Lassila *et al*. 10.1073/pnas.0607691103.

Supporting Information

Files in this Data Supplement:

Supporting Appendix
Supporting Table 3
Supporting Figure 5
Supporting Figure 6

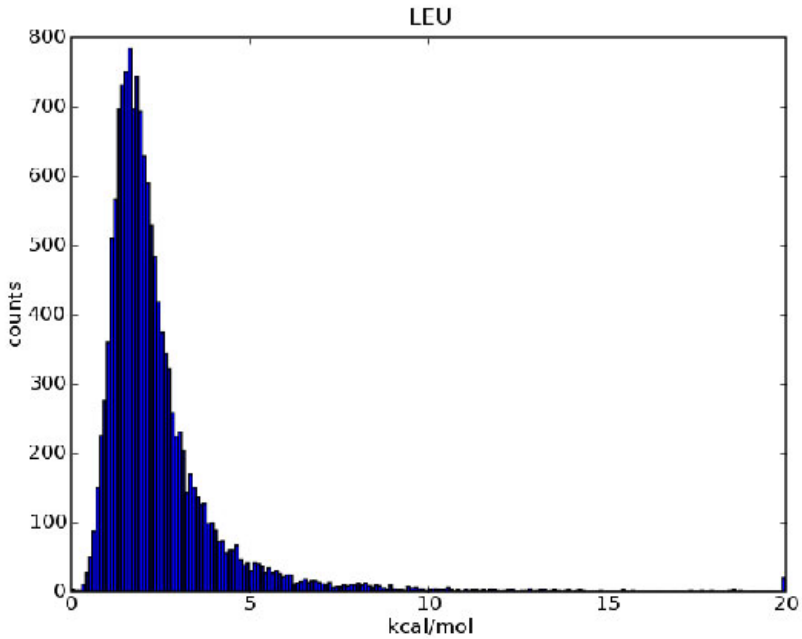

Fig. 5.
Sample histogram for leucine, indicating numbers of conformers in each 0.1 kcal/mol energy bin. A cutoff of 10 kcal/mol was applied to all amino acids, eliminating only the highest-energy outliers.

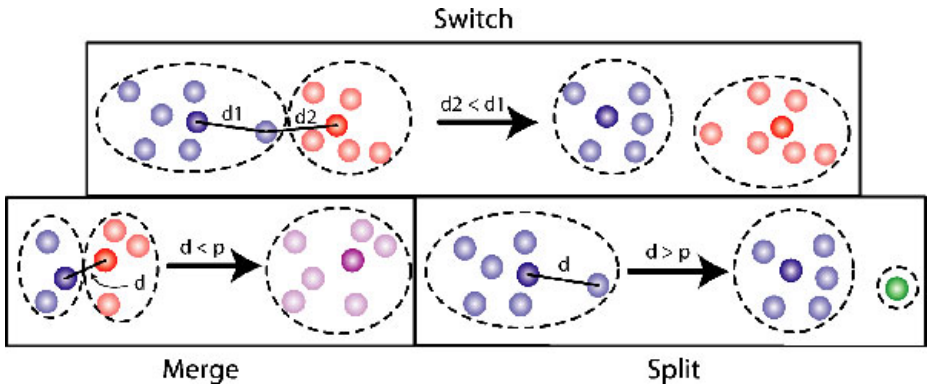

Fig. 6. The three clustering moves are illustrated by showing the state of a sample system before and after the move is performed. Each dot represents a single side-chain conformation taken from the Protein Data Bank (PDB). Distances represent side-chain rmsds between pairs of conformers. Dots sequestered together by a dashed line and colored the same are members of the same cluster. Darker-colored dots denote cluster representatives.

Table 3. rmsd and number of wild-type contacts as a function of rotational and translational step sizes

Chorismate mutase						
Translational step size, Å	**Rotational step size**					**Time (10°, hours)***
	30°	**20°**	**15°**	**10°**	**5°**	
0.6	1.69 ± 1.54 (2.3)	2.61 ± 1.67 (1.3)	0.77 ± 0.10 (4.3)	0.73 ± 0.02 (4.0)	0.61 ± 0.06 (4.7)	3
0.5	0.91 ± 0.20 (3.7)	0.72 ± 0.07 (4.0)	0.83 ± 0.06 (3.3)	0.74 ± 0.05 (4.0)	0.60 ± 0.13 (4.3)	10
0.4	2.02 ± 1.99 (2.3)	0.60 ± 0.04 (4.7)	0.59 ± 0.13 (4.0)	0.57 ± 0.12 (4.3)	0.53 ± 0.13 (4.3)	11
0.3	1.73 ± 1.51 (2.3)	0.61 ± 0.07 (4.3)	0.62 ± 0.15 (4.3)	0.58 ± 0.07 (4.0)	0.65 ± 0.04 (4.0)	12
0.2	1.71 ± 1.53 (2.3)	0.62 ± 0.10 (4.0)	0.60 ± 0.09 (4.0)	0.54 ± 0.07 (4.0)	0.56 ± 0.05 (4.0)	33
Streptavidin-biotin						
Translational step size, Å		**Rotational step size**				**Time (10°, hours)***
	30°	**20°**	**15°**	**10°**	**5°**	
0.6	-	1.16 ± 0.60 (3.7)	1.67 ± 1.02 (3.7)	0.88 ± 0.44 (4.3)	0.84 ± 0.48 (4.3)	5
0.5	2.05 ± 0.59 (1.7)	0.91 ± 0.44 (5.0)	0.84 ± 0.61 (5.0)	0.99 ± 0.91 (3.7)	-	18
0.4	1.32 ± 1.39 (3.7)	0.80 ± 0.09 (5.0)	0.67 ± 0.28 (5.0)	0.96 ± 0.72 (3.7)	-	19
0.3	0.63 ± 0.16 (5.0)	1.08 ± 0.49 (5.0)	0.57 ± 0.21 (5.0)	1.03 ± 0.48 (4.3)	-	18
0.2	0.60 ± 0.32 (5.0)	0.70 ± 0.34 (5.0)	0.80 ± 0.24 (5.0)	-	-	-
Triosephosphate isomerase						
Translational	**Rotational step size**					**Time**
	30°	20°	15°	10°	5°	

						(10°, hours)*	step size, Å
0.6	3.80 ± 2.14 (0.3)	5.22 ± 0.32 (0.0)	1.29 ± 0.91 (1.3)	2.39 ± 2.54 (1.7)	2.40 ± 2.58 (2.0)	0.4	
0.5	3.92 ± 1.94 (0.0)	5.64 ± 0.45 (0.3)	4.47 ± 1.45 (0.0)	1.33 ± 1.01 (1.7)	-	2	
0.4	3.13 ± 1.77 (0.3)	1.96 ± 1.05 (2.0)	0.47 ± 0.24 (1.7)	0.78 ± 0.66 (3.0)	-	2	
0.3	3.44 ± 1.96 (0.3)	0.59 ± 0.18 (2.0)	0.60 ± 0.29 (2.3)	0.46 ± 0.11 (3.0)	-	2	
0.2	2.33 ± 1.80 (0.7)	0.68 ± 0.10 (2.3)	0.49 ± 0.12 (3.0)	0.44 ± 0.11 (3.0)	-	5	

Dashes indicate that required contacts were not satisfied in at least one of three trials or that the calculation was too large to complete. Values are nonhydrogen atom rmsd in Ångstroms relative to crystallographic ligands or bicyclic atom rmsd relative to crystallographic ligand for biotin (i.e., the pentanoic acid moiety was not considered in biotin rmsds). Averages and standard deviations from three random initial positions are reported. Numbers in parentheses are the number of contacts where the amino acid position was the same as in the wild-type structure, averaged over the three trials. Maximum possible number of wild-type contacts: chorismate mutase, five; streptavidin, five; triosephosphate isomerase, three.

*Wall clock time; calculations performed on a 16-processor cluster.