1.7 Å with ARP[20] after 5% of the data had been set aside to calculate the free *R*-factor. Additional calculations were performed with the CCP4 suite of programs[21]. The model was refined with REFMAC[22] and water molecules were added with ARP. Model building was performed using the program O[23]. The final model has been refined at 1.7 Å to an *R*-factor of 0.175 with an R_{free} of 0.208 (Table 1).

ATP and acyl-adenylate complexes

Crystals of the apo complex were soaked for 24 h in a solution consisting of 1.7 M Li_2SO_4, 100 mM HEPES, pH 7.5, and 20 mM ATP. Diffraction data were collected at beamline X26C (99.7% complete, 6.3-fold redundancy, R_{sym} = 12.9%), and the structure was solved using difference Fourier methods. The ATP-bound model has been refined at 2.9 Å to an *R*-factor of 0.203 (R_{free} = 0.267). No water molecules were added owing to the limited resolution. Residues 167–188 and 241–248 appear to be disordered, including the zinc-binding motifs and the previously missing surface loop of MoeB. In the apo complex, the polypeptide segments containing the zinc-binding motifs have higher average B-factors compared with the remainder of the molecule. At 2.9 Å the quality of the electron density maps for the ATP complex is reduced making it impossible to observe these more mobile regions. To obtain the acyl-adenylate complex, apo crystals were soaked for 24 h in a solution consisting of 1.7 M Li_2SO_4, 100 mM HEPES, pH 7.5, 20 mM ATP, and 20 mM $MgSO_4$. Diffraction data were collected at beamline X26C (98.7% complete, 3.5-fold redundancy, R_{sym} = 8.6%), and the structure was solved using difference Fourier methods. The acyl-adenylate model has been refined at 2.1 Å resolution to an *R*-factor of 0.188 (R_{free} = 0.225) following the same protocol described for the apo complex. The residues in the zinc-binding motif of MoeB are present in the electron density maps in a conformation identical to that found in the apo complex, but residues 182–188 are again disordered.

MoeB variants and activity measurements

The QuickChange kit from STRATAGENE was used to generate the Arg14Ala, Arg14Lys, Arg73Ala, Arg73Lys, Asp130Ala and Asp130Glu variants of MoeB as well as the double mutants Arg14Ala and Arg73Ala, and Arg14Lys and Arg73Ala. Nucleic acid sequences were verified by automated sequencing of both strands. *MoeB*$^-$ cells[6] transformed with plasmids[15] expressing either the wild-type or a mutated version of MoeB were grown aerobically for 16 h at 37 °C on Luria Broth plates. After anaerobic growth for several hours at 22 °C, an overlay assay for nitrate reductase activity was performed as described[24].

Received 19 July; accepted 11 September 2001.

1. Hochstrasser, M. All in the ubiquitin family. *Science* **289,** 563–564 (2000).
2. Hochstrasser, M. Evolution and function of ubiquitin-like protein-conjugation systems. *Nature Cell Biol.* **2,** E153–E157 (2000).
3. Rajagopalan, K. V. in *Escherichia coli and Salmonella typhimurium: Cellular and Molecular Biology* (ed. Neidhardt, F. C.) 674–679 (ASM Press, Washington DC, 1996).
4. Rajagopalan, K. V. Biosynthesis and processing of the molybdenum cofactors. *Biochem. Soc. Trans.* **25,** 757–761 (1997).
5. Rudolph, M. J., Wuebbens, M. M., Rajagopalan, K. V. & Schindelin, H. Crystal structure of molybdopterin synthase and its evolutionary relationship to ubiquitin activation. *Nature Struct. Biol.* **8,** 42–46 (2001).
6. Leimkühler, S., Wuebbens, M. M. & Rajagopalan, K. V. Characterization of *Escherichia coli* MoeB and its involvement in the activation of MPT synthase for the biosynthesis of the molybdenum cofactor. *J. Biol. Chem.* **276,** 34695–34701 (2001).
7. Pitterle, D. M., Johnson, J. L. & Rajagopalan, K. V. *In vitro* synthesis of molybdopterin from precursor Z using purified converting factor. *J. Biol. Chem.* **268,** 13506–13509 (1993).
8. Walker, J. E., Saraste, M., Runswick, M. J. & Gay, N. J. Distantly related sequences in the alpha- and beta-subunits of ATP synthase, myosin, kinases and other ATP-requiring enzymes and a common nucleotide binding fold. *EMBO J.* **1,** 945–951 (1982).
9. Burch, T. J. & Haas, A. L. Site-directed mutagenesis of ubiquitin. Differential roles for arginine in the interaction with ubiquitin-activating enzyme. *Biochemistry* **33,** 7300–7308 (1994).
10. Arnez, J. G., Dock-Bregeon, A. C. & Moras, D. Glycyl-tRNA synthetase uses a negatively charged pit for specific recognition and activation of glycine. *J. Mol. Biol.* **286,** 1449–1459 (1999).
11. Hatfield, P. M. & Vierstra, R. D. Multiple forms of ubiquitin-activating enzyme *E*1 from wheat. *J. Biol. Chem.* **267,** 14799–14803 (1992).
12. Lauhon, C. T. & Kambampati, R. The *iscS* gene in *Escherichia coli* is required for the biosynthesis of 4-thiouridine, thiamin, and NAD. *J. Biol. Chem.* **275,** 20096–20103 (2000).
13. Palenchar, P. M., Buck, C. J., Cheng, H., Larson, T. J. & Mueller, E. G. Evidence that ThiI, an enzyme shared between thiamin and 4-thiouridine biosynthesis, may be a sulfurtransferase that proceeds through a persulfide intermediate. *J. Biol. Chem.* **275,** 8283–8286 (2000).
14. Xi, J., Ge, Y., Kinsland, C., McLafferty, F. W. & Begley, T. P. Biosynthesis of the thiazole moiety of thiamin in *Escherichia coli*: identification of an acyldisulfide-linked protein-protein conjugate that is functionally analogous to the ubiquitin/E1 complex. *Proc. Natl Acad. Sci. USA* **98,** 8513–8518 (2001).
15. Leimkühler, S. & Rajagopalan, K. V. An *Escherichia coli* NifS-like sulfurtransferase is required for the transfer of cysteine sulfur in the *in vitro* synthesis of molybdopterin from precursor Z. *J. Biol. Chem.* **276,** 22024–22031 (2001).
16. Otwinowski, Z. & Minor, W. in *Methods in Enzymology: Macromolecular Crystallography* (eds Carter, C. W. & Sweet, R. M.) 307–326 (Academic, San Diego, 1997).
17. Sheldrick, G. M. & Schneider, T. R. in *Methods in Enzymology: Macromolecular Crystallography* (eds Carter, C. W. & Sweet, R. M.) 319–343 (Academic, San Diego, 1997).
18. DeLaFortelle, E. & Bricogne, G. in *Methods in Enzymology: Macromolecular Crystallography* (eds Carter, C. W. & Sweet, R. M.) 472–494 (Academic, San Diego, 1997).
19. Abrahams, J. P. & Leslie, A. G. W. Methods used in the structure determination of bovine mitochondrial F_1 ATPase. *Acta Crystallogr. D* **52,** 30–42 (1996).
20. Perrakis, A., Morris, R. & Lamzin, V. S. Automated protein model building combined with iterative structure refinement. *Nature Struct. Biol.* **6,** 458–463 (1999).
21. Bailey, S. The CCP4 suite: programs for protein crystallography. *Acta Crystallogr. D* **50,** 760–763 (1994).
22. Murshudov, G., Vagin, A. & Dodson, E. Refinement of macromolecular structures by the maximum likelihood method. *Acta Crystallogr. D* **53,** 240–255 (1997).
23. Jones, T. A., Zou, J. Y., Cowan, S. W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and the location of errors in these models. *Acta Crystallogr. A* **47,** 110–119 (1991).
24. Johnson, M. E. & Rajagopalan, K. V. *In vitro* system for molybdopterin biosynthesis. *J. Bacteriol.* **169,** 110–116 (1987).
25. Laskowski, R. A., Moss, D. S. & Thornton, J. M. Main-chain bond lengths and bond angles in protein structures. *J. Mol. Biol.* **231,** 1049–1067 (1993).
26. Kraulis, P. J. MOLSCRIPT: a program to produce both detailed and schematic plots of protein structures. *J. Appl. Crystallogr.* **24,** 946–950 (1991).
27. Barton, G. J. ALSCRIPT: a tool to format multiple sequence alignments. *Protein Eng.* **6,** 37–40 (1993).
28. Nicholls, A., Sharp, K. A. & Honig, B. Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. *Proteins* **11,** 281–296 (1991).

Acknowledgements

We thank M. J. Rudolph for initial help with crystallization and data collection, J. Daniels for technical assistance, and D. Schneider for support at beamline X26C. This work was supported by National Institutes of Health (NIH) grants to H.S. and K.V.R.. The National Synchrotron Light Source in Brookhaven is supported by DOE and NIH, and beamline X26C is supported in part by the State University of New York at Stony Brook and its Research Foundation.

Correspondence and requests for materials should be addressed to H.S. (e-mail: hermann.schindelin@sunysb.edu). The atomic coordinates have been deposited in the Protein Data Bank under accessions numbers 1JW9, 1JWA and 1JWB.

correction

Antibacterial agents based on the cyclic D,L-α-peptide architecture

Sara Fernandez-Lopez, Hui-Sun Kim, Ellen C. Choi, Mercedes Delgado, Juan R. Granja, Alisher Khasanov, Karin Kraehenbuehl, Georgina Long, Dana A. Weinberger, Keith M. Wilcoxen & M. Reza Ghadiri

Nature **412,** 452–455 (2001).

The two organisms *Streptococcus pneumonieae* and *Enterococcus faecalis* are mislabelled as Gram-negative strains (paragraph 3 and Table 1), whereas they are Gram-positive. This error does not alter our conclusions. □

erratum

Transmission intensity and impact of control policies on the foot and mouth epidemic in Great Britain

Neil M. Ferguson, Christl A. Donnelly & Roy M. Anderson

Nature **413,** 542–548 (2001).

In this Letter, the key to Figure 4b contained two errors. The description of the green curve should be “no non-IP culling” (not “non-IP culling”) and the description of the orange curve should be “69% case increase” (not “69% case decrease”). □

© 2001 Macmillan Magazines Ltd