



STRUCTURAL  
BIOLOGY

**Volume 75 (2019)**

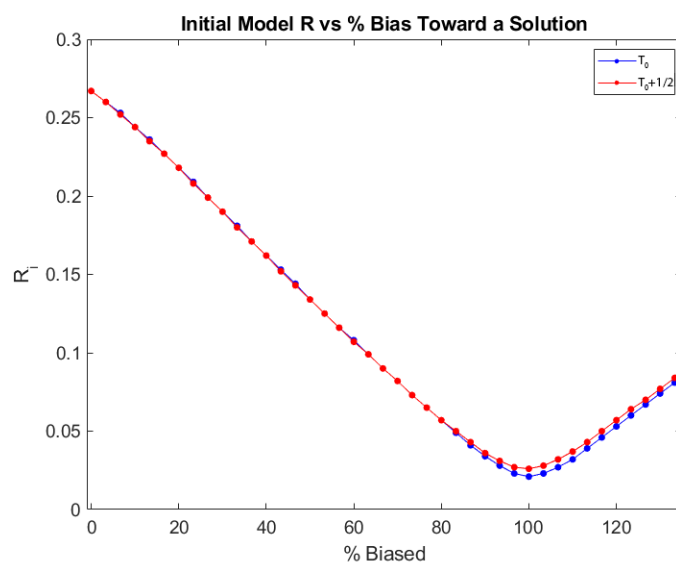
**Supporting information for article:**

**Supercell refinement: a cautionary tale**

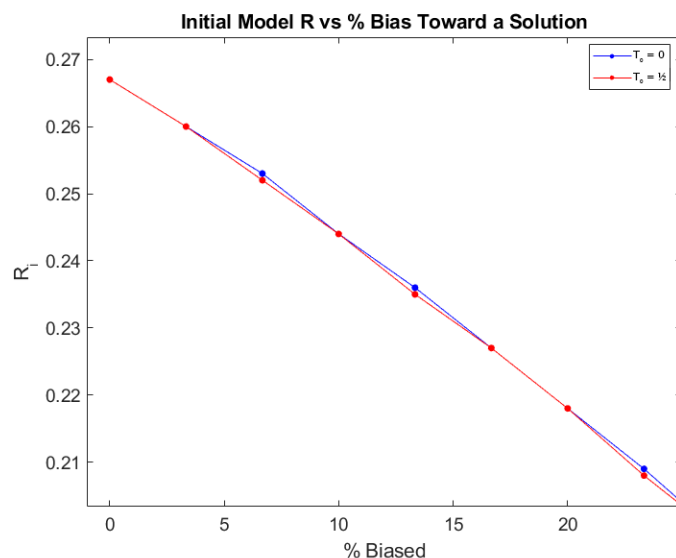
**Jeffrey Lovelace, Václav Petříček, Garib Murshudov and Gloria E. O. Borgstahl**

In the paper we argued that the  $T_0=1/2$  solution will have a shallower error well leading to a broader well that when it combines with the error well for the correct solution (deeper and have steeper sides) will cause refinements starting near the average to favor the  $T_0=1/2$  solution.

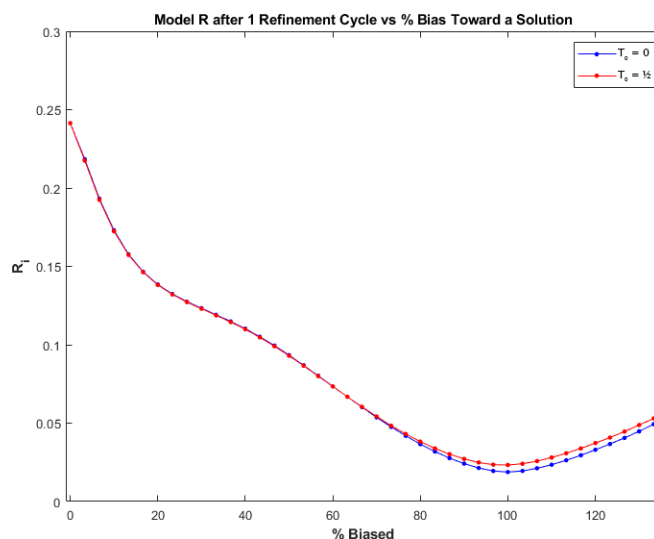
The error space was approximated by using the initially calculated R values for molecular states that were biased toward one of the two solutions ( $T_0=0$  or  $T_0=1/2$ ). Figure S1a shows that  $T_0=1/2$  seems to provide evidence supporting our view about the shape of the error space.



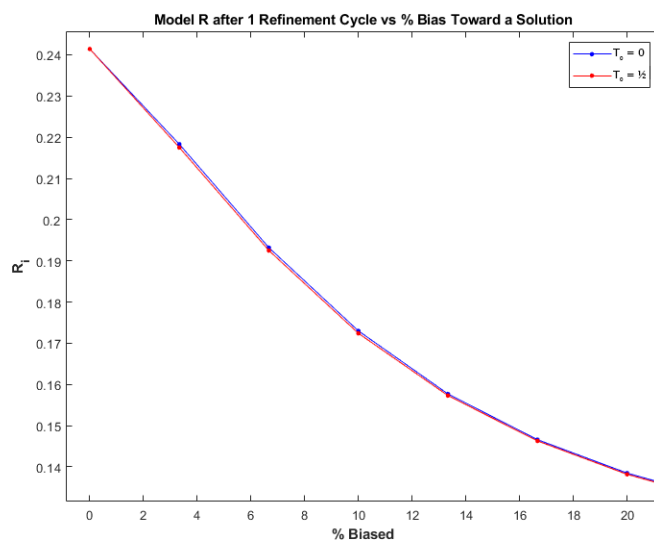
**Figure S1(a):** Plot of the initial R values as a function of the % bias toward the  $T_0=0$  or the  $T_0=1/2$  solutions. The  $T_0$  solution can achieve a lower R value. A bias of 0% is the average structure 100% represents one of the two solutions and >100% represents an overshooting of the rotation.



**Figure S1(b):** Zoomed in region of Fig. S1a near the starting point of refinement. Although  $T_0=0$  has the lowest final R value,  $T_0=1/2$  has (slightly) lower R values for states near the average structure which may cause refinement approaches to favor the  $T_0=1/2$  because of these locally more favorable R values.



**Figure S1(c):** Plot of the R values after one cycle of refinement as a function of the % bias toward the  $T_0=0$  or the  $T_0=1/2$  solutions. The  $T_0=0$  solution can achieve a lower R value. A bias of 0% is the average structure 100% represents one of the two solutions and >100% represents an overshooting of the rotation.



**Figure S1(d):** Zoomed in region of Fig. S1c near the starting point of refinement. Although  $T_0=0$  has the lowest R value,  $T_0=1/2$  has (slightly) lower R values for states near the average structure which may cause refinement approaches to favor the  $T_0=1/2$  because of these locally more favorable R values.