Signal Peptide

CPase domain

C-terminal domain

Amphipilic helix

PBP6b ....MKR**RL**IIAAS**L**FVFNLS**S**GFA..AENIPFS**P**QP**PE**I**H**A**G**SWVL**M**DY**TTG**Q**IL** *29*
PBP5 MNTIFSARIMKR**RL**ALTTAL**L**CTAFI**S**AAHA**DD**LNIKTMI**P**GV**PQ**I**D**A**ES**YIL**IDY**NS**G**KV**L** *31*

PBP6b TAG**N**EHQQ**R**N**PA**S**LTK**LMTGYVVDRA**I**DSHRITPDD**I**V**T**VGR**DAWA**K**D**NPVF**VGSSLMFL** *89*
PBP5 AEQ**N**ADVR**R**D**PA**S**LTK**MMTSYVIGQA**M**KAGKFKET**D**L**VT**IGN**DAWA**T**G**NPVF**KGSSLMFL** *91*

PBP6b **K**EG**D**RV**S**V**R**D**L**SRG**LIVD**SGN**DACVAL**AD**YIAG**GQR**QFVEM**MN**N**Y**AEK**L**H**LK**D**THFE**T**VH** *149*
PBP5 **K**PG**M**QV**P**V**S**Q**L**IRG**INLQ**SGN**DACVAM**AD**FAAG**SQD**AFVGLM**NS**Y**VNAL**G**L**KN**T**HFQ**T**VH** *151*

PBP6b **GLDA**P**GQ**H**SSA**Y**D**LAVLSRA**I**HGE**P**E**F**Y**HM**Y**S**EK**S**L**T**WNGITQ**Q**NRNGLLWD**KTM**NVDG** *209*
PBP5 **GLDA**D**GQ**Y**SSA**R**D**MALIGQA**L**IRDVP**N**E**Y**S**IY**K**EK**E**F**T**FNGIR**Q**L**NRNGLLWD**NSL**NVDG** *211*

PBP6b **L**KTGH**TSGAG**F**N**L**IASAVDGQ**R**R**L**I**AVVMGADSA**KGREE**EARKLL**RWG**Q**QN**F**T**TVQ**IL**HR** *269*
PBP5 **I**KTGH**TDKAG**Y**N**L**VASATEGQM**R**L**I**SAVMGGRTF**KGREA**ESKKLL**TWG**F**RFF**E**T**VNP**L**KV** *271*

PBP6b **GK**KVGTERIWY**GD**KENID**LG**TEQEFWMVL**P**KAEIPHI**KAK**Y**TL**DGK**EL**T**AP**ISAHQ**RVG**E** *329*
PBP5 **GK**EFASEPVWF**GD**SDRAS**LG**VDKDVYLTIP**R**GRMKDL**KAS**Y**VL**NSS**EL**H**AP**LQKNQ**VVG**T** *331*

PBP6b **I**ELYDRD**K**QVAHW**PLV**T**L**ESVG**EG**SM**F**SRLS**DY**FHHKA..... *367*
PBP5 **I**NFQLDG**K**TIEQR**PLV**VL**QEIP**EG**NF**F**GKII**DY**IKLMFHHWFG *374*

Figure S6. Sequence alignment of full-length PBP6b with PBP5 (UniProt codes: P33013 and P0AEB2, respectively). Domains are shown as coloured bars: CPase domain in green and the C-terminal domain in dark blue. Active site sequences motifs essential for catalysis are highlighted in green. Secondary structure based on the solved crystal structure of PBP6b is depicted above the corresponding residues as blue arrows (beta-sheets) and pink cylinders (alpha-helices). The C-terminal amphiphilic helix is shown in orange. Sequence alignment was generated and annotated using Clustal Omega [Sievers *et al*. (2011) Mol Sys Biol **7**: 539] and Aline [Bond and Schüttelkopf (2009) Acta Cryst **D65**: 510-512], respectively.