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Supporting information for article:

The 1.1 Å resolution structure of a periplasmic phosphate-binding protein from Stenotrophomonas maltophilia: a crystallization contaminant identified by molecular replacement using the entire protein database

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Fig. S1. A photomicrograph of the largest phosphate-binding protein crystal which was approximately 0.3 mm in length.

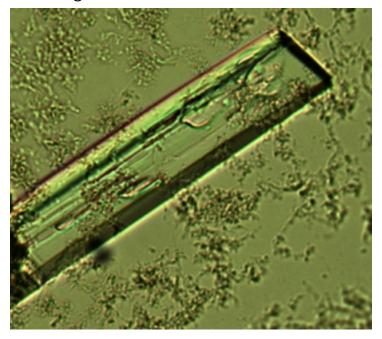


Fig. S2. Part of one of the diffraction images obtained at ESRF with circles corresponding to two resolution limits in Å shown.

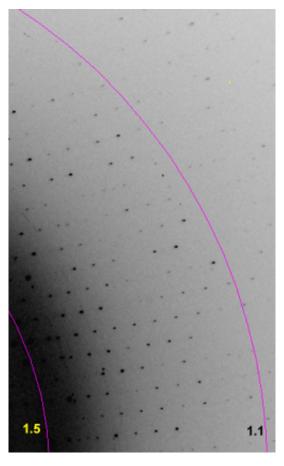


Fig. S3. A region from the centre of the first diffraction image of the high resolution pass is shown using the threshold map function in *dials.image_viewer*. Top panel: default spot-finding parameters led to noise around the backstop and between detector modules that may contaminate the strong spot list. Lower panel: modified parameters (see main text) produce a cleaner threshold map for spot-finding.

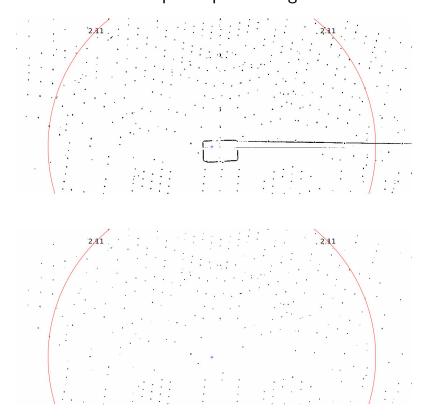


Fig. S4. A sample of the map obtained after molecular replacement with the *P. fluorescens* phosphate binding protein. Blue contours indicate the 2Fo-Fc map while green and red contours indicate the positive and negative Fo-Fc difference density.

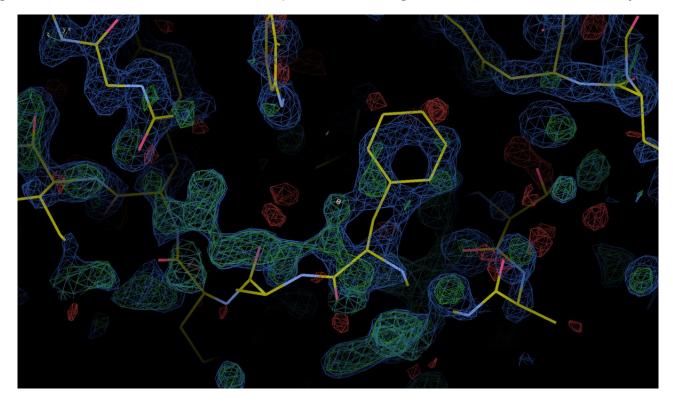
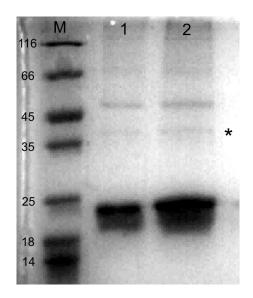


Fig. S5. A reducing SDS-PAGE gel showing the presence of a faint band at the molecular weight expected for the phosphate binding protein (38 kDa) shown by an asterisk. The dominant band at around 20 kDa is due to the dioxygenase which we intended to crystallise. The lane labelled M corresponds to the standards with molecular masses shown in kilo-Daltons and the protein was loaded into lanes 1 and 2 (two aliquots were loaded in the latter).



Note that in a more heavily over-loaded gel that was used for LC-MS analysis, an additional band at 36 kDa was also visible.

Table S1. Identification of proteins present in gel pieces close to the expected molecular weight of the phosphate binding protein (36 and 38 kDa). The Mascot score is a measure of the probability that the protein has been correctly identified.

36 kDa band

Uniprot identifier	Mascot score	Origin
RSGA_ECOBW	2908	E. coli putative ribosome biogenesis GTPase RsgA
LDHD_ECOLI	2769	E. coli D-lactate dehydrogenase ldhA
NDPA_ECOBW	1221	E. coli nucleoid-associated protein YejK

38 kDa band

Uniprot identifier	Mascot score	Origin
DHAK_ECOLI	8883	E. coli PEP-dependent dihydroxyacetone kinase DhaK
GSA_ECOBW	2126	E. coli glutamate-1-semialdehyde 2,1-aminomutase
EFTU_SALAR	1091	Salmonella arizonae elongation factor Tu