

Supplementary Material

Table S1. IMGT indices of conserved framework residues. The table shows the residues that were used for model superimposition.

Receptor type	Chain type	IMGT indices
BCR	heavy	2, 3, 4, 5, 6, 7, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 39, 40, 41, 42, 43, 44, 45, 49, 50, 51, 52, 53, 54, 55, 67, 68, 71, 72, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 118, 119, 120, 121, 122, 123, 124, 125, 126
BCR	light	3, 4, 5, 6, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 66, 67, 68, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 80, 82, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 118, 119, 120, 121, 122, 123, 124, 125
TCR	beta	3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 39, 40, 41, 42, 43, 44, 45, 50, 51, 52, 53, 54, 55, 76, 77, 78, 79, 80, 86, 87, 88, 89, 90, 91, 92, 93, 97, 98, 99, 100, 101, 102, 103, 104, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127
TCR	alpha	4, 5, 6, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 39, 40, 41, 42, 43, 44, 45, 50, 51, 52, 53, 54, 55, 76, 77, 78, 79, 80, 81, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127

Table S2. Comparison between 80 and 90% template blacklisting. The table summarizes the all-atom RMSDs and, in brackets, variances for the two benchmarks, one in which templates were blacklisted if they had a sequence identity of 80% or more and another in which templates were blacklisted if they had a sequence identity of 90% or

BCR 80% Blacklist	Rep. Builder	ABodyBuilder	P Value
CDR-H3	4.32 (3.30)	4.57 (4.59)	7.48E-04
ALL	1.92 (0.18)	1.96 (0.32)	8.62E-01
	Rep. Builder	Lyra	P Value
CDR-H3	4.32 (3.30)	5.06 (4.64)	2.20E-16
ALL	1.92 (0.18)	2.10 (0.29)	2.20E-16
	Rep. Builder	PIGSPro	P Value
CDR-H3	4.32 (3.30)	4.88 (4.97)	2.78E-13
ALL	1.92 (0.18)	2.09 (0.38)	5.42E-16

BCR 90% Blacklist	Rep. Builder	ABodyBuilder	P Value
CDR-H3	4.14 (3.41)	4.38 (4.31)	3.53E-04
ALL	1.85 (0.18)	1.87 (0.24)	4.74E-01
	Rep. Builder	Lyra	P Value
CDR-H3	4.14 (3.41)	4.94 (4.80)	2.20E-16
ALL	1.85 (0.18)	2.03 (0.30)	2.20E-16
	Rep. Builder	PIGSPro	P Value
CDR-H3	4.14 (3.41)	4.71 (5.37)	4.79E-12
ALL	1.85 (0.18)	1.97 (0.30)	1.45E-09

TCR 80% Blacklist	Rep. Builder	TCRmodel	P
CDR-B3	3.23 (1.67)	3.93 (2.70)	9.30E-04
ALL	2.04 (0.08)	2.64 (4.16)	9.17E-09
	Rep. Builder	Lyra	P
CDR-B3	3.23 (1.67)	3.77 (1.63)	2.47E-03
ALL	2.04 (0.08)	2.31 (0.15)	1.14E-07

TCR 90% Blacklist	Rep. Builder	TCRmodel	P Value
CDR-B3	3.26 (1.70)	4.01 (6.04)	4.69E-03
ALL	2.00 (0.11)	2.60 (4.21)	8.16E-07
	Rep. Builder	Lyra	P Value
CDR-B3	3.26 (1.70)	3.86 (1.87)	5.25E-03
ALL	2.00 (0.11)	2.17 (0.17)	9.17E-05

Table S3. Comparison between Repertoire Builder and Kotai Antibody Builder. Repertoire Builder and Kotai Antibody Builder were compared for 15 queries in three representative groups taken from the Kotai Antibody Builder benchmark: Best-5, Median-5 and Worst-5. Columns 3-4 show the CDRH3 RMSDs; Columns 5-6 show all-residue RMSDs; Column 7 shows the Repertoire Builder query-template CDRH3 score. Data corresponds to that plotted in **Figure 2G**.

Group	Query	RB CDRH3	KAB CDRH3	RB ALL	KAB ALL	CDRH3 Score
Best-5	4bh8BA	1.02	1.43	1.51	1.59	1.00
	4xvsHL	1.02	2.81	1.78	2.22	0.95
	4rdqGF	1.27	1.71	1.21	1.73	0.54
	5ikcBA	1.36	2.63	1.32	1.44	0.61
	4xxdBA	1.36	4.06	1.55	2.52	0.33
Median-5	5b8cBA	4.51	4.05	1.72	2.00	0.22
	5jueHL	4.51	5.99	1.93	2.81	0.16
	5l6yHL	4.51	6.75	1.86	2.58	0.24
	5e94BA	4.53	5.98	1.78	2.04	0.07
	5tz2HL	4.54	3.76	1.60	1.50	-0.25
Worst-5	4zfoAB	9.48	10.99	2.78	3.27	0.10
	4rwyHL	10.40	5.69	3.51	2.42	-0.06
	4mwfAB	12.35	6.01	4.28	2.78	-0.03
	5tplHL	12.81	8.98	4.07	3.48	-0.16
	4lkcBA	13.88	4.00	4.61	5.74	-0.11

Table S4. Average RMSD of Repertoire Builder and Rosetta Antibody Refined models. A total of 15 queries in three representative groups were defined from the high-throughput blacklisted BCR benchmark: Worst-5, Median-5 and Best-5. Columns 3-4 show CDRH3 RMSDs for Repertoire Builder (RB) and Refined Rosetta Antibody (RA) models; Columns 5-6 show the all-residue RMSDs. Column 7 shows the Repertoire Builder query-template CDRH3 score. Data corresponds to that plotted in **Figure 2H**.

Group	Query	RB CDRH3	RA CDRH3	RB ALL	RA ALL	CDRH3 Score
Best-5	4xxdBA	0.52	2.14	1.06	1.29	1.00
	5e2tHL	1.19	1.52	1.39	1.63	0.36
	1c08BA	1.22	1.44	1.04	1.28	1.00
	1kcrHL	1.32	2.29	1.27	1.41	0.24
	1kcsHL	1.35	2.92	1.15	1.43	0.22
Median-5	1ck0HL	4.08	3.37	1.73	1.73	-0.02
	1pkqBA	4.09	6.22	1.76	2.17	-0.07
	3mlxHL	4.09	16.08	1.82	5.22	0.07
	4hc1HL	4.09	3.25	1.71	1.79	-0.05
	4hpyHL	4.10	4.92	2.12	3.82	-0.04
Worst-5	1dlfHL	9.65	8.00	3.23	4.55	-0.18
	4imkAD	9.70	9.26	3.34	3.29	-0.08
	1a3rHL	9.99	6.95	2.76	2.16	-0.02
	1dqdHL	10.84	9.23	3.12	2.77	-0.20
	4ogxHL	11.69	11.54	3.82	3.93	0.09