabeta chain1_type: : alpha chain2_type: : beta	CDR1: SVFSS CDR2: VVTGGEV CDR3: AGAGSQGNLI	CDR1: LNHDA CDR2: SQIVND CDR3: ASSSRSSYEQY	V gene: : TRAV27*01 D gene: : J gene: : TRAJ42*01	V gene: : TRBV19*01 D gene: : J gene: : TRBJ2-7*01	C: G1, I2, L3, G4, F5, V6, F7, T8, L9;	9.0
4.A1_B1.a1	<a href="#">1005001</a> <a href="#">View 3D Structure</a>	<a href="#">20354</a>	<a href="#">8684</a>	Epitope: GILGFVFTL Core Epitope: GILGFVFTL Antigen: Matrix protein 1 (58-66) Organism: Influenza A virus	pdb_id: <a href="#">1OGA</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C	Resolution: 1.4 R Free: 0.2 Missing residues in CDR: 0	Class: I Allele: HLA-A*02:01 Organism: human (Homo sapiens)	receptor_type: : alphabeta chain1_type: : alpha chain2_type: : beta	CDR1: SVFSS CDR2: VVTGGEV CDR3: AGAGSQGNLI	CDR1: LNHDA CDR2: SQIVND CDR3: ASSSRSSYEQY	V gene: : TRAV27*01 D gene: : J gene: : TRAJ42*01	V gene: : TRBV19*01 D gene: : J gene: : TRBJ2-7*01	C: G1, I2, L3, G4, F5, V6, F7, T8, L9;	9.0
4.A1_B1.a1	<a href="#">1005001</a> <a href="#">View 3D Structure</a>	<a href="#">20354</a>	<a href="#">819</a>	Epitope: GILGFVFTL Core Epitope: GILGFVFTL Antigen: Matrix protein 1 (58-66) Organism: Influenza A virus	pdb_id: <a href="#">1OGA</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C	Resolution: 1.4 R Free: 0.2 Missing residues in CDR: 0	Class: I Allele: HLA-A*02:01 Organism: human (Homo sapiens)	receptor_type: : alphabeta chain1_type: : alpha chain2_type: : beta	CDR1: SVFSS CDR2: VVTGGEV CDR3: AGAGSQGNLI	CDR1: LNHDA CDR2: SQIVND CDR3: ASSSRSSYEQY	V gene: : TRAV27*01 D gene: : J gene: : TRAJ42*01	V gene: : TRBV19*01 D gene: : J gene: : TRBJ2-7*01	C: G1, I2, L3, G4, F5, V6, F7, T8, L9;	9.0
2.A2_B2.a2b1	<a href="#">1005014</a> <a href="#">View 3D Structure</a>	<a href="#">48237</a>	<a href="#">1819</a>	Epitope: PKYVKQNTLKLAT Core Epitope: PKYVKQNTLKLAT Antigen: Hemagglutinin precursor (322-334) Organism: Influenza A virus	pdb_id: <a href="#">1FYT</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C	Resolution: 2.6 R Free: 0.2 Missing residues in CDR: 0	Class: II Allele: HLA-DRB1*01:01 Organism: human (Homo sapiens)	receptor_type: : alphabeta chain1_type: : alpha chain2_type: : beta	CDR1: SSVPPY CDR2: YTSAATLV CDR3: AVSESPFGNEKLT	CDR1: MDHEN CDR2: SYDVKM CDR3: ASSSTGLPYGYT	V gene: : TRAV9-4*01 D gene: : J gene: : TRAJ48*01	V gene: : TRBV28*01 D gene: : J gene: : TRBJ1-2*01	C: P306, K307, Y308, V309, K310, Q311, N312, T313, L314, K315, L316, A317, T318;	13.0
2.A2_B2.a2b2	<a href="#">1005016</a> <a href="#">View 3D Structure</a>	<a href="#">48237</a>	<a href="#">18522</a>	Epitope: PKYVKQNTLKLAT Core Epitope: PKYVKQNTLKLAT Antigen: Hemagglutinin precursor (322-334) Organism: Influenza A virus	pdb_id: <a href="#">1JRH</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C	Resolution: 2.4 R Free: 0.2 Missing residues in CDR: 0	Class: II Allele: HLA-DRB1*04:01 Organism: human (Homo sapiens)	receptor_type: : alphabeta chain1_type: : alpha chain2_type: : beta	CDR1: SSVPPY CDR2: YTSAATLV CDR3: AVSESPFGNEKLT	CDR1: MDHEN CDR2: SYDVKM CDR3: ASSSTGLPYGYT	V gene: : TRAV9-4*01 D gene: : J gene: : TRAJ48*01	V gene: : TRBV28*01 D gene: : J gene: : TRBJ1-2*01	C: P306, K307, Y308, V309, K310, Q311, N312, T313, L314, K315, L316, A317, T318;	13.0
43.A3_B3.a3	<a href="#">1404662</a> <a href="#">View 3D Structure</a>	<a href="#">16878</a>	<a href="#">1412</a>	Epitope: FLRGRAYGL Core Epitope: FLRGRAYGL Antigen: nuclear antigen EBNA-3 (11-19) Organism: Human herpesvirus 4 (Epstein Barr virus)	pdb_id: <a href="#">1MIS</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C	Resolution: 2.5 R Free: 0.2 Missing residues in CDR: 0	Class: I Allele: HLA-B*08:01 Organism: human (Homo sapiens)	receptor_type: : alphabeta chain1_type: : alpha chain2_type: : beta	CDR1: TISGTDY CDR2: GLTSN CDR3: ILPLAGGTSYGKLT	CDR1: SGHVS CDR2: FQNEAQ CDR3: ASSLGQAYEQY	V gene: : TRAV26-2*01 D gene: : J gene: : TRAJ52*01	V gene: : TRBV7-8*01 D gene: : J gene: : TRBD1*01 TRBJ2-7*01	C: F1, L2, R3, G4, R5, A6, Y7, G8, L9	9.0

# SCEptRe: TCR-pMHC 3D complexes -results

<http://tools.iedb.org/sceptre/tcr/>

IEDB Analysis Resource - Labs



Home TCR MHC BCR Help Reference Contact

## Structural Complexes of Epitope Receptor: TCR - Results

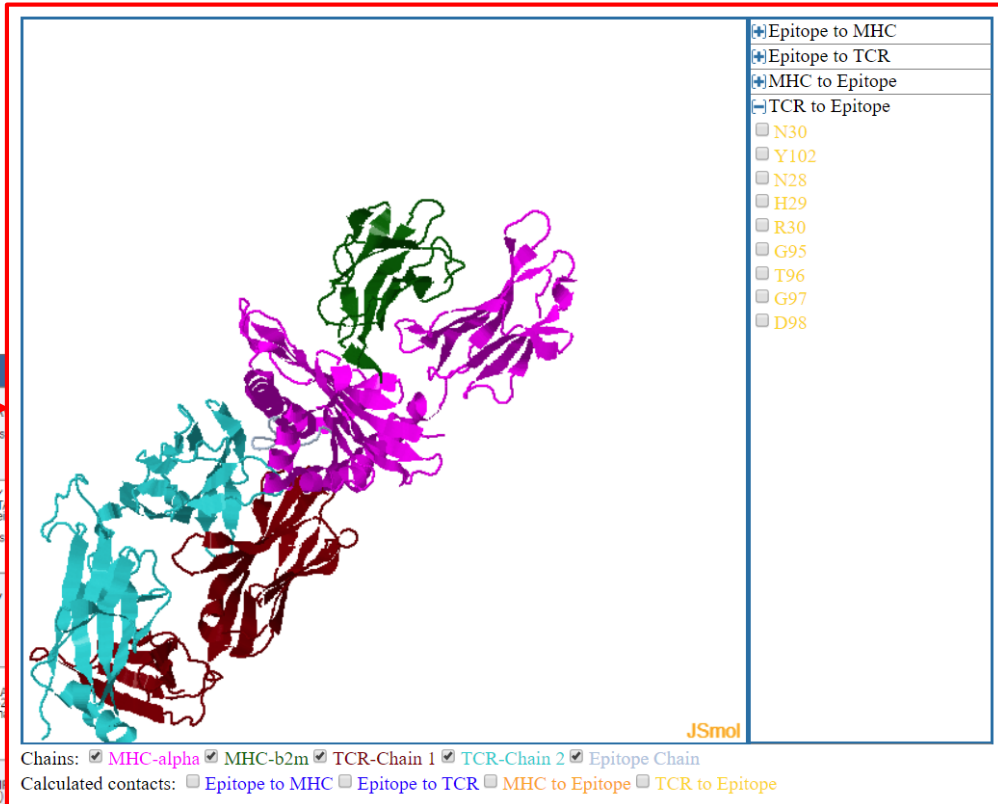
Input Parameters

Parameter	Value
Resolution <=	3.0
Include TCRs with missing CDR residues	no
Molecule type	peptidic
Length >=	10
Identity >=	0.90
Clustering based on	core_epitope
Organism	human (Homo sapiens)
MHC Class	I

Download result

Show 10 entries

Cluster	Assay_id	Epitope_ids	Receptor_ids	Antigen
2.A6_B6.a5	15105 <a href="#">(View 3D Structure)</a>	13701	18523	Epitope: EPLPQGQLTAY Core Epitope: EPLPQGQLTAY Antigen: BZLF1 (54-64) Organism: Human herpesvirus (Epstein Barr virus)
2.A24_B24.a17	1619817 <a href="#">(View 3D Structure)</a>	38458	116	Epitope: LPEPLPQGQLTAY Core Epitope: LPEPLPQGQLTAY Antigen: Trans-activator protein BZLF1 (52-64) Organism: Human herpesvirus (Epstein Barr virus)
5.A36_B38.a1	1883845 <a href="#">(View 3D Structure)</a>	12941	227	Epitope: ELAGIGILTV Core Epitope: ELAGIGILTV Antigen: Organism:
10.A37_B39.a1	1930414 <a href="#">(View 3D Structure)</a>	103041	330	Epitope: ALWGFDPAAAL Core Epitope: ALWGFDPAAAL Antigen: Insulin precursor (15-2 Organism: Homo sapiens (hum
6.A42_B44.a24	1966214 <a href="#">(View 3D Structure)</a>	29804	408	Epitope: KAFSPEVIPMIF Core Epitope: KAFSPEVIPMIF Antigen: p24 protein (17-27) Organism: Human immunodeficiency virus 1
2.A24_B47.a17	1981437 <a href="#">(View 3D Structure)</a>	38458	452	Epitope: LPEPLPQGQLTAY Core Epitope: LPEPLPQGQLTAY Antigen: Trans-activator protein BZLF1 (52-64) Organism: Human herpesvirus 4 (Epstein Barr virus)



- Epitope to MHC
- Epitope to TCR
- MHC to Epitope
- TCR to Epitope
- N30
- Y102
- N28
- H29
- R30
- G95
- T96
- G97
- D98

Search:

calc_epitope_residues	ep_len
C: E1, P2, L3, P4, Q5, G6, Q7, L8, T9, A10, Y11;	10.0
C: L1, P2, E3, P4, L5, P6, Q7, Q8, Q9, L10, T11, A12, Y13;	13.0
C: E1, L2, A3, Q4, I5, O6, I7, L8, T9, V10	10.0
C: A1, L2, W3, G4, P5, D6, P7, A8, A9, A10	10.0
C: K1, A2, F3, S4, P5, E6, V7, I8, P9, M10, F11	11.0
C: L1, P2, E3, P4, L5, P6, Q7, Q8, Q9, L10, T11, A12, Y13	13.0

mhc_chain2: B epitope_chain: C	chain2_type: beta	Resolution: 2.3 R Free: 0.2 Missing residues in CDR: 0	Class: I Allele: HLA-B*35:08 Organism: human (Homo sapiens)	receptor_type: : alpha:beta chain1_type: alpha chain2_type: beta	CDR1: TRDTITYY CDR2: RNSFDEQN CDR3: ALSGFYNTDKLI	CDR1: MNHNS CDR2: SASEQT CDR3: ASPGETEAF	V_gene: : TRAV19*01 D_gene: : J_gene: TRAJ34*01	V_gene: : TRBV6-1*01 D_gene: : J_gene: TRBJ1-1*01	C: L1, P2, E3, P4, L5, P6, Q7, Q8, Q9, L10, T11, A12, Y13	13.0
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# SCEptRe: TCR-pMHC 3D complexes - results

<http://tools.iedb.org/sceptre/tcr/>

## IEDB Analysis Resource - Labs

Home TCR MHC BCR Help Reference Contact

### Structural Complexes of Epitope Receptor: TCR - Results


Input Parameters

Parameter	Value
Resolution <=	3.0
Include TCRs with missing CDR residues	no
Molecule type	peptidic
Length >=	10
Identity >=	0.90
Clustering based on	core_epitope
Organism	human (Homo sapiens)
MHC Class	I

Download result

Show 10 entries

Cluster	Assay_id	Epitope_ids	Receptor_ids	Antigen	Structure
2.A6_B6.a5	<a href="#">1510571 (View 3D Structure)</a>	13701	18523	Epitope: EPLPQGQLTAY Core Epitope: EPLPQGQLTAY Antigen: BZLF1 (54-64) Organism: Human herpesvirus 4 (Epstein Barr virus)	<a href="#">pdb_id: 2NX5</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C
2.A24_B24.a17	<a href="#">1619817 (View 3D Structure)</a>	38458	116	Epitope: LPEPLPQGQLTAY Core Epitope: LPEPLPQGQLTAY Antigen: Trans-activator protein BZLF1 (52-64) Organism: Human herpesvirus 4 (Epstein Barr virus)	<a href="#">pdb_id: 2AK4</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C
5.A36_B38.a1	<a href="#">1883845 (View 3D Structure)</a>	12941	227	Epitope: ELAIGIGILTV Core Epitope: ELAIGIGILTV Antigen: Organism:	<a href="#">pdb_id: 3HG1</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C
10.A37_B39.a1	<a href="#">1930414 (View 3D Structure)</a>	103041	330	Epitope: ALWGGPDAAA Core Epitope: ALWGGPDAAA Antigen: Insulin precursor (15-24) Organism: Homo sapiens (human)	<a href="#">pdb_id: 3UJT</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C
6.A42_B44.a24	<a href="#">1966214 (View 3D Structure)</a>	29804	409	Epitope: KAFSPEVIPMF Core Epitope: KAFSPEVIPMF Antigen: p24 protein (17-27) Organism: Human immunodeficiency virus 1	<a href="#">pdb_id: 2YPL</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C
2.A24_B47.a17	<a href="#">1981437 (View 3D Structure)</a>	38458	452	Epitope: LPEPLPQGQLTAY Core Epitope: LPEPLPQGQLTAY Antigen: Trans-activator protein BZLF1 (52-64) Organism: Human herpesvirus 4 (Epstein Barr virus)	<a href="#">pdb_id: 4JRX</a> tcr_chain1: D tcr_chain2: E mhc_chain1: A mhc_chain2: B epitope_chain: C



156767 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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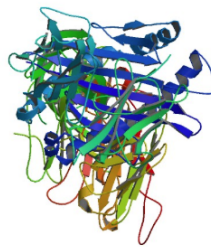
[Advanced Search](#) | [Browse by Annotations](#)

Structure Summary

3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment

Display Files Download Files

Biological Assembly 1



3D View: Structure

Standalone Viewers  
Protein Workshop | Ligand Explorer

Global Symmetry: Asymmetric - C1

Global Stoichiometry: Hetero 4-mer - ABCD

Biological assembly 1 assigned by authors.

## 2NX5

Crystal structure of ELS4 TCR bound to HLA-B\*3501 presenting EBV peptide EPLPQGQLTAY at 1.7A

DOI: 10.2210/pdb2NX5/pdb

Classification: **IMMUNE SYSTEM**

Organism(s): **Homo sapiens, Epstein-Barr virus (strain B95-9)**

Expression System: **Escherichia coli BL21(DE3)**

Deposited: 2006-11-16 Released: 2007-02-27

Deposition Author(s): **Tynan, F.E., Reid, H.H., Rossjohn, J.**

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 2.7 A

R-Value Free: 0.327

R-Value Work: 0.269

wwPDB Validation

Metric

Percentile Ranks

Value

Clashscore

7

Ramachandran outliers

1.3%

Sidechain outliers

4.8%

Worse | Percentile relative to all X-ray structures | Percentile relative to X-ray structures of similar resolution | Better


This is version 1.2 of the entry. See complete history.

Literature

Download Primary Citation

Missing residues in CDR:	Allele:	Class:	receptor_type:	CDR1:	CDR2:	D gene:	V gene:	C:	Ig
Missing residues in CDR: 0	HLA-B*57:03	I	alpha:beta	DSSSTY	RNSFDQGN	TRAJ12*01	TRAV5*01	C: K1, A2, F3, S4, P5, E6, V7, I8, P9, M10, F11	11.0
Missing residues in CDR: 0	HLA-B*35:08	I	alpha:beta	TRDITYY	RNSFDQGN	TRAJ13*01	TRAV19*01	C: L1, P2, E3, P4, L5, P6, O7, O8, O9, L10, T11, A12, Y13	13.0

# SCEptRe: MHC-ligand 3D complexes

IEDB Analysis Resource - Labs 

Home TCR **MHC** BCR Help Reference Contact

## Structural Complexes of Epitope Receptor: Dataset of MHC-ligand 3D complexes

**Select structural quality parameters**

Resolution <=

R free factor <=

**Select peptide features**

Ligand molecule type **Peptidic**

Peptide length >=

Peptide sequence identity >=

Clustering based on


**Select MHC features**

Organism

MHC Class

Submit Reset

<http://tools.iedb.org/sceptre/mhc/>

IEDB Analysis Resource - Labs 

Home TCR **MHC** BCR Help Reference Contact

## Structural Complexes of Epitope Receptor: Dataset of MHC-ligand 3D complexes

**Select structural quality parameters**

Resolution <=

R free factor <=

**Select peptide features**

Ligand molecule type **Non-peptidic**

**Select MHC features**

Organism

MHC Class

Submit Reset

Submit Reset

Submit Reset

# SCEptRe: MHC-ligand 3D complexes -results

<http://tools.iedb.org/sceptre/mhc/>

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## Structural Complexes of Epitope Receptor: MHC - Results

Input Parameters


Parameter	Value
Resolution <=	3.0
Molecule type	nonpeptidic
Organism	mouse (Mus musculus)
MHC Class	I

Download result

Show 10 entries Search:

Clust#	Assay_id	Epitope_id	Antigen	Structure	Structure_quality	MHC	calc_epitope_residues
	<a href="#">3838883</a> <a href="#">[View 3D Structure]</a>	<a href="#">766894</a>	Epitope: Core Epitope: Antigen: 1-O-[6-O-(3-phenylpropanoyl)-alpha-D-galactopyranosyl]-N-hexacosanoylsphinganine Organism:	pdb_id: <a href="#">6BNL</a> mhc_chain1: A mhc_chain2: B epitope_chain: A	Resolution: 2.6 R Free: 0.2	Class: non classical Allele: mouse CD1d Organism: mouse (Mus musculus)	A: (QWV)405
	<a href="#">1802187</a> <a href="#">[View 3D Structure]</a>	<a href="#">158632</a>	Epitope: Core Epitope: Antigen: glycolipid Organism:	pdb_id: <a href="#">3JVG</a> mhc_chain1: A mhc_chain2: C epitope_chain: A	Resolution: 2.2 R Free: 0.2	Class: non classical Allele: chicken CD1-1 Organism: chicken (Gallus gallus)	A: (UNL)1, (UNL)283;
	<a href="#">1848554</a> <a href="#">[View 3D Structure]</a>	<a href="#">153506</a>	Epitope: Core Epitope: Antigen: 1-O-(1-O-hexadecanoyl-2-O-heptadecanoyl-sn-glycero-3-phosphono)-1D-myo-inositol Organism:	pdb_id: <a href="#">3QI9</a> mhc_chain1: A mhc_chain2: B epitope_chain: A	Resolution: 2.3 R Free: 0.2	Class: non classical Allele: mouse CD1d Organism: mouse (Mus musculus)	A: (PII)405;
	<a href="#">1969015</a> <a href="#">[View 3D Structure]</a>	<a href="#">139426</a>	Epitope: Core Epitope: Antigen: 1-(3-O-sulfo-beta-D-galactosyl)sphingosine Organism:	pdb_id: <a href="#">4FLM</a> mhc_chain1: A mhc_chain2: B epitope_chain: A	Resolution: 3.5 R Free: 0.2	Class: non classical Allele: mouse CD1d Organism: mouse (Mus musculus)	A: (SGF)305, (PLM)306
	<a href="#">1976430</a> <a href="#">[View 3D Structure]</a>	<a href="#">164047</a>	Epitope: Core Epitope: Antigen: 1-O-(alpha-D-glucopyranosyl)-N-icoso-11,14-dienoylphytosphingosine Organism:	pdb_id: <a href="#">3RUG</a> mhc_chain1: A mhc_chain2: B epitope_chain: A	Resolution: 2.4 R Free: 0.2	Class: non classical Allele: mouse CD1d Organism: mouse (Mus musculus)	A: (DB6)303
	<a href="#">1971310</a> <a href="#">[View 3D Structure]</a>	<a href="#">181167</a>	Epitope: Core Epitope: Antigen: 1-elaidoyl-sn-glycero-3-phosphocholine	pdb_id: <a href="#">3TZV</a> mhc_chain1: C mhc_chain2: D	Resolution: 3.1 R Free: 0.2	Class: non classical Allele: human CD1d Organism: human	C: (LSC)303, (HEX)304, (D12)305

# SCEptRe: antibody-antigen 3D complexes

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## Structural Complexes of Epitope Receptor: Dataset of antibody-antigen 3D complexes

**Select structural quality parameters**

Resolution <=	<input type="text" value="2.0"/>
R free factor <=	<input type="text" value="optional"/>
Include BCRs with missing CDR residues	<input type="button" value="No"/>

**Select antigen features**

Epitope molecule type	<input type="button" value="Peptidic"/>
Antigen length >=	<input type="text" value="50"/>
Antigen sequence identity >=	<input type="button" value="70%"/>

<http://tools.iedb.org/sceptre/bcr/>



# SCEptRe: antibody-antigen 3D complexes -results

<http://tools.iedb.org/sceptre/bcr/>

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## Structural Complexes of Epitope Receptor: BCR - Results

Input Parameters

Parameter	Value
Resolution <=	2.0
Include BCRs with missing CDR residues	no
Molecule type	peptidic
Length >=	50
Identity >=	0.70

Download result

Show 10 entries Search:

Cluster	Assay_id	Epitope_id	Receptor_id	Antigen	Structure	Structure_quality	Receptor	Chain1 CDRs	Chain2 CDRs	Chain1 VDJ genes	Chain2 VDJ genes	calc_epitope_residues	ep_id
33.H23_L22.1	<a href="#">2213 [View 3D Structure]</a>	<a href="#">32990</a>	<a href="#">13</a>	Antigen: Major prion protein precursor (188-199) Organism: Ovis aries (domestic sheep)	pdb_id: 1TPX ab_chain1: B ab_chain2: C ag_chain: A	Resolution: 2.6 R Free: 0.3 Missing residues in CDR: 0	receptor_type: : heavy/light chain1_type: heavy chain2_type: light	CDR1: GYFTNYG CDR2: INTFTGEP CDR3: TRGTDY	CDR1: QSLLDSGKTY CDR2: LVS CDR3: WQGSHPQT	V gene: : IGHV3-3-1*01 D gene: : J gene: : IGKJ1*01 IGHJ2*01	V gene: : IGHV1-135*01 D gene: : J gene: : IGKJ1*01	A: G127, L128, N156, Y158, R159, I185, K188, Q189, T191, V192, T193, T194, T195, T196, K197, G198, E199, N200	18
33.H23_L22.1	<a href="#">376700 [View 3D Structure]</a>	<a href="#">32990</a>	<a href="#">13</a>	Antigen: Major prion protein precursor (188-199) Organism: Ovis aries (domestic sheep)	pdb_id: 1TQC ab_chain1: B ab_chain2: C ag_chain: A	Resolution: 2.8 R Free: 0.3 Missing residues in CDR: 0	receptor_type: : heavy/light chain1_type: heavy chain2_type: light	CDR1: GYFTNYG CDR2: INTFTGEP CDR3: TRGTDY	CDR1: QSLLDSGKTY CDR2: LVS CDR3: WQGSHPQT	V gene: : IGHV3-3-1*01 D gene: : J gene: : IGKJ1*01 IGHJ2*01	V gene: : IGHV1-135*01 D gene: : J gene: : IGKJ1*01	A: G127, L128, Y152, N156, Y158, R159, I185, K188, Q189, T191, V192, T193, T194, T195, T196, K197, G198, E199, N200	19
33.H23_L22.1	<a href="#">1376701 [View 3D Structure]</a>	<a href="#">32990</a>	<a href="#">13</a>	Antigen: Major prion protein precursor (188-199) Organism: Ovis aries (domestic sheep)	pdb_id: 1TQB ab_chain1: B ab_chain2: C ag_chain: A	Resolution: 2.5 R Free: 0.3 Missing residues in CDR: 0	receptor_type: : heavy/light chain1_type: heavy chain2_type: light	CDR1: GYFTNYG CDR2: INTFTGEP CDR3: TRGTDY	CDR1: QSLLDSGKTY CDR2: LVS CDR3: WQGSHPQT	V gene: : IGHV3-3-1*01 D gene: : J gene: : IGKJ1*01 IGHJ2*01	V gene: : IGHV1-135*01 D gene: : J gene: : IGKJ1*01	A: G127, L128, N156, Y158, R159, I185, K188, Q189, T191, V192, T193, T194, T195, T196, K197, G198, E199, N200	18
185.H298_L256.1	<a href="#">1929072 [View 3D Structure]</a>	<a href="#">59283</a>	<a href="#">247</a>	Antigen: Organism:	pdb_id: 3GJF ab_chain1: H ab_chain2: L ag_chain: AC	Resolution: 1.9 R Free: 0.3 Missing residues in CDR: 0	receptor_type: : heavy/light chain1_type: heavy chain2_type: light	CDR1: GFTFSTYQ CDR2: IVSSGGST CDR3: AGELLPYYGMDV	CDR1: SRDVGYYNY CDR2: DVI CDR3: WSFAGSYYV	V gene: : IGHV3-23*01 D gene: : IGHJ6*02	V gene: : IGLV2-11*01 D gene: : IGLJ1*01	A: E58, G62, R65, K66, A69, Q72, T73, A150, H151, Q155, A158, T163, E166, W167; C: M4, W5, I6, T7, Q8	19
185.H299_L256.1	<a href="#">1929073 [View 3D Structure]</a>	<a href="#">59283</a>	<a href="#">247</a>	Antigen: Organism:	pdb_id: 3HAE ab_chain1: H ab_chain2: H	Resolution: 2.9 R Free: 0.3 Missing residues in CDR: 0	receptor_type: : heavy/light chain1_type: heavy chain2_type: heavy	CDR1: GFTFSAYG CDR2: IGSSGGGT CDR3: AGELLPYYGMDV	CDR1: SRDVGYYNY CDR2: DVI CDR3: WSFAGSYYV	V gene: : IGHV3-23*01 D gene: : IGHJ6*02	V gene: : IGLV2-11*01 D gene: : IGLJ1*01	A: D61, R65, K66, K68, A69, Q72, T73, R75, T80, A150, Q155, T163, W167; C: S1, L2, M4, W5,	21

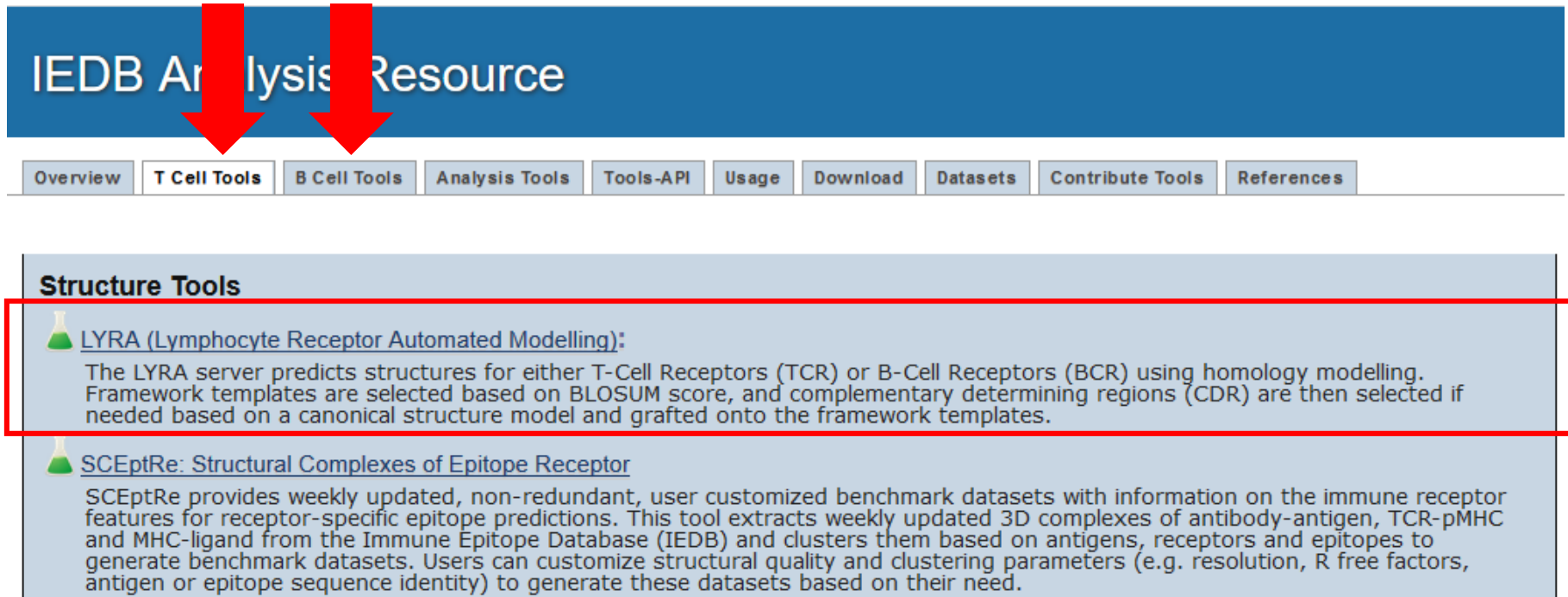
ClusterID: N.Hx\_Ly.M

Antigen BCR Epitope







# Tools accessible from both T Cell & B Cell tabs





IEDB Analysis Resource

Overview | **T Cell Tools** | B Cell Tools | Analysis Tools | Tools-API | Usage | Download | Datasets | Contribute Tools | References

### Structure Tools

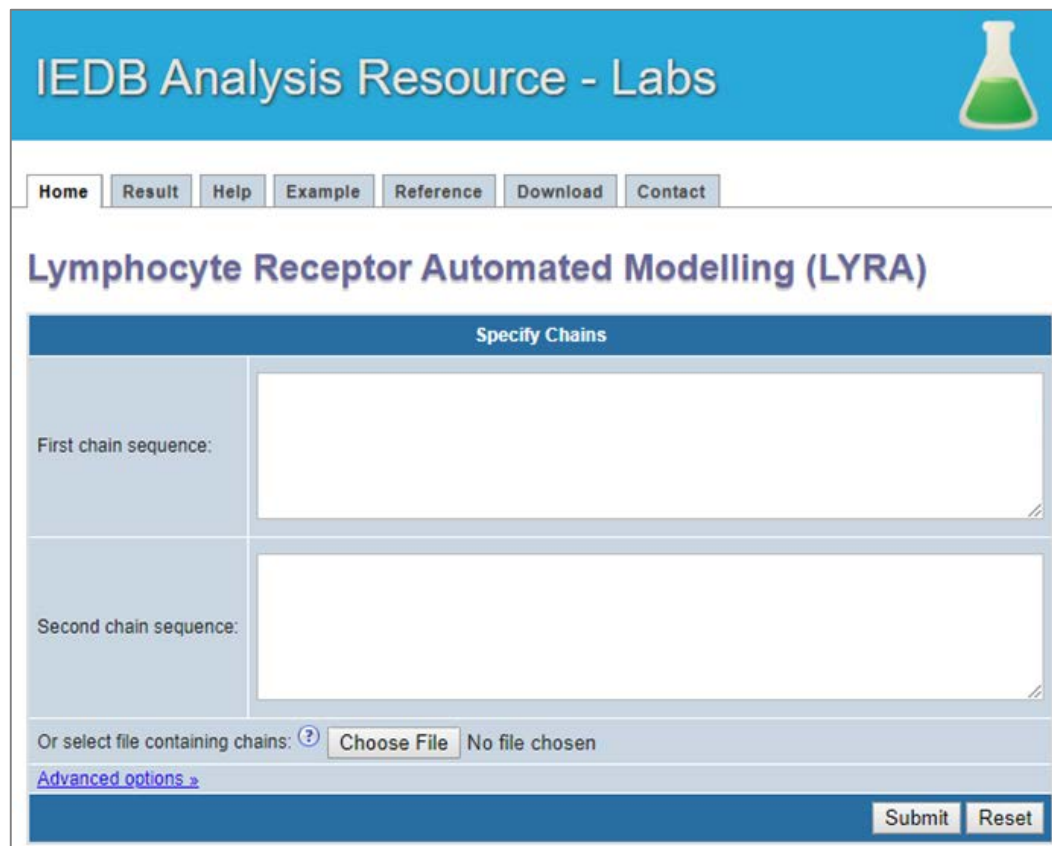
-  [LYRA \(Lymphocyte Receptor Automated Modelling\):](#)  
The LYRA server predicts structures for either T-Cell Receptors (TCR) or B-Cell Receptors (BCR) using homology modelling. Framework templates are selected based on BLOSUM score, and complementary determining regions (CDR) are then selected if needed based on a canonical structure model and grafted onto the framework templates.
-  [SCEptRe: Structural Complexes of Epitope Receptor](#)  
SCEptRe provides weekly updated, non-redundant, user customized benchmark datasets with information on the immune receptor features for receptor-specific epitope predictions. This tool extracts weekly updated 3D complexes of antibody-antigen, TCR-pMHC and MHC-ligand from the Immune Epitope Database (IEDB) and clusters them based on antigens, receptors and epitopes to generate benchmark datasets. Users can customize structural quality and clustering parameters (e.g. resolution, R free factors, antigen or epitope sequence identity) to generate these datasets based on their need.

# Why yet another specialized tool?

- Structure provides detailed information essential to access function of a protein
- Homology modeling is still the most reliable approach for accurate protein structure prediction
  - Works accurately if similar templates exist
  - Low accuracy of variable loops
- The fold of BCR and TCR is highly conserved (similar templates exist ), but the function is dictated by the highly sequence variable CDR loops. 
- However, the CDR loops share relative low structural diversity (canonical structures)

# LYRA: Lymphocyte Receptor Automated Modeling

<http://tools.iedb.org/lyra/>



- B- and T-cell receptor structure modeling
- Canonical structures (CS):
  - Hypervariable CDR loops only assume a limited number of conformations (*Chothia & Lesk, JMB 1987*)
  - Usually identified by specific sequence features

Nucleic Acids Res. 2015 Jul 1;43(W1):W349-55. doi: 10.1093/nar/gkv535. Epub 2015 May 24.

**LYRA, a webserver for lymphocyte receptor structural modeling.**

Klausen MS<sup>1</sup>, Anderson MV<sup>1</sup>, Jespersen MC<sup>1</sup>, Nielsen M<sup>2</sup>, Marcatili P<sup>3</sup>.

PMID: 26007650 PMCID: PMC4489227 DOI: 10.1093/nar/gkv535

# LYRA: Lymphocyte Receptor Automated Modeling

<http://tools.iedb.org/lyra/>

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### Lymphocyte Receptor Automated Modelling (LYRA)

Specify Chains

First chain sequence:

Second chain sequence:

Or select file containing chains:  No file chosen

[Advanced options >](#)

- Templates are identified using BLOSUM62 scores
- Loop modeling:  
If the CS of target and template loops do not match, then the highest scoring identical canonical structure loops from other structures are selected

Nucleic Acids Res. 2015 Jul 1;43(W1):W349-55. doi: 10.1093/nar/gkv535. Epub 2015 May 24.

**LYRA, a webserver for lymphocyte receptor structural modeling.**

Klausen MS<sup>1</sup>, Anderson MV<sup>1</sup>, Jespersen MC<sup>1</sup>, Nielsen M<sup>2</sup>, Marcatili P<sup>3</sup>.

PMID: 26007650 PMCID: PMC4489227 DOI: 10.1093/nar/gkv535

# LYRA – example (BCRs)

<http://tools.iedb.org/lyra/>

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## Lymphocyte Receptor Automated Modelling (LYRA)

**Specify Chains**

First chain sequence:

```
DIQMTQSPASLSASVIGATVTITCRTSENIDSYLAWYQQRQKSPQLLVYAATNLADGVP
SRFSGSGSGTQYSLKINSLQSEDVARYYCQHYSTTPWTFGGGTQLEIKRADAAPTVSIFP
PSSEQLTSGGASVVCFLNNFYPKDINVKWKIDGSERQNGVLNSWTDQDQSKDSTYSMSS
TLTLTKDEYERHNSYTCEATHKTSTSPIVKSFNRNECO
```

Second chain sequence:

```
EVQLQQSGPELVKPGASVKISKASGYSFTGYMNVWVKQSPEKSLEWIGEMSPSTGRT
TYNQNFKAKATLTDQSSSTAYMQLKSLTSEDSAVYYCARSVPLTTLIEDWYFDVWGT
GTTVTVSSAKTTPPSVYPLAPGSAQAQNTNSMVTGLCLVKGYFPEPVTVTVNSGSLSSGVH
TFPAVLQSDLYTLSSSVTVPSSTWPSETVTCNVAHPASSTKVDKDKIVPR
```

Or select file containing chains:  No file chosen

[Advanced options »](#)

Chain sequences  
(input or upload)

FASTA upload format:

>light chain header  
*sequence for light chain here...*

>heavy chain header  
*sequence for heavy chain here...*

# LYRA – example (BCRs)

<http://tools.iedb.org/lyra/>

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## Lymphocyte Receptor Automated Modelling (LYRA)

Specify Chains

First chain sequence:  
DIQMTQSPASLSASVIGATVITICRTSENIDSYLAWYQQRQKSPQLLVYAATNLADGV  
PSRFGSGSGTQYSLKINSLSQSEDEVARYYCQHYSTTPWTFGGGTQLEIKRADAAPTVSIF  
PPSSEQLTSGGASVVCFLNNFYPKDINVKWKIDGSRQNGVLNSWTDQDSDKDSTYSM  
SSTLTLTKDEYERHNSYTCEATHKTSTSPIVKSFNRECO

Second chain sequence:  
EVQLQQSGPELVKPGASVKISCKASGYSFTGYMNVKQSQPEKSLEWIGEMSPSTGRT  
TYNQNFKAKATLTVDDQSSTAYMQLKSLTSEDSAVYYCARVPLTLLIEDWYFDVWGT  
GTTVTVSSAKTTPSPVYPLAPGSAQTNSMVTLGCLVKGYFPEPVTVTWNSGSLSSGV  
HTFPAVLQSDLYTLSSVTPSSTWVPSSETVTCNVAHPASSTKVDKDKIVPR

Or select file containing chains:  No file chosen

[Advanced options >](#)

Side Chain Modeling Method:

Blacklisted PDBs (optional):

### Side Chain Modeling Method

HMMER + SCWRL  
HMMER

- HMMER – searches sequence databases for sequence homologs & makes sequence alignments
- SCWRL 4.0 models non conserved residues (uses conserved residue side chains as constraints)

Prevents use as framework or loop template for both chains



# LYRA – example (BCRs)

<http://tools.iedb.org/lyra/>

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## Lyra results

**Contents** [\[hide\]](#)

- [1 Input sequences](#)
- [2 Summary of modelled BCR](#)
- [3 Alignment](#)
  - [3.1 Heavy chain alignment](#)
  - [3.2 Kappa Light chain alignment](#)
- [4 Structure 3D View](#)
- [5 Download PDB file](#)

### Input Sequences

Name	Sequence
First chain sequence:	DIQMTQSPASLSASVIGATVITICRTSENIDSYLAWYQQRQKSPQLLVYAATNLADGVPSRFSGSGSGTQYSLKINSLQSEDEVARYYCQHYSTTPWTFGGGTQLEIKRADAAPTVISIFPPSSEQLTSGGASVVCFLNMFYPKDINVKWKIDGSERQNGVLNSWTDQDSKDYSTYSMSSTLTLTKDEYERHNSYTCETHKTSTSPIVKSFNREK
Second chain sequence:	EVQLQQSGPELVKPGASVKISCKASGYSTFGYYMNWVKQSPEKSLIEWIGEMSPSTGRRTYNQNFKAKATLTVDQSSSTAYMQLKSLTSEDSAVYYCARSVPLTLLIEDWYFDVWGTGTTVTVSSAKTTPPSVYPLAPGSAQAQNSMVTLGCLVKGYFPEPVTVTWNSGSLSSGVHTFPAVLQSDLYTLSSSVTPVSSSTWPSSETVTCNVAHPASSTKVDKIVPR

# LYRA – example (BCRs)

<http://tools.iedb.org/lyra/>

## Summary of modelled BCR

	Heavy chain			Kappa Light chain		
	Template	Template CS	Predicted CS	Template	Template CS	Predicted CS
Framework	<a href="#">1IQW</a>			<a href="#">1WEJ</a>		
Loop 1	<a href="#">1IQW</a>	1	1	<a href="#">1WEJ</a>	2	2
Loop 2	<a href="#">1IQW</a>	3	3	<a href="#">1WEJ</a>	1	1
Loop 3	<a href="#">3O0R</a>	31	31	<a href="#">1WEJ</a>	1	1
Packing	<a href="#">1VFB</a>					

## Alignment:

Heavy chain alignment:

```

1      10      20      30      33      43      55      65      75      92      110
|      |      |      | ABCDEFG |      |      |      |      |      |      |      |
Template: QVQLQQPGAELVKPGASVKLSCKASQGYFTFS-----YWMQWVKRPGQGLEWIGRIDP-----SDSYTNYNQKFKGKATLTVDTSSSTAYMQLSSLTSEDSAVYYCARNQLSLDGYVVKWNCF-----DQVWG
||||| | ||||| ||||| ||||| || || | ||| | ||||| || | | ||| || ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| |||||
Input:    EVQLQQSGPELVKPGASVKISCKASQGYSTFG-----YMNWVKQSPKSLWIGEMSP-----STGRTTYNQKFKKATLTVDSSTAYMQLKSLTSEDSAVYYCARSQVPLTTLIEDWYF-----DQVWG
           □ ─── H1 ─── □           □ ─── H2 ─── □           □ ─── H3 ─── □

```

Kappa Light chain alignment:

```

1      10      20      30      40      50      52      62      74      84      94      96      106
|      |      |      | ABCDEFGHIJ |      |      | ABCDEFGH |      |      | ABCDEFGH |      |      | ABCDEFGH |      | A
Template: DIQMTQSPASLSASVGETVTITCRASGNIH-----NYQLAWYQQKQKSPQLLVYQN-----AKQLADGVPSRFSGSGSG-----TQYSLKINSLQPEDFGSYQCQHFVSTP-----WTFGGGKLEIKRAD
||||| ||||| ||||| ||||| || || | ||| | ||||| || | | ||| || ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| ||||| |||||
Input:    DIQMTQSPASLSASVGATVTITCRTSENID-----SYQLAWYQQKQKSPQLLVYA-----ATNLADGVPSRFSGSGSG-----TQYSLKINSLQSEDAVRYQCQHYSTTP-----WTFGGGQLEIKRAD
           □ ─── K1 ─── □           □ ─── K2 ─── □           □ ─── K3 ─── □

```

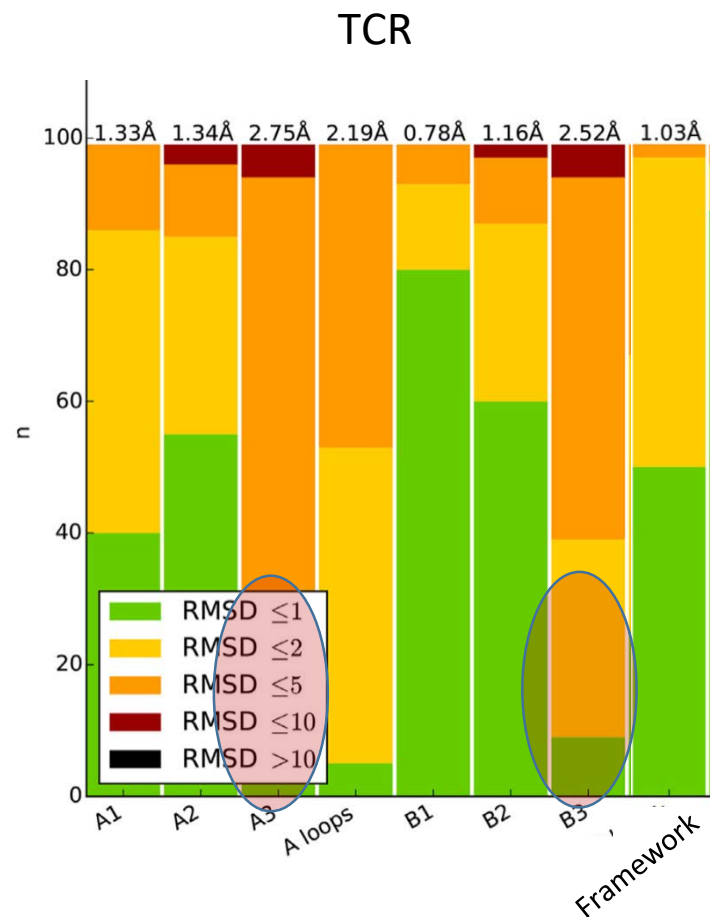
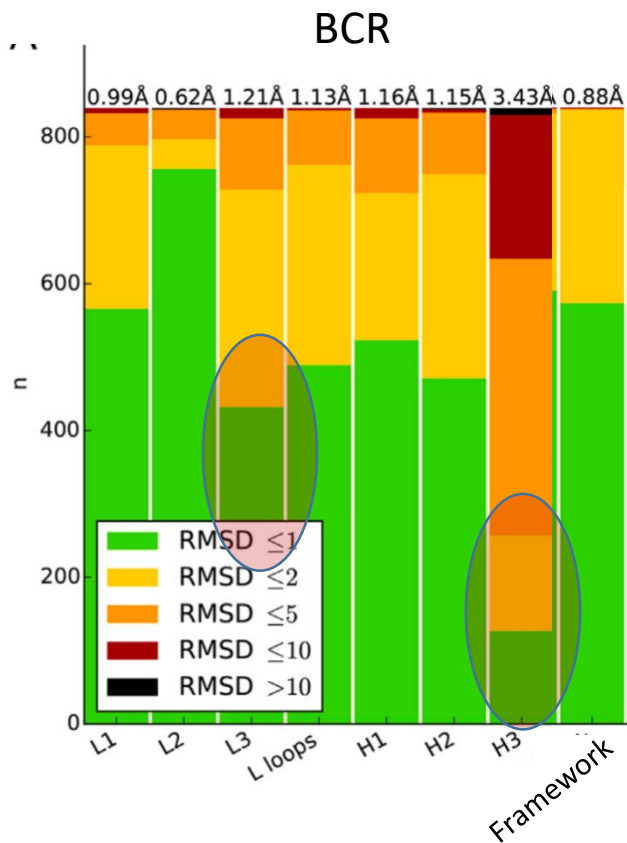


# LYRA – example (BCRs)

<http://tools.iedb.org/lyra/>



# Benchmark evaluation

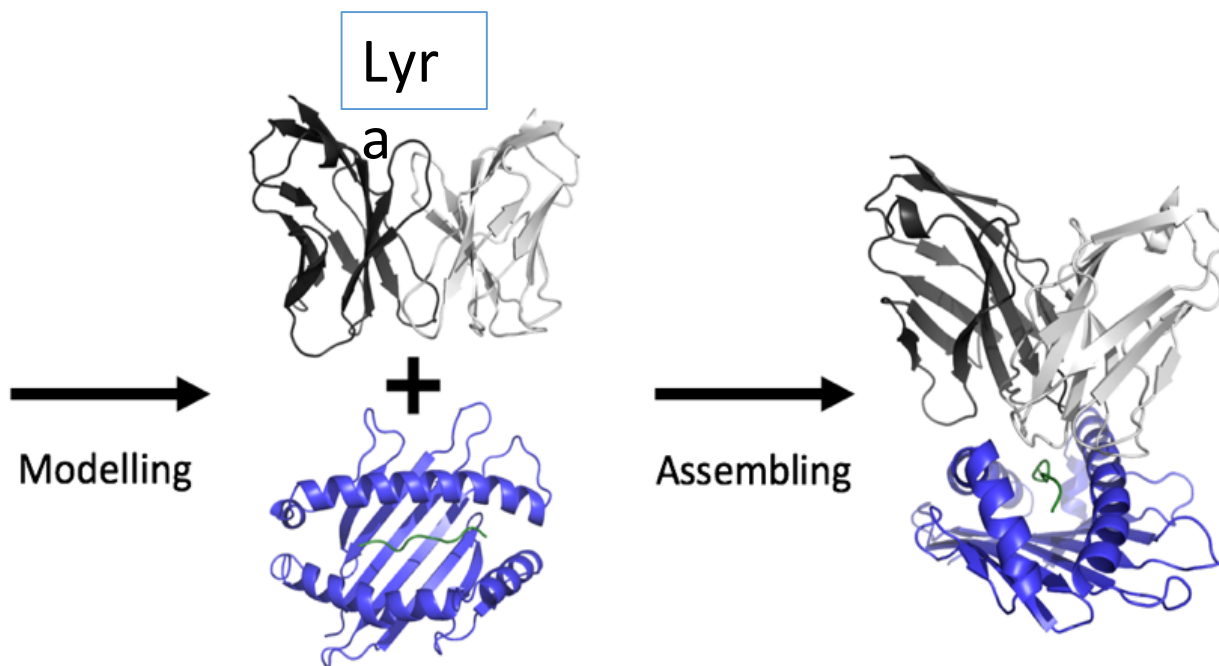


# Application: Modeling TCR – peptide:MHC interactions

```

>MHC
GPHSLRYFVTAVSRPGLGEPRYMEVGYYDDT
EFVRFSDAENPRYEPRARWMEQEGPEYWER
ETQKAKGNEQSFVLDLRTLGGYNNQSKGGSH
TIQVISGCEVGS DGRLLRGYQYAYDGC DYI
ALNEDLKTWTAADMAALITKHKWEQAGEAER
LRAYLEGTCVEWLRRL
>Peptide
SIYRYYGL
>TCR_alpha
QSVTQPDARVTVSEGASLQLRCKYSYSATPY
LFWYVQYPRQLQLLLKYSGDPVVQGVNGF
EAEFSKSNSSFHLRKASVHWSDSAVYFCAVS
GFASALTFGSGTKVIVLP
>TCR_beta
VTQSPRNKVAVTGGKVTLS CNQTNNHNMYW
YRQDTGHGLRLIHYSYGAGSTEKGDIPDGYK
ASRPSQENFSLILELATPSQTSVYFCASGGG
GTYLFGAGTRLSVL
    
```

Input sequence



TCR and pMHC models

Final model

*Sci Rep.* 2019 Oct 10;9(1):14530. doi: 10.1038/s41598-019-50932-4.

**TCRpMHCmodels: Structural modelling of TCR-pMHC class I complexes.**

Jensen KK<sup>1</sup>, Rantos V<sup>1,2</sup>, Jappe EC<sup>1,3</sup>, Olsen TH<sup>1</sup>, Jespersen MC<sup>1</sup>, Jurtz V<sup>4</sup>, Jessen LE<sup>1</sup>, Lanzarotti E<sup>5</sup>, Mahajan S<sup>6</sup>, Peters B<sup>6,7</sup>, Nielsen M<sup>1,5</sup>, Marcatili P<sup>8</sup>.

PMID: 31601838 PMCID: [PMC6787230](https://pubmed.ncbi.nlm.nih.gov/31601838/) DOI: [10.1038/s41598-019-50932-4](https://doi.org/10.1038/s41598-019-50932-4)

*Mol Immunol.* 2018 Feb;94:91-97. doi: 10.1016/j.molimm.2017.12.019. Epub 2017 Dec 27.

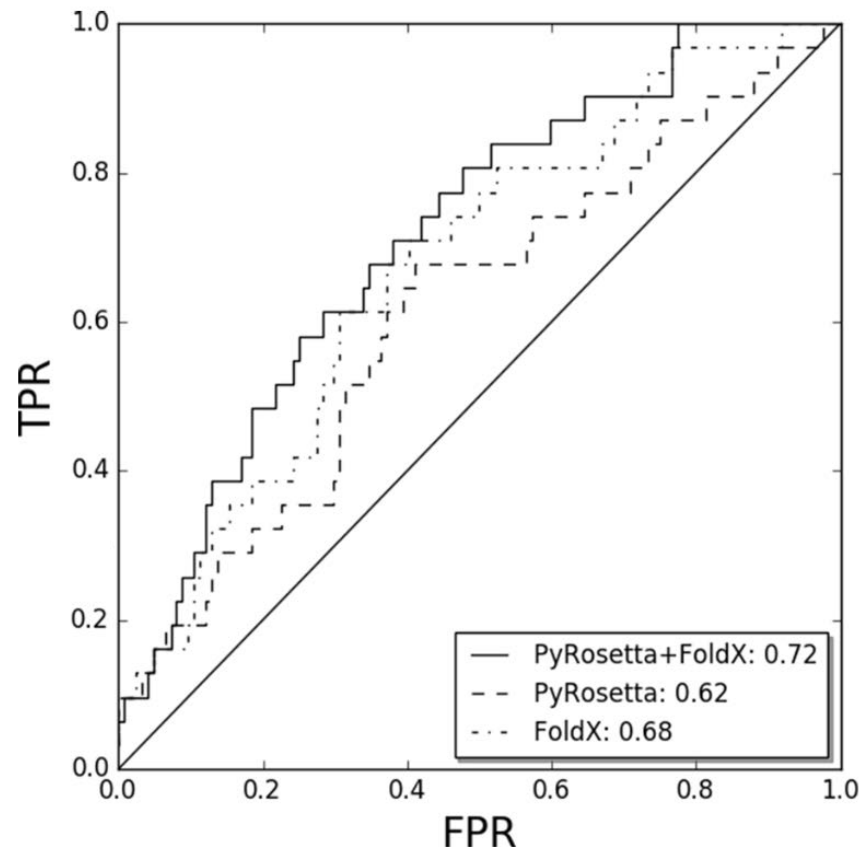
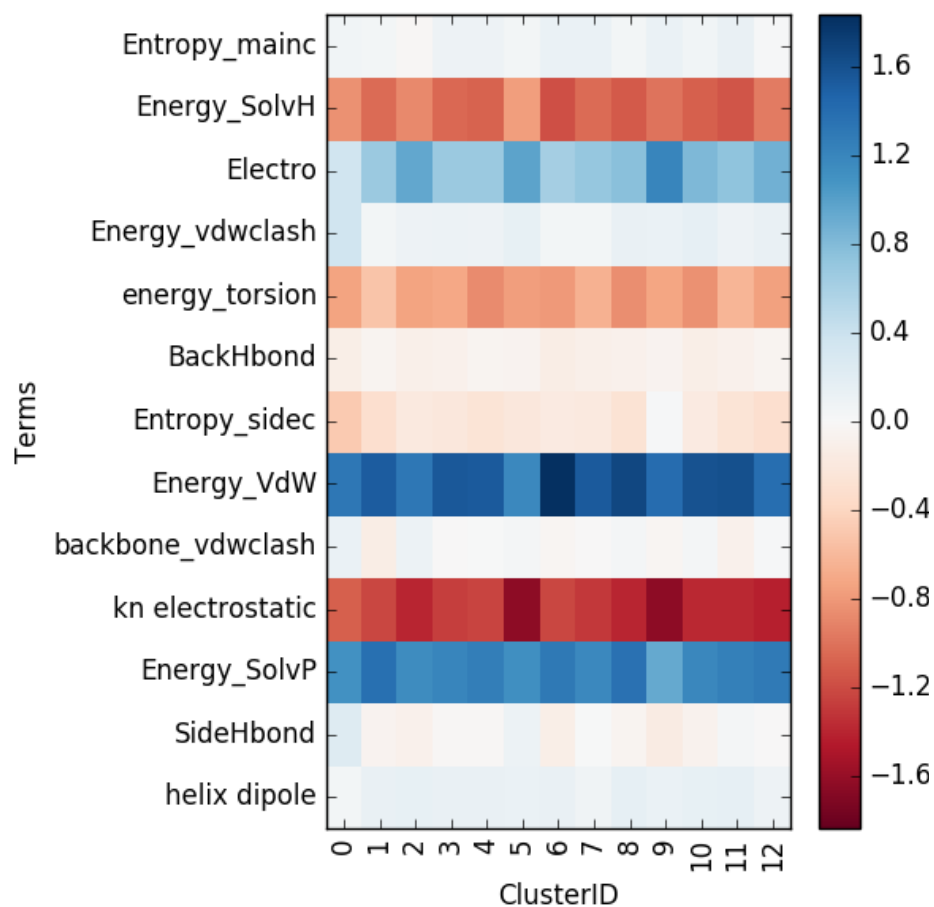
**Identification of the cognate peptide-MHC target of T cell receptors using molecular modeling and force field scoring.**

Lanzarotti E<sup>1</sup>, Marcatili P<sup>2</sup>, Nielsen M<sup>3</sup>.

PMID: 29288899 PMCID: [PMC5800965](https://pubmed.ncbi.nlm.nih.gov/29288899/) DOI: [10.1016/j.molimm.2017.12.019](https://doi.org/10.1016/j.molimm.2017.12.019)

# Modeling TCR – peptide:MHC interactions

## Optimized force field terms



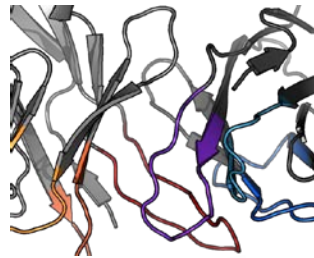
*Mol Immunol*. 2018 Feb;94:91-97. doi: 10.1016/j.molimm.2017.12.019. Epub 2017 Dec 27.

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PMID: 29288899 PMID: PMC5800965 DOI: 10.1016/j.molimm.2017.12.019

# Modeling TCR – peptide:MHC interactions



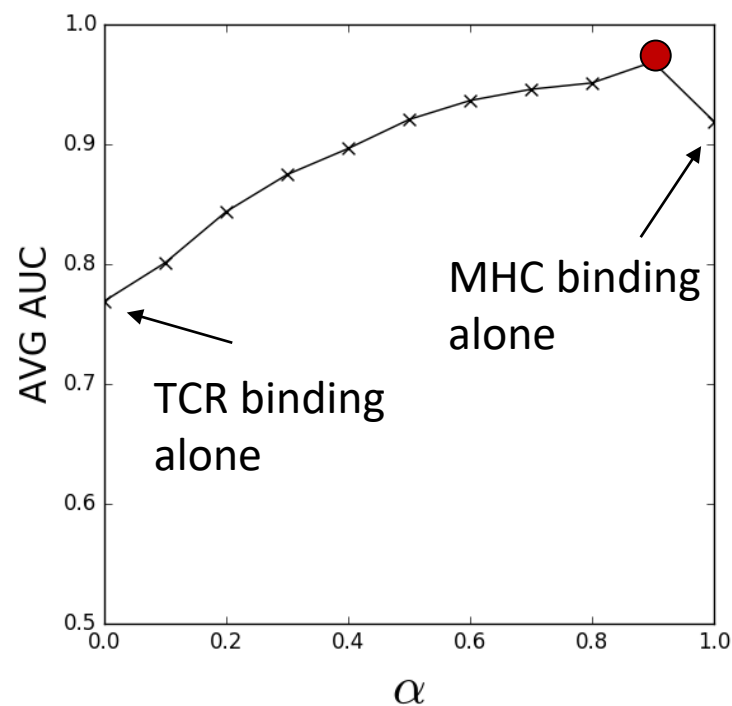
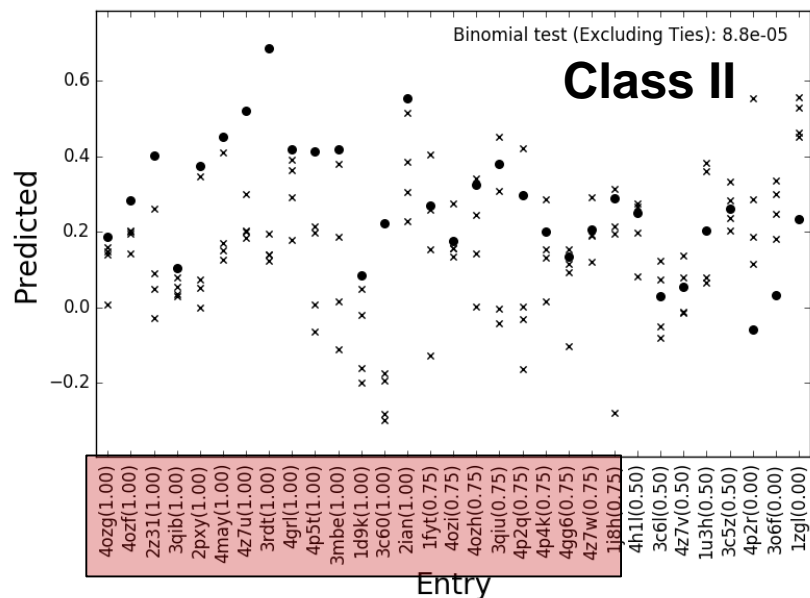
*Mol Immunol.* 2018 Feb;94:91-97. doi: 10.1016/j.molimm.2017.12.019. Epub 2017 Dec 27.

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PMID: 29288899 PMCID: PMC5800965 DOI: 10.1016/j.molimm.2017.12.019

# Modeling TCR – peptide:MHC interactions



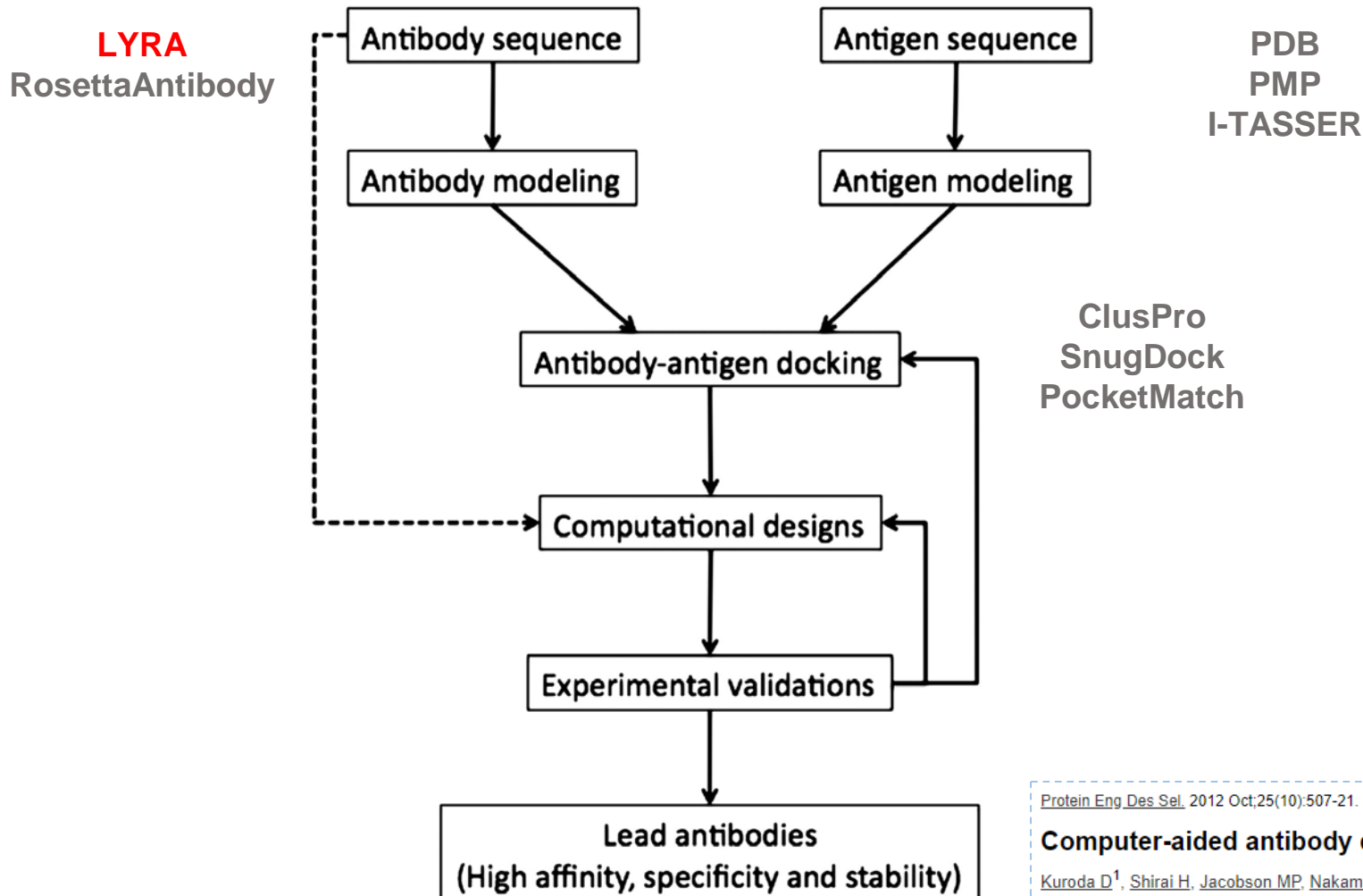
*Mol Immunol*. 2018 Feb;94:91-97. doi: 10.1016/j.molimm.2017.12.019. Epub 2017 Dec 27.

**Identification of the cognate peptide-MHC target of T cell receptors using molecular modeling and force field scoring.**

Lanzarotti E<sup>1</sup>, Marcatili P<sup>2</sup>, Nielsen M<sup>3</sup>.

PMID: 29288899 PMCID: [PMc5800965](https://pubmed.ncbi.nlm.nih.gov/29288899/) DOI: [10.1016/j.molimm.2017.12.019](https://doi.org/10.1016/j.molimm.2017.12.019)

# Application of LYRA in Computational Epitope discovery



[Protein Eng. Des. Sel.](#), 2012 Oct;25(10):507-21. Epub 2012 Jun 2.

## Computer-aided antibody design.

Kuroda D<sup>1</sup>, Shirai H, Jacobson MP, Nakamura H.

PMID: 22661385 PMCID: [PMC3449398](#) DOI: [10.1093/protein/gzs024](#)

# Summary

- **SCEptRE**

- Provides easy access to all BCR and TCR structures available from the IEDB
- The tool allows customized clustering of the data based on CDR and epitope information
- Next, step will be to develop a similar tool for BCR/TCR sequence data

- **LYRA**

- A tool for accurate modeling of BCR and TCR structures
- CDR loops are modeled based on canonical structures
- Accuracy high with the exception of CDR3b for BCR and CDR3a and b for TCR
- For these loops, further development of *ab-initio* modeling is needed