We searched the train dataset (see table S6) for CDRs unique residues and found 59 such residues. Table S4 lists the obtained CDRs unique residues.

Table S4. The list of CDRs unique residues within the train set for which we performed our in-silico alanine scan analysis.

PDB ID	Chain type	Location	Residue type
1A3R	HEAVY	93	D
1ADQ	HEAVY	26	G
1AHW	HEAVY	65	Q
1AR1	HEAVY	26	G
1BGX	HEAVY	63	K
1BGX	HEAVY	64	S
1BGX	HEAVY	61	S
1BGX	HEAVY	62	L
1BGX	HEAVY	26	G
1EO8	HEAVY	26	G
1FBI	HEAVY	65	K
1FSK	HEAVY	97	T
1HI6	HEAVY	97	T
1IQD	HEAVY	26	G
1JPS	HEAVY	65	Q
1JPS	HEAVY	62	P
1JRH	HEAVY	61	P
1KB5	HEAVY	64	K
1KB5	HEAVY	61	Q
1KB9	HEAVY	26	G
1KTR	HEAVY	107	E
1NCD	HEAVY	64	K
1NCD	HEAVY	61	E
1OAZ	HEAVY	26	G
1QFU	HEAVY	26	G
1S78	HEAVY	64	K
1S78	HEAVY	61	Q
1S78	HEAVY	60	N
1SM3	HEAVY	26	G
1UJ3	HEAVY	365	Q
1XCQ	HEAVY	26	G
1XGY	HEAVY	93	A
1YNT	HEAVY	562	Q
1ZA3	HEAVY	63	V
1ZA3	HEAVY	64	K
1ZA3	HEAVY	61	D
1ZA3	HEAVY	65	G
1ZA3	HEAVY	62	S
1ZTX	HEAVY	26	G
2A6I	HEAVY	97	A
2B2X	HEAVY	60	L
2B4C	HEAVY	64	R
2B4C	HEAVY	61	Q

2BDN	HEAVY	26	G
2BOC	HEAVY	62	E
2EH8	HEAVY	93	A
2HH0	HEAVY	137	D
2HH0	HEAVY	135	K
2HH0	HEAVY	108	R
2HH0	HEAVY	107	G
2HKF	HEAVY	26	G
2OZ4	HEAVY	65	K
2OZ4	HEAVY	26	G
2Q8A	HEAVY	26	G
2R0K	HEAVY	26	G
2R29	HEAVY	26	G
1TJI	LIGHT	26	S
1YY9	LIGHT	26	S
2OTU	LIGHT	25	S