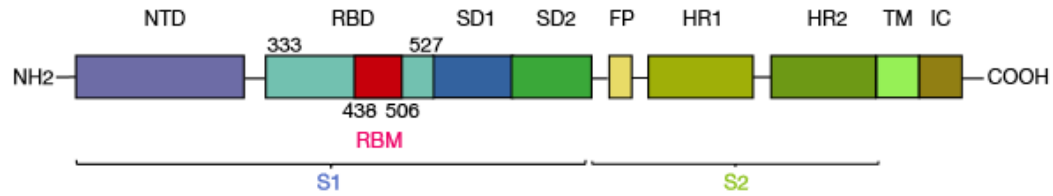
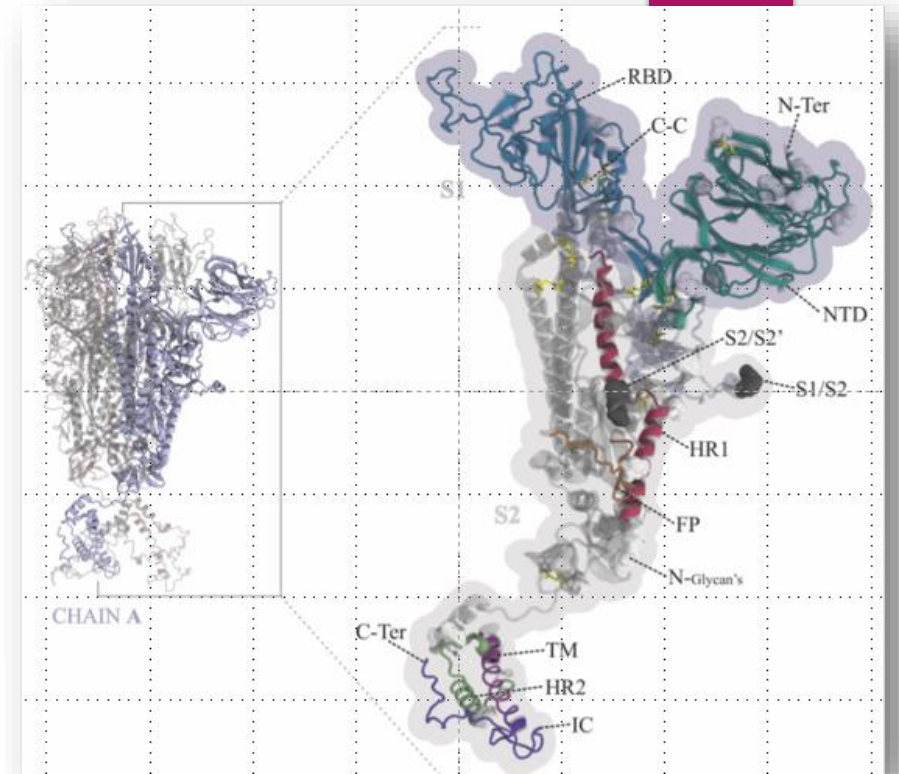
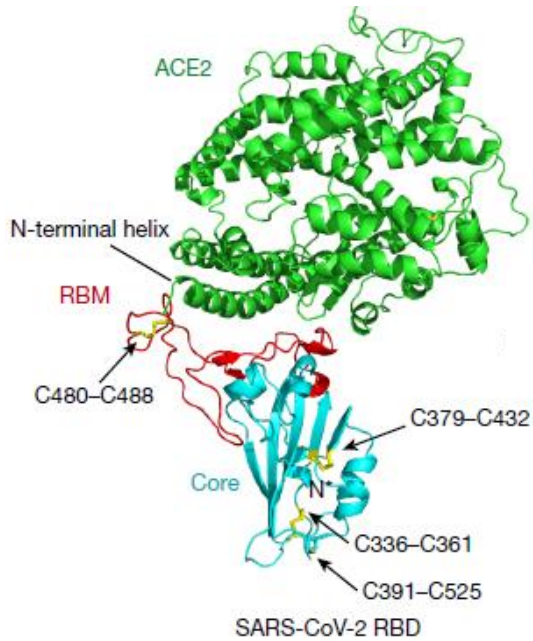
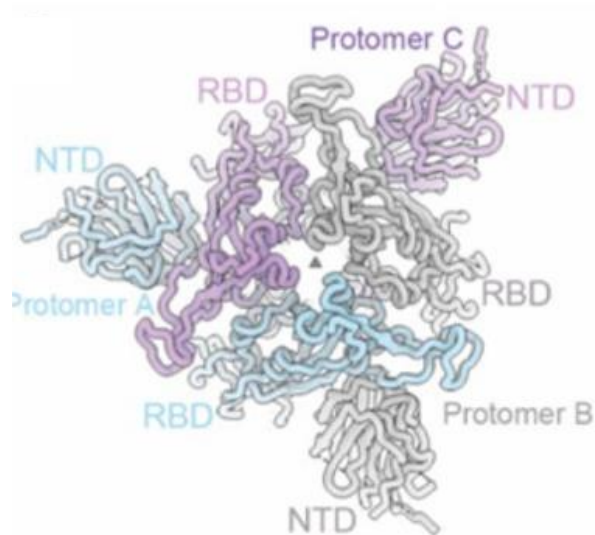


Proteina Spike



S1 = 13 – 685

S2 = 686-1213



Structure Summary

3D View

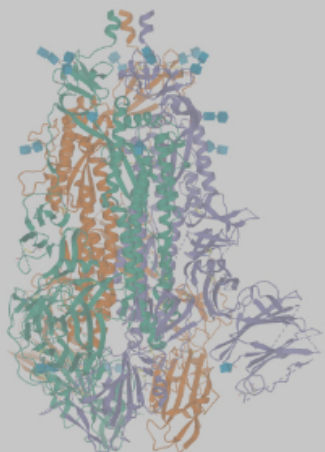
Annotations

Experiment

Sequence

Genome

Biological Assembly 1 ?



3D View: Structure | Ligand Interaction

Global Symmetry: Cyclic - C3 (3D View)

Global Stoichiometry: Homo 3-mer - A3

Find Similar Assemblies

Biological assembly 1 assigned by authors.

6VXX

Structure of the SARS-CoV-2 spike glycoprotein (closed state)

DOI: 10.2210/pdb6VXX/pdb EMDDataResource: EMD-21452

Classification: VIRAL PROTEIN

Organism(s): Severe acute respiratory syndrome coronavirus 2

Expression System: Homo sapiens

Mutation(s): No

Deposited: 2020-02-25 Released: 2020-03-11

Deposition Author(s): Walls, A.C., Park, Y.J., Tortorici, M.A., Wall, A., Seattle Structural Genomics Center for Infectious Disease (SSGCID), McGuire, A.T., Veessler, D.

Funding Organization(s): National Institutes of Health/National Institute of General Medical Sciences (NIH/NIGMS)

Experimental Data Snapshot

Method: ELECTRON MICROSCOPY

Resolution: 2.80 Å

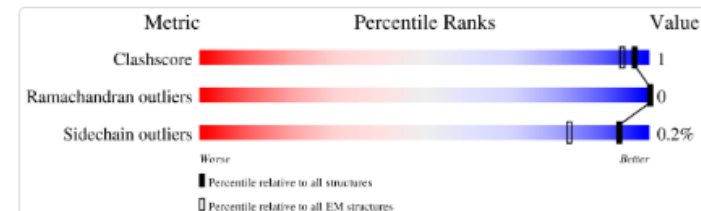
Aggregation State: PARTICLE

Reconstruction Method: SINGLE PARTICLE

wwPDB Validation

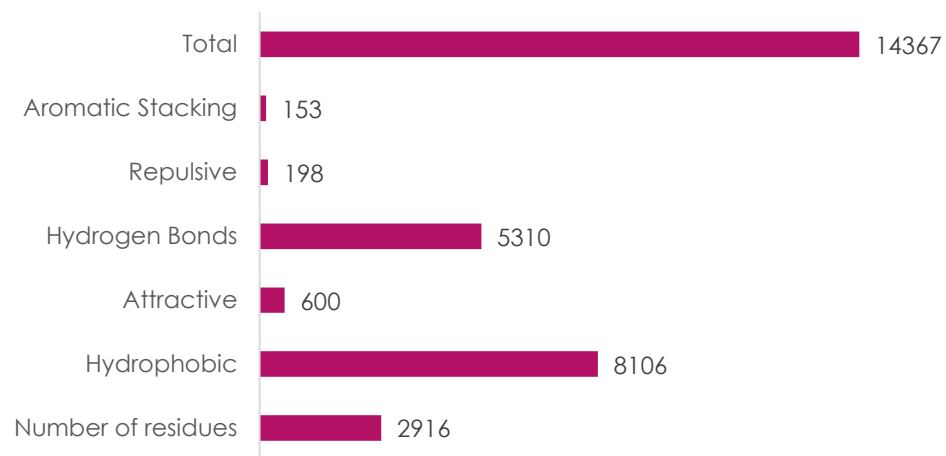
3D Report

Full Report

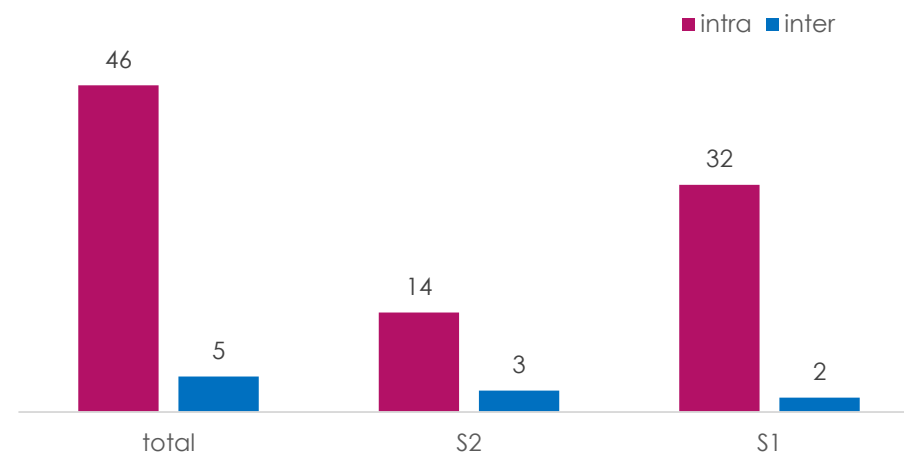


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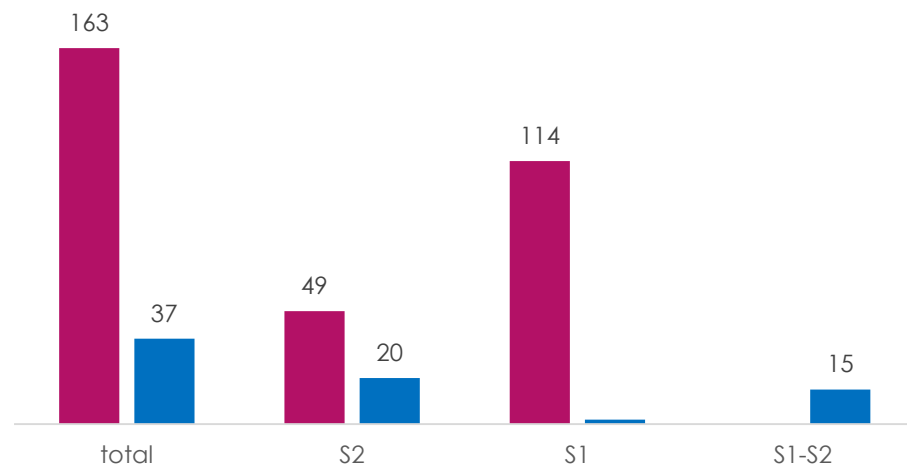
Tipos de contatos



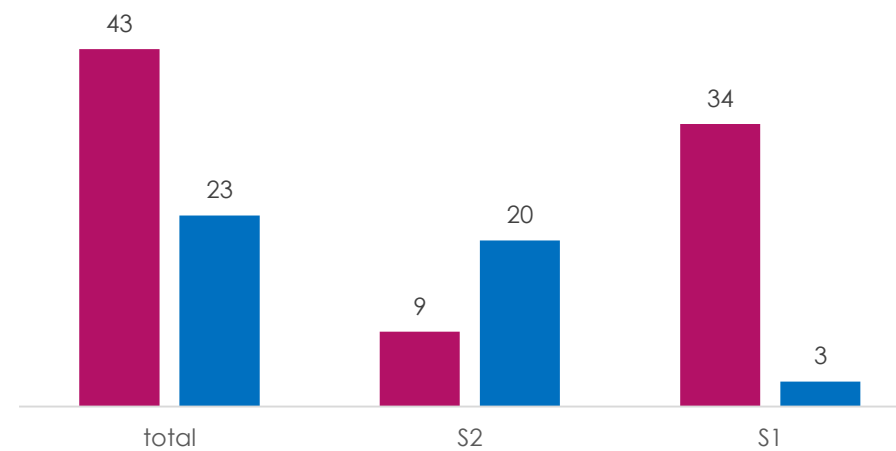
Empacotamento Aromático



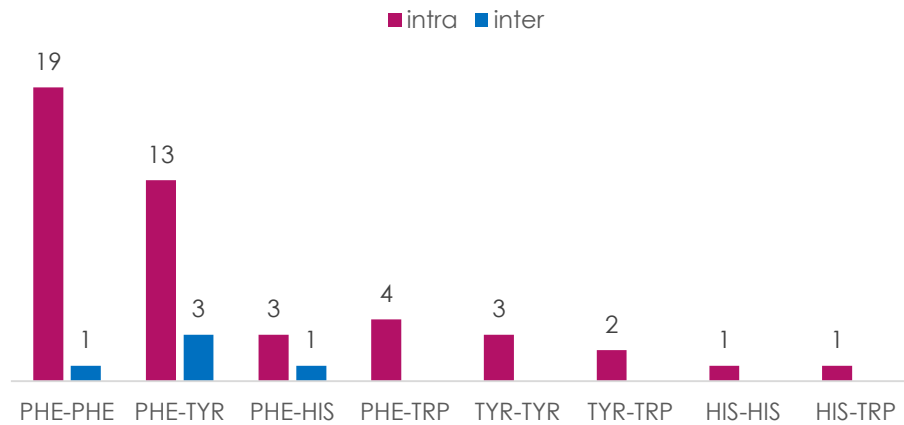
Atrativa



Repulsiva



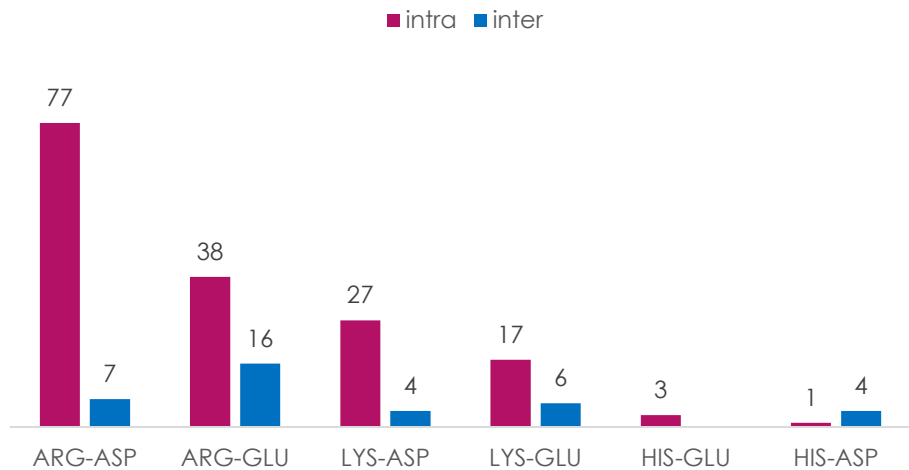
Contato por emparelhamento aromático



S2 PHE800 faz 58 contatos e a PHE802 38 contatos

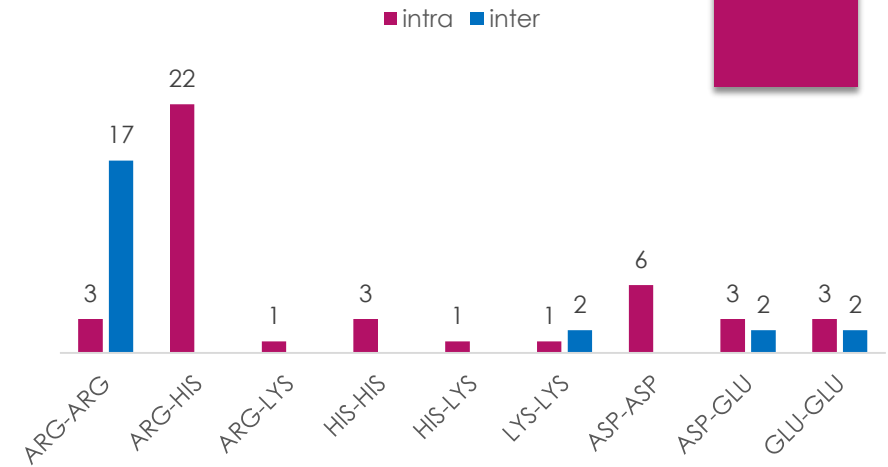
Não há PHE fazendo empilhamento aromático no RBM
Há TRP somente no S1

Contato por atrativa



Presente no S2 a ARG1039 faz interações intra e inter com o GLU103, sendo o segundo átomo com mais contatos 56.

Contato por repulsiva



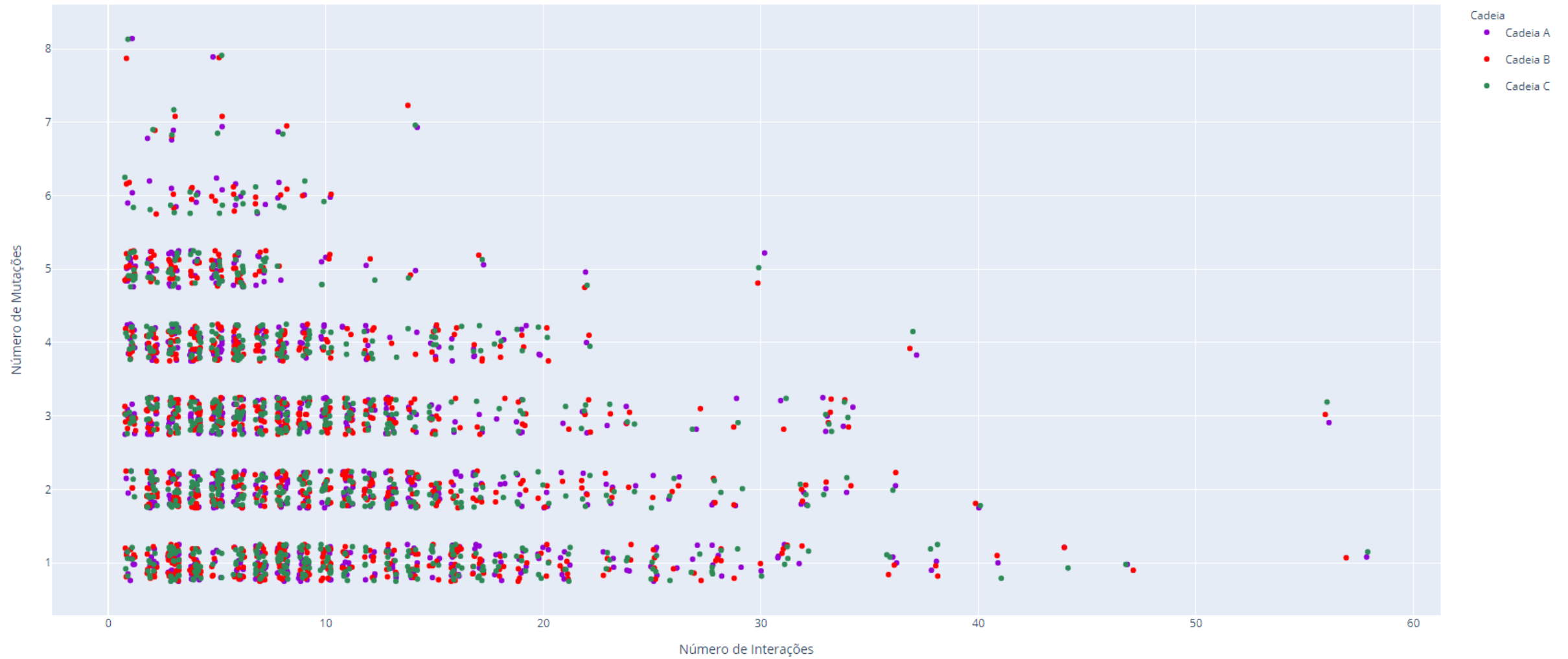
Só ARG-HIS forma repulsiva com ligação de hidrogênio e isso acontece intra ARG44-HIS49, HIS519-ARG567, ambos no S1

Não há repulsiva no RBD

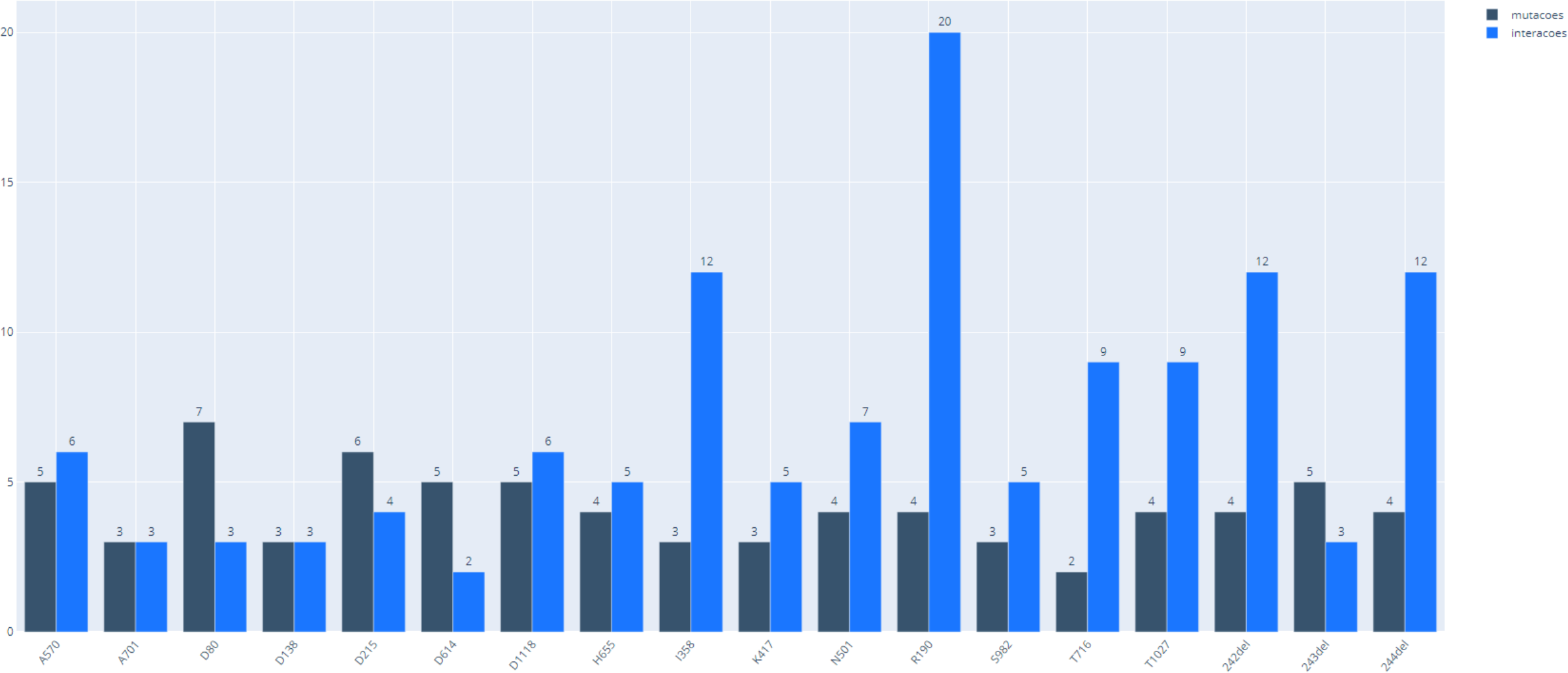
A LYS (2) só faz inter com ela mesmo, assim como ARG(17)

A HIS não forma contato inter, somente intra

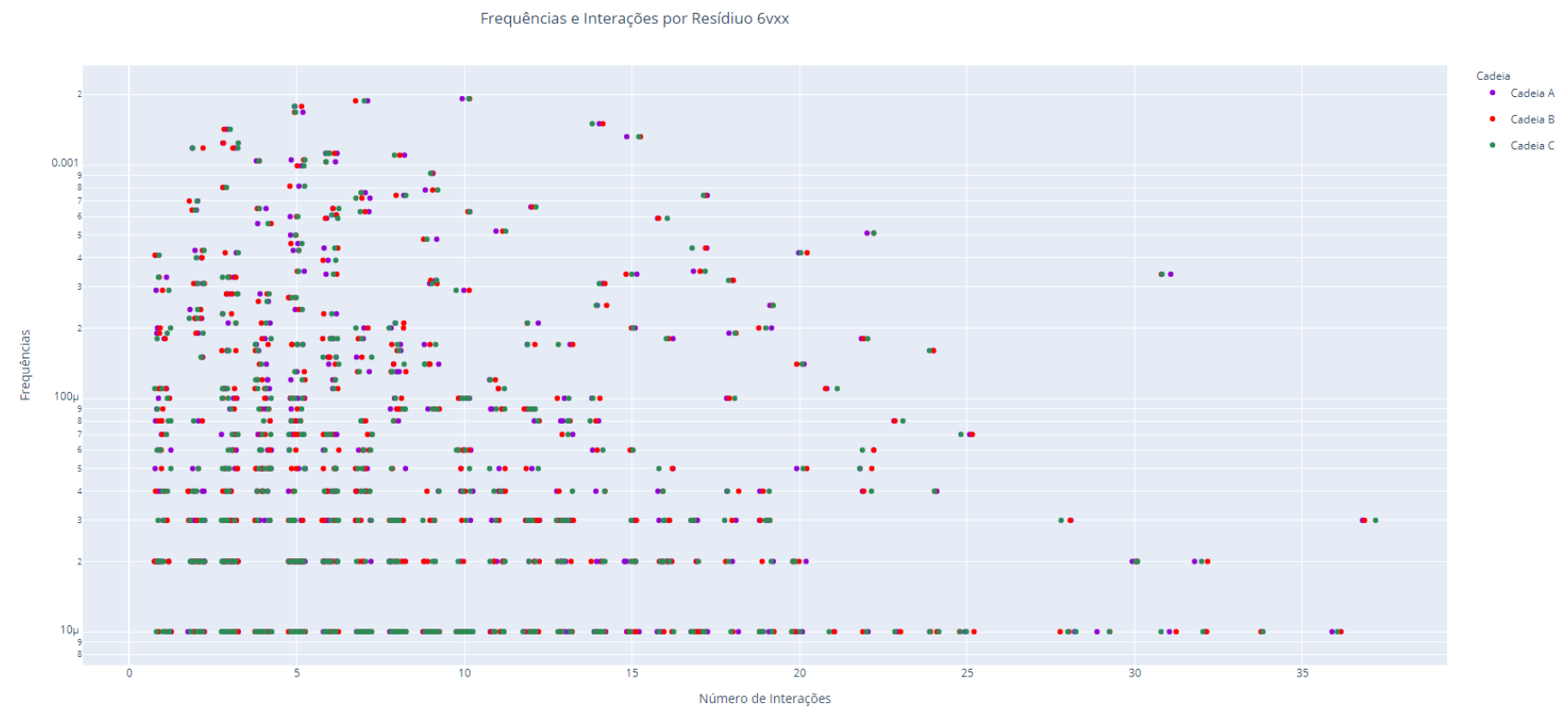
Mutações e Interações por Resíduo 6vxx



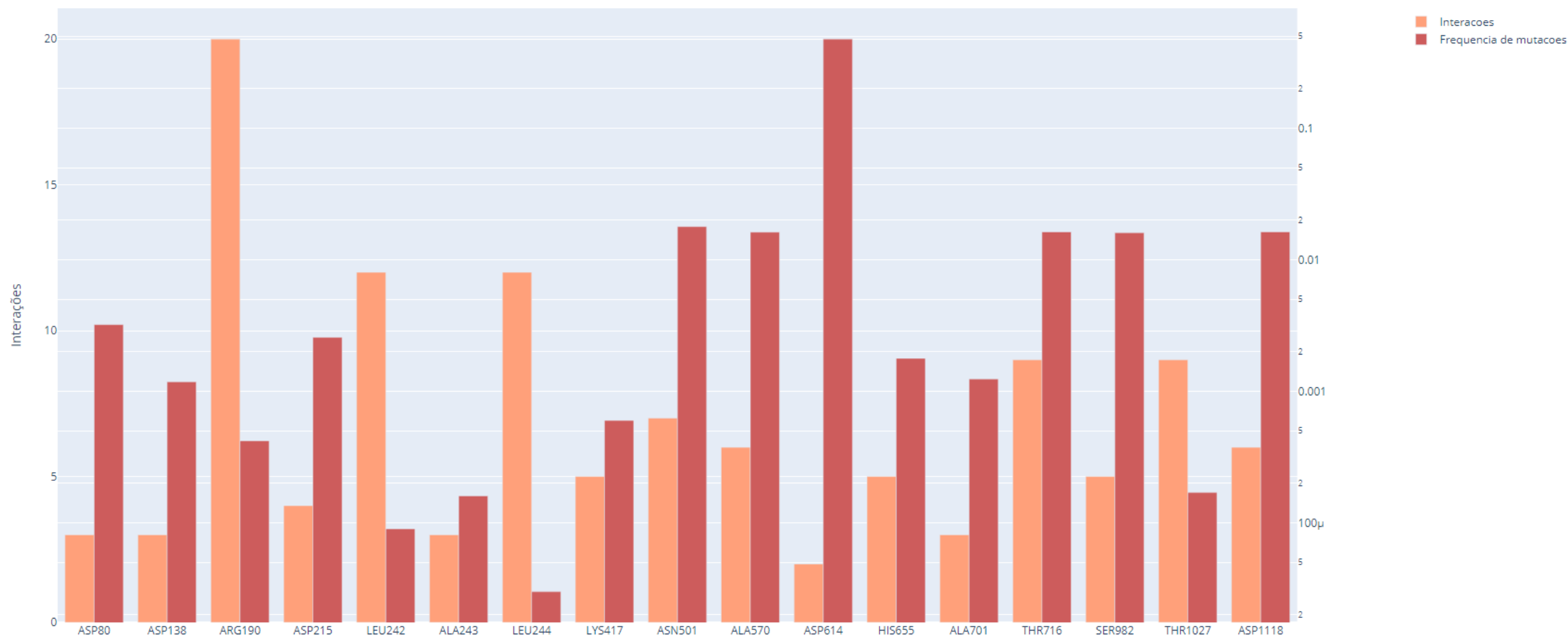
Interações e Mutações nas Cadeias A, B e C (6VXX)



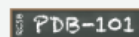
Região	Seq	frequência média
Peptide signal	1-133	0,0008054
S1	13-685	0,0018927
S2	686-1213	0,0003189
domínio transmemb.	1214-1234	0,0002740
citoplasmática	1234-1273	0,0002011
NTD	13-332	0,0009849
RBD	333-526	0,0006645
RBM	438-506	0,0016083
Spike	1-1273	0,0011599



Interações e Frequência de mutação na Cadeia (6VXX)



Enter search term(s)

[Advanced Search](#) | [Browse Annotations](#)[Help](#)Worldwide
Protein Data Bank
FoundationYEARS OF
Protein Data Bank

Structure Summary

3D View

Annotations

Experiment

Sequence

Genome

Biological Assembly 1 ?

[3D View: Structure](#) | [Electron Density](#) |
[Ligand Interaction](#)

Global Symmetry: Asymmetric - C1

Global Stoichiometry: Hetero 2-mer - A1B1

[Find Similar Assemblies](#)

Biological assembly 1 assigned by authors.

6MOJ

Crystal structure of SARS-CoV-2 spike receptor-binding domain bound with ACE2

DOI: [10.2210/pdb6MOJ/pdb](https://doi.org/10.2210/pdb6MOJ/pdb)Classification: **VIRAL PROTEIN/HYDROLASE**

Organism(s): Homo sapiens, Severe acute respiratory syndrome coronavirus 2

Expression System: Trichoplusia ni

Mutation(s): No

Deposited: 2020-02-21 Released: 2020-03-18

Deposition Author(s): Wang, X., Lan, J., Ge, J., Yu, J., Shan, S.

Display Files

Download Files

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 2.45 Å

R-Value Free: 0.227

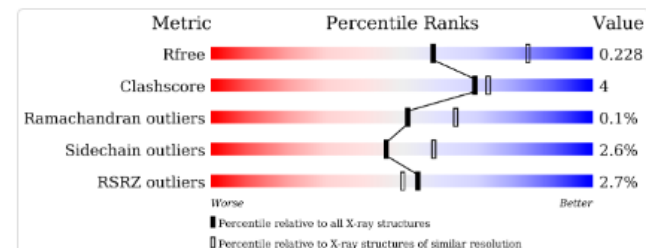
R-Value Work: 0.192

R-Value Observed: 0.194

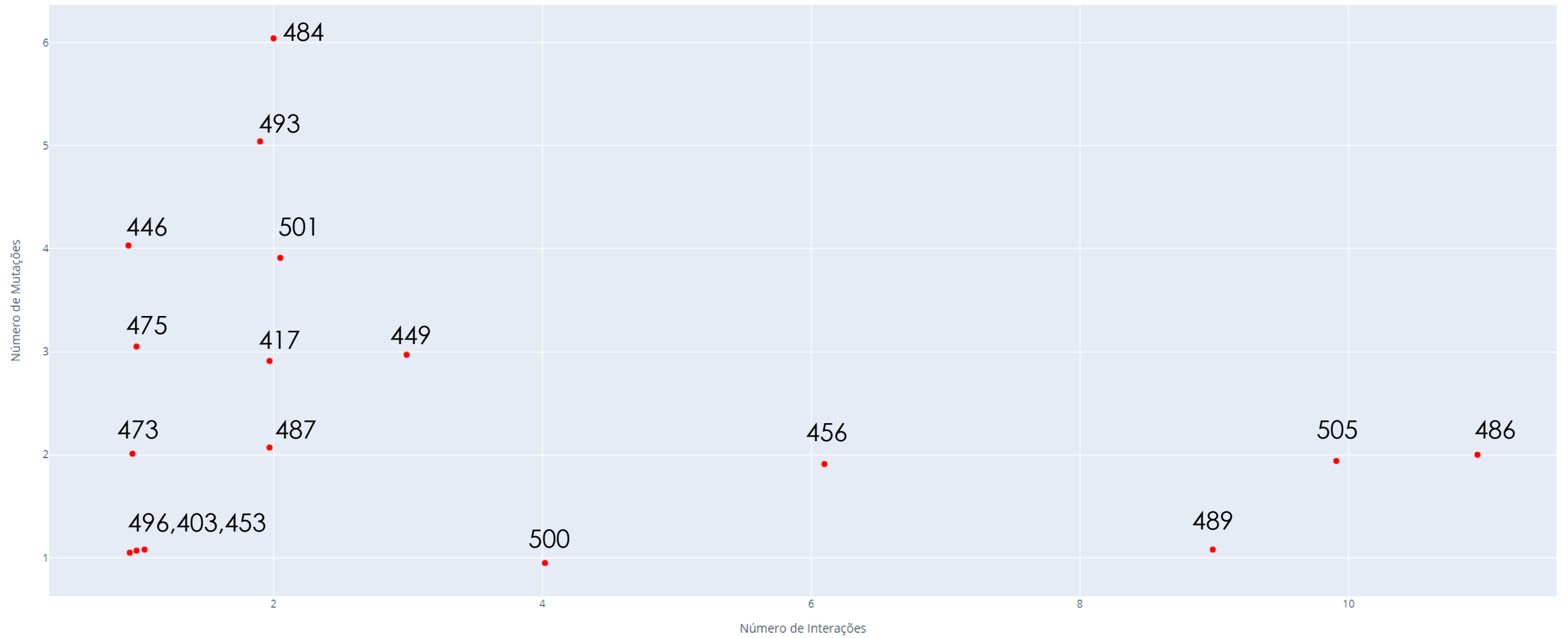
wwPDB Validation

3D Report

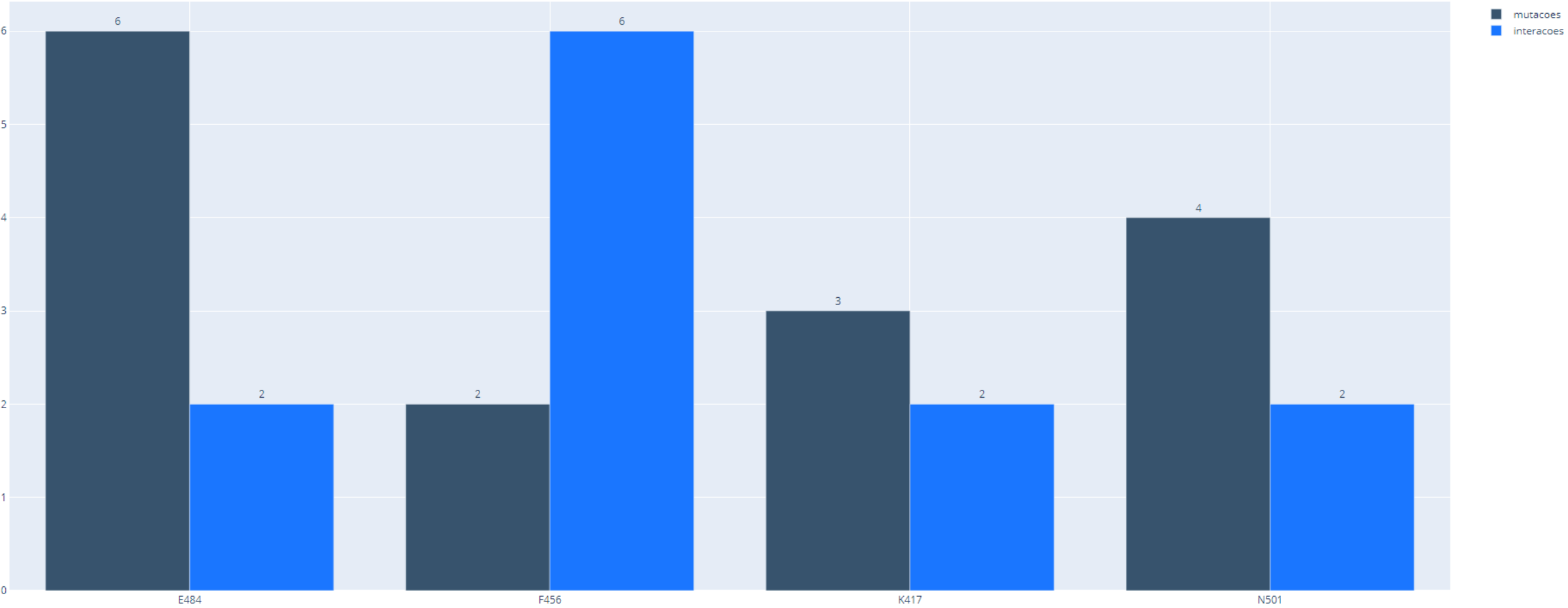
Full Report

This is version 2.5 of the entry. See complete [history](#).

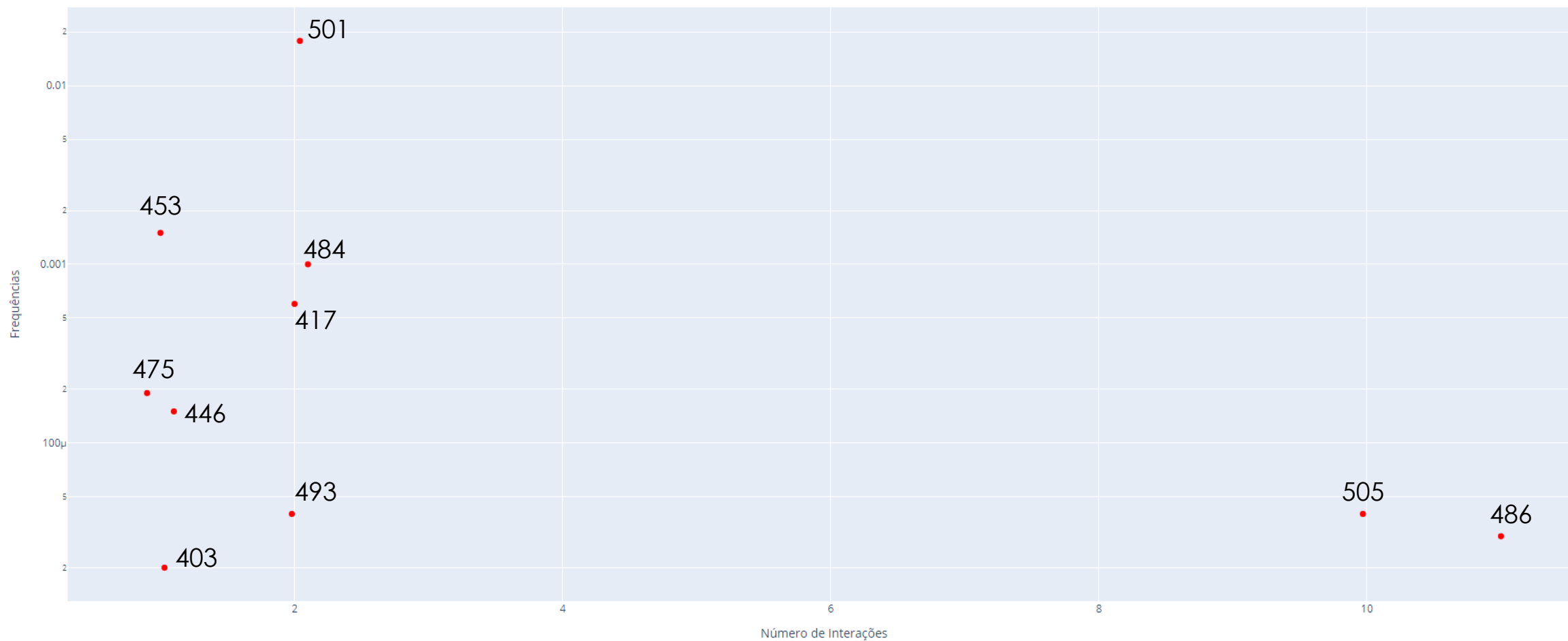
Mutações e Interações por Resíduo 6m0j



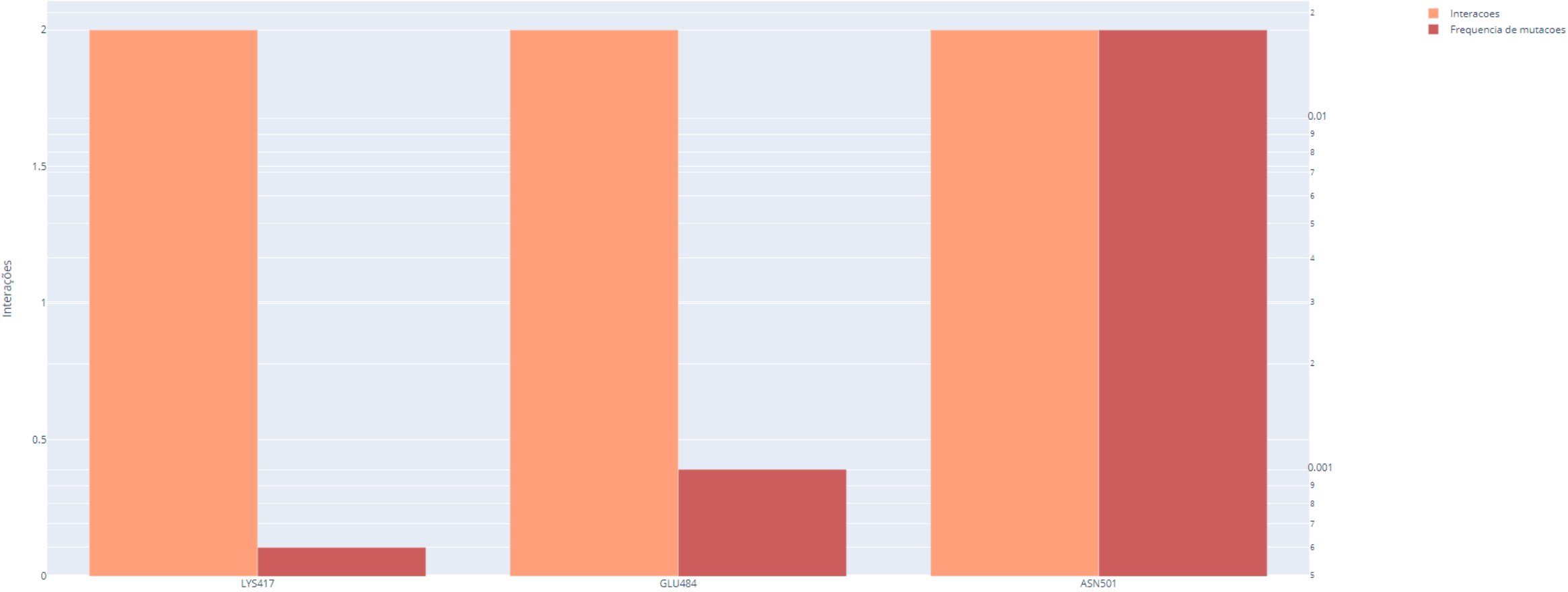
Interações e Mutações na Cadeia E (6M0J)



Frequências e Interações por Resíduo 6m0j



Interações e Frequência de mutação na Cadeia E (6M0J)



Considerações sobre as variantes P1, B.1.17(UK) e B.1.351 (África do Sul)

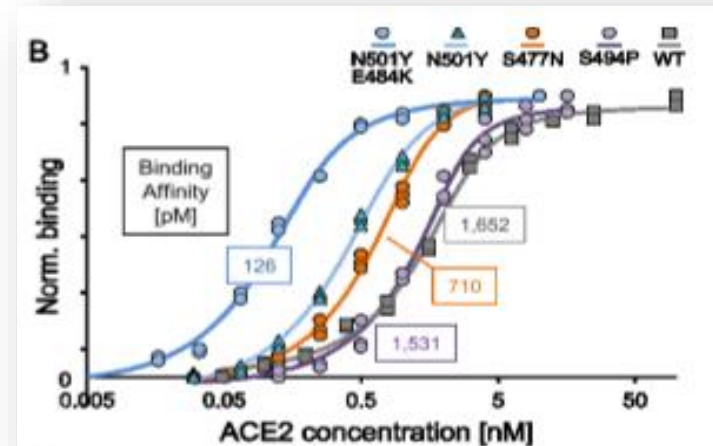
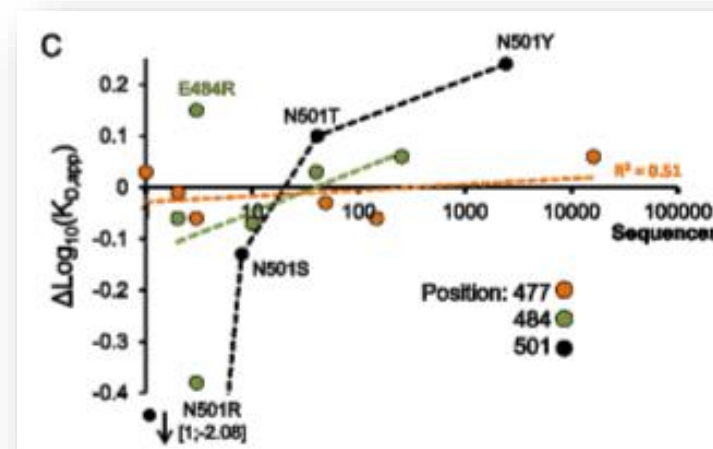
NTD

AA origem	Mutações					
L18	L18F	L18I				
T20	T20A	T20I	T20N	T20S		
I68	I68K	I68L	I68M	I68R	I68T	
H69	H69D	H69L	H69P	H69Q	H69R	H69S H69Y
Y144	Y144*	Y144C	Y144F	Y144H	Y144N	Y144S
L147	K147*	K147E	K147I	K147N	K147R	K147T
N148	N148*	N148D	N148K	N148S	N148T	N148Y
N211	N211D	N211K	N211S	N211T	N211Y	
R214	R214C	R214H	R214L	R214S		
L242	L242F	L242I	L242P	L242R		
A243	A243H	A243P	A243S	A243T	A243V	
L244	L244F	L244R	L244S	L244V		

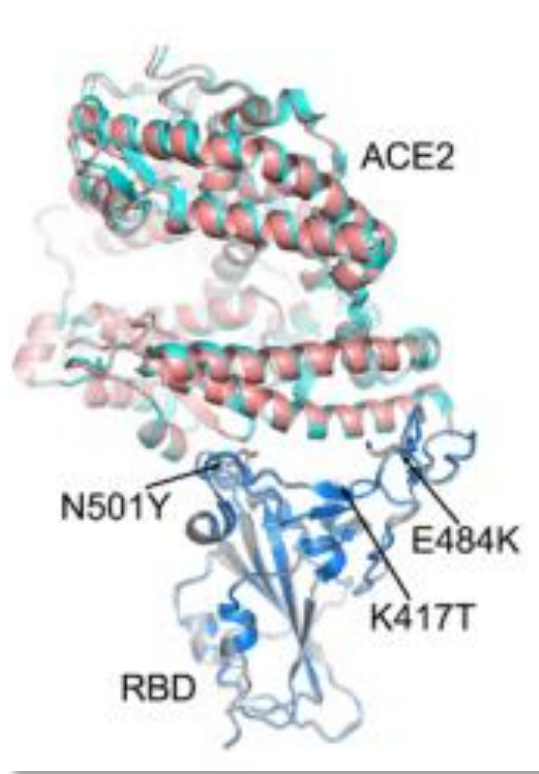
	AROM E POLAR
	AROMATICO
	NEGATIVO
	POSITIVO
	POLAR
	POLAR AMIDA
	PEQUENO
	HIDROFOBICO
	DELEÇÃO

RBD

AA origem	Mutações					
I358	I358L	I358T	I358V			
K417	K417N	K417R	K417T			
F456	F456*	F456L				
N460	N460I	N460K	N460S	N460T		
S477	S477G	S477I	S477N	S477R	S477T	
E484	E484A	E484D	E484G	E484K	E484Q	E484R
N460	N460I	N460K	N460S	N460T		
N501	N501I	N501S	N501T	N501Y		
D614	D614A	D614G	D614N	D614S	D614V	



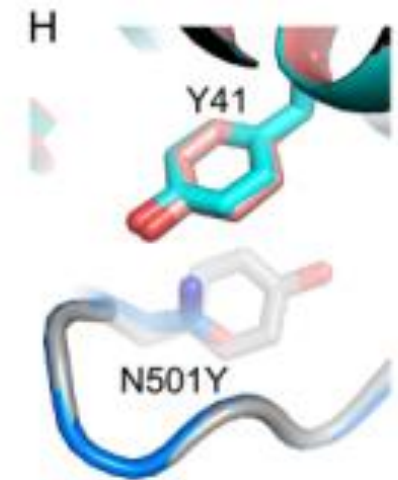
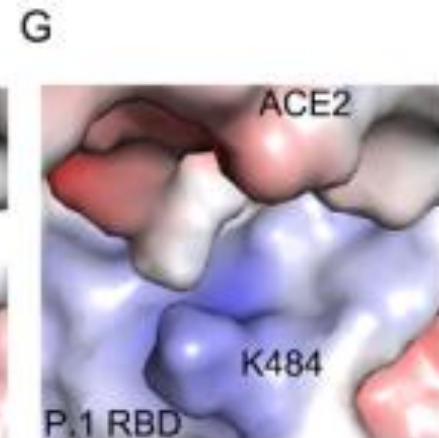
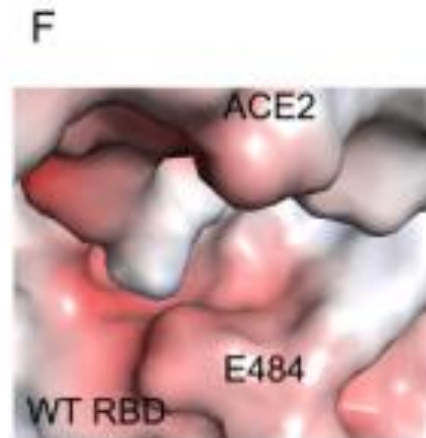
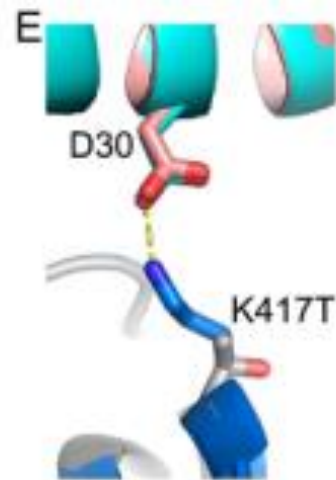
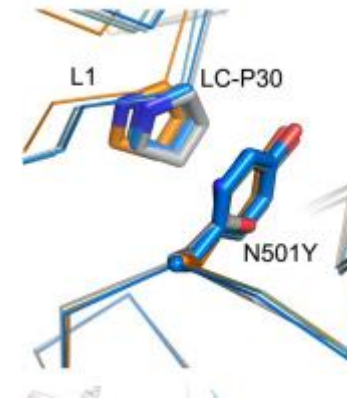
Jiri Zahradnik et al SARS-CoV-2 RBD *in vitro* evolution follows contagious mutation spread, yet generates an able infection inhibitor BioRxiv: <https://doi.org/10.1101/2021.01.06.425392>



□ K417T(P1)/ K417N(B.1.351)

□ E484K

□ N501Y



spreading in SARS-CoV-2.

<i>In vitro</i> evolution																		
RBD residue*	354	358	445	446	448	460	468	470	477	478	481	483	484	490	493	494	498	501
RBD wild-type	N	I	V	G	N	N	I	T	S	T	N	V	E	F	Q	S	Q	N
Library S2		F																
Library B3		F			S		T		N		Y	E	K	S				Y
Library B4		F		R		K	V		N	S			K	Y		P	R	Y
Library B5		F		R		K	V		N				K	Y	H	P	R	Y
Library B6(FA)	E	F	K			K	T	M	N				K			P	R	Y
Clone B62		F	K			K	T	M	N				K				R	Y
SARS-CoV2 var.	parental/lineage**					460	468	470	477	478	481	483	484	490	493	494	498	501
Europe	20E/EU1								N									
British	20I/501Y.V1																	Y
“South African”	20H/501Y.V2												K					Y
Brazilian	20J/501Y.V3												K					Y
Other detected mutations									I,R, G,T, K	A,I, R,K			Q,A, D,G, R,V	S,L, V	L,K, H,R	P,L, A	H,P	R,T, S

* The colored amino-acids are dominant (>50 %, red) or minor (<50 %, grey) at a given position. The red background highlights the emerging mutations both in clinical samples and yeast display.

** The lineage designation by NextStrain initiative ²⁰; alternative strain designation proposed by Rambaut et al. ²¹ - B.1.1.7 (501Y.V1), B.1.351 (501Y.V2), and P.1 (descendent of B.1.1.28, 501Y.V3)

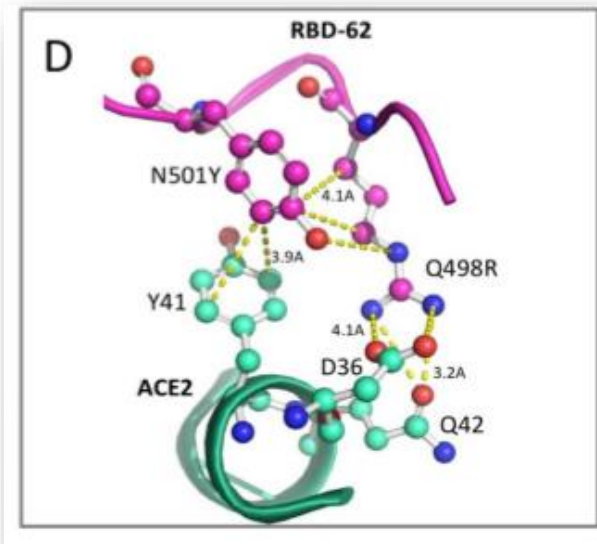
- Biophysical parameters of multiple selected mutant clones are shown in Table 2.

Mutações de
atenção

□ Q498R

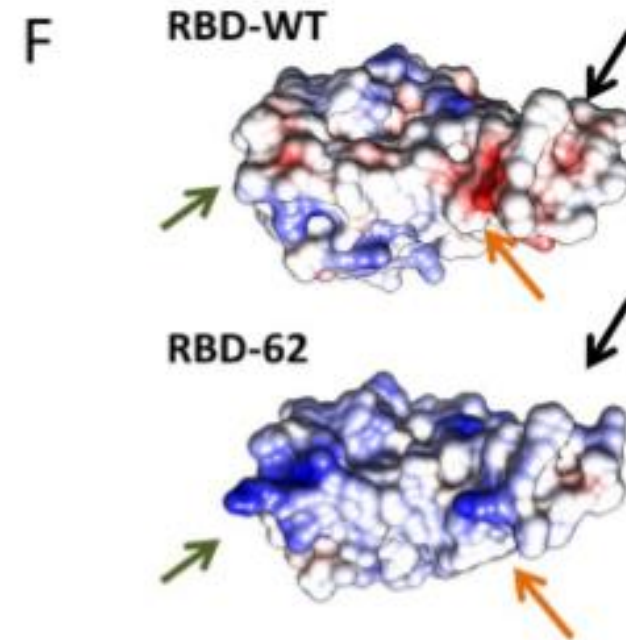
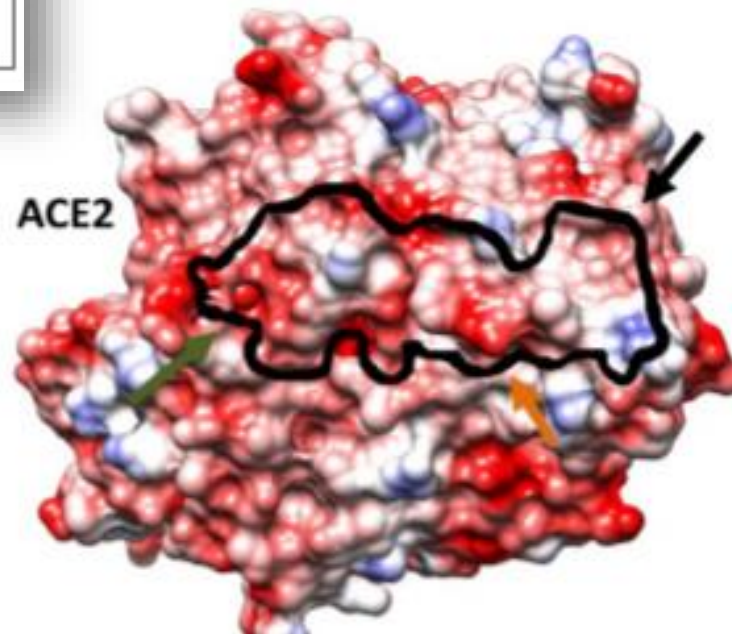
□ N460K

□ I358F



Mutações de atenção

□ Q498R



Referências

Lan, Jun, et al. "Structure of the SARS-CoV-2 spike receptor-binding domain bound to the ACE2 receptor."
Nature 581.7807 (2020): 215-220

Jiri Zahradnik et al SARS-CoV-2 RBD *in vitro* evolution follows contagious mutation spread, yet generates an able infection inhibitor BioRxiv: <https://doi.org/10.1101/2021.01.06.425392>

Wanwisa Dejnirattisai et al. Antibody evasion by the Brazilian P.1 strain of SARS-CoV-2
BioRxiv : <https://doi.org/10.1101/2021.03.12.435194>

Paola C. Resende et al. The ongoing evolution of variants of concern and interest of SARS-CoV-2 in Brazil revealed by convergent indels in the amino (N)-terminal domain of the Spike protein
<https://www.medrxiv.org/content/10.1101/2021.03.19.21253946v1>