

Supplementary Information

Pox-AbDab: the Orthopoxvirus Antibody Database

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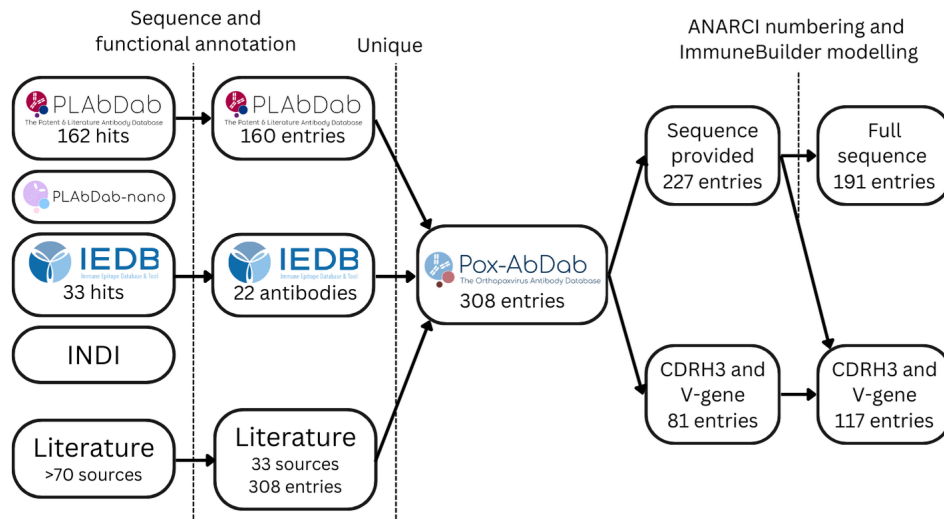


Figure S1. Data curation flow for Pox-AbDab. The publicly available databases PLaBdab (1), PLaBdab-nano (2), IEDB (3), and INDI (4) were searched for antibodies binding orthopoxvirus antigens. Additionally an exhaustive literature search on antibodies binding to orthopoxviruses was performed to collect additional antibodies for which sequence and binding/neutralisation information is available. No antibodies/nanobodies could be retrieved from PLaBdab-nano and INDI. The resulting database, Pox-AbDab contains 308 antibody entries. We filtered full sequence information based on if ANARCI (5) is able to number the sequence and ImmuneBuilder (6) is able to structurally model the sequence. This removed full sequence information for 36 antibodies as their provided sequences are incomplete.

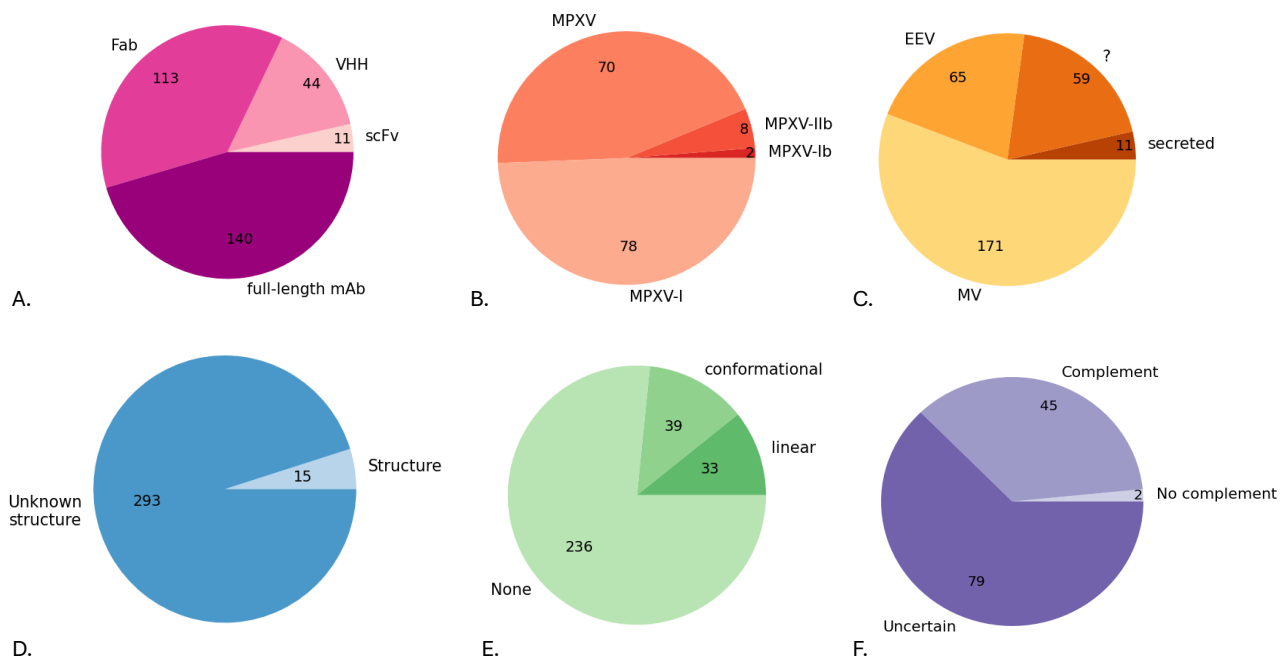
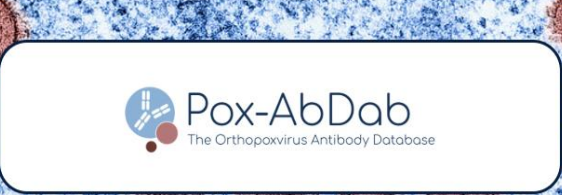


Figure S2. Pie charts showing (A) the ratios of conventional antibodies and single-domain antibodies in Pox-AbDab, with conventional antibodies split by format; (B) where a Pox-AbDab entry has been tested against MPXV, the clade that was tested (if specified, else 'MPXV'); (C) the location context of each entry, (if specified, else '?'); (D) the number of entries for which crystal structures are available; (E) the epitope information available for each Pox-AbDab entry. Linear epitope information is defined as a contiguous string of amino acids. (F) the contingency of neutralisation on an active complement system.

A.



B.

> Downloads

Database (CSV)

C.

> Search Database by Attribute

To view all entries, leave all search fields as 'All' and click 'Search'

Antibody construct: All
Species origin: All
Binds to: Virus: YACV, Clade: All, Strain: All, Location: mpox virus, Protein: L1
Does not bind to: Virus: All, Clade: All, Strain: All, Location: All, Protein: All
Neutralises: Virus: All, Clade: All, Strain: All, Location: All
Does not neutralise: Virus: All, Clade: All, Strain: All, Location: All
Protects against: Virus: All, Clade: All, Strain: All, Location: All
Does not protect against: Virus: All, Clade: All, Strain: All, Location: All
Epitope type: All
Heavy V gene: All
Heavy J gene: All
Light V gene: All
Light J gene: All
Added since: QMOMQOOS
Updated since: QMOMQOOS

Search

Downloads: CSV Excel

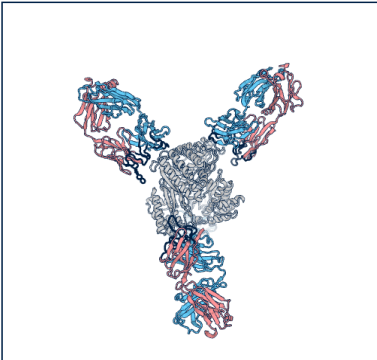
10 entries per page

Search:

| Name | Construct | Species origin | Binds to (virus=[clade]_strain_location_protein) | Does not bind to (virus=[clade]_strain_location_protein) | Neutralises (virus=[clade]_strain_location) | Does not neutralise (virus=[clade]_stra |
|-------|-----------------|----------------|--|---|--|--|
| T011 | Fab | mouse | YACV_MV_M2_7, YACV_T_MV_L1, MPXV-129_USA-2022-M6001_MV_M1(r) | | YACV_MND-3_7 | |
| RC3 | full-length mAb | mouse | YACV_T_MV_L1(r) | | | YACV_MV_MV |
| M12B9 | full-length mAb | mouse | YACV_T_MV_L1(r) | | YACV_MV_MV | |
| M2E9 | full-length mAb | mouse | YACV_T_MV_L1(r) | | YACV_MV_MV | |
| M7B0 | full-length mAb | mouse | YACV_T_MV_L1(r) | | YACV_MV_MV | |

D.

> Structure visualisation



E.

Key (Default Scheme):

- VH Chains
- VL Chains
- CDRs
- Antigen Chains

Display options:

- Spacefill
- Wire
- Ball&stick
- Cartoon
- Default colours
- Colour by B-factor
- Colour by chain
- Colour by sec. structure
- Colour by element
- Spin on/off

Figure S3. The Pox-AbDab Web Application. (A) The Pox-AbDab homepage logo (background image credit: NIAID, Mpox Virus, CC BY 2.0, <https://www.flickr.com/photos/niaid/52988422372/in/photostream/>). (B) All Pox-AbDab data can be downloaded. (C) The database can be queried by attribute (neutralisation profile, construct, germlines, etc.). (D) The result table of the attribute search. (E) The result table links the experimental solved antibody structures stored in SABDab (7) (PDB ID 2I9I visualised here) or modelled structures by ABodyBuilder2 (6).

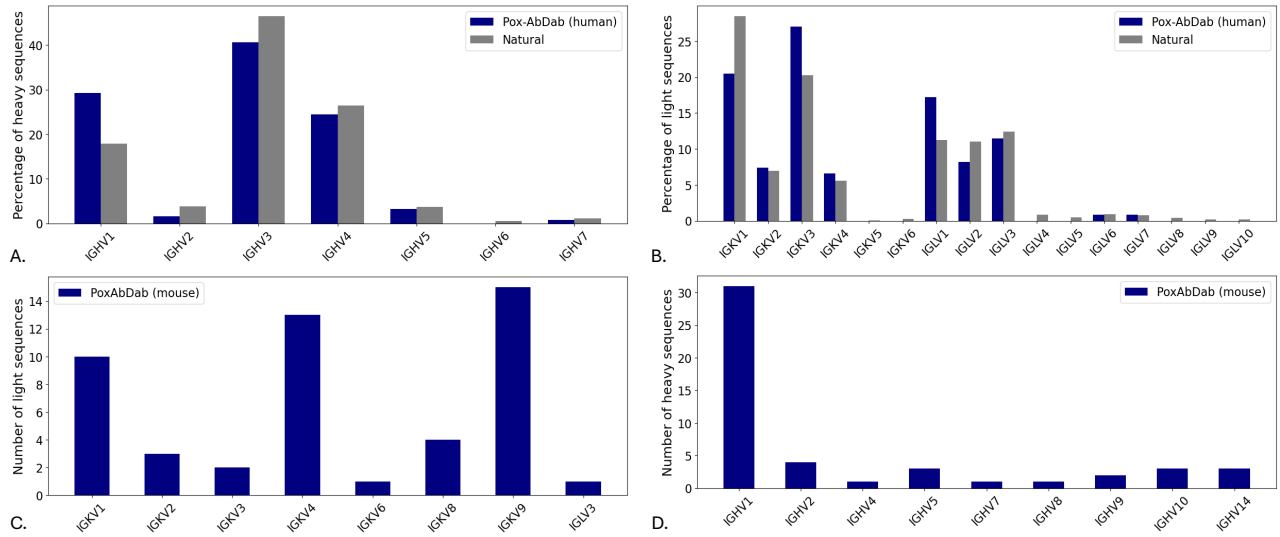


Figure S4. Bar charts showing (A) the distribution of heavy V gene family usage across the human antibodies in Pox-AbDab relative to a sample of the baseline natural repertoire from the Observed Antibody Space (OAS) database (8, 9); (B) the distribution of light V gene family usage across the human antibodies in Pox-AbDab relative to a sample of the baseline natural repertoire from the Observed Antibody Space (OAS) database (8, 9); (C) the distribution of heavy V gene family usage across the murine antibodies in Pox-AbDab; (D) the distribution of light V gene family usage across the murine antibodies in Pox-AbDab. Comparison against the natural human repertoire is based on 5000 randomly samples natural antibody sequence from the Jaffe et al., 2022 (10) as stored in OAS.

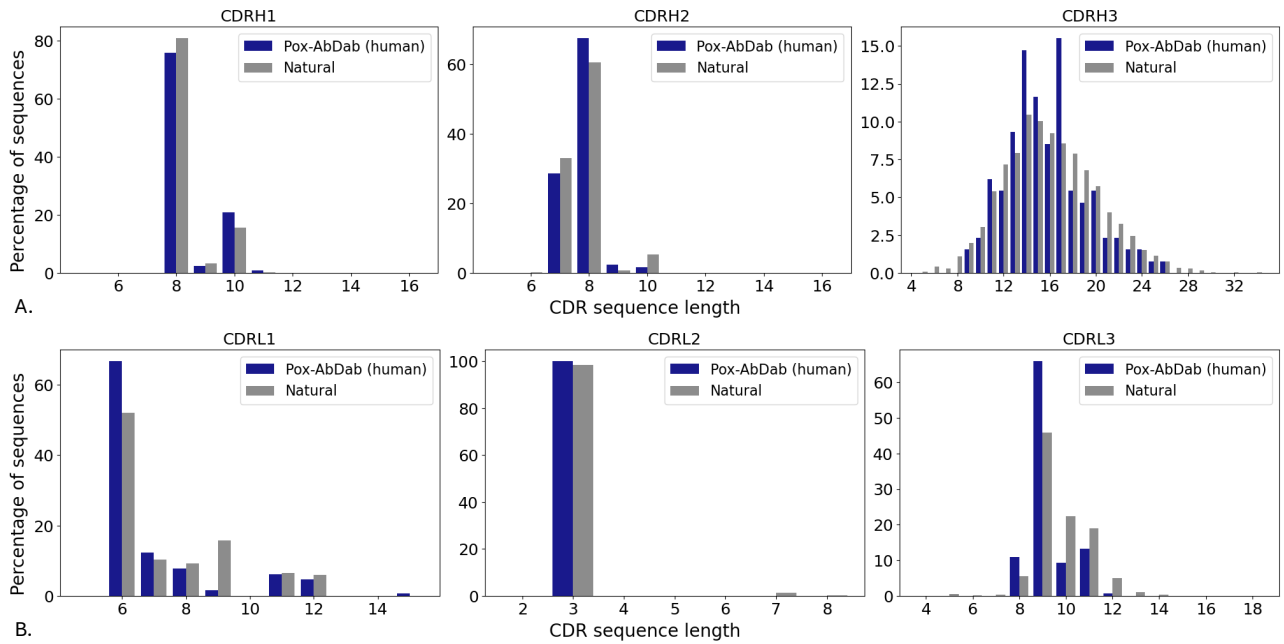


Figure S5. Bar charts showing the distributions of CDR lengths in the full-length sequenced, human antibodies in Pox-AbDab relative to a sample of the baseline natural repertoire from the Observed Antibody Space (OAS) database (8, 9): (A) across heavy chain CDRs, and (B) across light chain CDRs. Comparison against the natural human repertoire is based on 5000 randomly samples natural antibody sequence from the Jaffe et al., 2022 (10) as stored in OAS.

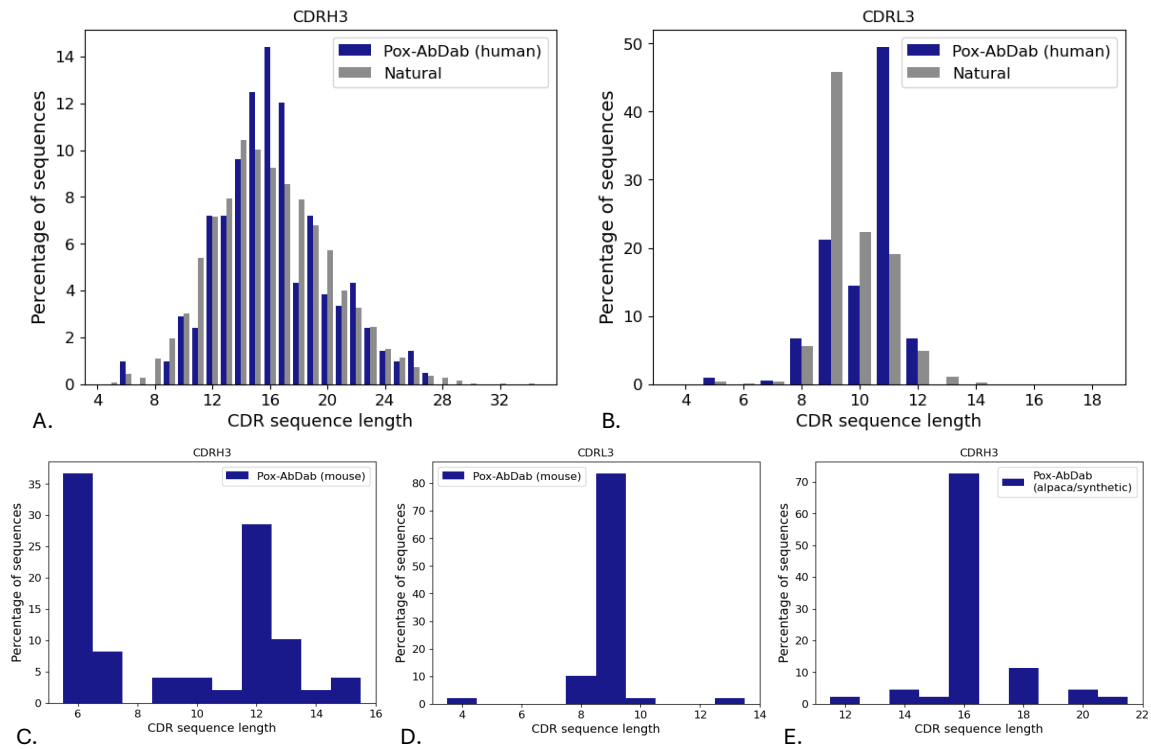


Figure S6. Bar charts showing (A) the CDRH3 and (B) the CDRL3 distributions of all the human antibodies in Pox-AbDab (including those that only have clonotype information) relative to a sample of the baseline natural repertoire from the Observed Antibody Space (OAS) database (8, 9); (C) the CDRH3 and (D) the CDRL3 distributions of all the murine antibodies in Pox-AbDab (including those that only have clonotype information); (E) the CDRH3 distribution of all single-domain antibodies in Pox-AbDab. Comparison against the natural human repertoire is based on 5000 randomly samples natural antibody sequence from the Jaffe et al., 2022 (10) as stored in OAS.

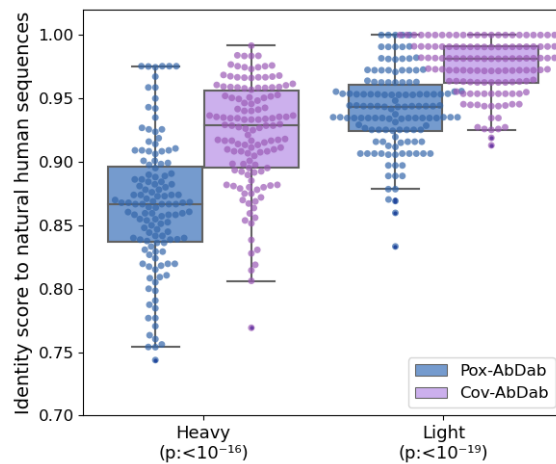


Figure S7. Antibody heavy and light sequence identity score to a set of human antibodies from naive B-cells. The 130 full-length human antibody sequences in Pox-AbDab (blue) and 130 randomly selected human antibody sequences from CoV-AbDab (purple) were compared against all human B cell receptor sequences from OAS using the "OAS-aligned" dataset provided with KA-Search (1.9Bn heavy chains from 69 studies, 350.5M light chains from 38 studies). The highest sequence identity observed was recorded. P-values of the Mann-Whitney U test are indicated on the x-axis.

| Protein in VACV Nomenclature (Strain if not Copenhagen) | Location | Function | Surface protein | Number of targeting antibody sequences | Number of targeting antibody crystal structures |
|---|----------|----------------------------------|-----------------|--|---|
| A10 | MV | Assembly (11) | No | 1 | |
| A13 | MV | Assembly (12) | Yes | | |
| A14 | MV | Morphogenesis (13) | Yes | 5 | |
| A16 | MV | Entry/Fusion | Yes | 4 | |
| A17 | MV | Assembly, Fusion | Yes | | |
| A21 | MV | Entry/Fusion | Yes | 1 | |
| WR148 (WR) | MV | Fusion Suppressor | No | 7 | |
| A26 | MV | Attachment | Yes | | |
| A27 | MV | Attachment | Yes | 27 | 2 |
| A28 | MV | Attachment | Yes | 1 | |
| A33 | EEV | Spread | Yes | 33 | 3 |
| A34 | EEV | Spread, Attachment (14) | Yes | | |
| A56 | EEV | Fusion (15), Immune Evasion (16) | Yes | | |
| B5 | EEV | Spread, Morphogenesis | Yes | 27 | 1 |
| C3 | Secreted | Immune evasion | No | 11 | |
| D8 | MV | Attachment | Yes | 32 | 5 |
| F5 | EEV | Plaque morphology (17) | Yes | | |
| F9 | MV | Entry/Fusion | Yes | 1 | |
| F13 | EEV | Spread (18), Morphogenesis (18) | Yes | 1 | |
| G3 | MV | Entry/Fusion | Yes | | |
| G9 | MV | Entry/Fusion | Yes | | |
| H2 | MV | Entry/Fusion | Yes | | |
| H3 | MV | Assembly, Attachment | Yes | 39 | |
| H5 | MV | Morphogenesis (19) | No | 2 | |
| I1 | MV | Assembly (20) | No | 5 | |
| J5 | MV | Entry/Fusion | Yes | | |
| L1 | MV | Entry/Fusion | Yes | 15 | 2 |
| L5 | MV | Entry/Fusion | Yes | | |
| O3 | MV | Entry/Fusion | Yes | | |

Table S1. VACV proteins with known roles in orthopoxvirus function alongside the data availability for antibodies engaging each protein in Pok-AbDab. For the proteins highlighted in bold no antibody sequence is publicly available. All function annotations derive from Moss et al. 2011 (21), except where otherwise indicated.

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