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Supporting information for article:

Crystallographic and kinetic study of riboflavin synthase from *Brucella abortus*, a chemotherapeutic target with an enhanced intrinsic flexibility

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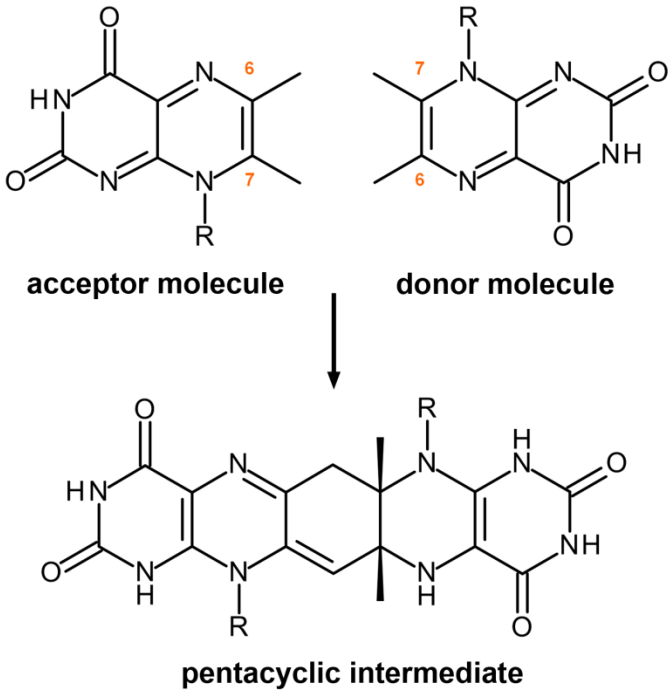

Figure S1 Proposed relative orientation of the 6- and 7-methyl groups from both substrate molecules, giving rise to a pentacyclic intermediate after an initial hydride transfer step.

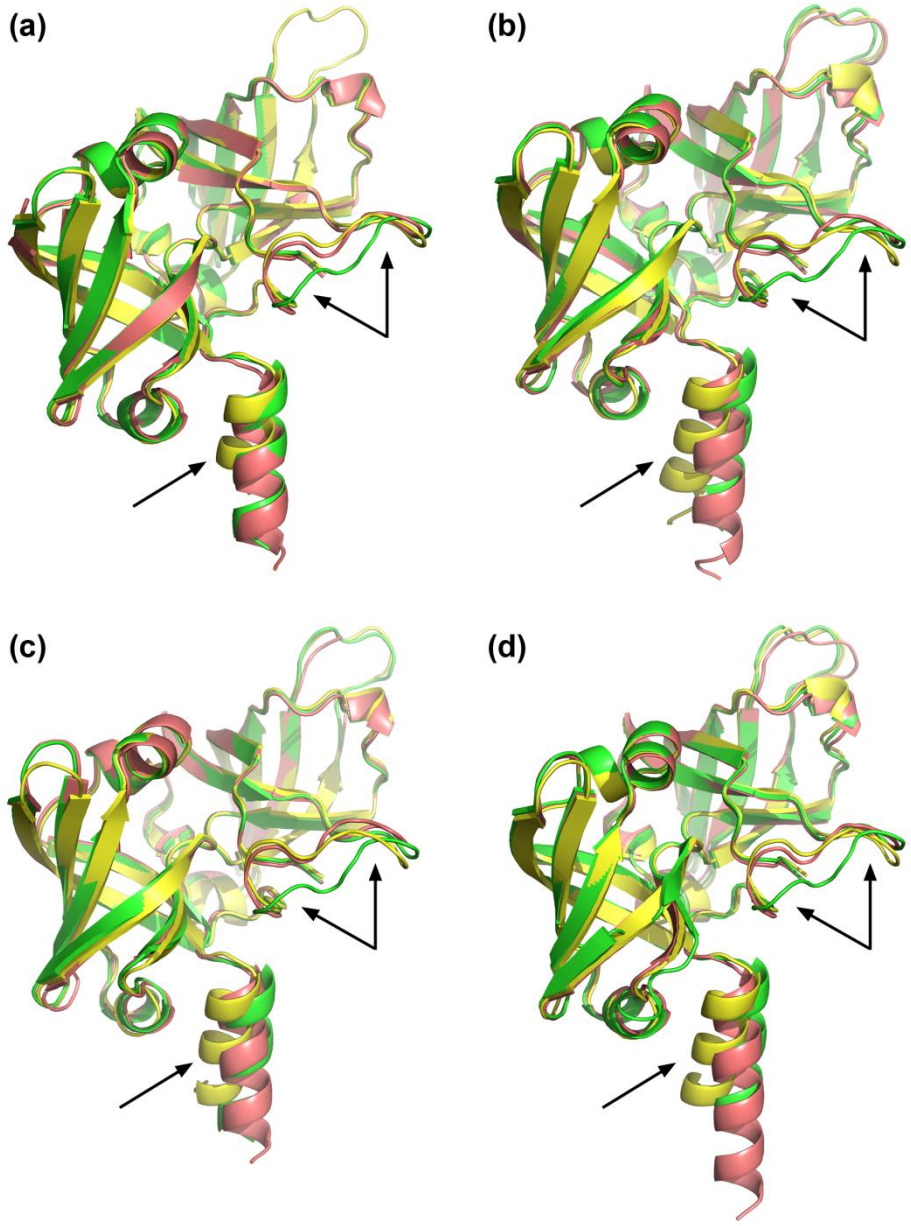

Figure S2 Superposition of the monomers A (green), B (pink) and C (yellow) in the four structures solved in this work. Single arrows point at the deviated C-terminal α-helices from chain C. Double arrows identify the residue range 96-101A in each case. Ligands were omitted for clarity. (a) RS-APO. (b) RS-RBF. (c) RS-ROS. (d) RS-NRP.

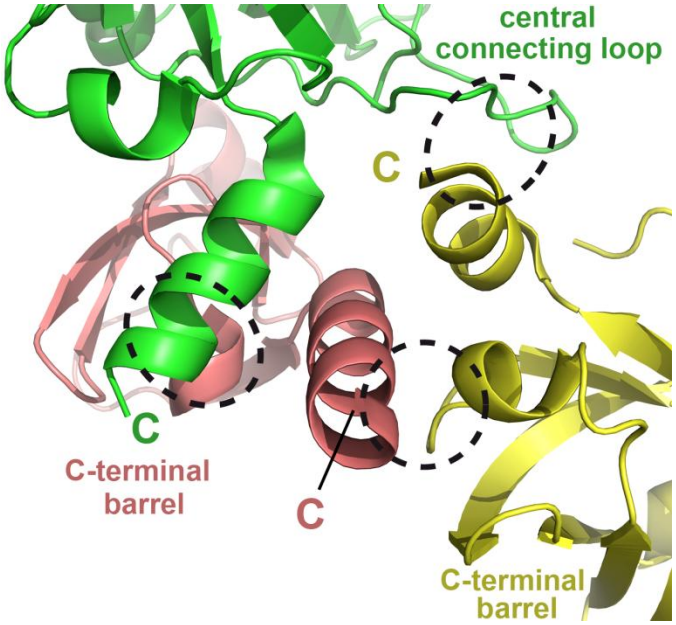

Figure S3 Interactions between the three-helix bundle and other structural elements in the RS trimer. Monomers are depicted in green (chain A), pink (chain B), and yellow (chain C). The interacting regions are highlighted with black dashed ovals (see text for details), and the C-termini are indicated for each chain. The figure is drawn in an opposite orientation with respect to Figure 2a for clarity

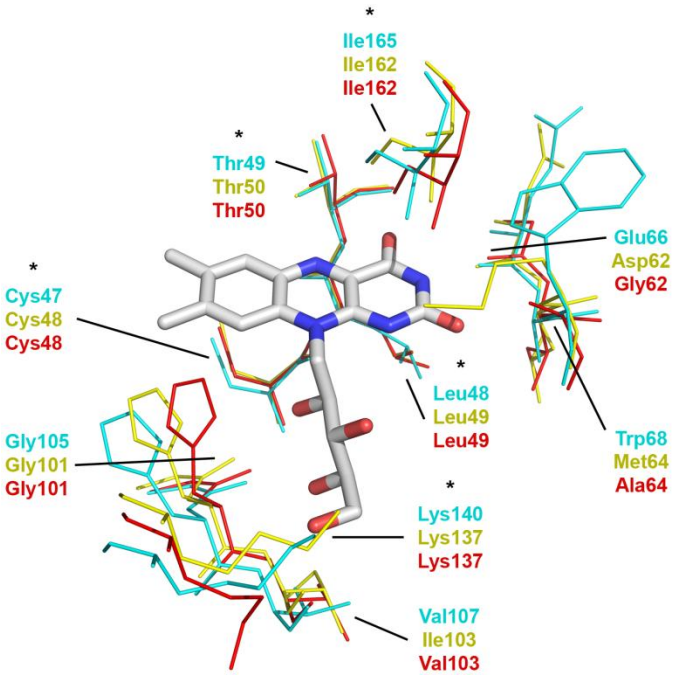

Figure S4 Superposition of the most relevant residues involved in riboflavin binding in RS from *B. abortus* (blue, this work), *E. coli* (yellow) (Liao *et al.*, 2001), and *S. pombe* (red) (Gerhardt, Schott, *et al.*, 2002). Residue triplets that contact riboflavin with their side chains are marked with a star.

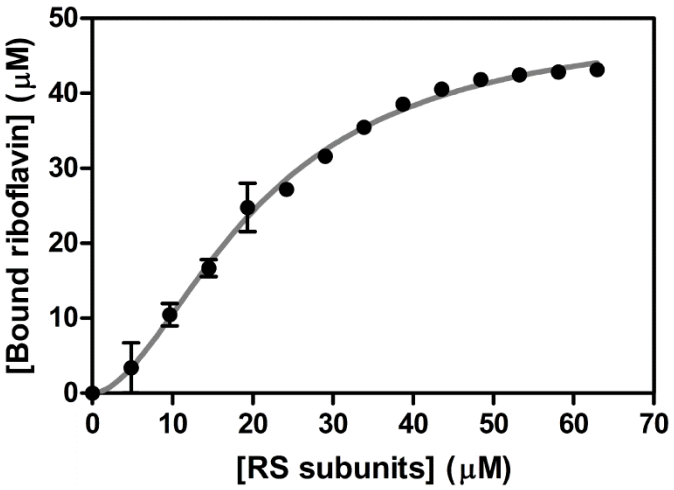

Figure S5 Binding curve of riboflavin to RS. The curve shows a sigmoidal shape with a Hill coefficient of 1.8 (positive cooperativity).

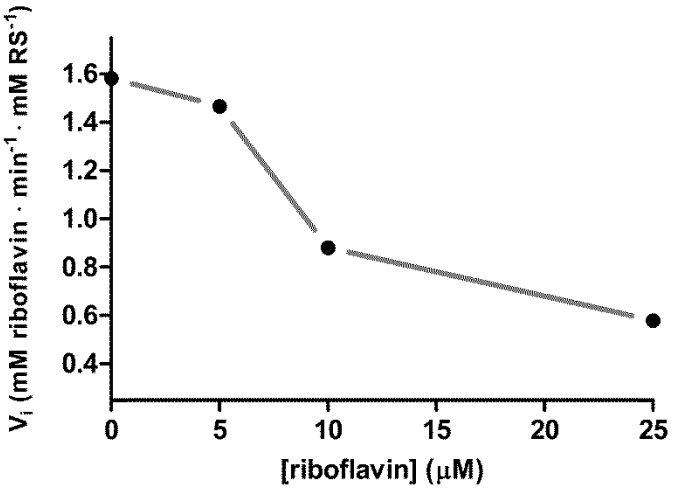

Figure S6 Product inhibition. The initial velocities of riboflavin formation (V_i) at different riboflavin concentrations were determined using a fixed concentration of 6,7-dimethyl-8-ribityllumazine (5 μM, see Materials and Methods for details).