

Figure S1. The radius of one molecule of (a) ethylbenzene, (b) toluene, (c) 1,3-dibutadiene, and (d) trichloroethylene.

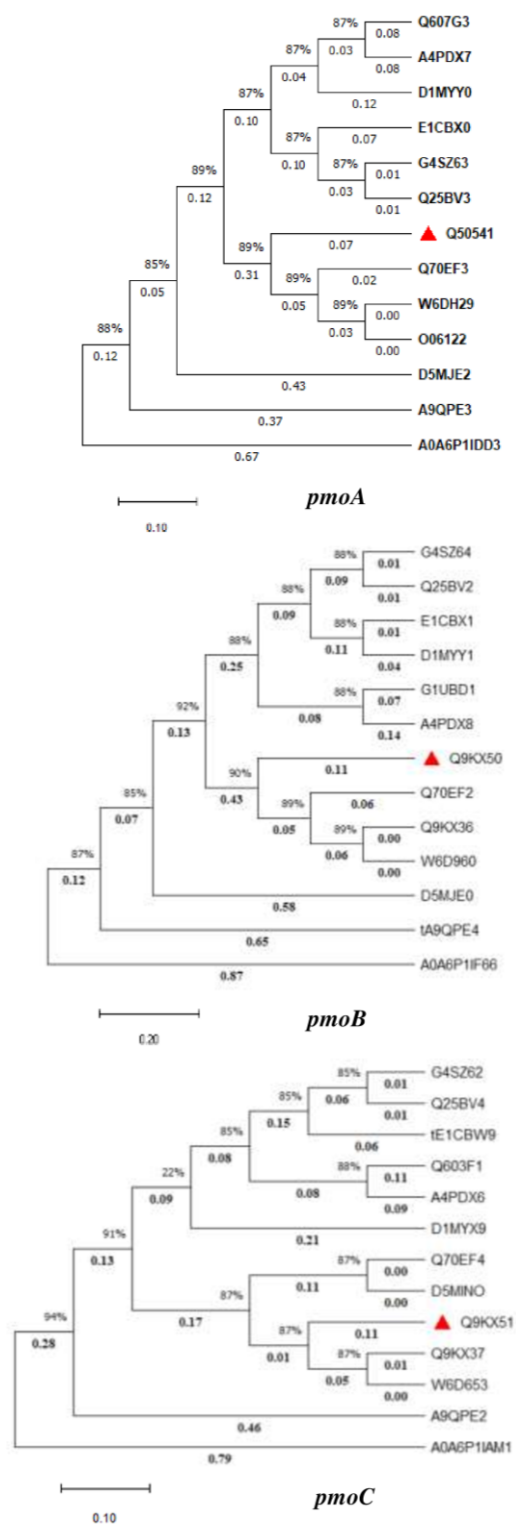


Figure S2. Phylogenetic dendrograms between the 13 methanotrophs, each for *pmoA*, *pmoB*, and *pmoC*, individually.

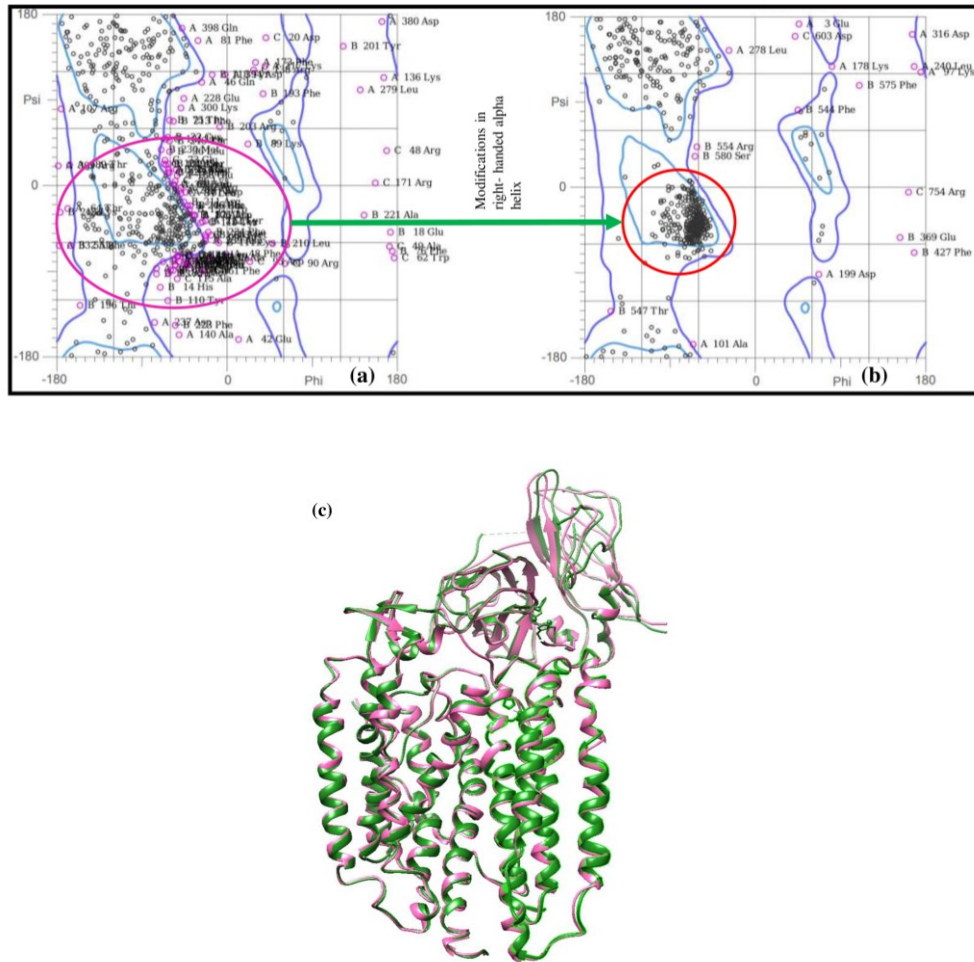


Figure S3. Ramachandran plots showing the stereochemical features of (a) the template structure and (b) the modeled structure. The magenta color circle represents the poor geometry of the right-handed alpha helix within the template (3CHX) and the red color circle represents the improved geometry of the region within the modeled structure, and (c) the superimposition of the template and the modeled structure. The template and the modeled structure are shown in pink and green,

respectively.

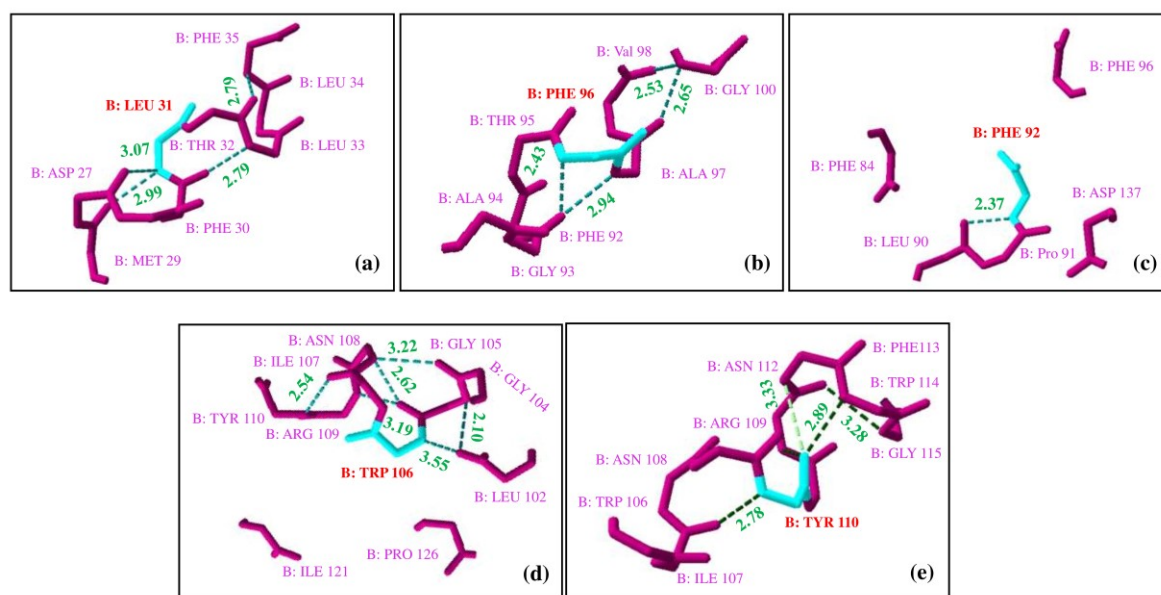


Figure S4. Hydrogen bond interactions of the wild-type residues (a) B:Leu31, (b) B:Phe96, (c) B:Phe92, (d) B:Trp106, and (e) B:Tyr110 with their neighbor residues. The wild-type residues are marked in sky-blue color, the neighbor residues are marked in red color, and the hydrogen bonds are shown in green color.

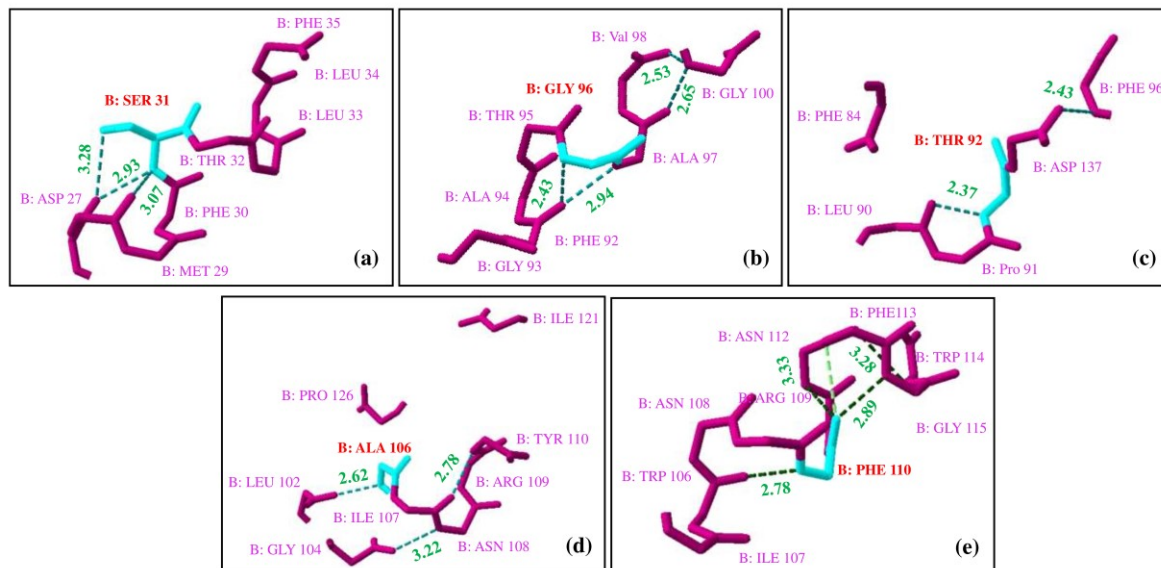


Figure S5. Hydrogen bond interactions of the mutants (a) B:Leu31Ser, (b) B:Phe96Gly, (c) B:Phe92Thr, (d) B:Trp106Ala, and (e) B:Tyr110Phe, with their neighbor residues. The mutant residues are marked in sky-blue, the neighbor residues are marked in red, and the hydrogen bonds are shown in green.