

Abstract Submitted
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**Structural and functional
allostery wiring diagrams in GroEL/GroES**¹ RIINA TEHVER, JIE CHEN,
D. THIRUMALAI, University of Maryland — Repeated cycling between distinct
allosteric states is required for the functions of numerous biological nanomachines.
Determining the specific residues that are responsible for transmitting allosteric sig-
nals is needed to understand their operation. Using structural perturbation analysis
and evolutionary correlations of mutations of residues, we determine networks of key
residues in molecular chaperonin GroEL and its cochaperonin GroES. GroEL is a
molecular machine that rescues aggregation-prone misfolded proteins. Its functional
cycle consists of a series of large-scale allosteric transitions between the T, R, R' and
R'' states. The corresponding structural rearrangements facilitate substrate protein
capture, refolding, and release. The networks of residues we find provide a micro-
scopic foundation for the cooperativity of the allosteric transitions and a linkage
between substrate protein binding and ATPase activity of GroEL.

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Riina Tehver
University of Maryland

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