STRUCTURAL BIOLOGY COMMUNICATIONS

Volume 76 (2020)

Supporting information for article:

Detecting the nature and solving the crystal structure of a contaminant protein from an opportunistic pathogen

Riccardo Pederzoli, Delia Tarantino, Louise J. Gourlay, Antonio Chaves-Sanjuan and Martino Bolognesi

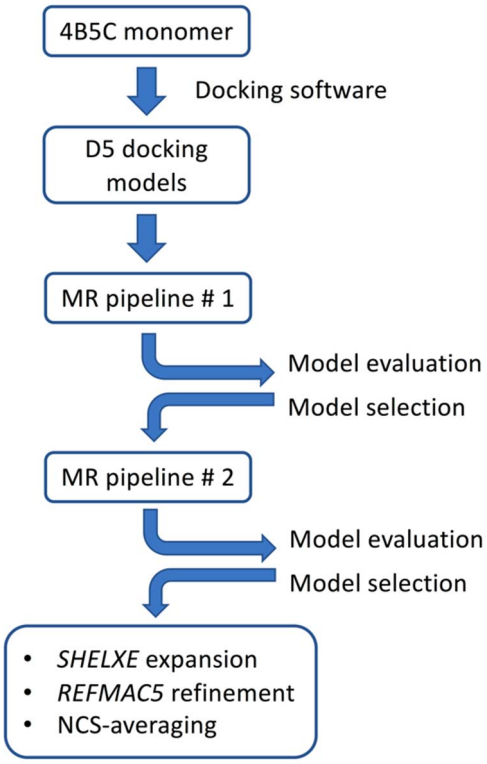

Figure S1 Work-flow used to generate the D5 docking models and to test them in Molecular Replacement. In the first step of the pipeline, several docking packages are used to generate a number of assemblies with the desired D5 symmetry starting from chain A of BPSL2765 (PDB 4B5C). The D5 assemblies are used as search-models in the first MR pipeline, which uses *PHASER* and *MolRep* with default settings. The solutions are filtered based on standard indicators and only the most promising are retained and used in a second MR-search. For this, a more sophisticated search is performed using again *PHASER* and *MolRep*, but varying some of the critical parameters that are known to be important for MR. The solutions are again filtered and only the most promising are subjected to additional verification through *REFMAC5* restrained refinement, *SHELXE* expansion and/or NCS-averaging. See the main text for details.