Instructions for generating the atomic coordinates of the new haemoglobin tetramers presented at WATOC08 by Don Vanselow.

Download crystal structure 1A3N (Tame and Vallone) from PDB. Separate chain A (alpha) and chain D (beta).

Rotate A with $\begin{bmatrix} 0.489 & 0.488 & -0.723 \\ -0.669 & -0.323 & -0.670 \\ -0.560 & 0.811 & 0.169 \end{bmatrix}$. Then add the vector $\begin{bmatrix} 19.607 \\ 31.603 \\ 1.334 \end{bmatrix}$.

Rotate D with $\begin{bmatrix} 0.387 & 0.740 & 0.549 \\ 0.633 & 0.220 & -0.742 \\ -0.670 & 0.635 & -0.384 \end{bmatrix}$. Then add the vector $\begin{bmatrix} -31.214 \\ 13.345 \\ 21.084 \end{bmatrix}$.

Rotate a copy of the pair 180° about x axis → T-state. Rotate a copy of the pair 180° about z axis → R-state.