

Correction to Structure of a Sedoheptulose 7-Phosphate Cyclase: ValA from *Streptomyces hygroscopicus*

Kelsey M. Kean, Sara J. Coddling, Shumpei Asamizu, Taifo Mahmud, and P. Andrew Karplus*

Biochemistry 2014, 53 (26), 4250–4260. DOI: 10.1021/bi5003508

Shortly after this article describing the crystal structure of ValA from *Streptomyces hygroscopicus* was accepted for publication, we were able to determine the structure of the related enzyme desmethyl-4-deoxygadusol synthase from *Anabaena variabilis* (AvDDGS) at a higher (~ 1.7 Å) resolution (work still in progress). In light of the new structure, we are now able to satisfactorily interpret what we had described as a difficult to fit β -hairpin turn at residues 32 and 33 of ValA that collided with its symmetry mate across the crystallographic 2-fold axis. Rather than these residues forming a β -hairpin to match the chain topology seen

in dehydroquionate synthase structures, a domain-swapped arrangement exists in which the residues N-terminal to position 33 continue in a linear direction, making an extended β -strand that participates in the core β -sheet in the other subunit of the dimer. We have updated the Protein Data Bank deposition to reflect this altered topology and provide here an updated version of our original Figure 3 that provides a corrected overview of the topology of ValA. Further details of this new topology will be reported in a future publication of the AvDDGS structure.

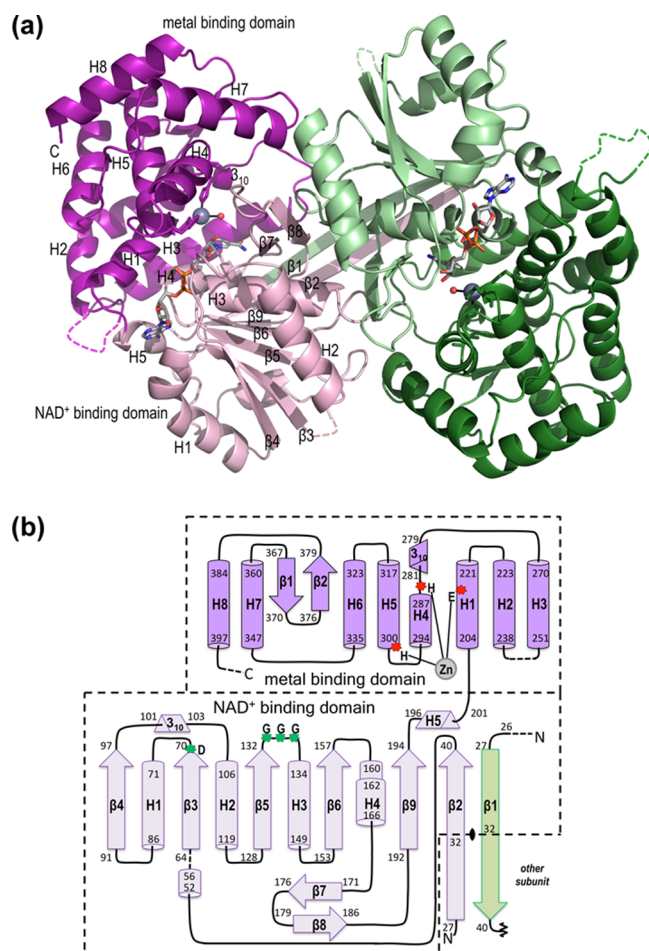


Figure 3. continued

Figure 3. Overall structure and topology of ValA. (a) Ribbon diagrams of the two chains of the ValA dimer are colored in purple and green tones, with the N-terminal NAD⁺-binding domains in light hues and the C-terminal metal-binding domains in dark hues. The extended β -strands of each subunit involved in the domain-swapped arrangement are visible in the back of the dimer. Dashed lines indicate internal unmodeled backbone segments. The NAD⁺ and the Zn²⁺ with its coordinating ligands are shown (colored as in Figure 1). Secondary structural elements in each domain of one monomer are labeled. (b) Topology diagram showing α -helices (cylinders), β -stands (arrows), 3_{10} -helices (triangular prisms), and π -helices (wider cylinder) with their respective first and last residues given. The minimal length α - and 3_{10} -helices (five and three residues, respectively) are left out of the secondary structure family nomenclature. The domains are colored light and dark purple as indicated, and helices (H) and strands (β) common to the SPCs are named sequentially within each domain. The domain-swapped β -strand containing residues 27–32 from the other subunit of the dimer, but contributing to the purple domain, is colored light green. The crystallographic 2-fold rotation axis (indicated as a black vertical ellipse) relates this β -strand to the residues extending from residue 32 of the purple domain to be part of the β -sheet of the other subunit. We retain the $\beta 1$ and $\beta 2$ names for the two parts of the long N-terminal β -strand because they participate in different β -sheets and to maintain in this report a consensus secondary structure nomenclature relevant to the sugar phosphate cyclase superfamily. Dashed lines denote unmodeled backbone segments. The three Zn²⁺-binding residues (red asterisks) and the glycine-rich turn and acidic residue (green asterisks) that are important for NAD⁺ binding are indicated.

Received: June 13, 2014

Published: June 27, 2014