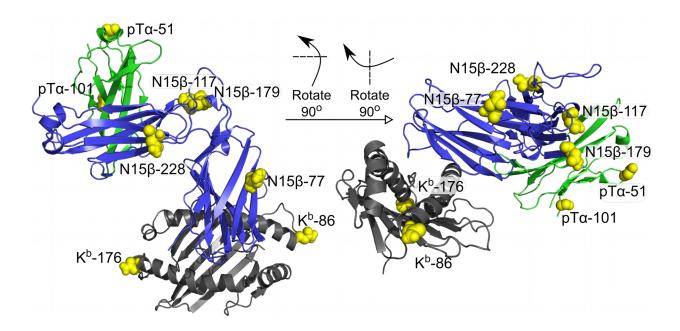
NMR-Directed Design of PreTCR β and pMHC Molecules Implies a Distinct Geometry for preTCR Relative to $\alpha\beta$ TCR Recognition of pMHC

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Figure S1

Supplementary References



SUPPLEMENTARY FIGURE 1. Glycosylation sites and pT α location relative to proposed interaction surfaces. Two views of the complex model conformer 1 (Fig. 10D) illustrating the position of pT α , added by superposition of C β from 3OF6 (1) onto the C β of N15 β , and the conserved glycosylation acceptor Asn residues. Eight conserved glycosylation sites are found in this complex, two on H-2K b (2) , four on N15 β (3), and two on pT α (1,4). Colors are as in Fig 10D with pT α in green and Asn sites in yellow spheres.

SUPPLEMENTARY REFERENCES

- 1. Pang, S.S., Berry, R., Chen, Z., Kjer-Nielsen, L., Perugini, M.A., King, G.F., Wang, C., Chew, S.H., La Gruta, N.L., Williams, N.K., Beddoe, T., Tiganis, T., Cowieson, N.P., Godfrey, D.I., Purcell, A.W., Wilce, M.C.J., McCluskey, J., Rossjohn, J. (2010) The structural basis for autonomous dimerization of the pre-T-cell antigen receptor. *Nature* **467**, 844-8.
- 2. Powell, L.D., Smith, K., Hart, G.W. (1987) Site specific glycosylation patterns of H-2K: effects of allelic polymorphism and mitogenic stimulation. *Journal of Immunology* **139**, 1206-1213.
- 3. Wang, J., Lim, K., Smolyar, A., Teng, M., Liu, J., Tse, A.G., Liu, J., Hussey, R.E., Chishti, Y., Thomson, C.T., Sweet, R.M., Nathenson, S.G., Chang, H.C., Sacchettini, J.C., Reinherz, E.L. (1998) Atomic structure of an alphabeta T cell receptor (TCR) heterodimer in complex with an anti-TCR fab fragment derived from a mitogenic antibody. *EMBO J.* **17**, 10-26.
- 4. Zhou, B., Chen, Q., Mallis, R.J., Zhang, H., Liu, J.-H., Reinherz, E.L., Wang, J.-H. (2011) A Conserved Hydrophobic Patch on Vβ Domains Revealed by TCRβ Chain Crystal Structures: Implications for Pre-TCR Dimerization. *Front. Immunol.* **2**, 5.