

Table S6. Train dataset. Contains the list of PDB structures used to construct Paratome.

PDB ID	Heavy chain	Light chain	Ag chain
2HH0	H	L	P
1NAK	H	L	P
3DGV	B	A	X
2B1A	H	L	P
1JHL	H	L	A
1XGY	H	L	P
1CFT	B	A	C
1AR1	C	D	A
2A6I	B	A	P
1SY6	H	L	A
1W72	H	L	A
2R4S	H	L	A
1ZA3	B	A	S
2CMR	H	L	A
3C09	H	L	D
2GDT	A	B	E
1U8N	B	A	C
2JEL	H	L	P
1TZH	B	A	W
1H0D	B	A	C
2QR0	B	A	C
2J88	H	L	A
1RJL	B	A	C
1TPX	B	C	A
2OQJ	B	A	F
2FJH	H	L	V
1ACY	H	L	P
1RZK	H	L	C
2QAD	D	C	A
1ORS	B	A	C
1N8Z	B	A	C
1PKQ	B	A	E
1E4X	H	L	P
2J4W	H	L	D
2CXD	H	L	P

2QSC	H	L	P
3C2A	H	L	P
2NZ9	D	C	A
2B2X	H	L	A
2JIX	H	L	E
1P4B	H	L	P
2E58	H	L	P
2R0L	H	L	A
1U95	B	A	C
3BKY	H	L	P
1QFW	H	H	A
1NDG	B	A	C
1U8M	B	A	C
1HYS	D	C	A
2QQL	H	L	A
1FSK	C	B	A
1MPA	H	L	P
2NR6	D	C	A
1U8Q	B	A	C
1JPS	H	L	T
2AP2	B	A	F
1TZI	B	A	V
1A3R	H	L	P
1PZ5	B	A	C
1UJ3	B	A	C
1DQJ	B	A	C
1CZ8	H	L	W
1CU4	H	L	P
2OZ4	H	L	A
1YQV	H	L	Y
2B0S	H	L	P
2ADF	H	L	A
2OR9	H	L	P
1ZTX	H	L	E
1CF5	B	A	C
1AFV	H	L	A
1BGX	H	L	T
1HI6	B	A	C
1NFD	H	G	C

3CK0	H	L	P
2UZI	H	L	R
1EO8	H	L	A
2R0W	H	L	Q
2FJG	B	A	W
1MHP	H	L	A
2CK0	H	L	P
2VWE	E	C	A
2BOC	A	B	C
1NSN	H	L	S
2I9L	B	A	I
1EGJ	H	L	A
2GSI	B	A	W
1S78	D	C	A
1QKZ	H	L	A
1XGU	B	A	C
1BVK	B	A	C
1U92	B	A	C
1KC5	H	L	P
2NY7	H	L	G
1FPT	H	L	P
1FBI	H	L	X
1GGI	H	L	P
1KTR	H	L	P
1P2C	B	A	C
1VFB	B	A	C
1I8K	B	A	C
2R0K	H	L	A
1JRH	H	L	I
1KEN	H	L	F
2J5L	C	B	A
2HFG	H	L	R
2B1H	H	L	P
1YNT	B	A	F
3B2U	H	L	A
1G9N	H	L	C
1BOG	B	A	C
1E4W	H	L	P
1OSP	H	L	O

1OAZ	H	L	A
2Q8A	H	L	A
2OSL	H	L	P
1FJ1	B	A	F
1KCS	H	L	P
1CE1	H	L	P
1FE8	H	L	A
1AHW	B	A	F
1CFN	B	A	C
1XIW	D	C	A
1ADQ	H	L	A
2VDK	H	L	A
2B4C	H	L	C
1QFU	H	L	A
1N6Q	H	L	A
1WEJ	H	L	F
3BKJ	H	L	A
1LKR	H	L	A
1ORQ	B	A	C
2HRP	H	L	P
2IFF	H	L	Y
2EH8	H	L	P
1Q1J	H	L	Q
2QQN	H	L	A
1UWX	H	L	A
1MLC	B	A	E
1FRG	H	L	P
2J6E	H	L	A
1E6J	H	L	P
1N64	H	L	P
1KCR	H	L	P
2DD8	H	L	S
1NOX	H	L	R
2BDN	H	L	A
3CSY	A	B	N
2OTU	B	A	P
1U8P	B	A	C
1FNS	H	L	A
1YJD	H	L	C

2AEP	H	L	A
1F90	H	L	E
2FX7	H	L	P
2VIS	B	A	C
1IGC	H	L	A
2IGF	H	L	P
2H1P	H	L	P
1NCD	H	L	N
1Z3G	H	L	A
3BNT	D	C	B
1TET	H	L	P
2QHR	H	L	P
1XCQ	B	A	P
1J1P	H	L	Y
1YY9	D	C	A
1U8O	B	A	C
1HIM	L	H	P
2ZCK	L	H	P
1OTS	C	D	A
1KB9	J	K	F
1U93	B	A	C
2V17	H	L	A
1V7M	H	L	V
1F58	H	L	P
3D85	B	A	D
1UAC	H	L	Y
1TJI	H	L	P
2ARJ	H	L	Q
1IQD	B	A	C
1XCT	B	A	P
3CVH	H	L	A
2HKF	H	L	P
1SM3	H	L	P
1NL0	H	L	G
3BT2	H	L	A
1NDM	B	A	C
1KB5	H	L	A
1HH9	B	A	C
2H9G	B	A	R

1NMA	H	L	N
1U8L	B	A	C
2BRR	H	L	P
2G5B	B	A	I
2R56	H	L	A
2IPU	H	L	Q
1OB1	B	A	F
2R29	H	L	A
1I9R	H	L	A