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EDUCATION

1975, **B.A.**, Biophysics, *Pomona College*, Claremont, CA.

1981, **Ph.D.**, Physics Dept., *University of California, San Diego*.

Dissertation Advisor: Xuong Nguyen-huu.

Dissertation title: *Techniques for Rapid and Precise Measurement of Crystallographic Intensities on the Multiwire Area Detector Diffractometer.*

Research specializations: software for crystallographic data acquisition and processing; low-temperature techniques; mammalian serine proteases.

1981-1983, **Postdoctoral Research**, *UC Los Angeles* .

Chemistry Dept. and Molecular Biology Institute. Advisor: David S. Eisenberg.

Research specializations: structure of ribulose biphosphate carboxylase / oxygenase; crystallographic methods development.

1983-1984, **Postdoctoral Research**, *Inhalation Toxicology Research Institute*,

Albuquerque, NM. Advisor: Charles Mitchell.

Research specializations: binding of toxicants to mouse lung DNA; mathematical modeling of toxicological risk; mechanisms of carcinogenesis.

EMPLOYMENT

1984-1991, *Genex Corporation*, Gaithersburg, MD, Corporate Research Scientist.

Wrote *XENGEN* software for processing Siemens Area Detector data. Solved or worked on structures of affinity proteins, Fab's, serine proteases, heme proteins. Executed Phase I NSF SBIR for development of detector-general crystallographic data processing software.

1991-1993, *Enzon Inc.*, Gaithersburg, MD, Principal Scientist.

Developed crystallographic software; studied structures of enzymes and immune-system proteins; managed research computers. Trained crystallographers worldwide in use of processing software.

1993-1995, *Molecular Simulations, Inc.*, Burlington, MA/ Rockville, MD

Senior Scientist, Life Sciences. Principal Investigator of NSF Phase II SBIR to develop X-GEN, a crystallographic data processing software package capable of handling data from several types of electronic detectors and image-plates. Managed two other SBIR projects.

Participated in crystallographic research at CARB, Rockville, MD as a Visiting Scientist.

1995-1996 *Advanced Photon Source*, Argonne National Laboratory

Associate Director, Industrial Macromolecular Crystallography Association Collaborative Access Team.

1995-1997 *Illinois Institute of Technology*, Chicago, IL.

Research Associate Professor, Department of Biological, Chemical, and Physical Sciences.

1996-2002; , *Advanced Photon Source*, Argonne National Laboratory

Director, Industrial Macromolecular Crystallography Association Collaborative Access Team.

1998- , *Illinois Institute of Technology*, Chicago, IL.

Associate Professor of Biology and Physics, Biological Sciences Department (tenured 2001)

TEACHING EXPERIENCE

1973-75 Teaching assistant in freshman physics at Pomona College

1975-79 Teaching assistant in freshman physics at UC San Diego

1981 Taught organic and biological chemistry at UC Los Angeles (175 students)

1987-93 Instructed users of *XENGEN* software worldwide, as needed

1994 Faculty, crystallography summer course in Mexico City;

Participating instructor and laboratory facilitator for a two-week postdoctoral course in macromolecular crystallography at the Universidad Autonoma de Mexico, Mexico, D.F.

1995-99 Faculty, crystallography course at Cold Spring Harbor;

Participating instructor for two-week graduate and postdoctoral course in macromolecular crystallography at Cold Spring Harbor Laboratory

1996-2000 Created and taught *Introduction to the Professions* at IIT;

This was a survey course taken by all freshman biology, chemistry, and physics majors. 1998-2016 Recreated and taught graduate course in radiation biophysics at IIT

1999, 2017 Taught freshman human biology to 61 students at IIT

1999- In charge of biology colloquium series at IIT.

This involves inviting and facilitating the visits of about twelve speakers per semester to the campus.

2001-02, 2019 Taught biological literature course (undergraduate/graduate)

2002-2020 Built and taught junior-level undergraduate biochemistry for majors,

chiefly to premedical students and molecular biology majors. Enrollment 20-40 students per year.

2005- Built and taught junior-level undergraduate biochemistry for non-majors,

chiefly to engineers and chemists. Enrollment 20-60 students per year.

2003- *ACA Summer School in Macromolecular Crystallography*

Lecturer, computer lab instructor, and beamline coordinator for the American Crystallographic Association's Summer School (see below).

2004-05 Co-taught *Case Studies in Health Physics*

Graduate student supervision:

- Ph.D. completed by Kyung-Jin Kim (2000; most supervision by Prof. D. Webster)
- Ph.D. completed by Kyung-Won Park (2002; some supervision by B. Stark)
- Ph.D. completed by Pauls Reinfelds, 2011
- Ph.D. completed by Sireesha Ratakonda, 2012
- Ph.D. completed by Yang Wang, 2013
- M.S. completed by Nisha Fernandes (1999), Shih-Chia Chang (2002 and 2014), Yifan Zhang (2015), Yumeng Pei (2015), Dongyang Bai (2016), Okba Hammadi (2021)
- Ph.D. underway for Jagriti Chander

MAJOR ACADEMIC ORGANIZATIONAL ACTIVITY: Current

2002- 2009 Co-Director, IIT Masters in Health Physics program

This is a professional science master's program in health physics, begun in 1998 at IIT. The program is taught primarily on-line, and is the only online PSM in health physics in the US. Current active enrollment: 82 students (largest HP master's program in US). Gross revenue for IIT: approx. \$370,000 / yr.

2003-10 Secretary, University Faculty Council, IIT.

Maintains website and takes minutes for Faculty Council and University Faculty meetings. A primary avenue of communication between university administration and Faculty Council.

2003-08 Director, *ACA Summer School in Macromolecular Crystallography*

This is a twelve-day annual summer in macromolecular crystallographic theory and practice, taught at IIT and the Advanced Photon Source in mid-July of each year. Total enrollment, 2003-05: 50 students. Includes extensive use of crystallographic beamlines at the APS. Prof.

Howard did most of the organization of the school, gave six lectures per year, and manages all the APS beamline activity for the school.

2010-22 IIT Representative, Illinois Board of Higher Education Faculty Advisory Council

This is a significant advisory body that includes representatives from public universities, community colleges, and independent universities and colleges.

RESEARCH SUPPORT: Past

1991-95 Principal Investigator, NSF Small Business Innovation Research Grant.

Grant was for development of crystallographic data processing software for multiple detector systems; culminated in development and successful marketing of X-GEN by Molecular Simulations, Inc. \$300,000 award. NSF SBIR was originally developed at Genex and Enzon

and was successfully transferred to Molecular Simulations in 1993.

1997-99 Co-PI, IITRI Institutional Research and Development Project.

with K. Stagliano at IIT. Project involved development of inhibitors of the enzymatic portion of cholera toxin and eventual crystallographic inquiries into the structures of enzyme-inhibitor complexes. \$10,000 award to IIT researchers. Research continued through the present without continuing funding.

1998-02, Principal Investigator, NIST contract,

"Structural Studies of Enzymes Involved in Aromatic Amino Acid Biosynthesis".

Project involved data collection and processing, and the potential of biochemical and structure-analysis studies, on enzymes in the chorismate pathway. IIT budget: approx. \$60,000 per year for three years.

1998-2004, Co-Principal Investigator, IIT-IMCA contract

This was the contract between IIT and the Industrial Macromolecular Crystallography Association (IMCA). Contract specifies IIT as developer and manager of experimental facilities for IMCA. Operating budget: approximately \$1,000,000 per year. Capital budget: \$250,000 - \$900,000 per year depending on requirements. The IMCA contract provided for employment of approx. 6 FTE employees of IIT at IMCA-CAT's facilities at the Advanced Photon Source at Argonne National Laboratory as well as half of Prof. Howard's academic-year salary and two months of summer salary per year. Contract renewed once during performance period.

1998-2008 Principal Investigator, NIH subcontract, GM57890

"X-ray diffraction measurements at the Advanced Photon Source". Part of multi-institution program project grant from the National Institutes of Health to the Maryland Biotechnology Institute, The Institute for Genomic Research, and IIT. IIT budget: \$250,833 for five years. Program project title: "From Genomic Sequences to Protein Structure and Function". IIT portion of project involves acquisition and processing of crystallographic data as part of a major proteomics project; recent modifications in project provide for molecular biology and biochemistry efforts at IIT as well. NIH grant and subcontract were renewed for five years in 2003.

2003-15 Co-PI / PI, IIT Subcontract to University of Georgia

Provides IIT support for the activities of Southeast Regional Collaborative Access Team (SER-CAT) at the Advanced Photon Source. Involves coordination of 3-5 IIT scientists involved in SER-CAT's activities. IIT budget: \$65,000 - \$92,000 / year.

2014-16 Participant / PI, NSF Education Grant to National Louis University & IIT;

A two-institution grant to develop ways of helping middle-school science teachers recognize the real dynamics of scientific research. Program included museum visits, research demonstrations at IIT, and extensive reviews to help teachers develop lesson plans. IIT budget: \$100,000 per year.

2015-20 PI, IIT Subcontract, US Dept. of Education TQP grant.

The primary recipient on this grant is National Louis University. The grant involves teacher training at AUSL schools in the Chicago Public

Schools; each year the NLU and IIT participants develop demonstration projects and curricular help for elementary- and middle-school science teachers. IIT budget: \$100,000 /year.

RESEARCH SUPPORT: Current

2022-2027 Co-PI, NSF Noyce Track I Scholarship Grant to National Louis University and IIT; a five-year grant providing scholarships to Illinois Tech students pursuing careers in high school STEM teaching by completing a Master of Arts in Teaching at NLU. Total budget for 5 years: \$1.1 million.

SCIENTIFIC COMMUNITY SERVICE

1991- , Member, NIH Special Study Section 6

Participates in reviews of Small Business Innovation Research and Small-business Technology Transfer Research grant applications, as well as some academic grants.

1992-93 NSF Small Business Innovation Research Grant proposal review; two sessions. 1997-99 Founder and first Chair, CAT Director's Council at the Advanced Photon Source.

Facilitated communication among directors of the APS Collaborative Access Teams and between the CAT Directors and the APS management.

1997-2001 Judge at Chicago Public Schools Science Fair competitions.

1998,2000 NASA proposal review

1998 Vice chair, Gordon Conference: Diffraction Methods in Molecular Biology
Proctor Academy, Andover, NH

1998- NIH *ad hoc* site-visit panels to review Research Resource grants.

1998- Editorial board, mmCIF

Editor for a few new entries related to the Macromolecular Crystallographic Information File (mmCIF) effort of the International Union of Crystallography (IUCr).

1998- co-founder, Crystallographic Binary File (CBF) effort; recognized by the IUCr.

2000 Chair, Gordon Conference: Diffraction Methods in Molecular Biology
Proctor Academy, Andover, NH

2015- Editorial board, *Cell Biochemistry & Biophysics* (Springer-Nature Journal)

2017- Editorial board, *The Protein Journal* (Springer-Nature Journal)

FACULTY SERVICE

1998-2003 Faculty advisor undergraduate Research Honors program

provided advice to students in Research Honors program and facilitate matchups between students and faculty sponsors. Created Research Honors courses. Provided sponsorship to first student in program (summer 2000).

1999-2001 IIT Undergraduate Studies Committee
and departmental Undergraduate Curriculum Committee at IIT

1999- Undergraduate academic advisor
Provide academic advising for biology and MBB majors at IIT. Typical portfolio: 60 students in the 2000's; fewer since then.

2000- Chair, new faculty search, biology division, BCPS Department, IIT.

2017-2019 Interim Chair, Biological Sciences Department, IIT.

OTHER COMMUNITY SERVICE

1970- active layman in church organizations, including choirs

1992-95 chorus member, Washington Revels, a nonprofit musical theater organization.

1998- founding Board member of Revels Chicago
a nonprofit musical theater organization; member of chorus beginning 1999.

1997-99 member, Choral Ensemble of Chicago.

2008- Cast member, Bristol Renaissance Festival, Kenosha, WI.

2014- Teacher, Bristol Academy of Performing Arts, Kenosha, WI.

2015-17 Music Institute of Chicago Chorus.

PUBLICATIONS

Weber, P.C., Bartsch, R.G., Cusanovich, M.A., Hamlin, R.C., Howard, A., Jordan, S.R., Kamen, M.D., Meyer, T.E., Weatherford, D.W., Xuong, Ng.-h., and Salemme, F.R. (1980) Structure of cytochrome c': A dimeric, high-spin haem protein. *Nature* **286**:302-304.

Weber, P.C., Howard, A., Xuong, Ng.-h and Salemme, F.R. (1981) Crystallographic structure of *Rhodospirillum molischianum* ferricytochrome c' at 2.5 Å resolution. *J. Mol. Biol.* **153**: 399-424.

Hamlin, R.C., Cork, C. Howard, A. Nielsen, C., Vernon, W., Matthews, D., and Xuong, Ng.-h. (1981) Characteristics of a flat multiwire area detector for protein crystallography, *J. Applied Crystallogr.***14**: 85-93.

Howard, A.J. (1982) Computing requirements for area detector data collection, in : *Computational Crystallography* (Sayre, D., ed.: Oxford, Clarendon Press), pp. 29-40.

Howard, A.J. Nielsen, C.P., Xuong, Ng.-h (1984) Software for a multiwire area detector. *Methods in Enzymology***114**: 452-472.

Howard, A.J. Mitchell, C.E., Dutcher, J.S., Henderson, T.R. and McClellan, R.O. (1986) Binding of nitropyrenes and benzo[a]pyrene to mouse

lung deoxyribonucleic acid after pretreatment with inducing agents. *Biochemical Pharmacology***35**: 2129-2134.

Howard, A.J. Gilliland, G.L., Finzel, B.C. Poulos, T.L. Ohlendorf, D.H. and Salemme, F.R. (1987) Use of an imaging proportional counter in macromolecular crystallography. *J. Applied Crystallogr.***20**: 383:387.

Poulos, T.L. and Howard, A.J. (1987) Crystal structures of metyrapone- and phenylimidazole-inhibited complexes of cytochrome P-450cam. *Biochemistry***26**: 8165-8174.

Poulos, T.L., Sheriff, S., and Howard, A.J. (1987) Cocrystals of yeast cytochrome c peroxidase and horse heart cytochrome c. *J. Biol. Chem.***262**: 13881-13884.

Poulos, T.L., Finzel, B.C. and Howard, A.J. (1987) High-resolution crystal structure of Cytochrome P-450cam. *J. Mol. Biol.***195**: 687-700.

Gilliland, G.L., Howard, A.J., Winborne, E.L., Poulos, T.L, Stewart, D.B., and Durham, D.R. (1987) Crystallization and Preliminary X-ray Diffraction Studies of Subtilisin GX from Bacillus sp. GX6644. *J. Biol. Chem.***262**: 4280-4283.

Whitlow, M., and Howard, A.J. (1989) 1.6Å Structures of xylose isomerase from *Streptomyces rubiginosus* with xylitol and xylose and their mechanistic implications. *Trans. Amer. Crystallogr. Assoc.***25**: 105-126.

Whitlow, M., Howard, A.J. Finzel, B.C. Poulos, T.L. Winborne, E., and Gilliland, G.L. (1991) A metal-mediated hydride shift mechanism for xylose isomerase based on 1.6Å *Streptomyces rubiginosus* structures with xylitol and D-xylose. *Proteins: Struct., Func., Genet.***9**: 153-173.

Achari, A., Hale, S.P. Howard, A.J. Clore, G.M. Gronenborn, A.M., Hardman, K.D., and Whitlow, M. (1992), the 1.67Å X-ray Structure of the B2 Immunoglobulin-Binding Domain of Streptococcal Protein G and Comparison to the NMR Structure of the B1 Domain. *Biochemistry* **31**: 10449-10457.

Howard, A.J. and Poulos, T.L., (1992) Methods in macromolecular crystallography. chapter in *Advances in Biophysical Chemistry***2**: 1-36.

Essig, N.Z. Wood, J.F., Howard, A.J., Raag, R., and Whitlow, M. (1993) Crystallization of Single-Chain Fv Proteins. *J. Mol. Biol.***234**: 897-901.

Whitlow, M., Howard, A.J., Wood, J.F., Voss, E.W., and Hardman, K.D. (1995) 1.85 Å Structure of anti-fluorescein 4-4-20 Fab. *Protein Engineering***8**: 749-761.

Howard, A.J. (2000) Data processing in macromolecular crystallography. Chapter in: *Crystallographic Computing 7: Proceedings from the Macromolecular Crystallographic Computing School, 1996*. P.E. Bourne and K.D. Watenpaugh, eds. Oxford: Oxford University Press.

Whitlow, M., Howard, A.J., Stewart, D., Hardman, K., Kuyper, L.F., Baccanari, D.P., Tansik, R.L., and Fling, M. (1997) X-ray crystallographic studies of *Candida albicans* dihydrofolate reductase: high resolution structures of the holoenzyme and an inhibited ternary complex. *J. Biol. Chem.***272** 30289-30298.

Thoden, J.B., Miran, S.G., Phillips, J.C., Howard, A.J., Raushel, F.M., Holden, H.M. (1998) Carbamoyl phosphate synthetase: Caught in the Act of Glutamine hydrolysis. *Biochemistry* **37**: 8825-8831.

Raves, M. L., Giles, K., Schrag, J. D., Schmid, M. F., Phillips Jr., G. N., Wah, C., Howard, A. J., Silman, I., Sussman, J. L. (1998) Quaternary Structure of Tetrameric Acetylcholinesterase. In: *Structure and Function of Cholinesterases and Related Proteins* (Doctor, B.P., Quinn, D.M., Rotundo, R.L. & Taylor, P., eds.).

Howard, A. (1998) Participation of pharmaceutical companies in synchrotron radiation research. *Nature Structural Biology* **5**: 623-626.

Eisenstein, E., Gilliland, G.L., Herzberg, O., Moulton, J., Orban, J., Poljak, R.J., Banerjee, L., Richardson, D., and Howard, A.J. (2000) Biological function made crystal clear - annotation of hypothetical proteins via structural genomics. *Current Opinions in Biotechnology* **11**: 25-30.

Mayhew, M.P., Holden, M.J., Howard, A.J., Gallagher, D.T., and Stover, C. (2000) Crystallization and 1.1-Å diffraction of chorismate lyase from *Escherichia coli*. *J. Structural Biology* **129**: 96-99.

Ladner, J.E., Reddy, P., Davis, A., Tordova, M., Howard, A.J., and Gilliland, G.L. (2000) The 1.30 Å resolution structure of the *Bacillus subtilis* chorismate mutase catalytic homotrimer. *Acta Crystallographica* **D56**: 673-683.

Gallagher, D.T., Mayhew, M., Holden, M.J., Howard, A., Kim, K.J., and Vilker, V.L. (2001) The crystal structure of chorismate lyase shows a new fold and a tightly retained product. *Proteins* **44**: 304-311.

Lim, K., Zhang, H., Tempczyk, A., Bonander, N., Toedt, J., Howard, A., Eisenstein, E., and Herzberg, O. (2001) Crystal structure of YecO from *Haemophilus influenzae* (HI0319) reveals a methyltransferase fold and a bound S-Adenosylhomocysteine. *Proteins* **45**: 397-407.

Sanders, D.A.R., Moothoo, D.N., Raftery, J., Howard, A.J., Helliwell, J.R., and Naismith, J.H. (2001). The 1.2 Å resolution structure of the con A-dimannose complex. *J. Mol. Biol.* **310**: 875-884.

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Parsons, J.F., Jensen, P.Y., Pachikara, A.S., Howard, A.J., Eisenstein, E., and Ladner J.E. (2002) Structure of *Escherichia coli* aminodeoxychorismate synthase: architectural conservation and diversity in chorismate-utilizing enzymes. *Biochemistry* **41**(7): 2198-2208.

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- Kim, K.-J. and Howard, A.J. (2002) Crystallization and preliminary X-ray diffraction analysis of the trigonal crystal form of *Saccharomyces cerevisiae* alcohol dehydrogenase I: evidence for the existence of Zn ions in the crystal. *Acta Crystallogr.* **D58**: 1332-1334.
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- Kim, K.J., Kim, Y., Park, K.W., Webster, D.A., and Howard, A.J. (2002) Purification, crystallization, and preliminary X-ray analysis of the soluble domain of the Na⁺-pumping cytochrome *bo* quinol oxidase from *Vitreoscilla*. *Acta Crystallogr.* **D.58**: 1329-1331.
- Willis, M.A., Krajewski, W., Chalamasetty, V.R., Reddy, P., Howard, A., Herzberg, O. (2002) Structure of HI1333 (YhbY), a putative RNA-binding protein from *Haemophilus*. *Proteins* **49**: 423-426.
- Lim, K., Tempczyk, A., Bonander, N., Toedt, J., Howard, A., Eisenstein, E., and Herzberg, O. (2003) A catalytic mechanism for D-Tyr-tRNA^{Tyr} deacylase based on the crystal structure of *Hemophilus influenzae* HI0670. *J. Biol. Chem.* **278**(15): 13496-13502.
- Gilliland, G.L., TePLYakov, A., Obmolova, G., Tordova, M., Thanki, N., Ladner, J., Herzberg, O., Lim, K., Zhang, H., Huang, K., Li, Z., Tempczyk, A., Krajewski, W., Parsons, L., Yeh, D.C., Orban, J., Howard, A.J., Eisenstein, E., Parsons, J.F., Bonander, N., Fisher, K.E., Toedt, J., Reddy, P., Rao, C.V., Melamud, E., and Moulton, J. (2003) Assisting functional assignment for hypothetical *Haemophilus influenzae* gene products through structural genomics. *Current Drug Targets - Infectious Disorders* **2**:339-353.
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Teplyakov, A., Obmolova, O., Chu, S.Y., Toedt, J., Eisenstein, E., Howard, A.J., and Gilliland, G.L. (2003) Crystal structure of YchF protein reveals binding sites for GTP and nucleic acid *J. Bacteriol.* **185**(14):4031-4037.

Lim, K., Tempczyk, A., Parsons, J. F., Bonander, N., Toedt, J., Kelman, Z., Howard, A., Eisenstein, E., Herzberg, O. (2003) Crystal structure of Ybab from *Haemophilus influenzae* (Hi0442), a protein of unknown function coexpressed with the recombinational DNA repair protein RecR. *Proteins: Struct.,Funct.,Genet.* **50**(2):375-79.

Lim, K., Zhang, H., Tempczyk, A., Krajewski, W., Bonander, N., Toedt, J., Howard, A., Eisenstein, E., and Herzberg, O. (2003) Structure of the YibK methyltransferase from *Haemophilus influenzae* (HI0766): a cofactor bound at a site formed by a knot. *Proteins: Struct., Func., Genet.* **51**:56-67.

Teplyakov, A., Obmolova, G., Bir, N., Reddy, P., Howard, A.J., and Gilliland, G.L. (2003) Crystal structure of YajQ protein from *Haemophilus influenzae* reveals a tandem of RNP-like domains. *J. Struct. Funct. Geno.* **4**: 1-9.

Hoang, Q., Sicheri, F., Howard, A., Yang, D. (2003) Bone recognition mechanism of porcine osteocalcin from crystal structure. *Nature* **425**: (October) 977-980.

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Park, K.-W., Webster, D.A., Stark, B.C., Howard, A.J., and Kim, K.-J. (2003) Fusion protein system designed to provide color to aid in the expression and purification of proteins in *Escherichia coli*. *Plasmid* **50**: 169-175.

Ladner, J.E., Obmolova, G., Teplyakov, A., Howard, A.J., Khil, P.P., Camerini-Otero, R.D., and Gilliland, G.L. (2003) Crystal structure of *Escherichia coli* protein ybgl, a toroidal structure with a dinuclear metal site. *BioMed Central Structural Biology* **3**: 7.

Lehmann, C., Doseeva, V., Pullalarevu, S., Krajewski, W., Howard, A., and Herzberg, O. (2004) YbdK is a carboxylate-amine ligase with a γ -glutamyl:cystein ligase activity: crystal structure and enzymatic assays. *Proteins: Struct., Func., Bioinform.* **56**: 376-383.

Khil, P. P., Obmolova, G., Teplyakov, A., Howard, A. J., Gilliland, G. L., Camerini-Otero, R. D. (2004) Crystal structure of the *Escherichia coli* Yjia protein suggests a GTP-dependent regulatory function. *Proteins: Struct., Funct., Bioinform.* **54**: 371-374.

Liu, S., Lu, Z., Han, Y., Jia, Y., Howard, A., Dunaway-Mariano, D., and Herzberg, O. (2004) Conformational flexibility of PEP Mutase. *Biochemistry* **43**: 4447-4453.

Lim, K., Sarikaya, E., Galkin, A., Krajewski, W., Pullalarevu, S., Shin, J-H., Kelman, Z., Howard, A., and Herzberg, O. (2004) Novel structure and

nucleotide binding properties of HI1480 from *Haemophilus influenzae*: A protein with no known sequence homologies. *Proteins: Struct., Func., Bioinform.* **56**: 564-571.

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