Conformational dynamics of the receptor-binding domain of the SARS-CoV-2 spike protein

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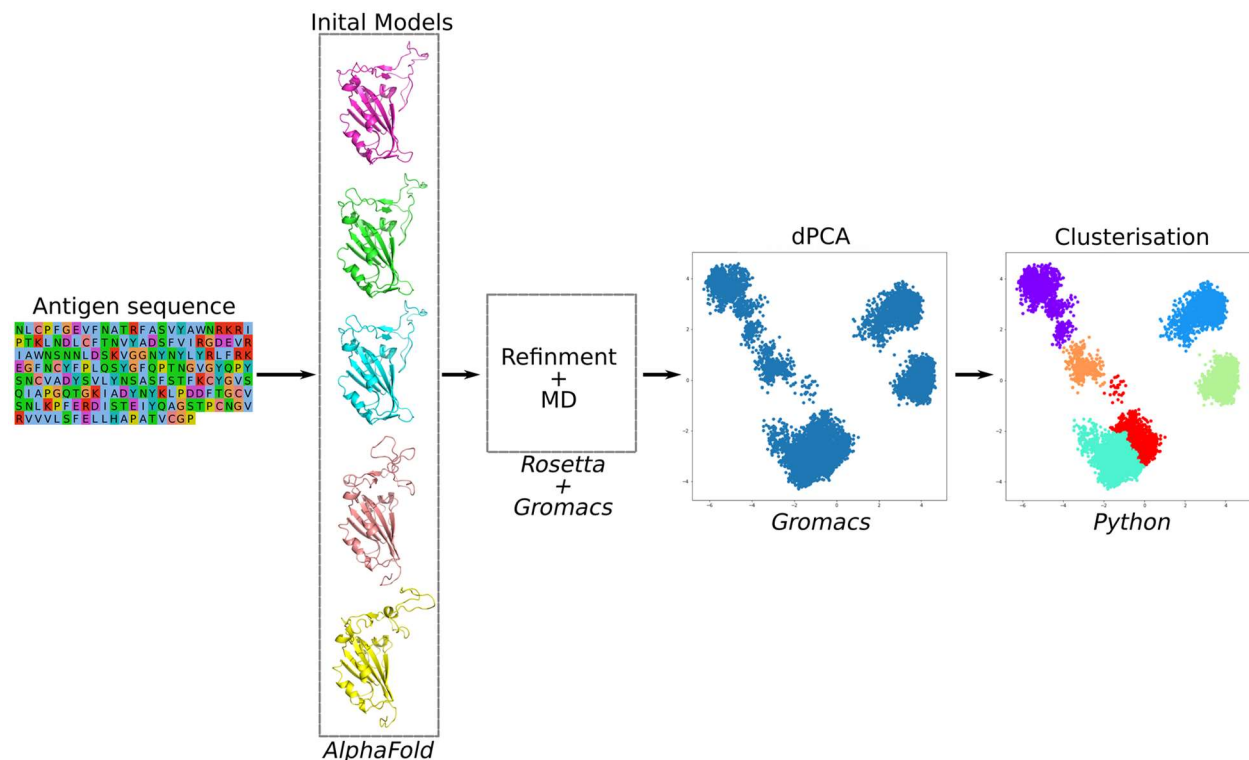   Moscow 119991, Russia
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Supplementary information

Computational workflow details

*SI Figure S1.* Representation of the computational workflow

Used amino acid sequences
Text S1. WT RBD amino acid sequence
*LCPFGEVFNATRFASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFV
IRGDEVRQIAPGQTGKIADYNYKLPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSNLKPFER
DISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVVLSFELLHAPATVCGP*

Text S2. Omicron RBD amino acid sequence
*LCPFDEVFNATRFASVYAWNRKRISNCVADYSVLYNLAPFFTFKCYGVSPTKLNDLCFTNVYADSF
VIRGDEVRQIAPGQTGNIADYNYKLPDDFTGCVIAWNSNKLDSKVSGNYNYLYRLFRKSNLKPFE
RISTEIYQAGNKPCNGVAGFNCYFPLRSYSFRPTYGVGHQPYRVVVLSFELLHAPATVCGP*
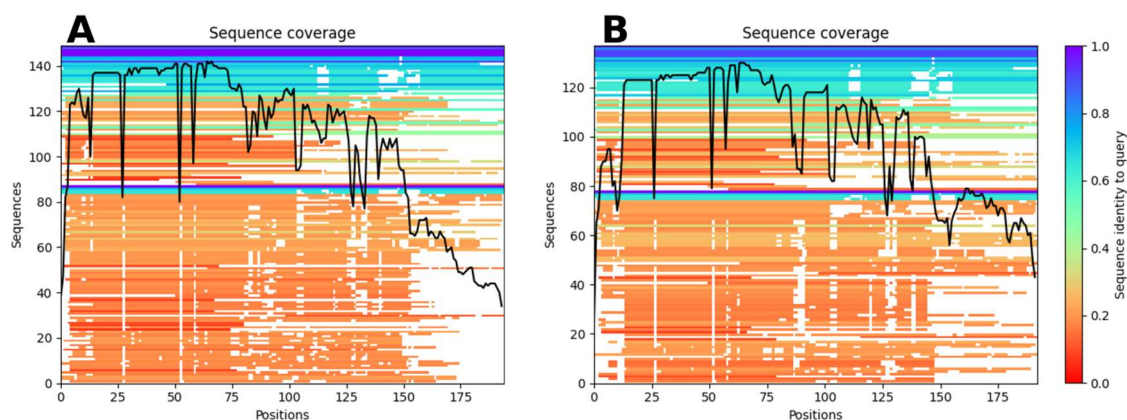
SI Figure S2. Sequence coverage for the modeling of WT (A) and OM (B) variants of RBD using Alpha Fold II.
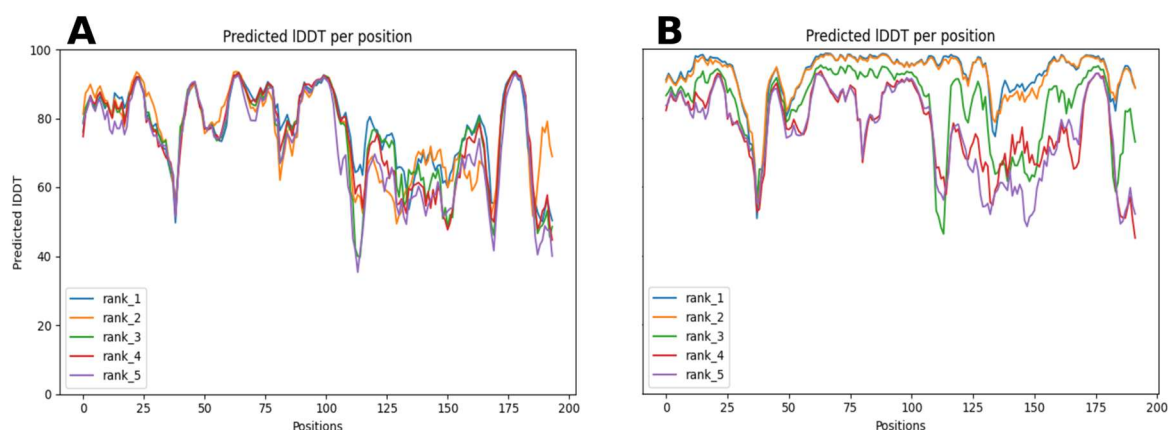
SI Figure S3. pLDDT score for five top ranking models obtained with Alpha Fold II for WT (A) and OM (B) variants of RBD.

Rosetta repack protocol details
Text S3. Rosetta repack protocol options

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            />
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            scorefxn="REF2015"
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            jump="0"
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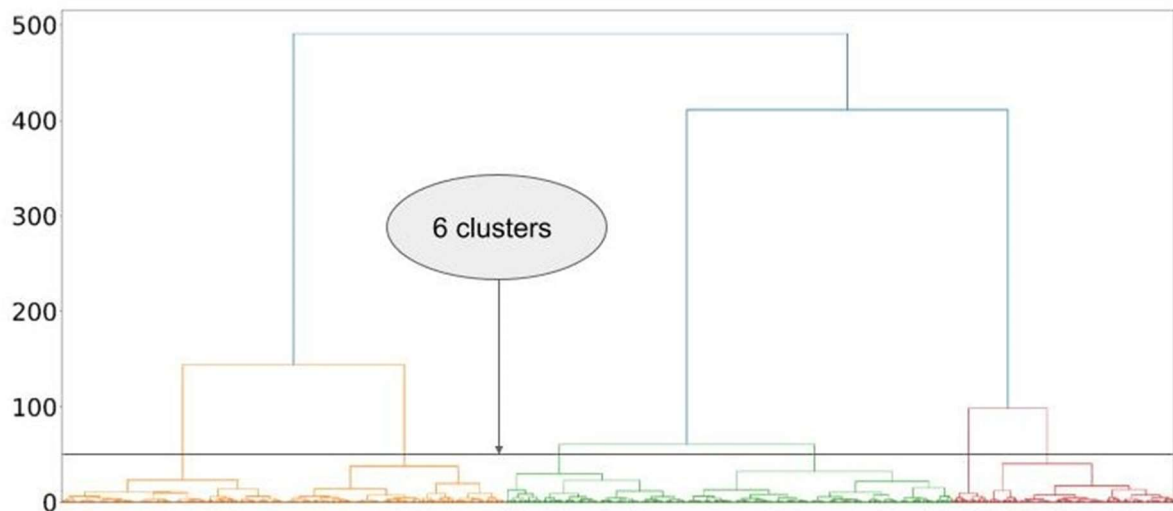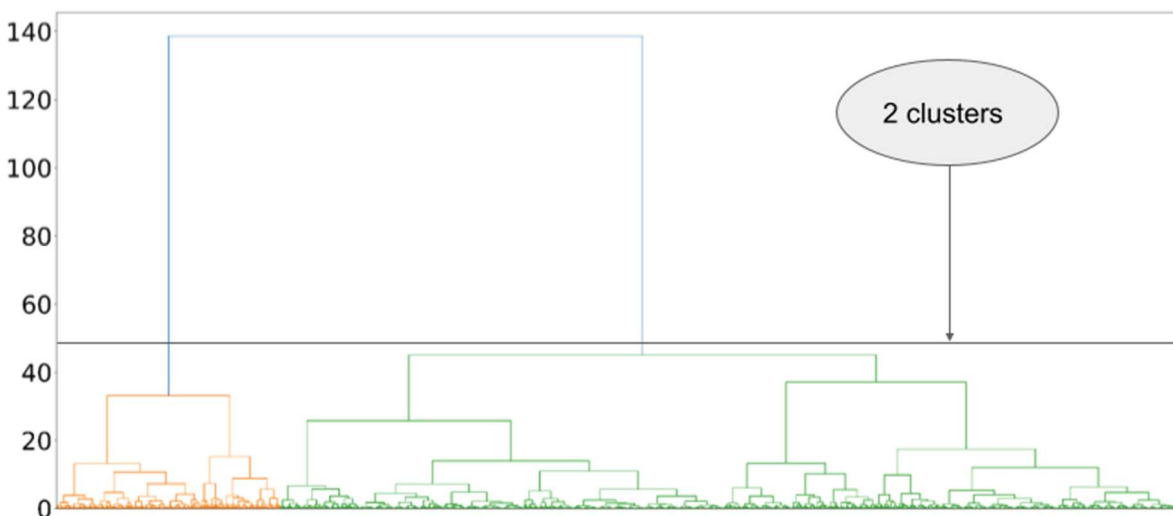
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-out:file:fullatom
-linmem_ig 10
-ex1
-ex2
-use_input_sc
-score:weights ref2015.wts

SI Figure S4. Results of clusterization of the WT trajectory in the basis of principal components. Cut-off line is added.

SI Figure S5. Results of clusterization of the omicron trajectory in the basis of principal components. Cut-off line is added.

SI Table S1. Description of RBD structures from Protein Data Bank

PDB code	Description	Method	Resolution
6acd	SARS-CoV spike glycoprotein in complex with ACE2	Cryo-EM	3.90 Å
7cjk	SARS-CoV-2 RBD in complex with a neutralizing antibody P4A1	X-RAY DIFFRACTION	2.11 Å
7e3k	SARS-CoV-2 RBD in complex with a neutralizing antibody 13G9	Cryo-EM	3.90 Å
7m6d	SARS-CoV-2 RBD in complex with neutralizing antibodies CR3022	X-RAY DIFFRACTION	3.10 Å

3D-structures for obtained clusters centroids are available upon request.