

S6 Table. Ligand binding affinity (kcal / mol) *.

Adenosine	Gs MutY (6u7t)	Marinosulfonomonas MutY	Rhodobacteraceae MutY	Thiotrichaceae MutY	Flavobacteriaceae MutY
Mode 1	-7.3	-6.8	-6.8	-7.0	-7.2
Mode 2	-6.9	-6.3	-6.5	-6.9	-7.1
Mode 3	-6.8	-6.2	-6.3	-6.3	-7.0
Mode 4	-6.7	-6.2	-6.3	-6.3	-6.9
Mode 5	-6.7	-6.2	-6.1	-6.3	-6.8
Mode 6	-6.7	-6.0	-6.0	-6.3	-6.6
Mode 7	-6.6	-5.9	-6.0	-6.2	6.5
Mode 8	-6.5	-5.8	-6.0	-6.2	-6.4
Mode 9	-6.5	-5.7	-5.8	-6.1	-6.3

OG	Gs MutY (6u7t)	Marinosulfonomonas MutY	Rhodobacteraceae MutY	Thiotrichaceae MutY	Flavobacteriaceae MutY
Mode 1	-7.7	-7.5	-7.7	-8.0	-8.0
Mode 2	-6.9	-6.8	-7.6	-7.5	-7.5
Mode 3	-6.9	-6.8	-7.5	-7.3	-7.4
Mode 4	-6.8	-6.8	-7.3	-7.0	-7.3
Mode 5	-6.7	-6.7	-7.1	-7.0	-7.2
Mode 6	-6.6	-6.7	-7.1	-6.8	-7.2
Mode 7	-6.5	-6.4	-7.1	-6.8	-7.2
Mode 8	-6.5	-6.2	-7.0	-6.6	-7.1
Mode 9	-6.3	-6.2	-6.9	-6.6	-7.0

* Binding affinities are reported for the binding modes generated by *AutoDock VINA*. Each mode represents a predicted ligand pose, which differs by a combination of position, orientation, and rotamer conformation. The receptor structure was obtained from PDB ID 6u7t for *Gs MutY* and through structure prediction for the LCHF *Marinosulfonomonas MutY*, *Rhodobacteraceae MutY*, *Thiotrichaceae MutY*, and *Flavobacteriaceae MutY*. The binding mode representing the starting complex for molecular dynamics analysis is highlighted.