Supporting Information

Xu et al. 10.1073/pnas.1015433108

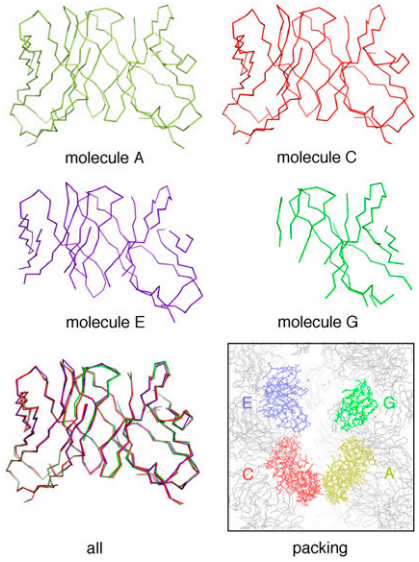

Fig. S1. Comparison of the four molecules (A, C, E, and G) within the asymmetric unit of δ1A/B-3 crystal and molecular packing in the crystal lattice. Each molecule is displayed in an identical orientation with different color traces. In the molecular packing panel, symmetry mates for the four molecules are shown in light gray as background (related to Fig. 1).

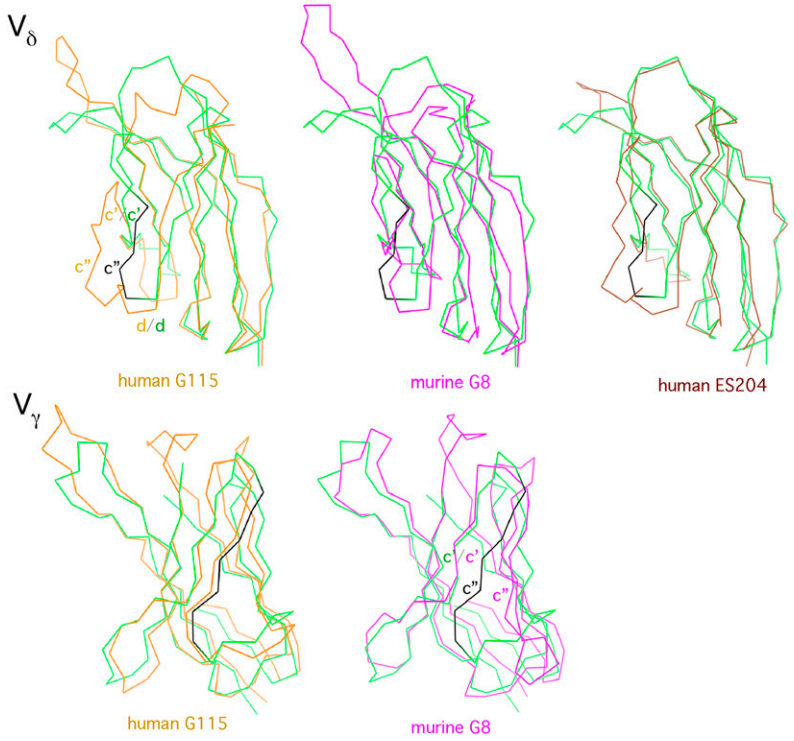

Fig. S2. Comparison of C″-strand positions in γδ T-cell receptor (TCR) structures. *Upper* shows V_{δ} domains, and *Lower* shows V_{γ} domains. γδ TCRs are color-coded: green is δ1A/B-3 single-chain Fv (scFv), orange is human G115, brown is $V_{\delta 3}$ δ chain ES204, and magenta is murine G8. C″ strands of δ1A/B-3 are shown in black. C′, C″, and D strands are selectively labeled (related to Fig. 2).

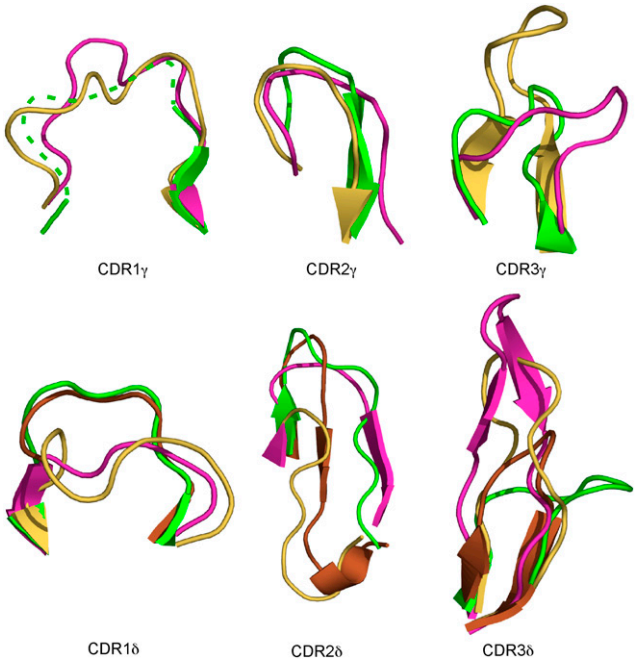

Fig. S3. Structural variations in complementary determining region (CDR) loops. Human G115, $V_{\delta 3}$ δ chain ES204, and murine G8 structures are superimposed onto the δ1A/B-3 structure using maximum likelihood-based algorithims. Only CDR loops are shown in the following color codes: green for δ1A/B-3, orange for G115, brown for $V_{\delta 3}$ δ chain ES204, and magenta for murine G8. The unmodeled segment of CDR1γ is shown as a dotted line (related to Fig. 2).

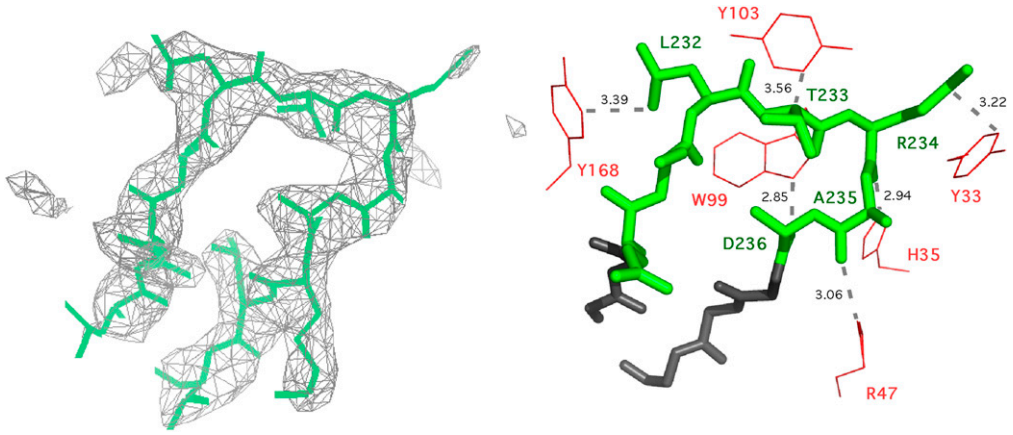

Fig. S4. Validation of CDR3δ structure in δ1A/B-3 (*Left*) and δ1A/B-3 CDR3δ and related neighboring residues in the structure (*Right*). A refined Fobserved–Fcalculated difference omit map for the CDR3δ loop shows strong positive density for the entire loop (compensating negative density is not shown for clarity). The map is contoured at 2.5 σ. Distances for interresidual noncovalent interactions are shown in angstroms. The stem of the loop is shown in backbone representation only (in gray for clarity; related to Table 1).

Table S1. Data collection and phasing statistics

	Native	SeMet peak	SeMet edge	SeMet remote
Space group	$P4_3$	$P4_3$	$P4_3$	$P4_3$
Cell dimensions				
a = *b*; *c* (Å)	112.4, 108.1	113.1, 108.8	113.8, 108.8	113.2, 108.7
Source	ALS 5.0.2	NSLS X29	NSLS X29	NSLS X29
Wavelength (Å)	1.0000	0.9790	0.9793	0.9600
Resolution (Å)	50–3.04 (3.16–3.04)	30–3.73 (3.88–3.73)	30–3.60 (3.73–3.60)	30–3.73 (3.88–3.73)
Unique reflections	25,563	14,399	15,396	15,235
Redundancy	4.1 (4.1)	13.1 (7.8)	13.9 (7.9)	13.7 (9.8)
Completeness (%)	99.8 (99.1)	89.9 (66.7)	95.2 (63.2)	95.5 (89.2)
I/σ (I)	48.4 (2.1)	31.9 (2.2)	41.8 (2.3)	37.9 (3.6)
R_{merge} (%)	5.4 (36.5)	8.8 (34.9)	7.0 (38.8)	8.5 (37.9)
Mean figure of merit	0.73	0.73	0.73	0.73
Phasing power		1.48	0.95	1.64

Highest resolution shell statistics are shown in parentheses. SeMet, selenomethionine.

Table S2. Refinement statistics

Statistic	Value
Resolution (Å)	32.8–3.04
Unique reflections	24,654
R_{cryst}/R_{free}	0.265/0.308
Average B factor	
Molecules 1, 2	75.2, 69.8
Molecules 3, 4	119.9, 119.5
rmsd	
Bond lengths (Å)	0.013
Bond angles	1.4
Ramachandran plot	
Most favored	82.7%/492
Additional allowed	16.5%/98
Generously allowed	0.8%/5
Disallowed	0
Estimated coordinate error [maximum likelihood ESU (Å)]	0.338