Supplementary Material

Crystallization and preliminary crystal structure analysis of the ligand-binding domain of PqsR (MvfR), the *Pseudomonas* Quinolone Signal (PQS) responsive quorum sensing transcription factor of *Pseudomonas aeruginosa*

Ningna Xu\textsuperscript{ab}, Shen Yu\textsuperscript{bc}, Sébastien Moniot\textsuperscript{a}, Michael Weyand\textsuperscript{a} and Wulf Blankenfeldt\textsuperscript{ab}\textsuperscript{*}

\textsuperscript{a}Lehrstuhl für Biochemie, Universität Bayreuth, Universitätsstraße 30, Bayreuth, 95447, Germany, \textsuperscript{b}previous address: Physikalische Biochemie, Max-Planck-Institut für Molekulare Physiologie, Otto-Hahn-Straße 11, Dortmund, 44227, Germany, and \textsuperscript{c}Department of Molecular Biology, Massachusetts General Hospital, Boston, MA 02114, USA

Correspondence email: wulf.blankenfeldt@uni-bayreuth.de
Fig. S1. Analytical size-exclusion chromatography of purified PqsR_91-319 (red). A gel filtration standard is shown for comparison (black); numbers refer to molecular weight in kDa. The column was a Superdex 75 10/300 GL from GE Healthcare, developed at 0.2 ml/min in 20 mM TRIS-HCl pH 8, 150 mM NaCl, 10% (v/v) glycerol, 1 mM TCEP. The expected molecular weight of a homodimer of PqsR_91-319 is 51 kDa.
Fig. S2. Effect of annealing by blocking the cryostream three times for six seconds. A diffraction image from approx. the same orientation is shown. Note that the spots seem less split and the diffraction pattern appears less diffuse. The procedure was only effective for the worst crystals and was not used for the data sets reported in Table 1.
Fig. S3. \( \kappa = 180^\circ \) section of a self-rotation function of the native data set (Tab. 1, column 2). Reflections to 4 Å resolution were included and an integration radius of 45 Å was used. The calculation was performed with MOLREP (Vagin & Teplyakov, 2010).