separate non-bonded groups using only X-ray terms in the target function. SigmaA-weighted electron-density maps[30] and the program EDEN[26] were used to check and to eliminate model bias. In the EDEN runs, the haem and its ligands were removed from the protein model and EDEN was used with a gentle solvent target to recover these missing molecules completely. In all cases shown here, the haem and its bound ligands were recovered and the electron density was at least as clear as in the starting maps, indicating that refinement proceeded without model bias. In order to perform further tests, the EDEN solution was perturbed by independently changing amplitudes and phases in the file of the calculated structure factor amplitudes (F_{calc}), using a 30% random gaussian perturbation; the resulting perturbed F_{calc} file served as the starting model for another EDEN run. The perturbation/recovery steps were repeated 10 times and the resulting 10 maps were then averaged. These maps showed excellent agreements with the starting maps. Occupancy of the ligands were refined in SHELXL (http://shelx.uni-ac.gwdg.de/SHELX).

Models were inspected with O (http://xray.bmc.uu.se/alwyn) and figures were rendered by POV-Ray (http://www.povray.org), using the Molray interface at http://xray.bmc.uu.se/markh.

Coordinates and structure factors have been deposited in the Protein Data Bank (accession codes 1h5m, 1h5d, 1h5e, 1h5f, 1h5g, 1h5h, 1h5i, 1h5j, 1h5k, 1h5l, for the structures in Table 1 of the Supplementary Information and 1h58, 1h5a, 1h57, 1h5c, 1hch and 1h55 for the structures in Table 2 of the Supplementary Information).

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Competing interests statement

The authors declare that they have no competing financial interests.

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retraction

Directed evolution of new catalytic activity using the α/β-barrel scaffold

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This laboratory reported the *in vitro* evolution of an enzyme with phosphoribosyl anthranilate isomerase activity (ivePRAI) from the α/β-barrel scaffold of indole-3-glycerol-phosphate synthase using a combination of rationally designed libraries, DNA shuffling, and selection with *Escherichia coli*, JA300, a strain that lacks an active PRAI gene. As part of the ongoing project to characterize the structure and properties of ivePRAI, we discovered that the protein expressed from a variety of vectors that contained a synthetic gene corresponding to the sequence of ivePRAI as published is insoluble and does not complement JA300 (R. L. Weinberg, C. M. Blair and A.R.F., unpublished results), as reported. We conclude that the results are unsound.

It appears that the discrepancy in the results is due to a combination of two episodes of cross-contamination. We are now repeating the directed evolution of ivePRAI using modified procedures to test the design strategy that should eliminate the source of errors of contamination.

The first author of this Article (M.M.A.), who was responsible for most of the analysis and design strategy involving loop transfer and most of the experimental work, wishes to be dissociated from this retraction because she believes that the experimental data are fundamentally sound. □