

## Supplementary Material

### ***In silico* Analysis of FtsZ Crystal Structures Towards a New Target for Antibiotics**

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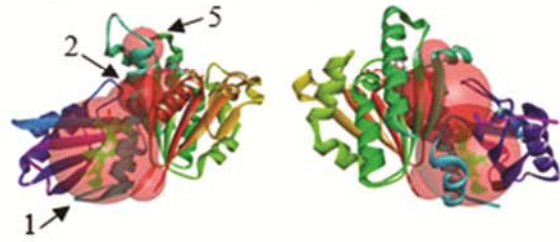
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<i>Helicobacter pylori</i>	RAEGLKELEQSSDSILVLPNDKILLT	MKKNASTTECYREVDDVLVRAVSGISTIITKPG	222
<i>Rickettsia typhi</i>	TADKGLIELQQFVDTLIVIPNQLFRJ	JANEQTTFADAFKMADDVLHAGVVRGVDLMIMPG	208
<i>Acinetobacter baumannii</i>	SAERGIEALEAHVDSLIIIPNQRLLSVYG-	DISMKDAYKKADDVLLNAVRSIFDLVVNRG	210
<i>Neisseria meningitidis</i>	VAQAGLEQLKEHVDSLIIIPNDKLMATA	LGEDVTMREAFRAADNVLRDAVAGISEVVTCPG	207
<i>Haemophilus influenzae</i>	FAELGIKDLQYVDSMIIIPNQIQKVL	PKNAKLIDAFAAAANDVLRNSVMGISMITSFG	229
<i>Pseudomonas aeruginosa</i>	IADEGIRALAESVDSLITIPNEKLLT	ILGKDASLLAAFAKADDVLAGAVRGISDIKRP	205
<i>Vibrio cholerae</i>	FAEQGIEELSKHVDSLITIPNEKLLKV	LGRGITLLEAFASANNVLKNAVQGGIAELITRPG	205
<i>Escherichia coli</i>	FAEQGITELSKHVDSLITIPNDKLLKV	LGRGISLLDAFGAANDVLKGAQQGIAELITRPG	204
<i>Shigella flexneri</i>	FAEQGITELSKHVDSLITIPNDKLLKV	LGRGISLLDAFGAANDVLKGAQQGIAELITRPG	204
<i>Salmonella enterica</i>	FAEQGITELSKHVDSLITIPNDKLLKV	LGRGISLLDAFGAANDVLKGAQQGIAELITRPG	204
<i>Yersinia pestis</i>	FAEQGIAELSKHVDSLITIPNDKLLKV	LGRGISLLDAFGAANDVLKGAQQGIAELITRPG	204
<i>Campylobacter jejuni</i>	LAESGELLEKESDSILVIQNEKLLSI	IDKKAGIKDAFRLVDDILARAVKGMVSILLDNG	208
<i>Thermotoga maritima</i>	KAIEGLKLRKHVDTLIKISNNKLMEE	LPRDVKIKDAFLKADETLHQGVKGISLITKRG	215
<i>Leptospira interrogans</i>	FARKGIEQLRSHVDTLILINNSIFRV	VDKNTFIDLAFQVIDDILLNAVRSIDIIINPG	206
<i>Mycobacterium tuberculosis</i>	QAENGIAALRESCDTLIVIPNDRLLQM	GDAAVSLMDAFRSADEVLLNGVQGITDLITTPG	202
<i>Streptococcus pneumoniae</i>	FAVEGINQLREHVDTLLIISNNNLEI	VDKKTPLLEALSEADNVLRQGVQGITDLITNPG	206
<i>Clostridium botulinum</i>	HAEMGINTLKERVDTLVTPNERLLSI	VDKKTSLMDSFKLADDVLRQGVQGISDLITIPG	205
<i>Staphylococcus aureus</i>	QAAGVEAMKAAVDTLIVIPNDRLLDI	VDKSTPMMEAFKEADNVLRQGVQGISDLIAVSG	205
<i>Listeria monocytogenes</i>	QALTGTEAMKEAVDTLIVIPNDRLLQI	VDKNTFMLLEAFREADNVLRQGVQGISDLIAVPG	205
<i>Bacillus anthracis</i>	QAASGIAAFKENVDTLIVIPNDRLLDI	VDKNTFMLLEAFREADNVLRQGVQGISDLIATPG	205
<i>Bacillus subtilis</i>	QAAGGISAMKEAVDTLIVIPNDRILEI	VDKNTFMLLEAFREADNVLRQGVQGISDLIATPG	205

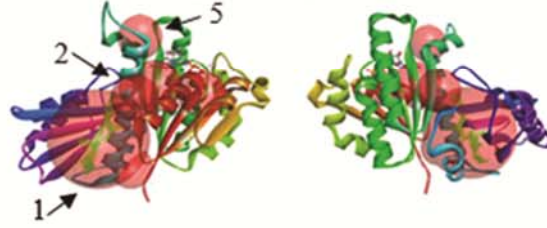
**Figure S1: Amino acid sequence alignment of the T6-loop from multiple bacterial species using Clustal Omega.** The T6-loop region (red box) consensus sequence was seen to be conserved within the Gram-negative  $\gamma$ -proteobacteria (pink) and Gram-positive firmicutes (cyan). The Gram-negative *Leptospira interrogans* has the same consensus sequence as the firmicutes. DS 4.5 identified the T6-loop as a possible binding site in all analysed FtsZ structures except in *B. subtilis* and *P. aeruginosa* FtsZ, suggesting the potential of this site as a target for broad-spectrum antibiotics.

## Staphylococcal FtsZ

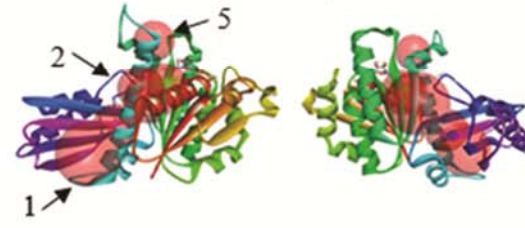
*S. epidermidis* (4M8I)



*S. aureus* (3VOA)

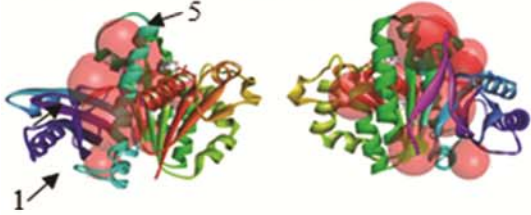


*S. aureus* (3VO8)

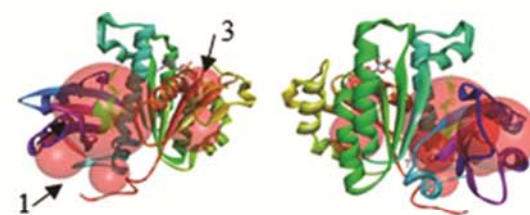


## Non-Staphylococcal FtsZ

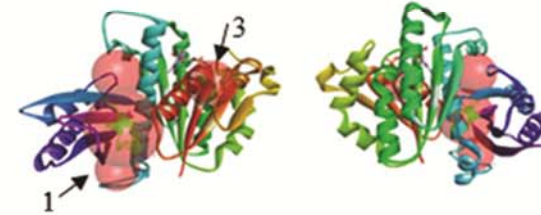
*A. aeolicus* (2R6R)



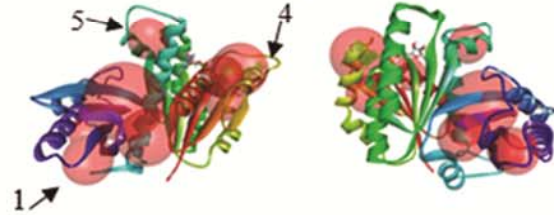
*P. aeruginosa* (2VAW)



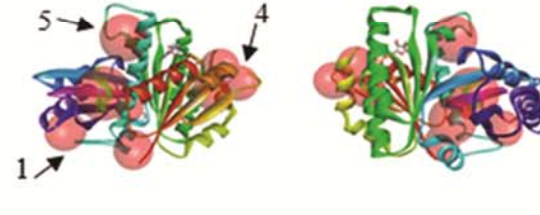
*B. subtilis* (2RHL)



*M. tuberculosis* (4KWE)



*M. tuberculosis* (1RQ7)



**Figure S2: Comparison of the accessible binding sites of various GDP-bound FtsZ structures.** The available binding sites as identified by Discovery Studio 4.5 are shown as red spheres. The locations of the spheres cover similar areas of the protein, but their sizes differ between the different FtsZ structures, especially in the area of the interdomain cleft (arrow 1). GDP was kept in the NBD; hence no sphere is shown in its binding pocket. See text for explanation of arrows 2-6.