*Supplementary file 3 for Kaltenbach at al., Reverse evolution leads to genotypic incompatibility despite functional and active-site convergence*

**Crystallographic information**

**Supplementary File 3A.** Data collection and refinement statistics for structures reported in this work.



[a]Values in parenthesis are for the highest-resolution shell.

[b[*R*merge(I) = (Σ*hkl* Σ*j* |*Ihkl,j -* 〈*Ihkl*〉|)/(Σ*hkl* Σ*j Ihkl,j*)where 〈*Ihkl*〉 is the average intensity of *j* symmetry-related observations of reflections with Miller indices *hkl*.

[c] CC1/2 = percentage of correlation between intensities from random half-datasets.

[d]*R*work = Σ*hkl*|F(obs)-F(calc)|/Σ*hkl*|F(obs)|; 5% of the data that were excluded from the refinement were used to calculate *R*free.