Structural Change and Nucleotide Dissociation of Myosin Motor Domain: Dual Gō Model Simulation

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Supplemental Material

Intermediate Structure

Figure1 shows the average structure of the intermediate state (2<dRMSD<3Å), which is superimposed on (a) the final structure and (b) the initial structure. Superposition is made so that 209-466th residues in U50kDa domain are fitted best. The intermediate structure is drawn with dark colors, and the final structure and the initial one with light colors. The figure clearly shows that the converter domain in the intermediate state is in between those in the initial structure and the final one.

Structural characteristics of the intermediate structure can be seen in detail in fig.2, in which the differences between the distance of ith and jth residues in the intermediate structure and that in the reference (initial or final) structure are shown. The upper triangle represents $r_{ij}^{\mathrm{im}} - r_{ij}^{\mathrm{i}}$, and the lower triangle represents $r_{ij}^{\mathrm{im}} - r_{ij}^{\mathrm{f}}$, where r_{ij}^{im}, r_{ij}^{i} and r_{ij}^{f} are the distance between ith and jth residues in the intermediate structure, the initial structure and the final struture, respectivery. Green indicates $r_{ij}^{\mathrm{im}} - r_{ij}^{\mathrm{ref}} \sim 0$ (ref=i or f). Intra-domain distances are roughly kept same. Thus N-terminal, U50kDa, L50kDa and convertor domain do not change their shape largely during the structural change. On the other hand, there are appreciable difference in inter-domain distances. The motion of the converter domain mentioned above is clearly recognized also in the figure. Furthermore, we found that the relative position of N-terminal domain to 50kDa domain in the intermediate state is very close to that in the initial state. Thus the final relaxation consists of a rearrangement of the N-terminal subdomain against the other part.

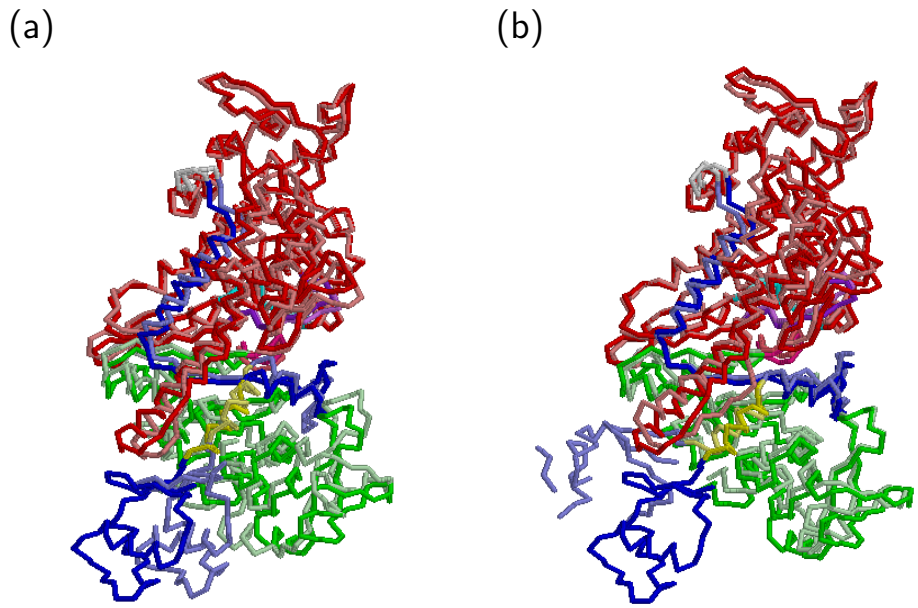

Figure 1: The average structure of intermedeate state superinmposed on (a) final (1Q5G) and (b) initial (1VOM) structure. Dark and light colors are corresponding to the intermediate structure and the final (a) or the initial (b) structures, respectively. Green, red and blue correspond to N-terminal, 50kDa and C-terminal subdomain, respectively.

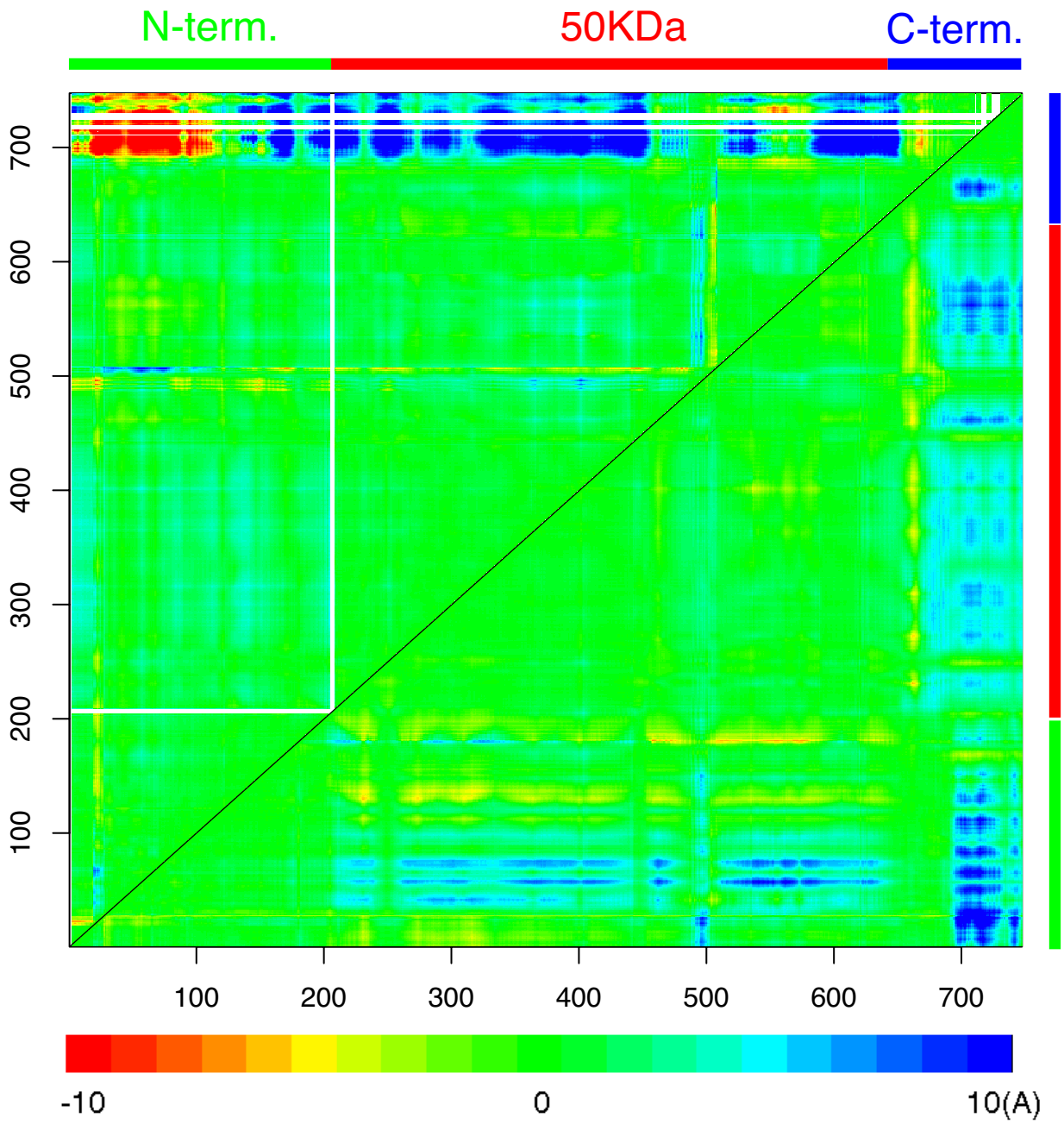

Figure 2: $r_{ij}^{\mathrm{im}} - r_{ij}^{\mathrm{ref}}$, ref=i or f. The white lines in upper triangle correspond to the gap region in the initial (1VOM) structure.

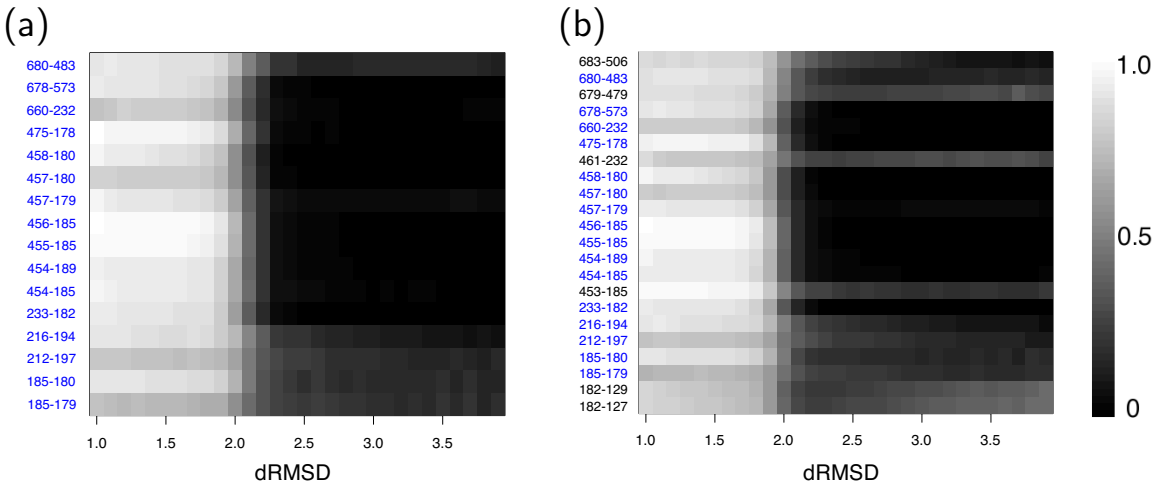

Figure 3: The contact formation rate, (a) $k_{\text{p-n}} = 0.6$, (b) $k_{\text{p-n}} = 0.7$. (b) is the same as Figure 7 of the main body. The contacts included common in both are written in blue.

Relaxation-Associated Contacts

dRMSD dendence of the contact formation rate for the relaxation-associated contacts (RAC) in $k_{\text{p-n}} = 0.6$ and 0.7 are shown in Figure 3. RAC are defined as the contacts which satisfy the conditions $P^{ij}(2\text{Å}, 3\text{Å}) < 0.3$ and $P^{ij}(0\text{Å}, 2\text{Å}) > 0.7$. The set of contacts are basically same for both figures (Some contacts that included in (b) dropped from (a), which are indicated in black letters. But they actually are ones that have the values of P^{ij} near the threshold to be identified as RAC). They are concentrated on the boundary between N-terminal and 50kDa domain. In this resolution, virtually all these contacts form at the same dRMSD, and thus simultaneously in time. Thus the native-contact formation take place cooperatively at the final relaxation irrespective of $k_{\text{p-n}}$.