Supporting Information

Impact of Phenylalanines Outside the Dimer Interface on Phosphotriesterase Stability and Function

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Figure S1: Over-expression gels of PTE and variants where (-) and (+) represent pre- and post-induction, respectively.



Figure S2: Purified protein gels of PTE and variants.

protein	expected molecular weight	observed molecular weight	
PTE	37779.10	37822.61	
F51L	37745.08	37706.46	
F150M	37763.11	37762.22	
F216L	37745.08	37719.88	
F304L	37745.08	37727.80	
F306L	37745.08	37721.46	
F327L	37745.08	37690.66	
F335M	37763.11	37791.71	
F357L	37745.08	37807.90	

Table S1: MALDI-TOF comparisons of PTE and variants.

Expected molecular weights were calculated in ExPASy



Figure S3: Lineweaver-Burk plots of PTE and variants kinetic assays.



Figure S4: ROSETTA score distributions for PTE and mutant conformational ensembles. (A) Ensembles with no substrate bound. (B) Ensembles with paraoxon bound to the active site of both chains. Each ensemble consists of 2000 structures per mutant generated with ROSETTA relax. Scores are given in ROSETTA Energy Units (REU).

Table S3: Hydrophobic solvent accessible surface areas (SASA) computed for mutant ensembles and their changes from PTE. Included are SASAs for individual residues that strongly contribute to the total SASA score $|\Delta WT| > 8 \text{ Å}^2$

Mutant	$\begin{array}{c} \text{Mean} \\ \text{SASA} \ (\text{\AA}^2) \end{array}$	Δ SASA (Å ²)	residue	SASA contribution
PTE	3915.1	0.0		
F51L	3890.0	-25.0	L51	-15.3
F150M	3927.1	12.0	F179	23.9
F216L	3918.5	3.4		
F304L	3957.9	42.8	A78	-9.0
			G86	10.6
			L304	24.5
			M325	8.4
F306L	3886.5	-28.6	W131	-13.4
			I274	-9.4
			L306	-13.5
F327L	3915.8	0.7	M314	-8.6
F335M	3913.1	-2.0	W277	9.8
			V320	-12.5
			M335	14.0
F357L	3902.1	-12.9		