Extended Data for:

Beyond Natural Antibodies: A novel anti-3CLpro Nanobody Nb01 using Large Language Model based on Segmented Generation

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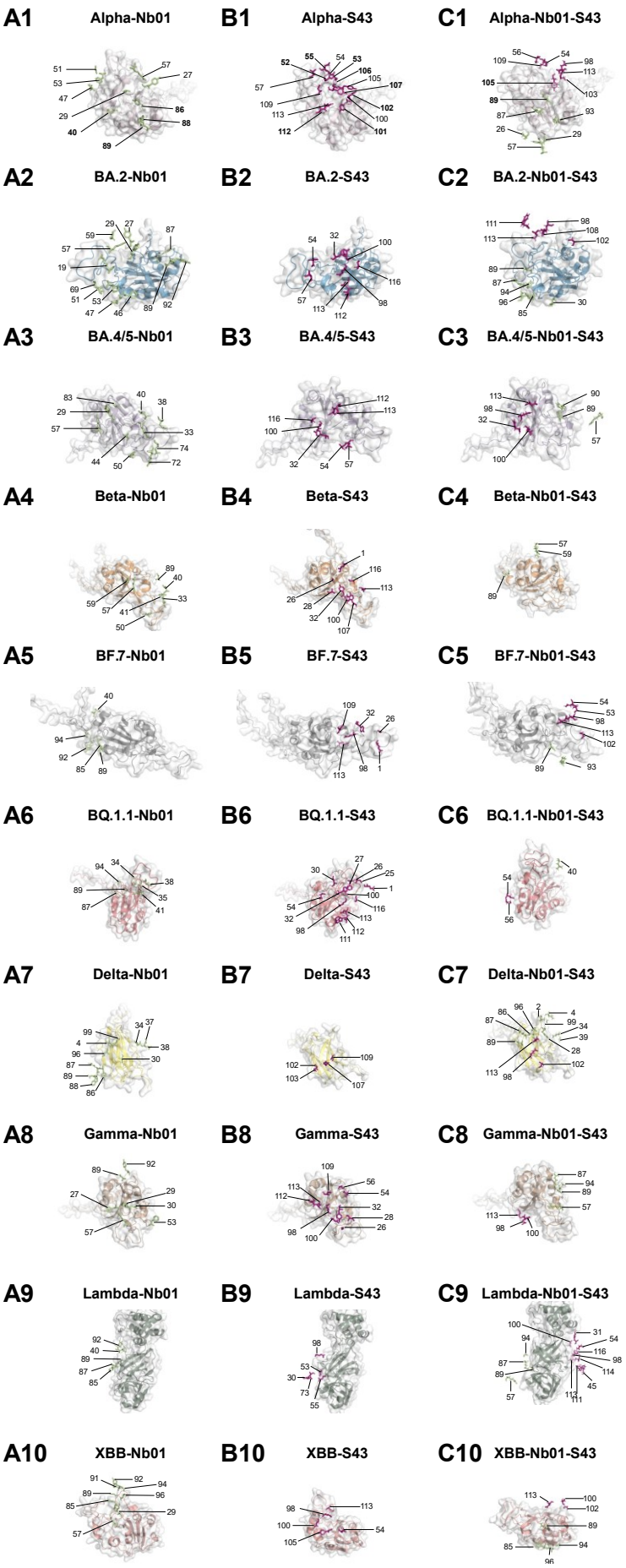
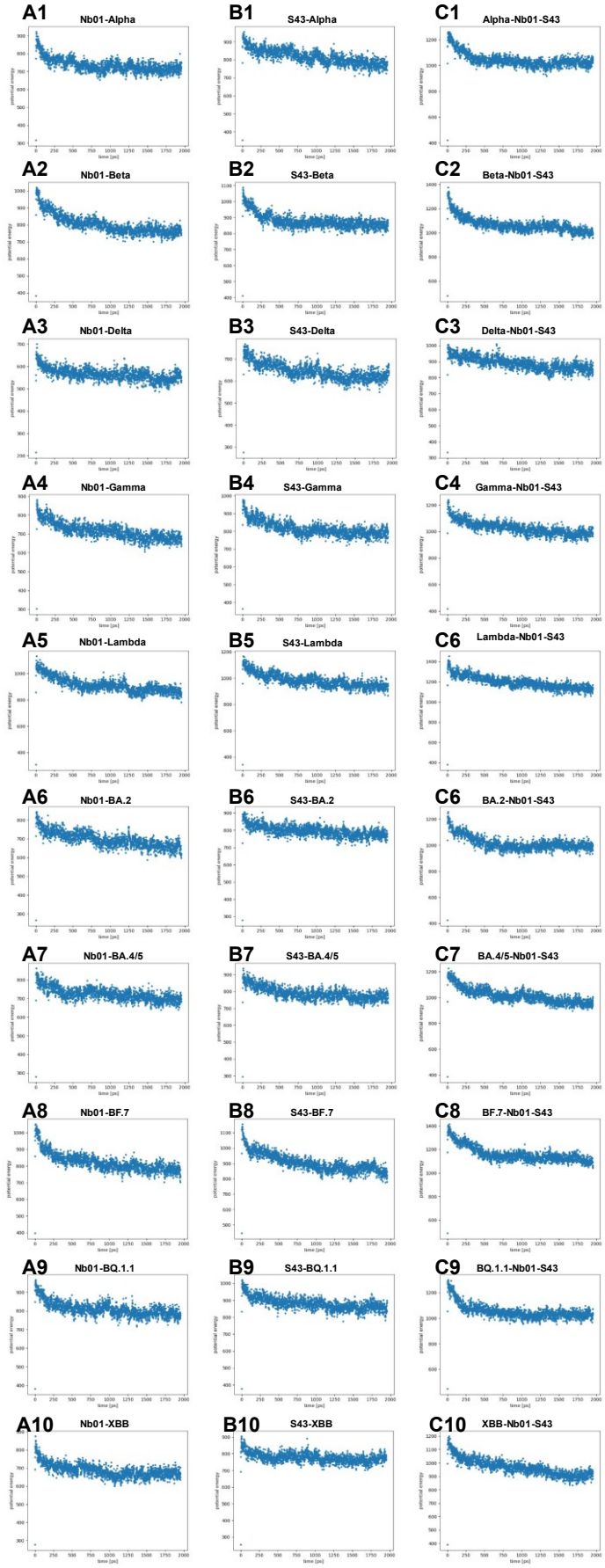


Extended Fig. 1 Details of the Interaction of NB01 and S43 in complex with the SARS-CoV2 variant, as well as of NB01 and S43 after simultaneous binding of the same antigen. Image generated with PyMOL.



Extended Fig. 2 Potential energy changes when Nb5 and S43 bind to the variants, respectively, and when they compete simultaneously for the same antigen. (A1-10) Potential energy changes when NB01 binds to a variant; (B1-10) Potential energy changes when S43 binds to a variant; (C1-10) Potential energy changes when NB01 and S43 compete to bind the same variant.

Extended Table. 1 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 ALPHA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR86[OH]	TYR128[O]	Hydrogen bond	2.53
TRP88[NE1]	TYR128[OH]	Hydrogen bond	3.85
LEU40[O]	GLN175[NE2]	Hydrogen bond	3.85
TRP88[O]	VAL180[N]	Hydrogen bond	2.31
ASN89[OD1]	VAL180[N]	Hydrogen bond	3.76

Extended Table. 2 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 BETA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR85[OH]	ASP87[OD2]	Hydrogen bond	3.22
TYR85[OH]	GLU88[OE1]	Hydrogen bond	3.84
ASN89[N]	ASN99[OD1]	Hydrogen bond	3.22
TYR86[OH]	TYR135[O]	Hydrogen bond	3.73
TRP88[N]	TYR135[OH]	Hydrogen bond	3.77
ARG33[NH2]	PHE168[O]	Hydrogen bond	3.44
SER48[N]	CYS170[O]	Hydrogen bond	3.75
ARG57[NH1]	TYR183[OH]	Hydrogen bond	2.10
ALA44[O]	GLN175[NE2]	Hydrogen bond	2.17
ILE45[O]	PHE172[N]	Hydrogen bond	3.41
GLU47[OE2]	GLY167[N]	Hydrogen bond	2.67
TYR86[O]	ASN99[ND2]	Hydrogen bond	2.63
TRP88[O]	TYR103[OH]	Hydrogen bond	3.28

Extended Table. 3 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 DELTA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
GLN100[N]	GLU48[OE1]	Hydrogen bond	3.37
SER30[OG]	GLY110[O]	Hydrogen bond	3.42
MET95[N]	TYR112[OH]	Hydrogen bond	2.15
TYR93[O]	SER39[OG]	Hydrogen bond	3.65
TYR93[O]	TYR112[OH]	Hydrogen bond	2.84

Extended Table. 4 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 GAMMA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR28[OH]	ASN127[OD1]	Hydrogen bond	2.04
ASN89[N]	PRO176[O]	Hydrogen bond	3.10
PHE90[N]	PRO176[O]	Hydrogen bond	2.31
TYR91[N]	THR177[O]	Hydrogen bond	3.44
ARG87[O]	THR177[N]	Hydrogen bond	3.32

Extended Table. 5 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 LAMBDA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ALA42[N]	THR169[O]	Hydrogen bond	3.74
TRP88[N]	LEU141[O]	Hydrogen bond	2.95
TRP88[NE1]	CYS145[SG]	Hydrogen bond	2.30
ASN89[N]	GLY143[O]	Hydrogen bond	3.52
TYR91[N]	SER139[OG]	Hydrogen bond	2.58
TYR91[N]	SER139[O]	Hydrogen bond	2.45
TYR92[OH]	GLU288[OE1]	Hydrogen bond	2.08
ASN89[O]	SER139[OG]	Hydrogen bond	3.51
ASN89[OD1]	GLY143[N]	Hydrogen bond	2.20
PHE90[O]	PHE140[N]	Hydrogen bond	2.89
TYR91[O]	SER139[OG]	Hydrogen bond	2.15

Extended Table. 6 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 OMICRON BA.2

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ASN89[N]	GLY121[O]	Hydrogen bond	2.40
ARG87[N]	ASN124[OD1]	Hydrogen bond	2.41
TYR93[OH]	ASN124[OD1]	Hydrogen bond	2.42
ASN59[ND2]	GLY156[O]	Hydrogen bond	2.43
ILE55[N]	GLY159[O]	Hydrogen bond	2.44
THR54[OG1]	ASN161[OD1]	Hydrogen bond	2.45
GLY51[N]	TYR163[OH]	Hydrogen bond	2.46
PHE90[N]	PHE171[O]	Hydrogen bond	2.47
PHE53[O]	TYR163[OH]	Hydrogen bond	2.48
ILE55[O]	TYR163[N]	Hydrogen bond	2.49
TYR86[OH]	TYR127[N]	Hydrogen bond	2.50
ARG87[O]	PHE171[N]	Hydrogen bond	2.51
TRP88[O]	ARG172[N]	Hydrogen bond	2.52
PHE90[O]	TYR175[OH]	Hydrogen bond	2.53
TYR92[O]	ASN122[ND2]	Hydrogen bond	2.54

Extended Table. 7 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 OMICRON BA.4/5

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TRP88[NE1]	TYR127[OH]	Hydrogen bond	3.03
GLU47[N]	CYS162[O]	Hydrogen bond	3.60
SER26[OG]	ASN122[ND2]	Hydrogen bond	3.80
LEU40[O]	TYR163[OH]	Hydrogen bond	3.66
GLU41[OE2]	ASN161[N]	Hydrogen bond	2.04
GLU41[OE2]	CYS162[N]	Hydrogen bond	3.61
ILE45[O]	PHE164[N]	Hydrogen bond	2.78
GLU47[OE2]	ALA158[N]	Hydrogen bond	3.23
SER48[OG]	VAL160[N]	Hydrogen bond	3.07
ILE55[O]	ARG172[NH1]	Hydrogen bond	2.98
ILE55[O]	ARG172[NH2]	Hydrogen bond	3.13

Extended Table. 8 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 OMICRON BF.7

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ARG87[N]	ASN70[O]	Hydrogen bond	2.70
TYR93[N]	ASP64[OD2]	Hydrogen bond	3.72
TYR93[N]	SER66[OG]	Hydrogen bond	3.39
TRP88[O]	GLU40[N]	Hydrogen bond	3.77
TYR92[O]	ASN70[ND2]	Hydrogen bond	2.58
TYR92[O]	SER66[OG]	Hydrogen bond	3.04

Extended Table. 9 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 OMICRON BQ.1.1

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
GLY39[N]	VAL162[O]	Hydrogen bond	3.38
LEU40[N]	TYR152[O]	Hydrogen bond	3.65
GLU41[N]	GLY164[O]	Hydrogen bond	3.64
GLU41[N]	CYS167[O]	Hydrogen bond	2.79
TYR86[OH]	GLN172[OE1]	Hydrogen bond	3.68
ARG87[NH1]	ASP99[OD2]	Hydrogen bond	2.65
ASN89[ND2]	GLY95[O]	Hydrogen bond	2.43
TYR91[OH]	GLU144[OE2]	Hydrogen bond	3.46
TYR92[N]	ASP99[O]	Hydrogen bond	2.53
GLN34[OE1]	TYR168[OH]	Hydrogen bond	3.33
ALA35[O]	VAL165[N]	Hydrogen bond	2.53
ALA35[O]	ASN166[N]	Hydrogen bond	3.29
GLN38[OE1]	ALA163[N]	Hydrogen bond	3.69
GLY39[O]	VAL165[N]	Hydrogen bond	3.08
LEU40[O]	PHE169[N]	Hydrogen bond	2.95
ARG87[NH1]	ASP99[OD2]	Salt bridge	2.65
ARG87[NH1]	ASP99[OD1]	Salt bridge	3.43

Extended Table. 10 THE INTERACTION BINDING SITE BETWEEN NB01 AND SARS-COV-2 OMICRON XBB

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR28[N]	THR167[O]	Hydrogen bond	3.86
TYR28[OH]	ARG165[O]	Hydrogen bond	3.35
TYR86[OH]	HIS172[O]	Hydrogen bond	3.45
ASN89[N]	ASN115[O]	Hydrogen bond	3.55
GLY94[N]	SER113[O]	Hydrogen bond	3.74
GLY84[O]	GLY171[N]	Hydrogen bond	3.71
TYR85[O]	TYR116[N]	Hydrogen bond	2.67
ASN89[O]	SER113[OG]	Hydrogen bond	2.76
ASN89[O]	GLY114[N]	Hydrogen bond	3.57
TYR92[O]	GLY114[N]	Hydrogen bond	3.11

Extended Table. 11 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 ALPHA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
SER102[N]	ASN125[O]	Hydrogen bond	3.19
TYR106[OH]	GLY159[O]	Hydrogen bond	3.21
ASN55[N]	GLU161[O]	Hydrogen bond	3.59
SER52[OG]	GLU161[O]	Hydrogen bond	2.55
SER53[N]	GLU161[O]	Hydrogen bond	3.77
SER53[OG]	GLU161[OE2]	Hydrogen bond	2.56
THR112[OG1]	GLN170[OE1]	Hydrogen bond	3.22
TYR107[OH]	ASN127[ND2]	Hydrogen bond	3.55
ASP100[OD1]	ASN127[ND2]	Hydrogen bond	3.82

Extended Table. 12 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 BETA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
SER102[OG]	SER176[O]	Hydrogen bond	2.51
SER102[OG]	SER176[OG]	Hydrogen bond	3.44
TYR101[OH]	PRO181[O]	Hydrogen bond	3.20
TYR32[OH]	ASN130[ND2]	Hydrogen bond	3.49
TYR105[O]	LYS166[NZ]	Hydrogen bond	3.22
TYR106[OH]	GLN175[NE2]	Hydrogen bond	2.53
VAL104[O]	GLY178[N]	Hydrogen bond	3.15
SER102[O]	PHE179[N]	Hydrogen bond	3.22
ASP100[O]	PHE179[N]	Hydrogen bond	2.23
TYR101[OH]	TYR183[N]	Hydrogen bond	3.34

Extended Table. 13 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 DELTA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR105[N]	GLY61[O]	Hydrogen bond	3.74
SER102[O]	SER58[OG]	Hydrogen bond	3.43
GLY103[O]	GLY59[N]	Hydrogen bond	3.76
GLY103[O]	ASP60[N]	Hydrogen bond	3.39
VAL104[O]	ARG57[N]	Hydrogen bond	2.04
VAL104[O]	SER58[N]	Hydrogen bond	3.12
TYR105[OH]	VAL54[N]	Hydrogen bond	3.60

Extended Table. 14 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 GAMMA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR105[OH]	GLY162[O]	Hydrogen bond	3.25
TYR31[OH]	ASN164[OD1]	Hydrogen bond	2.36
VAL104[N]	PHE167[O]	Hydrogen bond	3.55
CYS109[O]	TYR126[OH]	Hydrogen bond	3.45
TYR105[OH]	TYR166[N]	Hydrogen bond	2.56
TYR105[OH]	PHE167[N]	Hydrogen bond	3.49

Extended Table. 15 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 LAMBDA

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
SER53[OG]	GLN189[O]	Hydrogen bond	3.89
ASN54[ND2]	THR190[OG1]	Hydrogen bond	3.63
THR108[N]	ALA191[O]	Hydrogen bond	2.14
GLY103[O]	GLY170[N]	Hydrogen bond	2.96
GLY103[O]	VAL171[N]	Hydrogen bond	2.98
ASN54[OD1]	ARG188[NH1]	Hydrogen bond	3.86
TYR106[O]	ALA193[N]	Hydrogen bond	3.52

Extended Table. 16 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 OMICRON BA.2

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ASN54[ND2]	GLY159[O]	Hydrogen bond	2.10
ASN54[ND2]	CYS162[O]	Hydrogen bond	3.33
TYR105[N]	SER168[OG]	Hydrogen bond	3.46
SER102[OG]	TYR169[O]	Hydrogen bond	2.01
SER102[N]	PHE171[O]	Hydrogen bond	3.74
ASP100[O]	ASN122[ND2]	Hydrogen bond	2.12
TYR105[O]	ARG167[NH2]	Hydrogen bond	3.53
SER102[OG]	TYR169[N]	Hydrogen bond	2.94
SER102[OG]	GLY170[N]	Hydrogen bond	3.36
PHE114[O]	ARG172[NH1]	Hydrogen bond	3.54
ASP113[OD1]	ARG172[NE]	Salt bridge	2.79
ASP113[OD1]	ARG172[NH2]	Salt bridge	3.05
ASP113[OD2]	ARG172[NH2]	Salt bridge	3.89

Extended Table. 17 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 OMICRON BA.4/5

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
VAL104[N]	TRP27[O]	Hydrogen bond	3.79
TYR105[OH]	ARG126[O]	Hydrogen bond	2.56
TYR106[OH]	ILE142[O]	Hydrogen bond	3.83
TYR32[OH]	ARG20[NH1]	Hydrogen bond	3.16
SER56[OG]	GLY156[N]	Hydrogen bond	3.44
ASP100[O]	ARG20[NH1]	Hydrogen bond	3.37
SER102[O]	SER23[N]	Hydrogen bond	2.36
SER102[OG]	SER23[N]	Hydrogen bond	3.05
VAL104[O]	ARG128[NE]	Hydrogen bond	3.33
ASP113[OD1]	ARG126[NH2]	Hydrogen bond	2.70
ASP113[OD2]	ARG126[NH1]	Hydrogen bond	3.01
ASP100[OD2]	ARG20[NH1]	Salt bridge	3.70
ASP113[OD1]	ARG126[NE]	Salt bridge	3.79
ASP113[OD1]	ARG126[NH1]	Salt bridge	3.28
ASP113[OD1]	ARG126[NH2]	Salt bridge	2.70
ASP113[OD2]	ARG126[NH1]	Salt bridge	3.01
ASP113[OD2]	ARG126[NH2]	Salt bridge	3.92

Extended Table. 18 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 OMICRON BF.7

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR107[OH]	TYR201[OH]	Hydrogen bond	3.19
TRP111[N]	THR200[OG1]	Hydrogen bond	3.01
GLY26[O]	ASN187[N]	Hydrogen bond	3.26
GLU98[OE2]	TYR201[OH]	Hydrogen bond	2.51
PRO99[O]	ARG103[NH1]	Hydrogen bond	3.48
PRO99[O]	ARG103[NH2]	Hydrogen bond	3.90
TYR101[O]	ASN117[ND2]	Hydrogen bond	2.82
SER102[OG]	HIS205[NE2]	Hydrogen bond	3.20
VAL104[O]	ASN105[ND2]	Hydrogen bond	2.70
VAL104[O]	HIS205[NE2]	Hydrogen bond	3.43
GLY110[O]	ARG198[NH1]	Hydrogen bond	2.14
GLY110[O]	TYR201[OH]	Hydrogen bond	3.09
ASP113[OD1]	ARG198[NE]	Salt bridge	2.10
ASP113[OD1]	ARG198[NH2]	Salt bridge	3.44
ASP113[OD2]	ARG198[NE]	Salt bridge	2.83

Extended Table. 19 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 OMICRON BQ.1.1

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance(Å)
SER102[OG]	TYR132[O]	Hydrogen bond	2.05
VAL104[N]	TYR132[O]	Hydrogen bond	3.85
THR28[OG1]	ALA154[O]	Hydrogen bond	3.59
TYR31[N]	ASN166[OD1]	Hydrogen bond	3.51
VAL104[N]	TYR168[O]	Hydrogen bond	3.22
THR112[OG1]	ASN127[ND2]	Hydrogen bond	3.31
SER102[OG]	TYR132[N]	Hydrogen bond	3.59
PHE27[O]	LYS157[NZ]	Hydrogen bond	3.43
TYR101[O]	GLY164[N]	Hydrogen bond	3.17
TYR107[OH]	VAL165[N]	Hydrogen bond	2.04
ASP100[OD2]	ASN166[N]	Hydrogen bond	2.02
THR28[O]	ASN166[ND2]	Hydrogen bond	2.62
THR28[OG1]	ASN166[ND2]	Hydrogen bond	2.28
ASP100[OD1]	TYR168[N]	Hydrogen bond	3.49
ASP100[OD2]	TYR168[N]	Hydrogen bond	3.85
GLY103[O]	PHE169[N]	Hydrogen bond	2.53

Extended Table. 20 THE INTERACTION BINDING SITE BETWEEN S43 AND SARS-COV-2 OMICRON XBB

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ASN54[ND2]	ASN115[OD1]	Hydrogen bond	2.16
TYR101[OH]	VAL150[O]	Hydrogen bond	2.99
VAL104[N]	ARG165[O]	Hydrogen bond	2.75
TYR105[N]	PRO166[O]	Hydrogen bond	3.37
THR112[OG1]	ASN148[O]	Hydrogen bond	2.88
SER102[O]	THR167[N]	Hydrogen bond	2.41

Extended Table. 21 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ASN89[HD22]	GLY162[O]	Hydrogen bond	2.13
ASN89[HD21]	GLU161[O]	Hydrogen bond	2.04

Extended Table. 22 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ARG57[HH11]	ASN122[OD1]	Hydrogen bond	2.17
ARG57[HH21]	ASN122[OD1]	Hydrogen bond	2.50

Extended Table. 23 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
GLN34[OE1]	ARG49[HH22]	Hydrogen bond	2.23
TYR93[O]	TYR112[HH]	Hydrogen bond	1.83
GLN100[HE21]	GLY46[O]	Hydrogen bond	1.88
TRP98[H]	ARG49[O]	Hydrogen bond	2.42
ARG87[HH12]	ASP66[OD1]	Hydrogen bond	1.72
ARG87[HH22]	ASP66[OD2]	Hydrogen bond	1.73
TYR28[HH]	TYR108[O]	Hydrogen bond	1.84
ARG87[NH1]	ASP66[OD1]	Salt bridge	2.71
ARG87[NH2]	ASP66[OD1]	Salt bridge	3.43
ARG87[NH1]	ASP66[OD2]	Salt bridge	3.54
ARG87[NH2]	ASP66[OD2]	Salt bridge	2.72

Extended Table. 24 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
LYS50[HZ1]	SER154[OG]	Hydrogen bond	1.98
ASN89[HD22]	ASP82[OD2]	Hydrogen bond	2.24
PHE90[H]	TYR130[OH]	Hydrogen bond	2.31

Extended Table. 25 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
LYS50[HZ1]	SER154[OG]	Hydrogen bond	1.98
ASN89[HD22]	ASP82[OD2]	Hydrogen bond	2.24
PHE90[H]	TYR130[OH]	Hydrogen bond	2.31

Extended Table. 26 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR28[OH]	TYR175[HH]	Hydrogen bond	1.99
PHE90[O]	ARG167[HH22]	Hydrogen bond	1.94
PHE90[H]	ASN161[OD1]	Hydrogen bond	1.81
TYR91[HH]	VAL157[O]	Hydrogen bond	1.78
TYR92[H]	ASN161[OD1]	Hydrogen bond	1.72

Extended Table. 27 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR91[HH]	A:ASN 124[OD1]	Hydrogen bond	2.28

Extended Table. 28 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR85[OH]	GLY146[H]	Hydrogen bond	1.92
TYR86[O]	ASN150[HD21]	Hydrogen bond	2.29
TYR93[OH]	ARG152[HH22]	Hydrogen bond	2.36
TRP88[H]	GLY147[O]	Hydrogen bond	2.37

Extended Table. 29 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR86[OH]	ARG131[HH11]	Hydrogen bond	1.91

Extended Table. 30 THE INTERACTION BINDING SITE OF NB01 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR91[OH]	LYS111[H]	Hydrogen bond	2.23
TYR86[HH]	TYR168[O]	Hydrogen bond	2.32
ASN89[H]	GLY163[O]	Hydrogen bond	1.66
TYR91[H]	GLY114[O]	Hydrogen bond	2.47

Extended Table. 31 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR105[OH]	ALA25[H]	Hydrogen bond	2.22
TYR105[HH]	ARG23[O]	Hydrogen bond	1.78

Extended Table. 32 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR101[O]	ASN163[HD22]	Hydrogen bond	1.76
SER102[OG]	ARG28[HE]	Hydrogen bond	2.32
SER102[OG]	ARG28[HH21]	Hydrogen bond	1.95
THR108[OG1]	GLY167[H]	Hydrogen bond	1.98
ASP113[OD2]	THR160[H]	Hydrogen bond	1.76
TYR106[HH]	GLU22[OE1]	Hydrogen bond	1.71
GLY110[H]	SER159[O]	Hydrogen bond	2.47
TYR107[H]	CYS162[O]	Hydrogen bond	2.32
GLY103[H]	ASN163[OD1]	Hydrogen bond	2.48
SER53[H]	GLY164[O]	Hydrogen bond	2.42
THR108[H]	CYS170[SG]	Hydrogen bond	2.38

Extended Table. 33 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
GLU98[OE2]	TYR108[HH]	Hydrogen bond	1.68
VAL104[O]	THR106[H]	Hydrogen bond	2.18
TYR106[O]	PHE107[H]	Hydrogen bond	2.08
TYR106[H]	ASP105[O]	Hydrogen bond	1.77

Extended Table. 34 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ASP113[OD1]	ARG34[H]	Hydrogen bond	1.82

Extended Table. 35 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
GLU98[OE1]	LYS102[HZ2]	Hydrogen bond	2.03
GLU98[OE1]	LYS102[HZ3]	Hydrogen bond	2.33
GLU98[OE2]	LYS102[HZ3]	Hydrogen bond	2.29
ASP100[O]	ARG298[HH22]	Hydrogen bond	2.20
VAL104[O]	GLN110[HE22]	Hydrogen bond	2.27
THR108[O]	LYS102[HZ3]	Hydrogen bond	2.46
THR108[OG1]	ARG105[H]	Hydrogen bond	1.96
GLY110[O]	LYS102[HZ1]	Hydrogen bond	2.22
THR112[O]	LYS100[HZ2]	Hydrogen bond	1.74
ASP113[OD1]	CYS156[HG]	Hydrogen bond	1.76
VAL104[H]	GLY109[O]	Hydrogen bond	2.41
THR108[OG1]	ARG105[O]	Hydrogen bond	3.46
GLU98[OE1]	LYS102[NZ]	Salt bridge	2.71
GLU98[OE2]	LYS102[NZ]	Salt bridge	2.78
ASP113[OD2]	LYS102[NZ]	Salt bridge	3.28

Extended Table. 36 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
GLU98[OE1]	ASN155[HD22]	Hydrogen bond	1.74
TYR101[O]	ASN122[HD22]	Hydrogen bond	1.79
SER102[O]	ASN122[H]	Hydrogen bond	2.07
VAL104[O]	ARG20[HH21]	Hydrogen bond	1.84
VAL104[O]	ARG20[HE]	Hydrogen bond	2.12
ASP113[OD1]	ASN155[H]	Hydrogen bond	1.85
ASP113[OD2]	GLN148[HE22]	Hydrogen bond	2.05

Extended Table. 37 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR32[OH]	ARG20[HH11]	Hydrogen bond	2.06
TYR101[O]	ALA158[H]	Hydrogen bond	1.70
VAL104[H]	ALA158[O]	Hydrogen bond	2.07
TYR105[H]	ALA158[O]	Hydrogen bond	1.82

Extended Table. 38 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
TYR105[O]	GLN193[HE22]	Hydrogen bond	1.75
TYR106[O]	ARG198[HE]	Hydrogen bond	1.84
GLU98[OE1]	ARG198[HH11]	Hydrogen bond	1.87
TYR105[O]	ARG198[HH22]	Hydrogen bond	1.76
GLU98[OE1]	TYR201[HH]	Hydrogen bond	1.74
GLU98[OE1]	ARG198[NH1]	Salt bridge	2.68
GLU98[OE1]	ARG198[NH2]	Salt bridge	3.77
GLU98[OE2]	ARG198[NH2]	Salt bridge	3.94

Extended Table. 39 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
VAL104[O]	ASN96[HD21]	Hydrogen bond	1.77
TYR105[HH]	LEU134[O]	Hydrogen bond	2.17

Extended Table. 40 THE INTERACTION BINDING SITE OF S43 WHEN THE COMPLEX WITH THE VARIANT

Nanobody Res. Info.	Antigen Res. Info.	Interaction Info.	Distance (Å)
ASP100[O]	LYS111[HZ2]	Hydrogen bond	2.45
VAL104[O]	ASN21[HD22]	Hydrogen bond	1.84