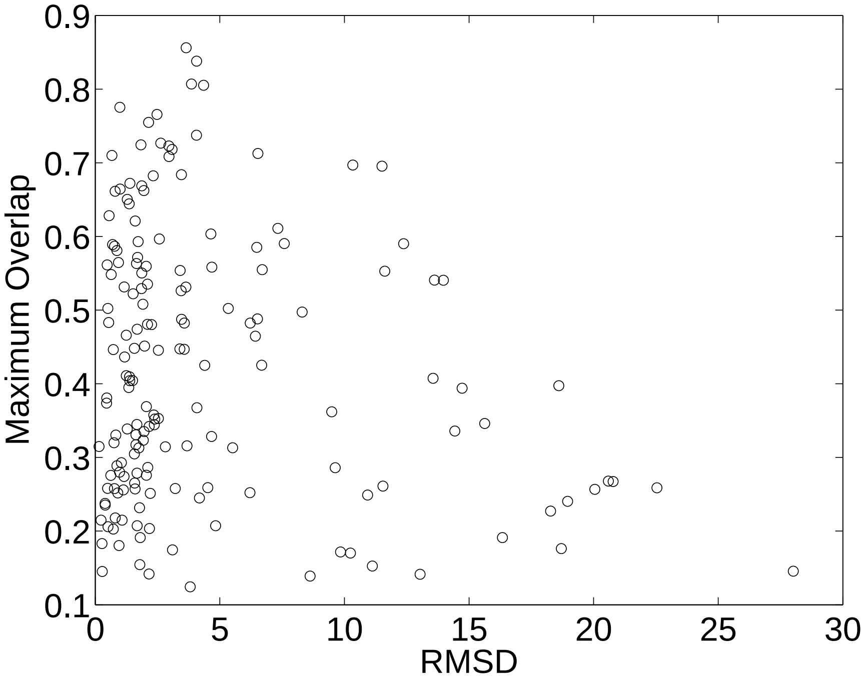
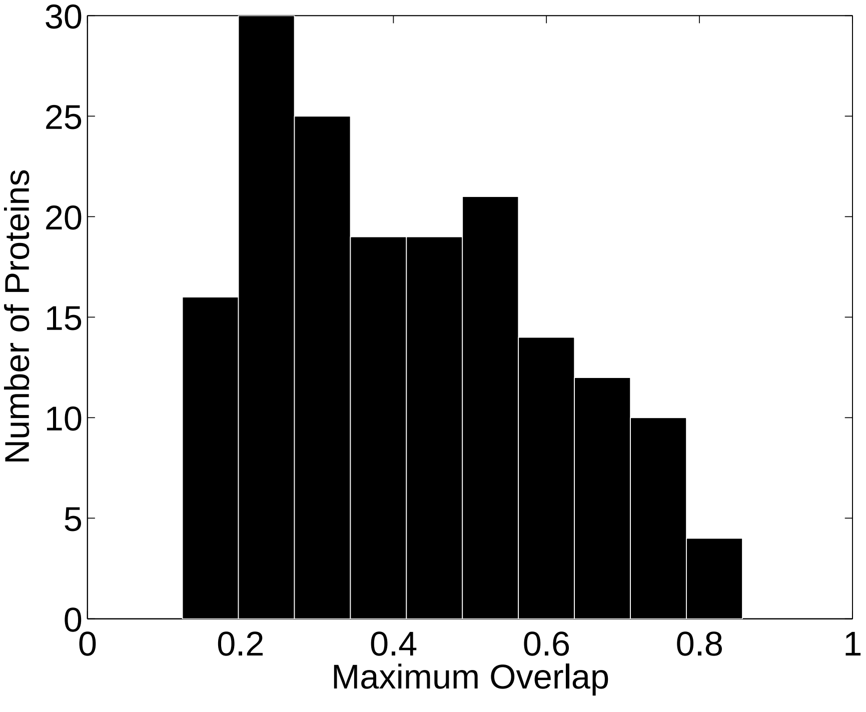
The table & figure numbers correspond to those in the paper except that these results are from the “closed” forms (the modes are calculated from the “closed” structures instead of the “open” structures).

Table 2: ("closed" results) Analyses of the conformational transitions by the motion types. The numbers shown are the mean values over all the structure pairs in each motion type.

Motion Type	**I. Fragments**	**II.A Shear**	**II.B Hinge**	**II. Other**	**III.**
Number of Pairs (170 total)	48	27	59	18	18
Concertedness (κ)	23.9	37.4	**99.7**	51.8	46.0
Reduced DOF $\delta_{reduced}$ ($6/\chi$)	81	107	68	79	113
Old Maximum Overlap	0.31	0.46	**0.51**	0.36	0.41
New Maximum Overlap	0.43	0.56	**0.63**	0.47	0.47
Old CSO(20)	0.27	0.50	**0.60**	0.36	0.43
New CSO(20)	0.53	0.68	**0.77**	0.55	0.62

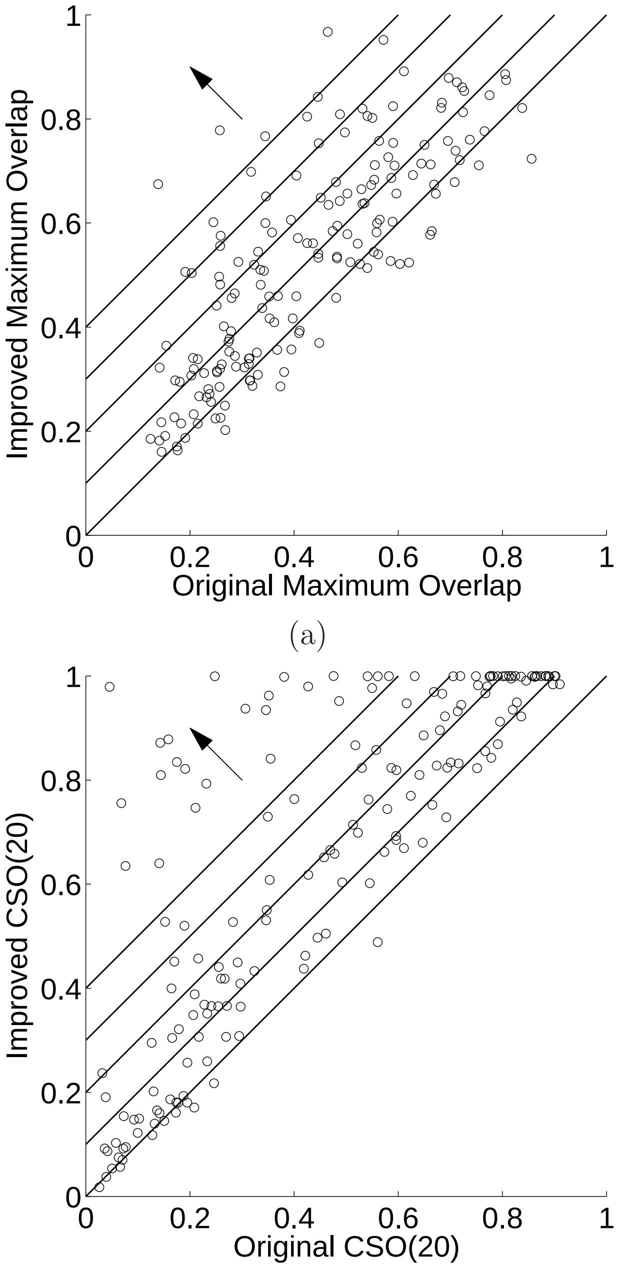


(a)



(b)

Figure 5: ("closed" results) Maximum overlaps using ENM. (a) Maximum overlap as a function of the transition scale, the RMSD between the "open" and "closed" structures. (b) Histogram of maximum overlaps.



(a)

(b)

Figure 6: ("closed" results) Comparison of the new model (domain-ENM) with the old (uniform ENM). (a) Scatter plot of the maximum overlaps. (b) Scatter plot of the CSO(20)s. The lines, along the direction of the arrow, indicate where the increasing scales of improvement are.

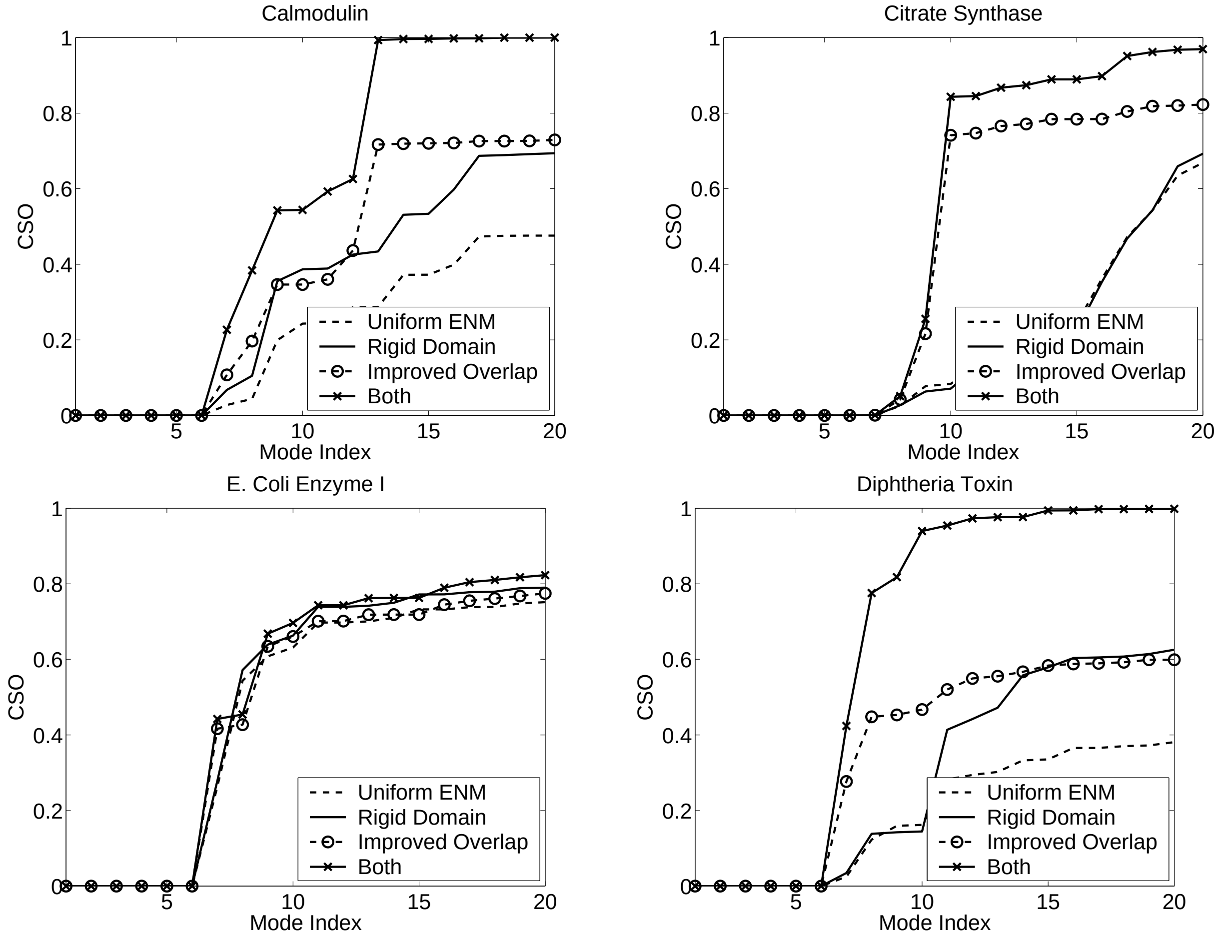
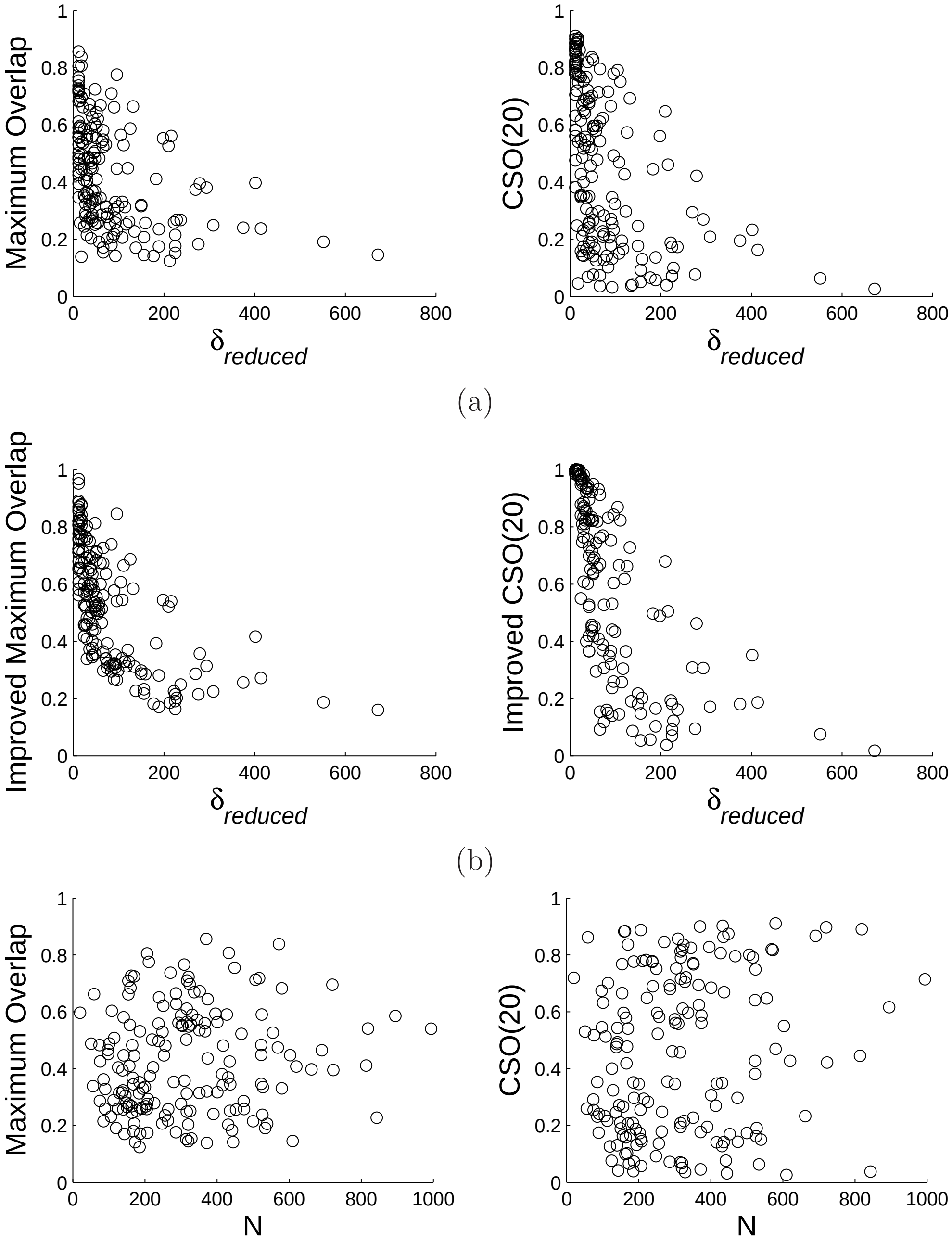


Figure 7: ("closed" results) CSOs (cumulative square overlaps) for some proteins using different models: uniform ENM, ENM with rigid domains, ENM with new overlap definition, and ENM with both rigid domains and new overlap definition (i.e., domain-ENM). The first 6 modes account for the rigid body translation and rotation of the system.



(a)

(b)

(c)

Figure 8: ("closed" results) Relationship between the overlap (maximum overlap or CSO(20)) and $\delta_{reduced}$ (the inverse of collectivity) using the original overlap definition and ENM (a), and the improved overlap definition and domain-ENM (b), and their dependence on protein size N (c). There is a strong correlation between overlap and collectivity (0.41 and 0.47 in (a) and 0.62 and 0.67 in (b), from left to right), while there is almost no correlation between overlap and the protein size (0.11 and 0.15 in (c), from left to right).