



IEDB-3D 2.0

A new way to visualize 3D structures in the IEDB

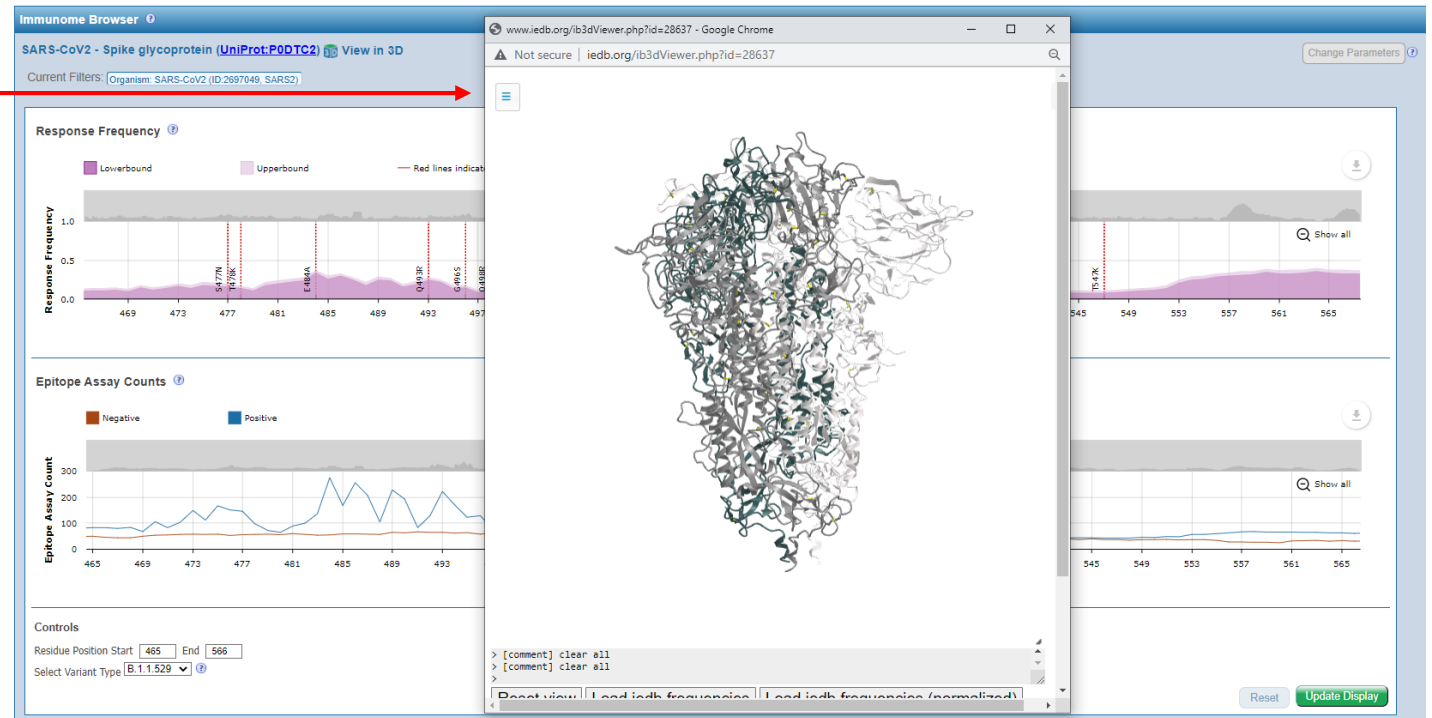
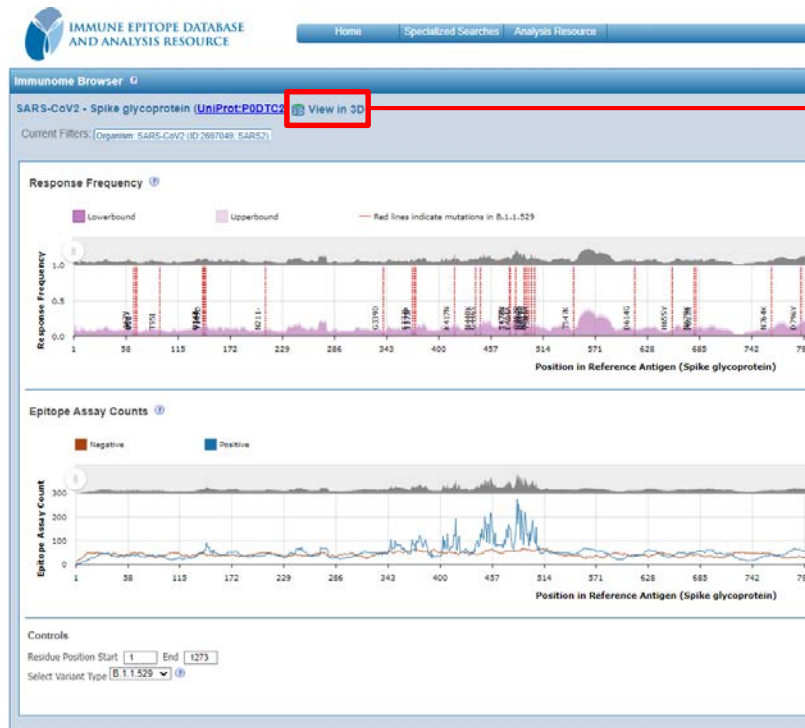
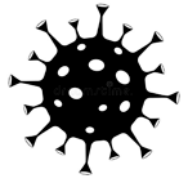
Presented by: Marcus Mendes, PhD, Bioinformatics Postdoc

IEDB-3D 2.0 Viewer Project

Background

NIH requested the IEDB to capture SARS-CoV-2 mutations:

- Displays each amino acid mutation on the Immunome Browser for the spike glycoprotein antigen
- Utilized iCn3D to display the spike glycoprotein (and the mutations) in the Immunome Browser



IEDB-3D 2.0 Viewer Project

(1) Assays Tab

Displays experimentally determined 3D structures from PDB, directly showing epitope recognition. Depending on the assay, it can show an epitope bound to MHC, MHC & TCR or an antibody with pre-calculated contacts

ID	Reference	Epitope	Host	Immunization	Assay Antigen
211922	Blag Y Borbolevych; Immunol 011	AAGIGILTV Melanoma antigen recognized by T-cells 1 (27-35) Homo sapiens (human)	Homo sapiens (human)	Occurrence of cancer (skin melanoma)	AAGIGILTV Melanoma antigen re by T-cells 1 (27-35) Homo sapiens (hum
534618	ance M Hellman; Mol Ther 019	AAGIGILTV Melanoma antigen recognized by T-cells 1 (27-35) Homo sapiens (human)	Homo sapiens (human)	Occurrence of cancer (skin melanoma)	AAGIGILTV Melanoma antigen re by T-cells 1 (27-35) Homo sapiens (hum
563758	orian Madura; Eur J Immunol 019	AAGIGILTV Melanoma antigen recognized by T-cells 1 (27-35) Homo sapiens (human)	Homo sapiens (human)	Primary induction in vitro with ELAGIGILTV (Structurally Related)	AAGIGILTV Melanoma antigen re by T-cells 1 (27-35) Homo sapiens (hum

(2) Epitopes Tab

Displays individual epitope in its source antigen, either from PDB or AlphaFold

IEDB ID	Epitope	Antigen	Organism
4002	ASNDGNETM	hemagglutinin	Influenza A virus
20864	GLGFWTE	hemagglutinin	Influenza A virus
26730	IPYEDPSV	hemagglutinin	Influenza A virus
61151	SGLEFTRAV	hemagglutinin	Influenza A virus
72826	WMAHSAAF	hemagglutinin	Influenza A virus
2137	AKNNTAV	hemagglutinin	Influenza A virus
3050	AKWMAAPY	hemagglutinin	Influenza A virus
42446	MGTLNPPY	hemagglutinin	Influenza A virus
66338	RLSLCHAF	hemagglutinin	Influenza A virus
76668	YLAGAGLAF	hemagglutinin	Influenza A virus
2643	ALPVGQYV	hemagglutinin	Influenza A virus
4803	ATAPWQYV	hemagglutinin	Influenza A virus
5554	AVTATFAF	hemagglutinin	Influenza A virus
14884	EVSMILTY	hemagglutinin	Influenza A virus
16733	FLKMGALG	hemagglutinin	Influenza A virus
17778	PLTSDSYV	hemagglutinin	Influenza A virus
18188	PKHGKFP	hemagglutinin	Influenza A virus

(3) ImmunomeBrowser

Maps set of epitopes to an antigen, highlighting immunogenic regions.

Overview of 3 Viewers

IEDB-3D 2.0 Viewer Project

- **Assay Viewer** - Displays experimentally determined 3D structures from PDB, directly showing epitope recognition.
- Depending on the assay, it can show an epitope bound to MHC, MHC & TCR or an antibody with pre-calculated contacts

(1) Assays Tab

IMMUNE EPITOPE DATABASE AND ANALYSIS RESOURCE

Home Specialized Searches Analysis Resource

Pending Filters:

Filter Options [?](#)

Default

Epitope [?](#)

Any

Linear peptide

Length

Sequence

Discontinuous

Non-peptidic

3D structure available

Amino acid modification

Epitope Source [?](#)

Organism

Current Filters: Include Positive Assays 3D structure available

Epitopes (3616) Antigens (896) Assays (5493)

T Cell Assays (387) B Cell Assays (3790) MHC Ligand Assays (1136)

Go To Records Starting At

367 Records Found Page 1 of 15

ID	Reference	Epitope	Host	Immunization	Assay Antigen
211922	Dleg Y Borbulevych; Immunol 011	AAGIGILTV Melanoma antigen recognized by T-cells 1 (27-35) Homo sapiens (human)	Homo sapiens (human)	Occurrence of cancer (skin melanoma)	AAGIGILTV Melanoma antigen re by T-cells 1 (27-35) Homo sapiens (hum
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The IEDB has just launched its updated 3D viewers! Learn more via our help article [here](#).

Welcome

The Immune Epitope Database (IEDB) is a freely available resource funded by NIAID. It catalogs experimental data on antibody and T cell epitopes studied in humans, non-human primates, and other animal species in the context of infectious disease, allergy, autoimmunity and transplantation. The IEDB also hosts tools to assist in the prediction and analysis of epitopes.

[Learn More](#)
Upcoming Events & News

AAI Exhibitor Booth	May 6-10
FOCIS Exhibitor Booth	June 21-24
Virtual User Workshop	Oct 26-28

* register [here](#)

[IEDB SARS-CoV-2 Epitope Analysis Videos](#)
Summary Metrics

Peptidic Epitopes	1,539,170
Non-Peptidic Epitopes	3,146
T Cell Assays	443,509
B Cell Assays	1,332,364
MHC Ligand Assays	4,631,827
Epitope Source Organisms	4,234
Restricting MHC Alleles	970
References	23,297

START YOUR SEARCH HERE
Epitope

- Any
- Linear peptide
- Discontinuous
- Non-peptidic

 Exact M

Assay

- T Cell
- B Cell
- MHC Ligand

 Ex: neutralization

 Outcome: Positive Negative

Epitope Source

Organism

 Ex: influenza, peanut

Antigen

 Ex: core, capsid, myosin

MHC Restriction

- Any
- Class I
- Class II
- Non-classical
- Ex: HLA-A*02:01


Host

- Any
- Human
- Mouse
- Non-human primate
- Ex: dog, camel


Disease

- Any
- Infectious
- Allergic
- Autoimmune
- Ex: asthma



Epitope Analysis Resource
T Cell Epitope Prediction

Scan an antigen sequence for amino acid patterns indicative of:

- MHC I Binding
- MHC II Binding
- MHC I Processing (Proteasome, TAP)
- MHC I Immunogenicity

B Cell Epitope Prediction

Predict linear B cell epitopes using:

 Antigen Sequence Properties

Predict discontinuous B cell epitopes using antigen structure via:

- Discotope
- ElliPro

Epitope Analysis Tools

Analyze epitope sets of:

- Population Coverage
- Conservation Across Antigens
- Clusters with Similar Sequences

IEDB-3D 2.0 Viewer Project

- **Epitope Viewer** - Displays where an **individual epitope** is located in its source antigen, using 3D models of the antigen either pulled from the PDB or from the [AlphaFold Protein Structure Database](#).

(2) Epitopes Tab

IMMUNE EPITOPE DATABASE AND ANALYSIS RESOURCE

Home Specialized Searches Analysis Resource Help More IEDB

Pending Filters: Include Positive Assays

Reset Search

Filter Options (?)
Default

Epitope (?)
 Any
 Linear peptide
Length
Sequence
 Discontinuous
 Non-peptidic
 3D structure available
Amino acid modification

Epitope Source (?)
Organism
Ex: influenza, peanut
Antigen
Ex: core, capsid, myosin
Include related structure
Select multiple options

Current Filters: Include Positive Assays

Epitopes (59743) Antigens (14816) Assays (90360) Receptors (2478) References (80)

Go To Records Starting At 1200 Export Results

59743 Records Found Page 1 of 2390 Per Page 25

IEDB ID	Epitope	Antigen	Organism	# References	# Assays
4602	ASNNEMETM	Nucleoprotein	Influenza A virus	7	32
20354	GILGFVFTL	Matrix protein 1	Influenza A virus	7	15
26730	IYERDFSY	Ribonucleoside-diphosphate reductase large subunit	Variola virus (small pox virus)	7	10
61151	SSLENFRAYV	Polymerase acidic protein	Influenza A virus	7	24
72636	WMACHSAAF	Nucleoprotein	Influenza A virus	7	11
2137	AIYKNTIAY	Uncharacterized protein (UniProt Q5NH73)	Francisella tularensis	6	6
3050	AMAAAAAPY	PPE family protein PPE56	Mycobacterium tuberculosis	6	6
42446	MQYLNPPPY	Matrix protein VP40	Marburg marburgvirus (Lake Victoria marburgvirus)	6	7
56338	RVLDCRTAF	Genome polyprotein	Yellow fever virus (Flavivirus febricis)	6	6
74568	YLAGAGLAF	Genome polyprotein	Dengue virus	6	6
2533	ALFHKVGSY	RNA-directed RNA polymerase L	Marburg marburgvirus (Lake Victoria marburgvirus)	5	5
4903	ATATWFQYY	Polymerase protein	Saaremaa hantavirus (Saaremaa virus)	5	5
5554	AVTALTIAY			5	5
14894	EVVDMISTY	mRNA-capping enzyme catalytic subunit	Vaccinia virus (vaccinia virus VV)	5	7
16733	FLLDALKL	Polymerase acidic protein	Influenza A virus	5	12
17778	FSLTSSSKY	Envelope polyprotein	Amur virus	5	5
18186	FVHSGRIYF	RNA-directed RNA polymerase L	Zaire ebolavirus (Zaire Ebola virus)	5	5

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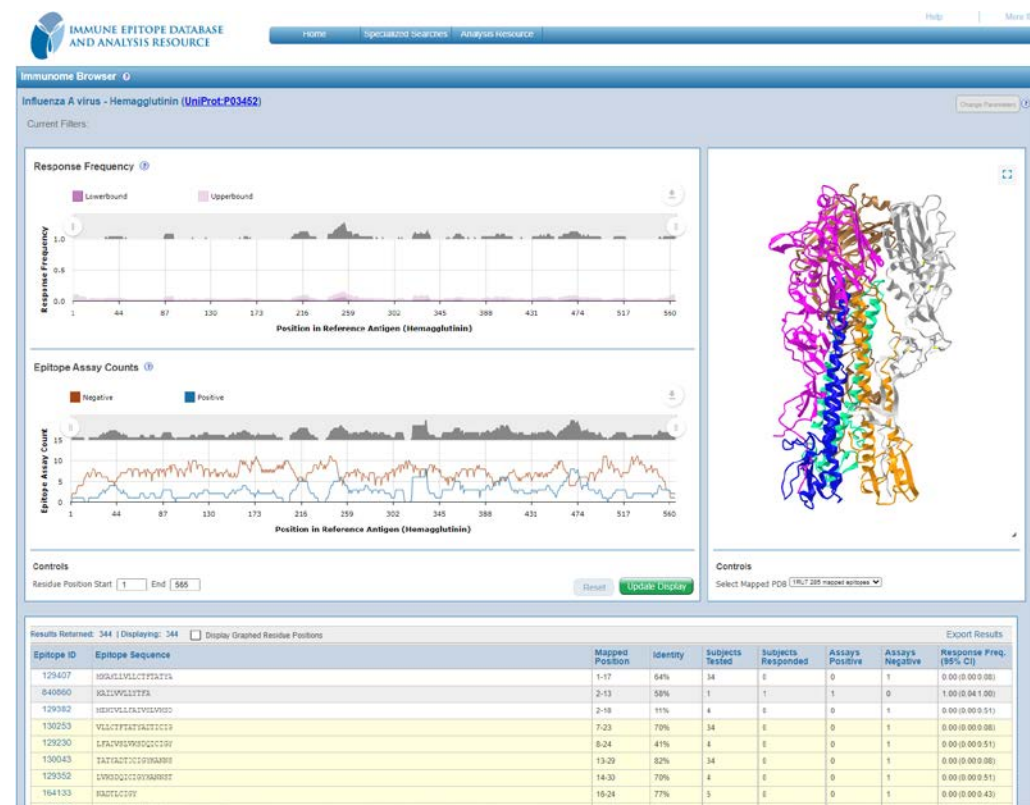
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IEDB-3D 2.0 Viewer Project

- **Immunome Browser Viewer** - works like the Epitope Viewer, but maps a **set of epitopes** to an antigen and highlights which antigen residues are frequently part of epitopes that are commonly recognized (i.e., immunogenic regions).

(3) Immunome Browser



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Search

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Epitope Source Organisms	4,241
Restricting MHC Alleles	971
References	23,343

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IEDB-3D 2.0 Help Article



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IEDB 3D Viewers (IEDB-3D 2.0)



Nina Blazeska

13 days ago · Updated

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The IEDB has been enhanced to enable **better visualization of 3D structures**. We are now using NCBI's [iCn3D viewer](#) to visualize the structures - please refer to the help resources available on the NCBI page for general introductions on how to utilize the viewer.

The IEDB has implemented three custom viewer applications that visualize different aspects of IEDB data:

1. **Assay Viewer** - Displays an experimentally determined 3D structure from the [Protein Data Bank \(PDB\)](#), which **directly shows epitope recognition**. Depending on the assay type, it displays an epitope being bound by MHC, an epitope bound by MHC and a TCR, or an epitope bound by an antibody, and provides consistent naming of chains and pre-calculated contacts.
2. **Epitope Viewer** - Displays where an **individual epitope** is located in its source antigen, using 3D models of the antigen either pulled from the PDB or the [AlphaFold Protein Structure Database](#).
3. **ImmunomeBrowser Viewer** - works like the Epitope Viewer but maps a **set of epitopes** to an antigen and highlights which antigen residues are frequently part of epitopes that are commonly recognized (i.e., immunogenic regions).

<https://help.iedb.org/hc/en-us/articles/6339160938523>

Thanks!

