

S5 Table. References to the TCR structures used for the analysis

Name	PDB	Ref.	Name	PDB	Ref.
1G4	2bnu	[1]	LC13	3kps	[2]
1G4	2bnq	[1]	MEL5	3hg1	[3]
1G4	2bnr	[1]	OB.1A12	2wbj	[4]
1G4 AV-wt	2f54	[5]	OB.1A12	lymm	[6]
1G4 c5c1	2pyf	[7]	RA14	3gsn	[8]
1G4 c5c1	2pye	[7]	SB27	2ak4	[9]
1G4 c49c50	2f53	[5]	SB27[K16Dα]	3kxf	[10]
1G4 c58c62	2p5w	[7]	TCR MS2-3C8	3o6f	[11]
1G4 c58c61	2p5e	[7]	TK3 wt	3mv7	[12]
3A6	1zgl	[13]	TK3 Q55H	3mv8	[12]
A6	2gi6	[14]	TK3 Q55A	3mv9	[12]
A6	1qsf	[15]	1934,4	2pxy	[16]
A6	1qse	[15]	1F1E8	3mff	[17]
A6	3d3v	[18]	226 TCR	3qiu	[19]
A6	3d39	[18]	226 TCR	3qiw	[19]
A6	1qrn	[15]	2B4	3qib	[19]
A6	1ao7	[20]	2B4	3qjf	[19]
A6	3h9s	[21]	2C	1tcr	[22]
A6	3pwp	[23]	2C	1g6r	[24]
AS01	3o4l	[25]	2C	1mwa	[26]
B7	1bd2	[27]	2C	2ckb	[28]
cf34	3ffc	[29]	2C T7	2icw	[30]
DM1	3dxa	[31]	2C [T7-wt-s] ^a	2oi9	[32]
DM1	3dx9	[31]	2C m13 [T7-s] ^a	3e3q	[33]
E8	2ian	[34]	2C m6 [T7-s] ^a	2e7l	[32]
E8	2iam	[34]	2C m67 [T7-s] ^a	3e2h	[33]
E8	2ial	[34]	2W20	3c6l	[35]
ELS4	2nx5	[36]	5c.c7	3qjh	[19]
ELS4	2nw2	[36]	AHIII12.2	2uwe	[37]
HA1.7	1fyt	[38]	AHIII12.2	2jcc	[37]
HA1.7	1j8h	[39]	AHIII12.2	1lp9	[40]
Hy.1B1	3pl6	[41]	B3K506	3c5z	[35]
JM22	2vlj	[42]	BM3.3	1nam	[43]
JM22	2vlk	[42]	BM3.3	1fo0	[44]
JM22	1oga	[45]	BM3.3	2ol3	[46]
JM22	2vlm	[42]	cl19	2z31	[16]
JM22	2xn9	[47]	D10	1d9k	[48]
JM22	2xna	[47]	KB5-C20	1kj2	[49]
JM22 [S99βA]	2vlr	[42]	N15	1nfd	[50]
KK50.4	2esv	[51]	TCR 21.30	3mbe	[52]
LC13	1mi5	[53]	TCR172.10	1u3h	[54]
LC13	1kgc	[55]	YAe62	3c60	[35]
LC13	3kpr	[2]			

^a) WT with solubility mutations acc. to ref. [32]. More detailed information is available in Table S2.

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