MOVIE. Morphing movie of structural rearrangements of Rab8 when binding to MSS4. The movie shows the structural changes in the nucleotide binding pocket of Rab8 when the GTPase binds to MSS4. It starts with Rab8 in the conformation bound to a guanosine nucleotide and then sequentially transforms into Rab8 in its nucleotide-free conformation bound to MSS4. Rab8 is drawn in cartoon representation (grey) with the P-loop in yellow, α_1-helix in orange, Switch I in red, and Switch II in purple. MSS4 is shown as a blue surface; the structure of MSS4 is taken from the MSS4:Rab8-complex structure. The movie demonstrates the steric clash of the α_1-helix of Rab8 (bound to nucleotide) with the surface of MSS4. The steric hindrance is released by displacement of the α_1-helix, concomitant with a structural rearrangement of the nucleotide-binding pocket. The structure of Rab8 bound to nucleotide is not known and has been modeled by sequence homology using Ypt1-Rab and Sec4-Rab structures as models (SWISS-MODEL (Automated Protein Modelling Server, http://swissmodel.expasy.org/SWISS-MODEL.html, (Guex & Peitsch, 1997; Schwede et al, 2003; Peitsch 1995)). Additionally, the conformation of residues Gly18 to Asp31 of Rab8 in the MSS4-bound structure is unknown because of lack of electron density. These loops have been modeled using Swiss PdbViewer (version 3.7, http://www.expasy.org/spdbv/, (Guex & Peitsch, 1997)). Morphing of structures between Rab8 bound to nucleotide and Rab8 bound to MSS4 was performed using the program lsqman (Jones et al, 1991; Kleywegt, 1996). Movie frames were prepared using the program pymol (DeLano 2002) and subsequently converted into a Quicktime-movie using Adobe ImageReady CS.

REFERENCES

DeLano WL The PyMOL Molecular Graphics System (2002) on World Wide Web http://www.pymol.org

Guex N and Peitsch MC (1997) SWISS-MODEL and the Swiss-PdbViewer: an environment for comparative protein modeling. *Electrophoresis* **18:** 2714-2723

Jones TA, Zou JY, Cowan SW, and Kjeldgaard (1991) Improved methods for building protein models in electron density maps and the location of errors in these models. *Acta Crystallogr A* **47 (Pt 2):** 110-119

Kleywegt GJ (1996) Use of non-crystallographic symmetry in protein structure refinement. *Acta Crystallogr D Biol Crystallogr* **52:** 842-857

Peitsch MC (1995) Protein modeling by E-mail *Bio/Technology* **13:** 658-660

Schwede T, Kopp J, Guex N, and Peitsch MC (2003) SWISS-MODEL: An automated protein homology-modeling server. *Nucleic Acids Res* **31:** 3381-3385