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Data Article

Dataset of SARS-CoV-2 spike protein receptor binding domain variants in complex with antigen-binding fragments targeting COVID-19 vaccine-referenced variants

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ABSTRACT

In this paper, we present a dataset of homology-modeled structures of SARS-CoV-2 Spike protein Receptor Binding Domain (RBD) variants complexed with antigen-binding fragments (Fab) derived from the PDB structures 8GPY (Omicron BA.4/5 RBD in complex with a neutralizing antibody scFv), 8H7Z (BA.2 RBD in complex with BA7535 Fab), and 8XE9 (XBB.1.5 RBD in complex with BD55–1205). The dataset consists of six sets of complex structures generated by combining 14 RBD variants with three different Fab pairs.

The SARS-CoV-2 Spike protein sequence variants included in the dataset are Wild Type, BETA, EPSILON, IOTA, ETA, GAMMA, LAMBDA, KAPPA, BA.2, BA.4, XBB.1.5, EG.5.1, and KP.2. Notably, the KP.2 variant, which has gained attention due to its inclusion in recent vaccine updates (https://www.ema.europa.eu/), is also part of this dataset.

The models were refined using the Schrödinger Bioluminate suite of software. For each variant, the homology-modeled RBDs were complexed with the Fab fragments from 8GPY, 8H7Z, and 8XE9 by grafting them onto the RBDs, followed by energy minimization, both individually and in combination. This process resulted in a comprehensive dataset of RBD-Fab

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complexes, suitable for comparative analysis and further investigations.
Binding affinities between the RBD-Fab pairs were calculated using the Prime MM-GBSA tool (VSGB solvation model and OPLS4 force field), enabling the ranking of antigen-antibody interactions. Structural minimizations were performed to accurately estimate interaction energies, providing insights into the efficacy of antibody binding across different variants.
This dataset provides high-quality structural data that can be reused for in-depth studies of antibody-antigen interactions, particularly in the context of vaccine efficacy and viral immune evasion strategies. The inclusion of the KP.2 variant, which is central to the latest COVID-19 vaccine updates, makes these homology models especially relevant. Supplementary files include the homology-modeled structures, computed binding affinities, and quality assessments (QMEANDisCo) for each model, ensuring reproducibility and reliability for further analyses.

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Specifications Table

Subject	Biology: structural biology.
Specific subject area	Structural biology and structural bioinformatics.
Type of data	Table .csv, Image .jpg, Protein structure .pdb, quality assessment visualization: .html, quality assessment results .json.
Data collection	Template sequences downloaded from https://www.ncbi.nlm.nih.gov/genbank/; Target structures downloaded from https://www.rcsb.org.
Data source location	ModelArchive.
Data accessibility	Repository name: ModelArchive Data identification number: 10.5452/ma-t6okf Direct URL to data: https://www.modelarchive.org/doi/10.5452/ma-t6okf
Related research article	none.

1. Value of the Data

- **Comprehensive Variant Coverage and Validated Structural Integrity**: This dataset offers homology models of multiple SARS-CoV-2 Spike protein Receptor Binding Domains (RBDs) complexed with antigen-binding fragments (Fab), covering a wide range of variants. These models provide crucial insights into the structural effects of mutations in the Spike protein, particularly regarding their impact on antibody binding and immune evasion. The accuracy of the models has been confirmed through quality assessment metrics (QMEANDisCo), ensuring their structural reliability.
- **Advanced Computational Analysis**: The high-quality, validated models of SARS-CoV-2 Spike protein RBD-Fab complexes offer a robust foundation for various computational studies. These models can be used as input for molecular dynamics simulations to explore the flexibility and conformational changes of antigen-antibody complexes over time. Additionally, they can be employed in virtual screening workflows to identify potential therapeutic candidates, perform free energy calculations to predict binding affinities, or support structure-based drug design efforts. The broad variant coverage enables assessments of mutation-induced structural changes, making the dataset a valuable tool for studying viral evolution and guiding future vaccine and therapeutic development.

- **Utility for Antibody Design and Optimization**: The dataset includes comprehensive binding affinity calculations between Spike protein variants and Fab fragments. The models may be employed by researchers to design or refine antibodies with enhanced efficacy by identifying key binding residues or regions prone to mutations. This resource has the potential to accelerate the development of therapeutic antibodies and optimize vaccines, thereby providing a valuable tool for research in computational immunology and structural biology research.
- **Potential for Comparative Analysis**: The dataset includes binding affinity data for a wide range of Spike protein-antibody complexes, enabling comparative analysis across different variants. The data may be employed by researchers to evaluate the impact of mutations on antibody neutralization, thereby facilitating the elucidation of viral escape mechanisms. This is of particular value in studies focusing on vaccine-resistant variants or emerging strains.

2. Background

The principal objective in assembling this dataset was the urgent need for real-time monitoring of the evolution of the SARS-CoV-2 Spike protein in the context of the ongoing global pandemic. The Spike protein, and in particular its Receptor Binding Domain (RBD), is highly susceptible to mutations, which can have a significant impact on viral infectivity, immune evasion, and vaccine efficacy. In light of the rapid emergence of new variants, there is pressing need for comprehensive structural data to elucidate the impact of these mutations on antibody recognition and neutralization mechanisms.

To address this need, homology models of various SARS-CoV-2 Spike protein RBD variants complexed with antigen-binding fragments (Fab) were produced [1]. These models provide essential insights into the structural consequences of mutations on antibody binding. By facilitating the examination of interactions between the Spike protein and neutralizing antibodies, this dataset serves as a crucial tool for monitoring the ongoing viral evolution and evaluating its implications for public health.

As the virus continues to mutate, particularly in regions critical for immune recognition such as the RBD, the availability of high-quality, validated models is essential for the advancement of research in this field [2–7]. These models allow for the evaluation of potential immune evasion mechanisms that may reduce the efficacy of existing vaccines or therapeutic antibodies. The dataset offers a reliable resource for researchers to analyze the structural effects of mutations, predict potential risks of immune evasion, and develop strategies to mitigate the impact of emerging variants.

The dataset is grounded in structural biology and computational modeling, thereby ensuring its versatility for reuse in a multitude of applications, including dynamics simulations, predictive analyses, and virtual screening efforts. This proactive approach enables the scientific community to remain at the forefront of viral evolution, thereby informing updates to vaccines and therapeutic interventions and contributing to global health security.

The provision of detailed and validated structural models by this dataset facilitates an understanding of the impact of viral mutations on the immune response, guiding the ongoing development of vaccines and therapeutics designed to counteract SARS-CoV-2 and its variants.

3. Data Description

3.1. Cover structure

The KP.2 RBD, complexed with the experimentally resolved Fab from the 8XE9 structure, was selected as the cover structure to emphasize both the novelty of the KP.2 variant and its

relevance to ongoing vaccine updates. This structure illustrates the binding affinity of the KP.2 variant to H and L chains, which were previously validated in prior variants used for COVID-19 vaccine updates. By emphasizing this resolved structure, the cover highlighted the importance of monitoring emerging variants like KP.2, particularly in terms of their potential impact on vaccine efficacy and antibody binding.

3.2. Complete dataset

The complete dataset is provided in the accompanying_data.zip file, which contains the following:

1. content.txt: A file that provides an organized list of all folders and files. The PDB files are named to represent the Spike RBD-antibody homology model (template filename format: [variant]_[target structure/structures]-[H & L chains experimentally resolved PDB structure].pdb).
2. PdBStructures.zip: This file contains all PDB files organized into subfolders based on sets of variant homology model complexes. The folders 8H7Z, 8GPY, and 8XE9 contain complexes generated using the respective PDB structure as the target, along with the corresponding H and L chains. Additionally, the folders 3–8H7Z, 3–8GPY, and 3–8XE9 contain complexes generated using all three PDB structures as targets, with the H and L chains grafted from the PDB structures mentioned in the folder titles.
3. Quality_Assessment.zip: This file includes two main directories:
   - HMSPIKE_RBD_VARIANTS_monotarget_complex_with_HL: Contains quality assessments for models generated using a single target.
   - HMSPIKE_RBD_VARIANTS_multitarget_complex_with_HL: Contains quality assessments for models generated using multiple targets.

   Each directory includes QMEANDisCo quality metrics for each homology model, with files such as results.json, qmean_bfactors.pdb, and visual representations like Ramachandran plots.

variant_quality_assessment.csv: A file organized into three columns, providing the correspondence between the quality assessment, the homology model, and links to the full quality evaluation for each model.

4. Experimental Design, Materials and Methods

4.1. Data acquisition process

The dataset was generated using a homology modeling approach based on the Receptor Binding Domain (RBD) of the SARS-CoV-2 Spike protein in complex with Fab. The experimentally resolved PDB templates were carefully selected for their validated structural integrity, ensuring both high structural quality and relevance to antigen-antibody interactions (visual flowchart shown in Fig. 1).

The computational workflow was designed in such a way as to capture structural variations driven by RBD mutations, while at the same time preserving the experimental orientation of the Fab-RBD interface. To maintain these orientations, the homology modeling workflow aligned the RBD variants to the experimental templates, retaining key structural features, particularly at the antigen-antibody interface. The energy minimization step, described in the

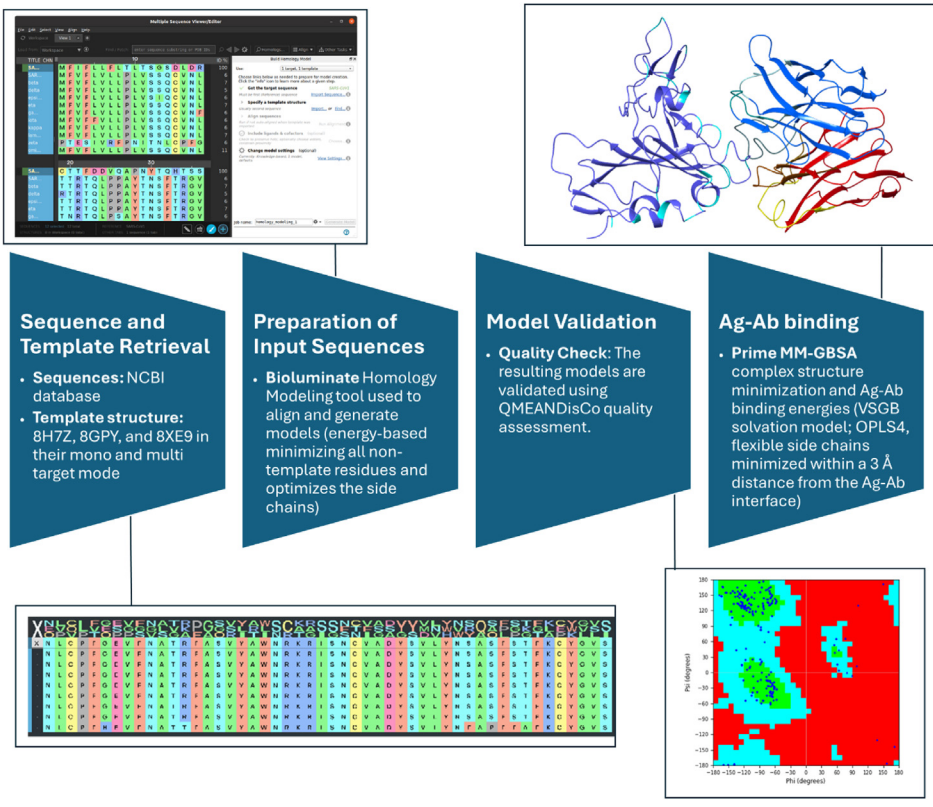


Fig. 1. Visual Flowchart of the experimental design. The flowchart summarizes the steps for sequence retrieval, homology modelling, model validation, and binding affinity calculations for SARS-CoV-2 Spike protein variant RBD-Fab complex pairs.

following pipeline, preserved the protein-protein orientation, thereby minimizing potential deviations from the original experimental structures as shown in Fig. 2.

Post-translational modifications (PTMs) were not explicitly modeled in this study, as the experimental reference templates do not include these features. While tools for modeling PTMs are available, we opted to remain faithful to the experimental structures, as they inherently account for the effects of PTMs in the observed binding modes. This decision ensures that the homology-derived models reflect the experimental conditions, which implicitly consider PTMs, particularly in regions distant from the RBD-Fab interaction interface analysed in this work. Although PTMs may influence binding interactions, their absence does not significantly impact the primary objective of comparing Fab-RBD binding affinities across variants. This approach ensures that the dataset remains consistent with the experimental data, thus providing robust structural models optimized for comparative analysis and downstream computational studies.

The dataset was generated, refined, and validated using a comprehensive pipeline designed to ensure methodological rigor, accuracy, and reproducibility. The binding energies were calculated directly from the experimentally resolved binding modes, with the experimental conformations employed as implicit constraints. This approach mitigated potential artifacts associated with al-

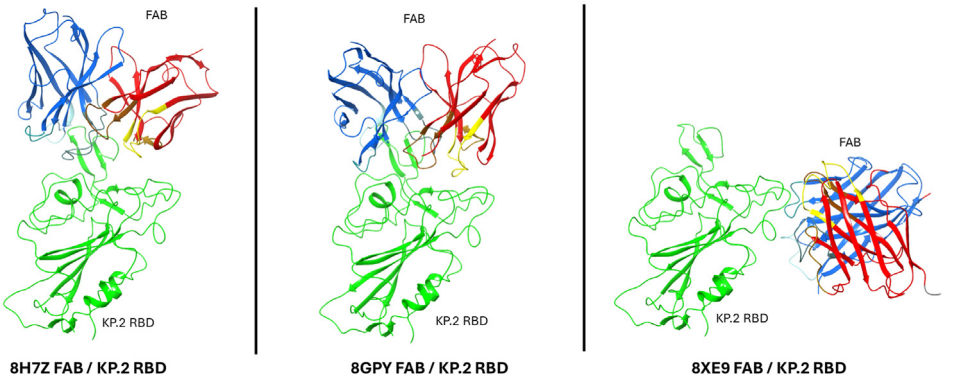


Fig. 2. Protein–protein orientation of the complex models. The figure illustrates the homology model of the KP.2 variant (green cartoon representation) in complex with the Fab fragments derived from PDB structures 8H7Z, 8GPY, and 8XE9. The heavy chain (H) is depicted in blue, while the light chain (L) is shown in red.

ternative poses that could arise from docking workflows or molecular dynamics simulations. The finalized models, which are now available for the download the Model Archive, are provided in a standard PDB format, ensuring full compatibility with open-source tools. This accessibility allows the scientific community to employ these models for in-depth investigations of alternative binding modes and dynamic interactions, thereby enhancing their versatility and scientific utility.

1. Protein Sequence Selection: The amino acid sequences of the following SARS-CoV-2 Spike protein variants were used: ETA B.1.351 (GenBank: QRN78347.1), DELTA B.1.617.2 (GenBank: QUD52764.1), ETA B.1.525 (GenBank: QRF70806.1), EPSILON B.1.429 (GenBank: QQM19141.1), GAMMA P.1 (GenBank: QRX39425.1), IOTA B.1.526 (GenBank: QRX49325.1), KAPPA B.1.617.1 (GenBank: QTY83052.1), LAMBDA B.1.1.1.C37 (GenBank: OT390974.1), OMICRON BA.2 (GenBank: 00,923,605.1), OMICRON BA.4 (GenBank: UPP14409.1), OMICRON EG.5.1 (GenBank: WGM84363.1), Omicron XBB.1.5 (GenBank: UZG29433.1), WILD TYPE (GenBank: QHD43416.1), and KP.2 (information available at https://outbreak.info).
2. Homology Modeling
   - Software Used: The Schrödinger Bioluminate Suite (v2024–1) was used to perform all homology modeling tasks [8].
   - Homology Modeling Workflow: The RBD regions of the Spike protein variants were modeled using three PDB templates—8GPY (Omicron BA.4/5 RBD-antibody complex), 8H7Z (BA.2 RBD with Fab), and 8XE9 (XBB.1.5 RBD with antibody BD55–1205)—selected because the resolved RBDs belong to variants used in recent COVID-19 vaccine updates (https://www.ema.europa.eu/). For each variant sequence, both individual and multiple-template approaches were applied, resulting in six sets of homology models. The models were further refined by grafting the Fab structures from the respective templates onto the modeled RBDs, generating six sets of models per variant.
     The obtained structures were then prepared for subsequent analysis through the following procedure:
     - Alignment with the experimental structures to standardize the spatial reference system.
     - Assignment of bonding orders and addition of hydrogen atoms according to the standards of the applied force field.

Table 1
MMGBSA DeltaG binding values. MMGBSA DeltaG binding values for SARS-CoV-2 Spike protein variants grafted to Fab across different PDB target structures (8H7Z, 8GPY, 8XE9). Lower DeltaG values represent stronger binding interactions. A 'Y' in the column 'Vaccine Reference Variant' indicates that the variant was used as a reference for COVID-19 vaccine development and/or updates. Specific data on the vaccine reference data available in https://www.ema.europa.eu/.

Rbd-hl pdb target structure	Vaccine reference variant	TARGETS						
Sars-CoV-2 variant		Date	8H7Z	8GPY	8XE9	8H7Z	8GPY	8XE9
Fab docked Spike protein Variant DBD			8H7Z BA 2	8GPY BA 4	8XE9 XBB 1.5	8H7Z BA 2	8GPY BA 4	8XE9 XBB 1.5
Wild Type	Y	Dec 2019	−78.05	−83.75	−125.47	−59.19	−73.85	−77.86
GAMMA		Jul 2020	−105.86	−75.03	−125.15	−53.52	−76.33	−70.73
BETA		Aug 2020	−100.65	−99.95	−106.44	−63.30	−79.34	−77.98
EPSILON		Sep 2020	−82.22	−49.58	−169.34	−68.13	−82.66	−85.53
IOTA		Nov 2020	−51.04	−76.55	−135.96	−60.98	−76.44	−79.04
DELTA		Dec 2020	−117.35	−88.18	−121.64	−64.85	−82.66	−91.11
ETA		Dec 2020	−51.04	−76.55	−129.64	−57.60	−76.63	−83.35
LAMBDA		Dec 2020	−96.82	−105.26	−111.95	−61.76	−78.17	−80.85
KAPPA		Oct 2021	−115.00	−101.95	−97.73	−60.28	−75.72	−80.10
BA 2	Y	Dec 2021	−160.78	−93.47	−155.75	−60.36	−74.22	−80.69
BA 4	Y	Jan 2022	−125.75	−85.46	−105.27	−60.98	−75.38	−76.95
XBB 1.5	Y	Nov 2022	−118.09	−103.95	−111.87	−56.05	−72.20	−62.96
EG 5,1		Mar 2023	−87.05	−108.11	−129.98	−57.44	−73.23	−77.42
KP.2	Y	Apr 2024	−82.39	−108.99	−119.13	−45.37	−60.22	−64.94

- Identification of disulfide bridges and annotation of the Fab according to the Chothia scheme [9].
- Generation of ionic states at pH 7.4 ± 2 using Epik [10].
- Identification and optimization of hydrogen bonds.

- Multiple Structure Alignment: All RBD structural models were aligned to enable comparative structural analysis.
- Energy Minimization: Energy minimization of non-template residues was performed using Prime [11], applying the OPLS4 force field [12]. This optimization was applied to side chains within a 3 Å cutoff from the protein-protein interface to enhance structural accuracy.

3. Binding Energy Calculations
   - Software Used: The Schrödinger Prime MM-GBSA tool was used to compute the binding free energies (ΔG Bind) for each modeled Spike variant-Fab complex [13].
   - Binding Affinity Calculation: Binding affinities were calculated using the VSGB solvation model and the OPLS4 force field. To ensure realistic interaction energies, the residues at the antigen-antibody interface were minimized within a 3 Å radius. The MM-GBSA ΔG Bind values are reported for each variant, providing insights into the strength of the antigen-antibody interactions (Table 1).
4. Structural Validation
   - Quality Metrics: Each homology model was assessed for structural quality using QMEANDisCo scores [14], a widely used metric for evaluating homology models. The results, along with structural data, are provided in supplementary tables.
5. Data Organization and Output
   - Data Format: The homology models for each variant are stored as .pdb files, accompanied by CSV files containing the calculated binding energy data.

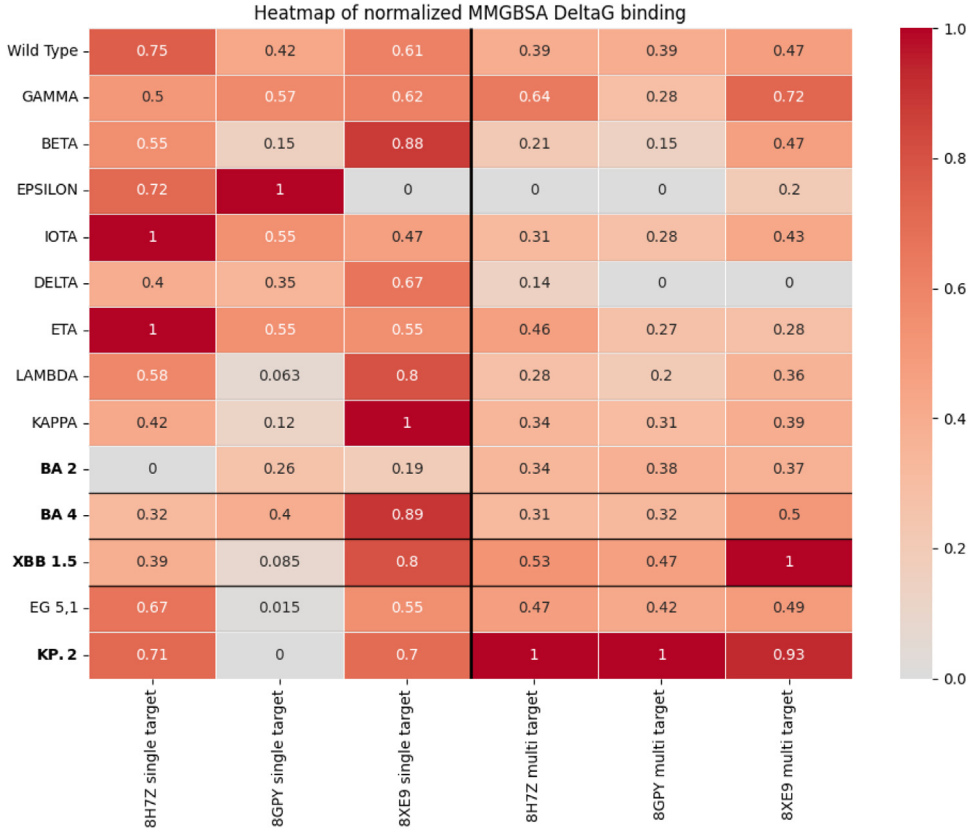


Fig. 3. Heatmap of normalized MMGBSA DeltaG binding values. Lower DeltaG values (darker red) indicate stronger binding interactions, while higher values (lighter shades) reflect weaker interactions within each set of RDB-Fab complexes ordered by column. The order of the variants in the rows corresponds to the chronological evolution of the variants over time, as indicated in Table 1. Bold lables refer to the variants template for COVID-19 vaccine production used to produce the presented dataset.

- Supporting Files: The dataset includes a README file that details the structure and usage of the data, as well as tables summarizing the mutations for each variant and their respective binding energy calculations. Additionally, comprehensive quality assessments for the models are provided in the supplementary data.

This pipeline facilitated the systematic modeling and analysis of SARS-CoV-2 Spike protein variants, providing detailed insights into antigen-antibody interactions across multiple variants and structures. The resulting dataset represent valuable resource for further investigations into viral evolution and the development of therapeutic antibodies.

To enable the use of binding energies as a comparative tool between the antigen-antibody pairs in the generated model sets, the DeltaG values have been normalized on a scale from 0 to 1, where 0 represents the least affine RBD-Fab pair and 1 represents the most affine pair, making the scale relative within the dataset. Figs. 3 and 4 display the normalized binding affinity (DeltaG) variations between the RBD regions of SARS-CoV-2 Spike protein variants and Fab by means of a heat plot and a radar plot.

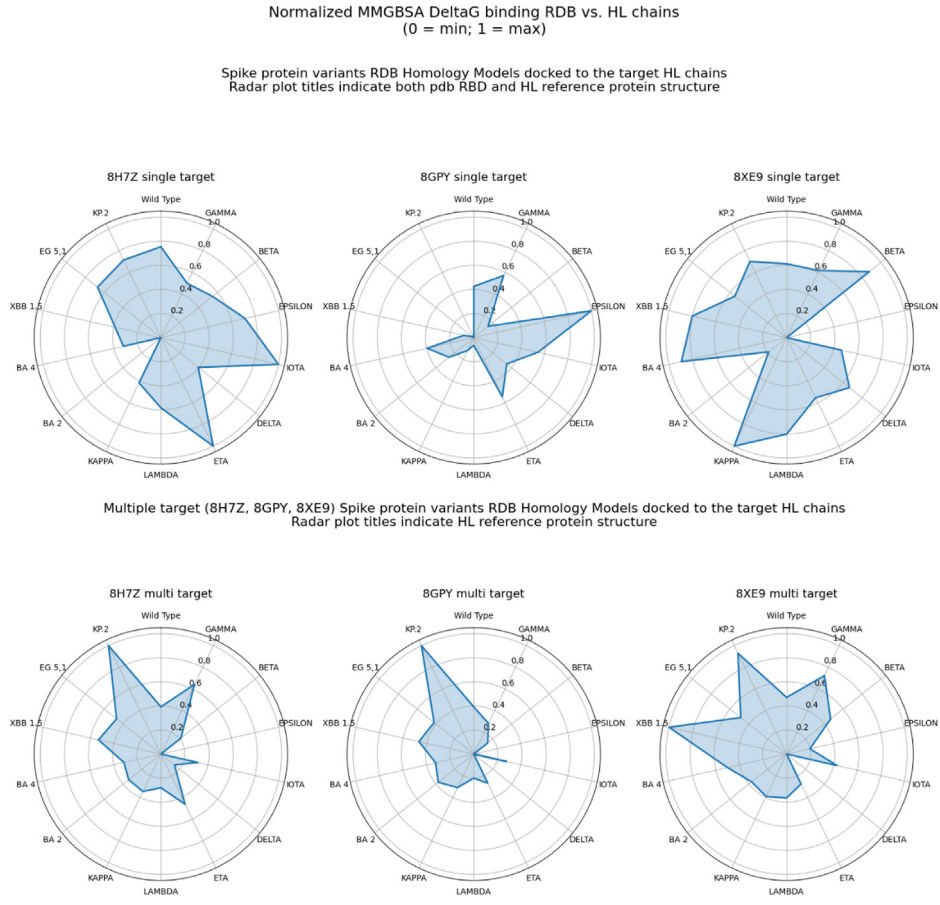


Fig. 4. Radar plots of normalized MMGBSA DeltaG binding values. Normalized DeltaG values range from 0, indicating the weakest interaction among RBD-Fab pairs, to 1, representing the strongest. The variants are labelled in a clockwise order, following Table 1 order. The first row of plots displays single-target Homology Models normalized DeltaG values (8H7Z, 8GPY, and 8XE9 used individually as target structures), and the second row showing multi-target Homology Models normalized DeltaG values (where 8H7Z, 8GPY, and 8XE9 are collectively considered as target structures).

Limitations

One limitation of this dataset is its reliance on homology modeling techniques, which, while powerful, may not fully capture the structural nuances present in experimentally determined protein-antibody complexes. The models are based on available template structures, which correspond to specific structural isoforms produced under experimental conditions. Consequently, they may not entirely reflect the dynamic conformational changes that occur in physiological environments, which could potentially impact the accuracy of structural predictions, particularly in flexible or mutation-prone regions.

Additionally, the predicted binding affinities (ΔG Bind) are dependent on the force fields (OPLS4) and solvation models (VSGB) used in the calculations. Despite the extensive validation of these computational tools, they may introduce certain biases that could influence the ranking of interactions, especially when comparing variants with complex mutations.

However, these structures provide an excellent foundation for subsequent investigations employing other computational tools, including open-source software. This enables researchers to

adapt analyses to their specific requirements. For example, the dataset can be utilized for molecular dynamics simulations, docking recalculations, or other advanced studies, making use of the distinctive capabilities of alternative computational platforms, whether commercial or open source.

Moreover, the dataset does not encompass all potential Spike protein variants. The data set focuses on a selected set of key variants, selected for the purpose of representing virus's temporal evolution up to June 2024. As the SARS-CoV-2 virus continues to evolve, new variants with potentially significant mutations may emerge that are not included in the current dataset. This could limit the dataset's applicability for future variant analysis unless it is updated regularly.

Ethics Statement

The authors have read and follow the ethical requirements for publication in Data in Brief and confirm that the current work does not involve human subjects, animal experiments, or any data collected from social media platforms.

CRediT Author Statement

Ferdinando Spagnolo: Conceptualization, Methodology, Software, Data Curation, Writing - Original Draft, Visualization. **Florigio Lista**: Supervision. **Claudia Curcio**: Conceptualization, Validation, Writing - Review & Editing, Supervision.

Data Availability

Homology Models of SARS-CoV-2 Spike Protein Variants RBD-HL Complexes (Original data) (Model Archive).

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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