

DynaDom: Structure-based prediction of TCR inter-domain and TCR-pMHC association angles - T. Hoffmann, A. Marion, and I. Antes
Additional File 8

Table S4: Angular deviations with respect to the crystal structures after DynaDom glutamine refinement.

PDB	CH ^a		Angular Deviation[°]				PDB	CH ^a		Angular Deviation[°]					
	ID	α	β	Single		Complex		ID	α	β	Single		Complex		
				α	β	α					β	α	β	α	β
1ao7	D	E	179.9	174.2	-168.3	-175.2	2vlr	I	J	11.4	7.9	7.7	5.7		
1fo0	A	B	-179.5	179.9	-176.9	-176.0	3e5z	A	B	13.5	-5.8	9.3	2.5		
1fyt	D	E	-11.5	-36.2	-135.3	-12.9	3e5z	E	F	13.7	-5.8	9.7	2.6		
1j8h	D	E	174.2	-37.5	23.6	-10.5	3c60	A	B	-2.0	-18.5	96.0	-54.9		
1kj2	A	B	-174.9	165.9	176.0	170.0	3c60	E	F	-3.2	-22.9	96.8	-56.9		
1kj2	D	E	-161.2	167.8	-177.9	169.3	3c6l	A	B	33.5	157.2	69.2	121.4		
1mi5	D	E	-168.6	5.6	8.0	6.4	3c6l	E	F	35.3	157.0	71.2	122.8		
1mwa	A	B	-108.5	-178.1	176.1	-163.8	3d39	D	E	-154.7	175.1	-153.4	-177.4		
1nam	A	B	179.9	158.8	168.1	174.0	3d3v	D	E	-165.6	174.2	-167.7	-172.0		
1oga	D	E	7.8	16.8	3.4	14.8	3dxa	D	E	-147.1	17.7	-163.7	14.9		
1qse	D	E	-173.3	157.0	-173.4	167.9	3dxa	I	J	-155.9	22.7	-172.6	19.9		
1u3h	A	B	25.6	138.8	26.3	127.0	3dxa	N	O	-150.5	20.5	-162.9	12.7		
1u3h	E	F	-2.2	134.1	-15.4	-149.7	3e2h	B	C	-2.8	-0.1	3.7	4.3		
2bnq	D	E	-174.8	168.5	-176.5	-178.9	3e3q	C	F	5.4	-0.1	10.7	4.2		
2bnr	D	E	-171.8	168.5	-173.5	-178.6	3e3q	d	e	2.3	-4.6	4.8	4.0		
2e7l	A	D	20.9	157.0	24.3	162.1	3e3q	D	E	3.5	-3.7	7.1	2.8		
2e7l	B	C	14.4	-4.3	22.1	-2.3	3e3q	I	J	5.7	-4.0	9.7	2.4		
2esv	D	E	11.4	n/a	-1.5	n/a	3e3q	M	N	5.2	-0.1	10.5	3.9		
2f53	D	E	0.8	-155.8	-9.0	-160.6	3e3q	R	S	1.2	-0.1	5.3	7.8		
2f54	D	E	3.9	174.2	-20.9	-170.2	3e3q	V	W	3.7	-5.8	5.6	2.0		
2f54	K	L	25.3	168.5	178.7	16.3	3e3q	Z	a	-5.8	0.2	-4.6	6.9		
2gj6	D	E	-173.5	179.9	-172.7	-173.0	3ffc	D	E	-3.0	8.4	-0.5	19.2		
2iam	C	D	-1.8	15.4	-9.0	17.4	3ffc	I	J	-5.2	17.2	-2.7	20.2		
2ian	D	E	-5.8	14.8	-7.6	27.3	3gsn	A	B	n/a	154.8	n/a	157.7		
2ian	I	J	-3.2	17.5	-3.7	18.8	3h9s	D	E	-180.0	174.2	-176.8	-177.8		
2ian	N	O	-5.8	-5.8	-8.3	1.7	3kpr	D	E	-2.4	3.3	-7.3	1.4		
2ian	S	T	-5.8	-5.8	4.1	-1.8	3kpr	I	J	180.0	-1.0	7.2	-2.7		
2nx5	I	J	2.4	1.1	-10.9	8.2	3kps	D	E	12.8	-13.2	-7.8	-14.5		
2nx5	N	P	21.1	11.4	12.9	7.3	3kxf	D	E	-2.0	-40.6	-5.1	-11.7		
2nx5	T	U	10.5	16.4	-1.1	25.9	3kxf	M	O	-3.8	-44.2	3.4	-49.2		
2oi9	B	C	5.3	-5.8	2.7	-3.5	3kxf	N	P	-166.3	-4.4	-166.0	14.7		
2ol3	A	B	3.6	-11.5	10.9	-8.0	3mbe	C	D	180.0	-30.6	149.2	-43.1		
2p5e	D	E	3.7	-157.6	-2.7	-159.2	3mbe	G	H	-180.0	-31.0	152.7	-38.2		
2p5w	D	E	-3.0	-157.0	-14.9	-159.9	3mv8	D	E	-172.2	50.9	-174.7	22.9		
2pxy	A	B	177.7	11.4	172.0	5.7	3pwp	D	E	5.6	2.3	3.7	9.4		
2pye	D	E	-6.3	-157.0	-18.4	-160.4	3qiu	C	D	n/a	-0.2	n/a	14.1		
2vll	D	E	-8.8	23.1	-11.3	19.8	3qiw	C	D	n/a	4.2	n/a	-6.4		
2vlr	D	E	3.7	9.4	0.8	7.6									

a) TCR chain ID contained in the same biological unit.