Supplemental information

Procedures

Modeling of the structure of Agl3 and its active site

A homology model of Agl3 was constructed using Swiss-Model in the automated mode (Guex and Peitsch 1997; Schwede et al. 2003; Arnold et al. 2006). As a template, the 1.6-Å resolution crystal structure of the SQD1 enzyme with Protein DataBank (Berman et al. 2000) identification code 1QRR was used (Mulichak et al. 1999). Coordinates for the NAD^+ cofactor and the substrate uridine 5'-diphospho-glucose were transferred from the template structure after a backbone superposition of the template and the model.

Results and Discussion

Model structure of Agl3

Since no crystal structure of Agl3 is available, we chose an approach for the prediction of functional epitopes similar to that used for SQD1 from *A. thaliana* (Essigmann et al. 1999) before a high resolution crystal structure of that protein was available (Mulichak et al. 1999). The 1.6-Å resolution structure of the UDP-sulfoquinovose synthase SQD1, co-crystallized with NAD^+ and UDP-D-glucose (Mulichak et al. 1999), served as a template for a homology model of the Agl3 enzyme (supplemental Figure S1). Agl3 showed 43% sequence identity with SQD1. The backbone root-mean-square deviation of the model with respect to the template structure amounts to 0.57 Å, indicating a very similar overall fold. This concurs with results when the unpublished 1.2-Å resolution structure with PDB identification code 1I24 was used as a template (data not shown).

References

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