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Supporting information for article:

The third structural switch in the molecule of archaeal translation initiation factor 2 and its possible role in initiation of GTP hydrolysis and removal of aIF2 from the ribosome

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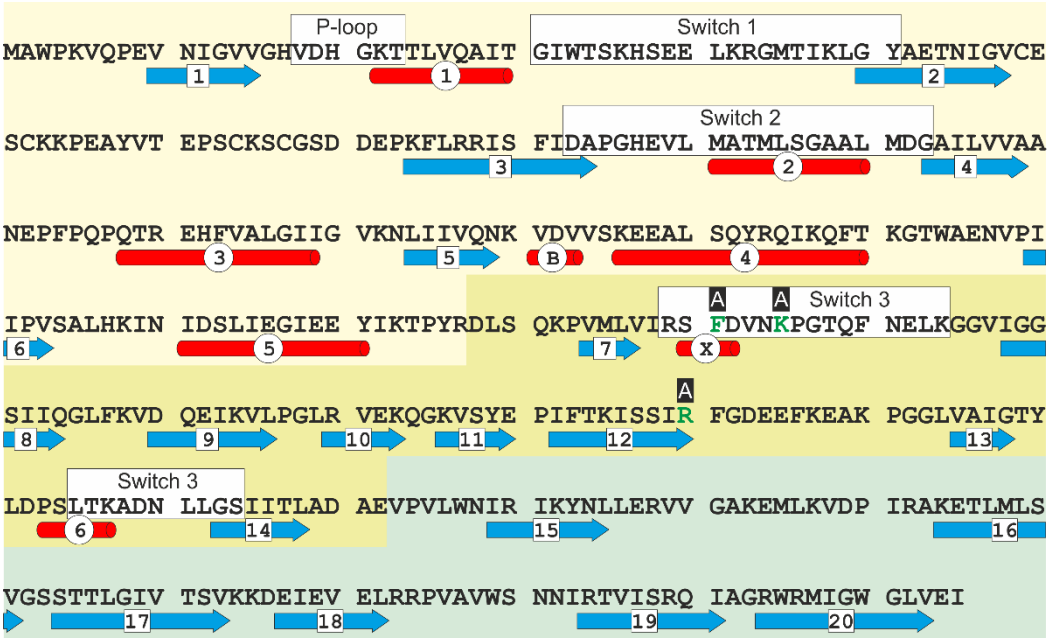

Figure S1 Amino acid sequence and elements of secondary structure of SsoIF2γ. Mutated residues (Phe221Ala, Lys225Ala, Arg280Ala) are indicated. Residues of domain I are shown with light yellow, residues of domain 2 with yellow and residues of domain 3 with light green. α-helices are shown as red cylinders and β-strands as blue arrows.

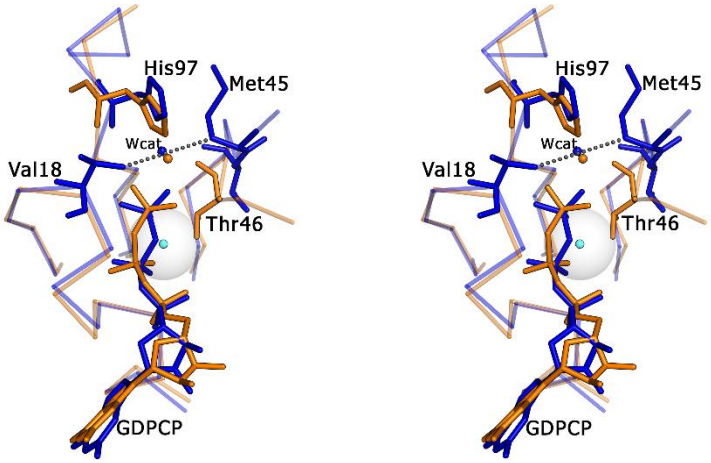

Figure S2 Superposition of nucleotide-binding pockets of EF-Tu in the active state [22], orange) and molecule A (blue) of the presented structure. Mg^{2+} of EF-Tu is shown in light blue. Side chains of His85 of EF-Tu and His97 of molecule A occupy a close position relative to the molecule of catalytic water.

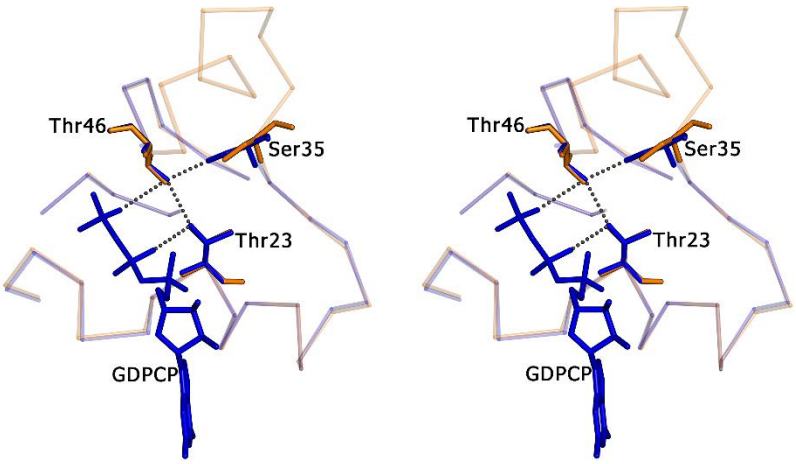

Figure S3 Superposition of the nucleotide-binding pockets of the molecule E (blue) of the presented structure and the SsoIF2γ-GDPCP complex obtained in the presence of Mg^{2+} (PDB code 4rjl, orange). The nucleotide, residues Thr23, Ser35, Thr46 and the hydrogen bonds formed by them are shown only for molecule E. Side chains of Ser35 and Thr46 approach, distorting the portion of switch 1 located between them.

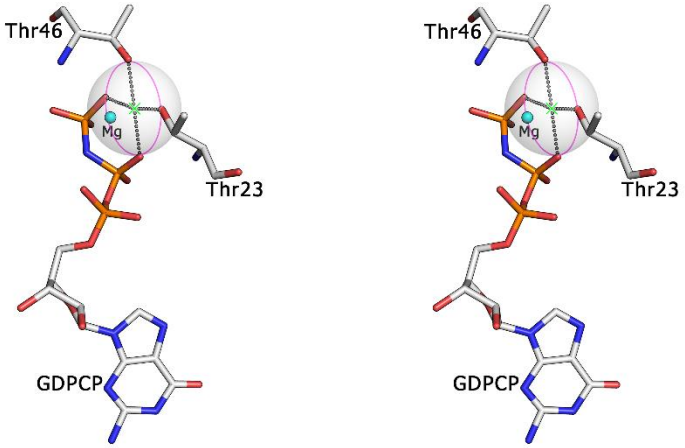

Figure S4 Nucleotide-binding pocket in the structure of αγ-heterodimer (PDB code 2aho). Usually the equatorial plane of the coordinating sphere of Mg^{2+} (shown with a cross) is formed by the O2G and O2B atoms of the nucleotide and the OG1 atoms of Thr23 and Thr46. The magnesium ion in αγ-heterodimer is removed from the equatorial plane by approximately 1.1 Å, which is typical for the water molecule.

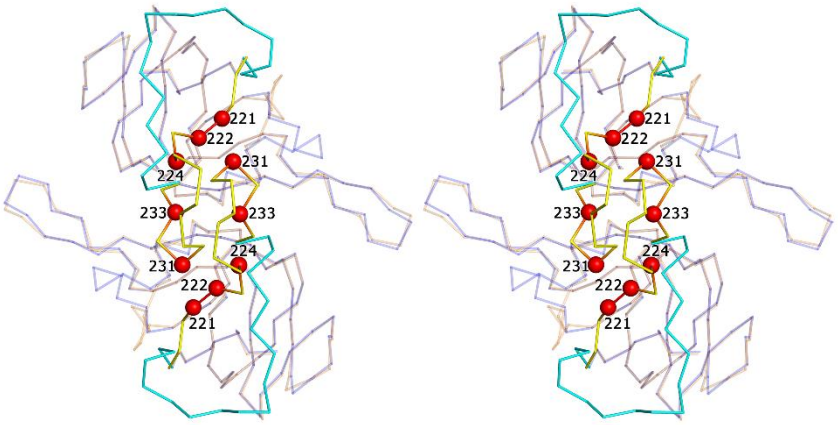

Figure S5 The mutual arrangement of the domains II of two symmetrically related molecules in the structure of SsoIF2γ-GDP (PDB code 4m4s, translucent blue) with switch 3 in a closed conformation (shown in cyan). The structure of SsoIF2γ-GDPCP (PDB-code 4rjl, translucent orange) with switch 3 in an open conformation (shown in yellow) is superimposed on both structures of the domain II β-sheet. The collision of Asp222, Asn224 and L233 with Asn224, Asn231 and Leu233 of the symmetric molecule excludes the existence of a L1 loop in the form of a β-hairpin for the considered packing of molecules in the crystal.