Supplementary Material

1 ROSETTA COMMANDS

We used the following command for RosettaAntibody grafting stage:

```
antibody.linuxgccrelease -n_multi_templates 1 -vhh_only
-exclude_homologs true -fasta nb_fasta
```

and the following command for the H3 loop modeling using the recommended abH3.flags file:

```
antibody_H3.linuxgccrelease @abH3.flags -s grafting/model-0.relaxed.pdb
-nstruct 100
```

We used the following command for Rosetta TCRmodel:

```
tcrmodel.linuxgccrelease -alpha <alpha_sequence> -beta <beta_sequence>
-template_identity_cutoff 95 -blastp_identity_cutoff 95
```

2 SUPPLEMENTARY TABLES

PDB	VHH	Fr	CDR1	CDR2	CDR3	CDR3 Length	Max train identity
6ocd	2.70	2.70	1.31	3.01	3.06	14	0.84
6z6v	1.09	0.73	1.34	0.63	2.19	17	0.79
7a4t	1.25	1.04	2.13	1.29	1.91	12	0.89
7c8v	0.84	0.56	0.84	2.03	1.87	6	0.89
6yu8	1.44	0.89	3.48	2.26	2.19	13	0.83
6xw5	1.52	0.94	4.08	0.52	2.72	9	0.84
7n0i	1.44	1.32	1.92	0.85	1.93	17	0.85
6waq	1.15	0.63	1.82	0.67	2.53	16	0.89
6xyf	1.67	0.95	3.56	1.00	3.17	17	0.85
7a0v	1.34	0.73	2.77	0.98	2.82	14	0.82
7d30	2.35	1.12	2.93	1.98	6.20	12	0.88
7mfv	0.95	0.58	1.15	2.39	1.98	6	0.88
7a50	1.56	0.84	1.80	2.82	3.31	17	0.86
7ldj	2.19	1.08	4.62	1.86	4.11	21	0.88
7kn5	2.39	1.13	5.02	1.57	4.67	20	0.87
6uht	2.30	2.09	4.13	0.97	2.46	16	0.83
7kjh	1.62	1.03	3.73	2.58	2.68	11	0.87
6xxo	1.57	1.13	4.01	2.73	1.36	15	0.78
7aqg	1.47	0.75	1.63	3.10	3.29	12	0.86
6x05	2.47	1.43	3.61	2.48	5.60	13	0.75
6xw7	0.74	0.58	0.78	1.31	1.50	8	0.86
6lz2	1.12	0.60	2.27	0.69	3.35	6	0.88
6z10	2.60	1.34	2.59	1.15	5.65	20	0.81
6obm	1.85	1.20	4.16	1.21	3.49	12	0.88
6lr7	1.16	0.57	2.94	0.61	2.08	18	0.78
6xzu	1.87	1.00	1.97	1.23	5.31	10	0.88
7mfu	1.25	0.63	1.08	4.55	1.12	6	0.88
6xw4	2.33	1.21	5.23	1.50	4.94	13	0.83
6obg	1.65	0.90	3.59	1.02	3.53	12	0.86
6zrv	1.44	0.77	1.96	1.78	3.32	14	0.90
7now	1.58	1.05	3.35	0.87	2.64	19	0.89
6obo	1.51	0.77	3.38	1.00	3.30	12	0.89
7k84	2.20	1.03	1.15	2.10	5.20	17	0.84
6oca	2.11	1.19	4.18	3.10	3.02	16	0.82
6ui1	2.10	1.22	2.49	0.93	4.73	16	0.76
7a48	1.35	0.86	2.37	1.82	3.07	9	0.84
6obc	1.25	0.86	2.46	1.21	2.42	11	0.76
6z1v	1.20	0.93	1.87	0.78	2.22	14	0.83
7kgj	1.81	0.81	2.46	4.20	3.90	12	0.89
6xw6	1.09	0.79	1.66	1.46	1.77	19	0.82
6obe	1.72	1.24	4.12	2.02	2.39	11	0.79
7d2z	1.59	1.59	1.62	1.66	1.50	6	0.89
7n0r	2.44	1.14	1.13	2.29	6.82	12	0.87
7lvu	1.15	0.88	2.04	1.76	1.73	14	0.86
Mean	**1.65**	**1.02**	**2.65**	**1.73**	**3.16**	**13.30**	**0.85**
STD	**0.51**	**0.40**	**1.20**	**0.94**	**1.39**	**4.07**	**0.04**
Median	**1.57**	**0.94**	**2.46**	**1.54**	**2.92**	**13**	**0.86**

Table S1. NanoNet results for the Nb test set. RMSDs (Å) for the whole VHH domain, followed by frame and CDRs1-3, CDR3 length, and maximal sequence identity to a Nb in the training set.

PDB	VH	FR	CDR1	CDR2	CDR3	CDR3 Length	Max train identity
1mtq	0.59	0.39	0.50	0.42	1.61	9	0.90
2r8s	1.28	0.66	0.90	2.59	3.02	12	0.96
3nps	1.75	1.21	2.93	1.41	3.19	17	0.95
2v17	1.10	0.68	0.47	0.98	2.93	11	0.88
1seq	1.34	0.54	0.88	0.87	3.62	14	0.88
1fns	1.23	0.86	0.64	0.83	2.77	14	0.91
3go1	1.36	0.74	1.98	1.97	3.00	14	0.75
2adf	0.73	0.60	0.49	0.49	1.69	9	0.91
1mfa	0.67	0.55	0.56	0.76	1.41	9	0.97
3eo9	0.84	0.57	0.81	0.74	1.98	12	0.87
4nzu	1.26	0.57	1.01	0.50	3.15	16	0.80
2e27	1.18	0.57	1.03	0.85	4.11	7	0.89
3gnm	0.87	0.61	0.70	0.69	2.31	9	0.85
2ypv	1.22	1.08	0.43	0.85	2.45	10	0.84
3p0y	0.75	0.54	1.05	1.19	1.38	12	0.90
3t65	0.59	0.46	0.73	0.70	1.14	11	0.95
2xwt	1.02	0.55	1.47	0.74	2.75	10	0.87
3umt	0.86	0.57	0.53	0.95	2.21	10	0.88
1dlf	1.25	0.63	1.29	0.89	3.65	10	0.91
3e8u	0.67	0.59	0.42	0.57	1.42	8	0.83
3mxw	0.88	0.58	0.74	1.26	2.15	10	0.86
3mlr	1.51	0.90	0.66	0.92	3.61	15	0.75
4h20	0.82	0.67	0.45	0.87	1.78	10	0.87
1gig	1.22	0.62	1.01	0.64	3.13	14	0.88
3liz	1.49	0.49	0.71	0.49	4.84	10	0.87
2vxv	0.99	0.56	0.47	1.10	2.57	12	0.89
3g5y	0.52	0.49	0.60	0.44	0.80	7	0.96
3lmj	2.18	0.97	3.53	5.70	3.73	16	0.83
4h0h	0.84	0.81	0.34	0.29	1.44	10	0.88
3oz9	0.79	0.53	0.50	0.99	1.98	10	0.89
3giz	0.78	0.51	0.47	0.45	1.91	13	0.91
1oaq	0.67	0.49	0.62	0.54	1.52	11	0.95
2d7t	0.95	0.74	0.80	0.54	2.53	7	0.93
1jfq	0.76	0.75	0.58	0.54	1.02	12	0.98
3hc4	0.95	0.96	0.48	0.92	1.25	7	0.86
1mlb	0.60	0.48	0.47	0.78	1.45	7	0.96
2w60	0.59	0.47	0.39	0.39	1.39	9	0.92
2fb4	1.65	0.62	0.62	0.78	4.19	17	0.82
2fbj	0.72	0.60	0.50	0.68	1.54	9	0.90
3vow	0.71	0.58	0.91	1.11	1.10	11	0.84
1jpt	0.67	0.56	0.70	0.59	1.46	8	0.83
4f57	1.35	0.60	0.85	1.51	3.31	16	0.79
3i9g	1.54	0.69	0.93	1.24	4.35	12	0.80
1nlb	0.49	0.46	0.38	0.55	0.79	9	0.91
3hnt	0.56	0.44	0.35	0.81	1.21	9	0.88
3m8o	1.82	0.98	1.74	1.25	5.81	8	0.76
4hpy	0.85	0.49	2.52	0.50	1.21	11	0.93
Mean	**1.01**	**0.64**	**0.88**	**0.95**	**2.38**	**10.94**	**0.88**
STD	**0.39**	**0.18**	**0.67**	**0.82**	**1.17**	**2.79**	**0.06**
Median	**0.87**	**0.58**	**0.66**	**0.78**	**2.15**	**10**	**0.88**

Table S2. NanoNet results on the mAb test set. RMSDs (Å) for the whole VH domain, followed by frame and CDRs1-3, CDR3 length, and maximal sequence identity to a mAb VH in the training set.

PDB	Vβ	Fr	CDR1	CDR2	CDR3	CDR3 Length	Max train identity
6vrn	1.00	0.63	0.58	0.62	2.24	15	0.92
6c61	1.81	1.69	0.92	1.02	2.88	16	0.90
2ial	0.85	0.72	0.53	0.50	1.72	11	0.93
6fr8	0.80	0.66	0.42	0.74	1.49	14	0.93
4ww1	1.01	0.88	0.55	0.91	1.83	12	0.82
1kgc	0.80	0.61	0.90	0.87	1.39	13	0.81
6ovn	2.01	1.81	0.88	2.50	2.89	17	0.93
4ei6	1.61	1.75	1.24	1.32	1.13	14	0.71
6r2l	2.28	1.24	1.33	5.34	2.97	18	0.86
2cdf	1.33	0.91	0.73	0.58	2.92	15	0.93
6frb	0.88	0.72	1.27	0.66	1.40	12	0.64
6lir	1.19	1.15	0.61	0.80	1.83	14	0.58
6ovo	2.08	1.40	2.36	1.37	4.00	17	0.93
3vxq	0.89	0.78	0.64	0.68	1.58	13	0.93
5d2n	1.12	0.68	0.69	1.08	2.39	16	0.92
Mean	**1.31**	**1.04**	**0.91**	**1.27**	**2.18**	**14.47**	**0.85**
STD	**0.51**	**0.43**	**0.49**	**1.23**	**0.81**	**2.07**	**0.12**
Median	**1.12**	**0.88**	**0.73**	**0.87**	**1.83**	**14.00**	**0.92**

Table S3. NanoNet results for the TCR test set. RMSDs (Å) for the whole Vβ domain, followed by frame and CDRs1-3, CDR3 length, and maximal sequence identity to a TCR Vβ in the training set.

PDB	Antigen	Min ligand	Min interface
6yu8	Ebola RNA methyltransferase	9.56	4.87
6xw5	MNV capsid protein P-domain	4.31	2.19
6xw7	MNV capsid protein P-domain	3.13	1.30
6xw4	MNV capsid protein P-domain	6.46	3.66
6xw6	MNV capsid protein P-domain	5.40	2.16
6waq	SARS-CoV-1 RBD	4.25	2.51
7n0i	SARS-CoV-2 N protein	5.29	1.79
7n0r	SARS-CoV-2 N protein	5.28	3.11
7c8v	SARS-CoV-2 RBD	3.55	4.60
7d30	SARS-CoV-2 RBD	3.63	2.55
7ldj	SARS-CoV-2 RBD	4.28	4.75
7kn5	SARS-CoV-2 RBD	4.50	4.68
7mfu	SARS-CoV-2 RBD	3.45	4.30
7kgj	SARS-CoV-2 RBD	8.18	5.69
7d2z	SARS-CoV-2 RBD	7.82	4.00
nb105	SARS-CoV-2 RBD	7.40	3.84
nb21	SARS-CoV-2 RBD	5.67	4.85
Mean	-	**5.42**	**3.58**
STD	-	**1.87**	**1.30**
Median	-	**5.28**	**3.84**

Table S4. Docking results for NanoNet generated models. Minimal ligand and interface RMSDs (Å) for docking models generated by PatchDock.

Model	**VH**	**Fr**	**CDR1**	**CDR2**	**CDR3**
#1	1.24	0.77	1.20	1.18	2.72
#2	1.05	0.70	1.00	1.11	2.34
#3	1.26	0.76	1.12	1.21	2.86
#4	1.22	0.75	1.12	1.07	2.79
#5	1.20	0.71	1.18	1.15	2.77
Mean	**1.20**	**0.74**	**1.12**	**1.14**	**2.69**
STD	**0.08**	**0.03**	**0.08**	**0.06**	**0.21**

Model	**VHH**	**Fr**	**CDR1**	**CDR2**	**CDR3**
#1	1.61	0.90	2.29	1.50	3.42
#2	1.75	1.11	2.19	1.57	3.45
#3	1.60	0.95	2.37	1.71	3.24
#4	1.75	0.97	2.50	1.65	3.63
#5	1.77	1.11	2.19	1.53	3.66
Mean	**1.69**	**1.01**	**2.31**	**1.59**	**3.48**
STD	**0.08**	**0.10**	**0.13**	**0.09**	**0.17**

Table S5. 5-Fold Cross Validation Results. Mean RMSDs (Å) for the whole VH/VHH domain, followed by frame and CDRs1-3 for each validation split. Top - mAb (mean of 100 mAb structures), Bottom - Nb (mean of 50 Nb structures) .

3 SUPPLEMENTARY FIGURES

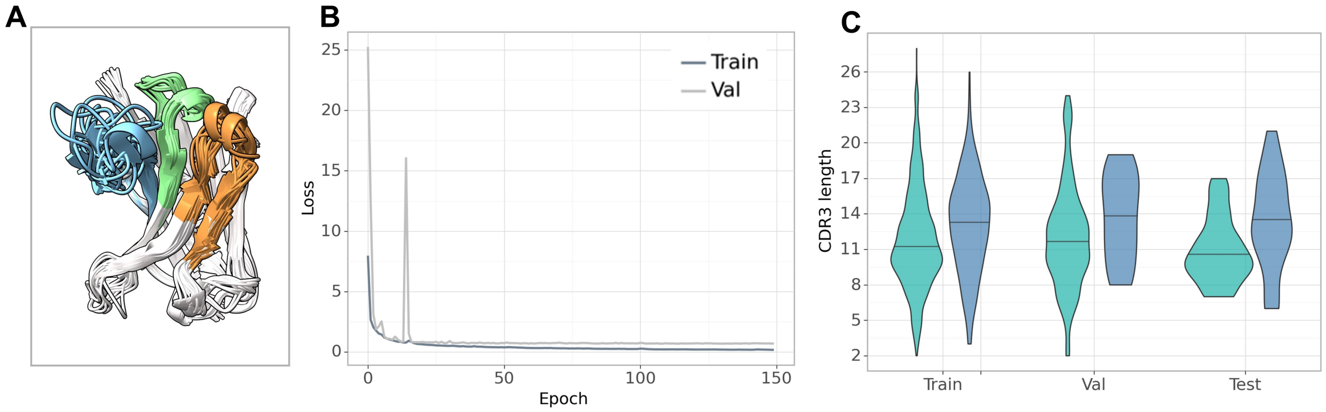

Fig. S1. **(A)** Structural alignment of the antibodies from the training set prior to coordinate extraction for training the network, **(B)** Training and validation loss during the training process, **(C)** CDR3 lengths of the training, validation, and test sets (mAb green, Nb blue).

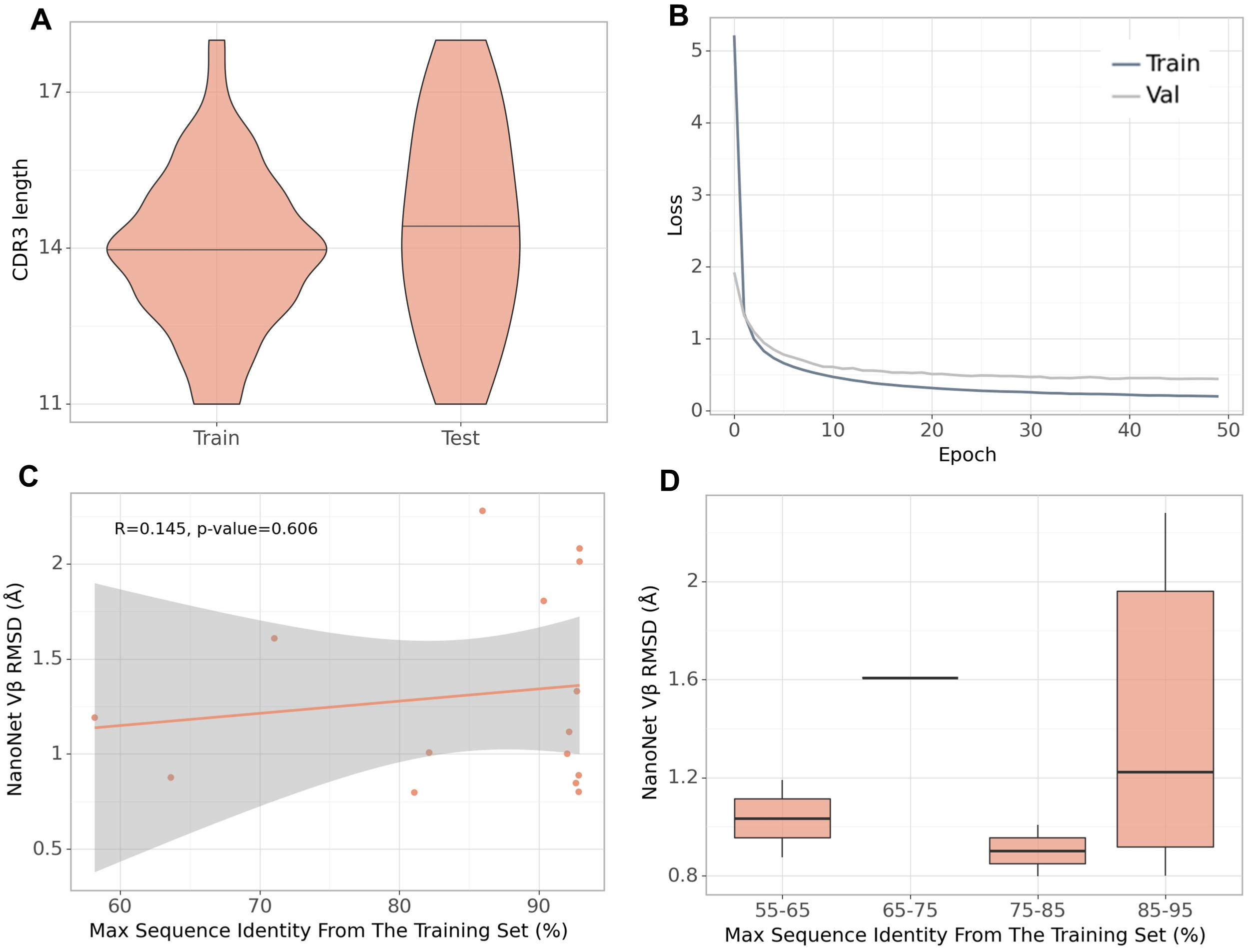

Fig. S2. TCR β chain test set. **(A)** CDR3 lengths of the training and test sets, **(B)** Training and validation loss during the training process, **(C)** Test set performance (measured as Vβ RMSD) as a function of maximal sequence identity to the train set, each dot represents a structure from the TCR test set (15 structures), **(D)** Test set performance with boxplots for sequence identity ranges.

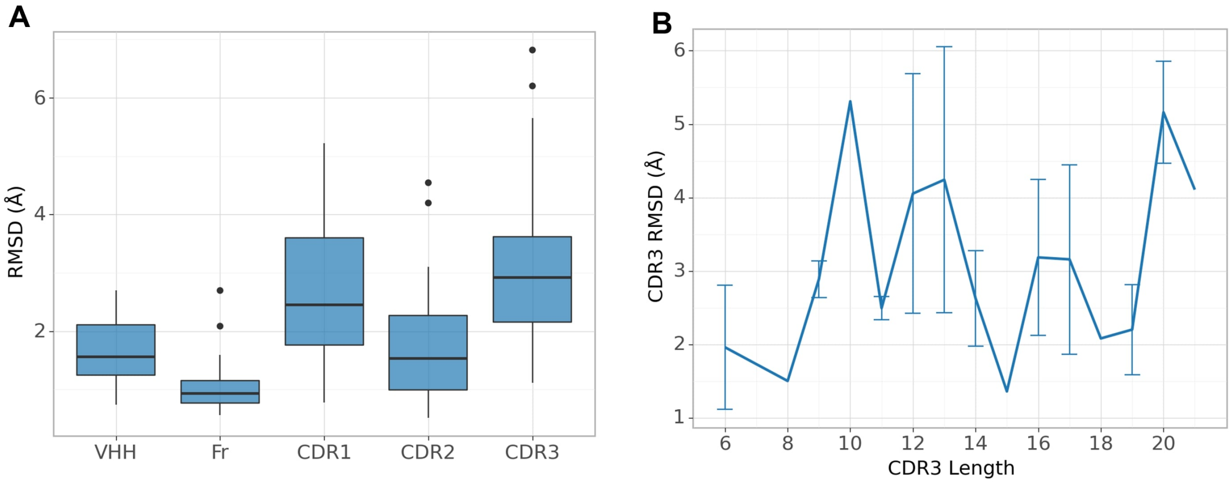

Fig. S3. NanoNet results for the entire Nb test set (44 structures). **(A)** Boxplots of RMSDs of the whole VHH region, framework, CDR1-3 loops, **(B)** RMSD of CDR3 loop as a function of loop length.

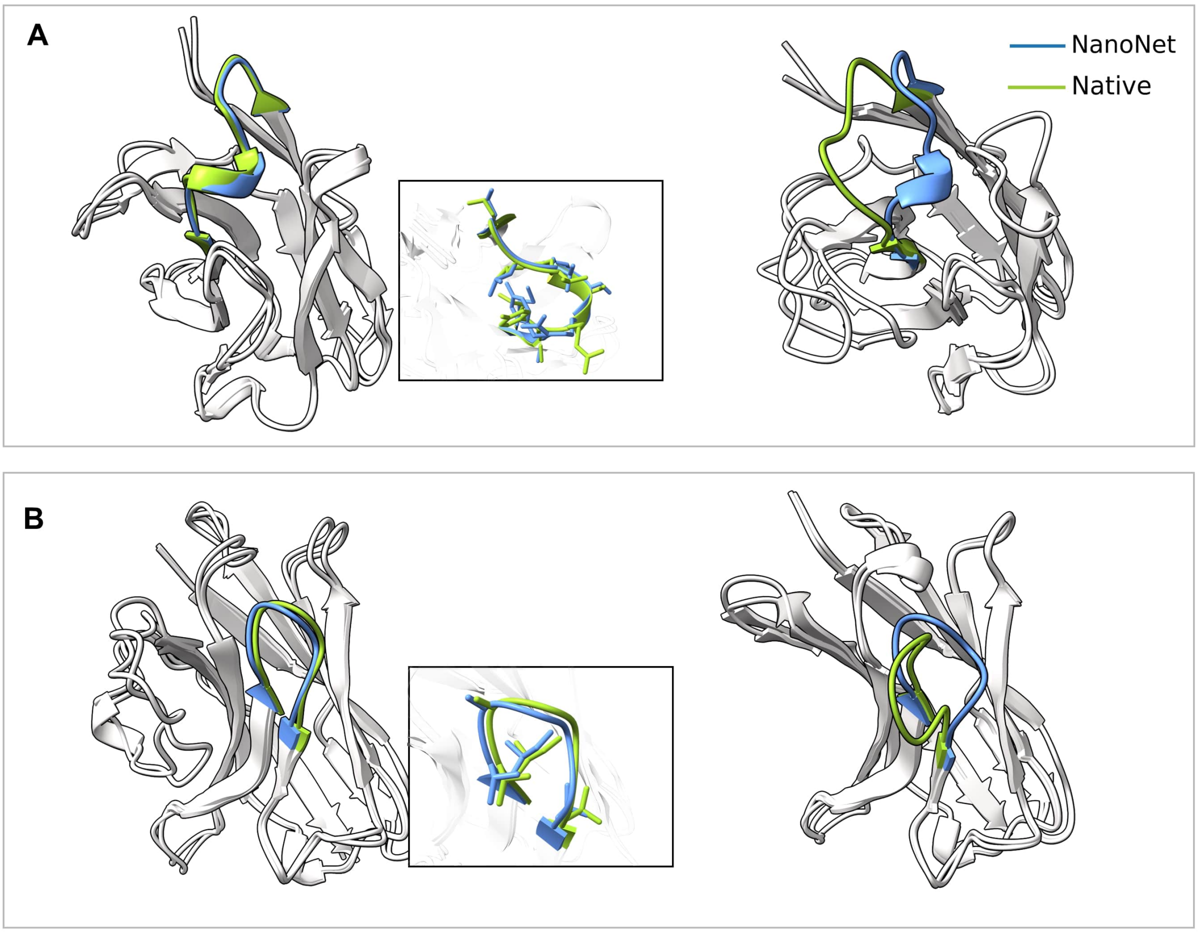

Fig. S4. CDR1 and CDR2 modeling examples of the Nb test set. **(A)** CDR1 modeling: PDB 6xw7 (left) and 6xw4 (right), CDR1 RMSDs 0.78Åand 5.23Årespectively, **(B)** CDR2 modeling: PDB 6z6v (left) and 7mfu (right), CDR2 RMSDs 0.63Åand 4.55Årespectively.

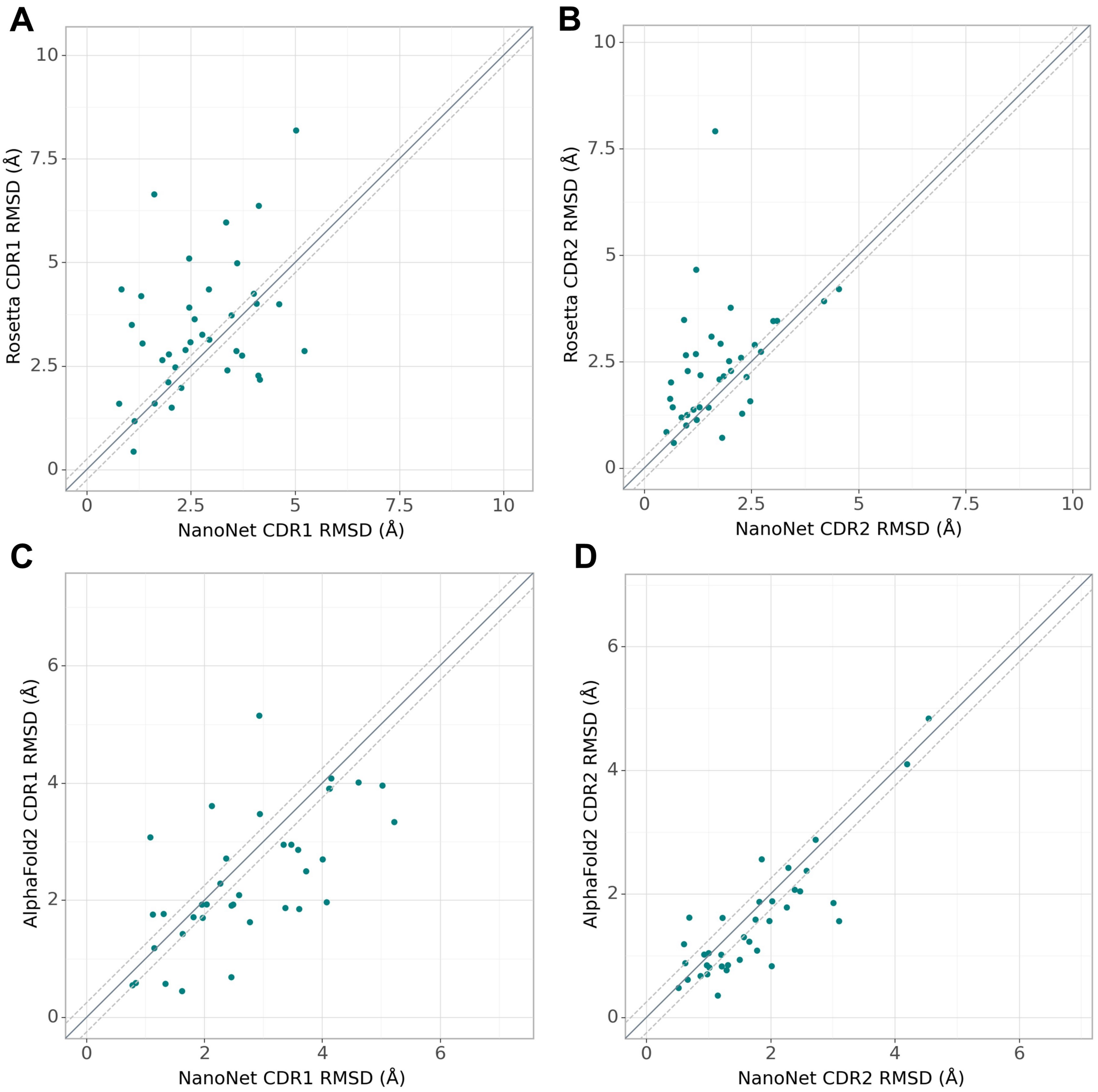

Fig. S5. CDR1 and CDR2 Nb results (37 structures). **(A)** CDR1 loop RMSD for NanoNet vs. RosettaAntibody, each dot represents a structure from the Nb test set. The dotted line corresponds to 0.25Å RMSD, **(B)** CDR2 loop RMSD for NanoNet vs. RosettaAntibody, each dot represents a structure from the Nb test set. The dotted line corresponds to 0.25Å RMSD, **(C)** Same as (A) but for NanoNet vs. AlphaFold2, **(D)** Same as (B) but for NanoNet vs. AlphaFold2

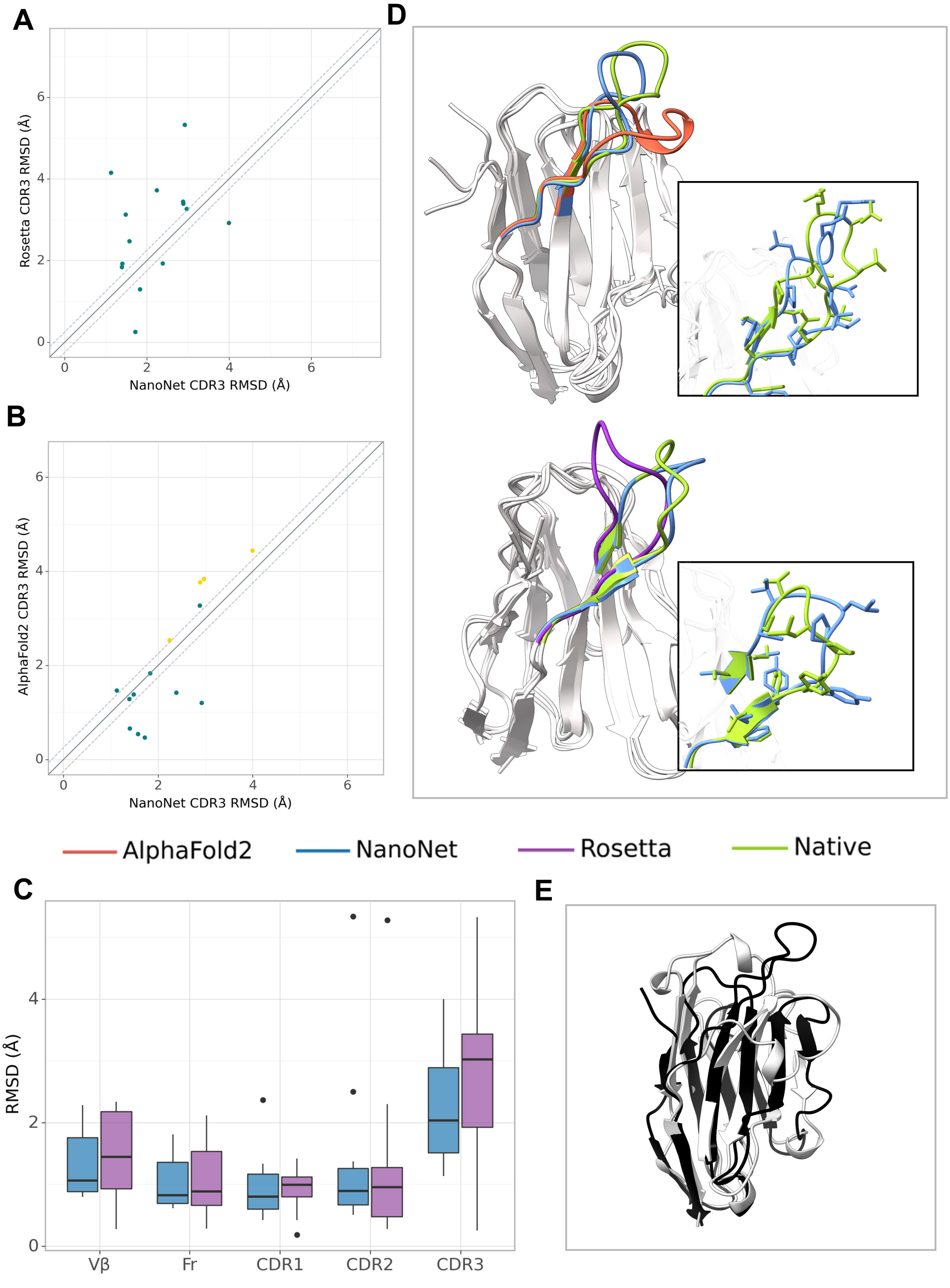

Fig. S6. TCR Vβ chain modeling (14 structures). **(A)** CDR3 loop RMSD for NanoNet vs. Rosetta TCRmodel, each dot represents a structure from the TCR test set. The dotted line corresponds to 0.25 A RMSD, **(B)** Same as (A) but for NanoNet vs. AlphaFold2, structures not in AlphaFold training set are highlighted in yellow. **(C)** Boxplots of RMSDs of the whole Vβ region, framework, CDR1-3 loops for the test set TCRs, **(D)** Test set examples of modeled structures by NanoNet (blue), Rosetta TCRmodel (purple), AlphaFold2 (red) vs. experimental (green): PDB 6ovn (top) - CDR3 RMSD 2.89Å, 3.76Å for NanoNet and AlphaFold2, respectively and 6fr8 (bottom) - CDR3 RMSD 1.49Å ,3.12Å for NanoNet and Rosetta TCRmodel, respectively, **(E)** TCR Vβ (PDB 6r2l, black) aligned to an Nb (PDB 6uht, white).