

## Petrus H. Zwart

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CONTACT INFORMATION	1 Cyclotron Road ALS, Bldg 6, Room 2134 Berkeley Nat. Laboratories Berkeley, 94720 CA, USA	<i>home phone:</i> +1 510 717 0169 <i>work phone:</i> +1 510 486 4214 <i>work fax:</i> +1 510 486 5664 <i>email:</i> PHZwart@lbl.gov
STATUS	Date and place of birth Sex Marital Status Nationality	May 10, 1976, Anna Paulowna, The Netherlands Male Married Dutch
RESEARCH INTERESTS	Experimental and theoretial crystallographic mehods, (Bayesian) Statistics, Protein and Small Molecule Crystallography, Powder Diffraction, Structural Biology.	
EDUCATION AND RESEARCH	September 1994 – August 1999	M.Sc. Chemistry, University of Amsterdam, Faculty of Chemistry, Laboratory of Crystallography.
	November 1997 – February 1998	Research project at the European Molecular Biology Laboratory (EMBL) in the group of Dr. V.S. Lamzin on the structure solution and refinement of SS-LADH.
	December 1998 – March 1999	Research project at the European Synchrotron Radiation Facility (ESRF) in the group of Dr. H. Graafsma on the crystal structure of deuterated Potassium Phosphate in a static electric field.
	September 1999 – August 2003	PhD-student at European Molecular Biology Laboratory (EMBL), Hamburg Outstation, in the group of Dr. V.S. Lamzin.  Home institute and supervisor: University of Amsterdam, Prof. Dr. H. Schenk. Defense date: December 17, 2003.
	September 2003 – October 2003	Postdoctoral fellow at European Molecular Biology Laboratory (EMBL), Hamburg Outstation, in the group of Dr. V.S. Lamzin.
	February 2004 – November 2005	Postdoctoral fellow with SAIC-Frederick Inc. in the group of Dr. Z. Dauter located at the NSLS, Brookhaven National Laboratories, Upton NY, USA
	November 2004 – March 2005	Postdoctoral fellow with SAIC-Frederick Inc. in the group of Dr. Z. Dauter located at the Argonne National Laboratories, Argonne, IL, USA
	March 2005 – Februari 2007	Postdoctoral fellow in the group of Dr. Adams, Lawrence Berkeley National Laboratories, Berkeley, CA, USA
	March 2007 – Present	Beamline scientist for BCSB beamlines 5.0.1, 5.0.2 and 5.0.3 ( <a href="http://bcsb.als.lbl.gov">http://bcsb.als.lbl.gov</a> ), Advanced Light Source, Berkeley National Laboratories, CA, USA

## AWARDS AND FELLOWSHIPS

June 1999

EMBL Fellowship to carry out PhD-research in the group of Dr. Lamzin.

October 2000

Unilever Research Price for undergraduate work.

## PUBLICATIONS

- Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adams, P.D. (2007). Handling of twinned data in the PHENIX software package. *in preparation*.
- Zwart, P.H.**, Afonine, P.V., Grosse-Kunstleve, R.W., Hung, L-W., Ioerger, T.R., McCoy, A.J., McKee, E., Moriarty, N.W., Read, R.J., Richardson, D., Richardson, J., Sacchettini, J.C., Sauter, N.K., Storoni, L.C., Terwilliger, T.C. & Adams, P.D. (2007) Automated structure solution with the Phenix suite. Chapter in: *Methods in molecular biology*, in the press.
- Zwart, P.H.**, Grosse-Kunstleve, R.W., Lebedev, A., Murshudov, G. & Adams, P.D. (2007). Suprises and pitfalls due to broken symmetry. *submitted*.
- Terwilliger, T.C., Grosse-Kunstleve, R. , Afonine, P.V., Adams, P.D., Moriarty, N.W., **Zwart, P.H.** , Read, R.J., Turk, D. & Hung, L-W. (2007). Interpretation of ensembles created by multiple iterative rebuilding of macromolecular models, *Acta Cryst* **D63**, 597–610.
- Zwart, P.H.** (2005). Anomalous signal indicators in protein crystallography, *Acta Cryst.* **D61**, 1437–1448.
- Zwart, P.H.**, Langer G.G. & Lamzin, V.S. (2004). Modeling Bound ligands in protein crystal structures, *Acta Cryst.* **D60**, 2230–39
- Zwart, P.H.**, Banumathi, S. , Dauter, M. & Dauter, Z. (2004). Radiation-damage-induced phasing with anomalous scattering: substructure solution and phasing, *Acta Cryst.* **D60**, 1958–63.
- Banumathi, S., **Zwart, P.H.**, Ramagopal, U.A., Dauter, M. & Dauter Z. (2004). Structural effects of radiation damage and its potential for phasing, *Acta Cryst.* **D60**, 1085–93.
- Zwart, P.H.** & Lamzin, V.S. (2004). The influence of positional errors on the Debye effects, *Acta Cryst.* **D60**, 220–6.
- Zwart, P.H.** (2003). Error Estimation and Pattern Recognition Techniques in Protein Crystallography. (PhD Thesis).
- Zwart, P.H.** & Lamzin, V.S. (2003). Distance distributions and electron density characteristics of protein models, *Acta Cryst.* **D59**, 2104–13..
- Morris, R.J., **Zwart, P.H.**, Cohen, S., Fernandez, F.J., Kakaris M., Kirillova, O., Vornrhein, C., Perrakis, A. & Lamzin, V.S. (2003). Breaking good resolutions with ARP/wARP, *J. Synch. Rad.* **11**, 56–9.
- Lorentzen, E., Pohl, E., **Zwart, P.**, Stark, A., Russell, R.B., Knura, T., Hensel, R., Siebers, B. (2003). Crystal structure of an archaeal class I aldolase and the evolution of ( $\beta\alpha$ )<sub>8</sub> barrel proteins. *J Biol Chem.* **278**, 47253–60
- Pegasova, T.V., **Zwart P.H.**, Koroleva O.V., Stepanova E.V., Rebrikov D.V. & Lamzin V.S. (2003). Crystallization and preliminary X-ray analysis of a four-copper laccase from *Coriolus hirsutus*. *Acta Cryst.* **D59**, 1459–61.
- Van Langevelde, A., Van Malssen, K., Driessen, R., Goubitz, K., Hollander, F., Peschar R., **Zwart P.**, & Schenk H. (2000). Structure of CnCn+2Cn-type (n = even) beta'-triacylglycerols. *Acta Cryst.* **B56** 1103–11.
- Adolph H.W., **Zwart, P.**, Meijers, R., Hubatsch, I., Kiefer, M., Lamzin, V., Cedergren-Zeppezauer, E. (2000). Structural basis for substrate specificity differences of horse liver alcohol dehydrogenase isozymes. *Biochemistry* **39** 12885–97.

NON  
PEER-REVIEWED  
ARTICLES

Banumathi, S., **Zwart, P.H.**, Dauter, M., Dauter, Z., (2004) Structural effects of radiation damage and its potential for phasing, *National Synchrotron Light Source Science Highlights*, November 5, 2004. (<http://www.nsls.bnl.gov/newsroom/science/2004/11-Dauter.htm>).

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adam, P.D. (2005) Characterization of X-ray data sets. *CCP4 Newsletter No. 42*.

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adam, P.D. (2005) Xtrriage and Fest: automatic assessment of X-ray data and substructure structure factor estimation. *CCP4 newsletter No. 43*

**Zwart, P.H.**, Grosse-Kunstleve, R.W. & Adam, P.D. (2006) Exploring Metric Symmetry. *CCP4 newsletter No. 44*

NOTEWORTHY AC-  
KNOWLEDGMENTS

Kim, J., Sitaraman, S., Hierro, A., Beach, B.M., Odorizzi, G. & Hurley J.H. (2005). Structural Basis for Endosomal Targeting by the Bro1 Domain. *Developmental Cell* **8**,937–47.

ORAL  
PRESENTATIONS

*Coordinate Error estimation of a set of free atoms*, XIXth International Union of Crystallography Conference and General Assembly, August 6–15, 2002, Geneva, Switzerland (**Invited Speaker**).

*Automated Ligand building in ARP/wARP*, Current Trends in Structure Aided Drug Design, May 22–24, 2003, Lund, Sweden (**Invited Speaker**).

*Ligand Fitting*, CCP4 Study Weekend 2004, January 4–5, 2004, Leeds, United Kingdom (**Invited Speaker**).

*Anomalous signal indicators in protein crystallography*, January 21, 2005, University of Madras (host: Prof. Dr. D. Velmurugan), Chennai, India.

*Anomalous signal indicators in protein crystallography*, CCP4 workshop on computational crystallographic methods, March 15–20, 2005, IISc, Bangalore, India (**Invited speaker**).

*Radiation damage induced phasing with anomalous scattering*, ACA annual meeting, May 28 – June 2, 2005, Orlando, USA (**Invited speaker**).

*Data quality assessment with Xtrriage & Automated structure solution with PHENIX*, National University of Singapore (host: Prof. Dr. K. Swaminathan), June 30, 2005, Singapore.

*First aid and Pathology; Data quality assessment with Xtrriage* International Symposium on Recent Trends in Macromolecular Structure and Function, January 18–20, 2006, Chennai, Tamil Nadu, India (**Invited speaker**; Member of organizing committee).

*Data quality assessment with Xtrriage*, Gordon research conference on Diffraction Methods in Structural Biology, June 16–21, 2006, Lewiston, USA.

*General Pathologies*, CCP4 Study Weekend, Januari 4–6, 2007, Leeds, United Kingdom (**Invited speaker**)

*Twinning and PHENIX*, ACA anual meeting, July 21–26, 2007, Salt Lake City, UT, USA.

TEACHING AND  
TUTORIALS

Tutor at beam line X9B during the NSLS *Rapidata 2004* course, April 25–30, 2004, NSLS, Brookhaven, NY, USA.

Tutor in CCP4 workshop on computational crystallographic methods, March 15–20, 2005, IISc, Bangalore, India.

*Automated structure solution with PHENIX*, ALS user meeting workshop, October 20–22, 2005, ALS, Berkeley, USA.

*Data quality assessment with Xtriage*, International Conference on Structural Genomics, October 19–21, 2006, Riken, Yokohama, Japan.

Tutor at beam line X3A during the NSLS *Rapidata 2007* course, April 22–27, 2007, NSLS, Brookhave, NY, USA.

POSTER  
PRESENTATIONS

*Modeling bound ligands in protein crystal structures.* Gordon Research Conference on Diffraction Methods in Structural Biology, June 11–16, Lewiston, USA.

*Radiation-damage induced phasing with anomalous scattering.* Gordon Research Conference on Diffraction Methods in Structural Biology, June 11–16, Lewiston, USA.

*Characterizing X-ray data sets with Xtrriage.* Gordon research conference on Diffraction Methods in Structural Biology, June 16–21, Lewiston, USA.

SKILLS

**Languages**

Dutch: Mother tongue, English: Fluent, German: Good

**Operating systems**

working knowledge of UNIX, LINUX, Windows and Mac OSX

**Programming**

Working knowledge of C++ and python, Limited knowledge of Fortran and Java.

Over two experience with the open source CCTBX crystallographic libraries (<http://cctbx.sf.net>).

**Crystallographic Software**

Experience with most Crystallographic software, notably HKL2000/Denzo/Scalepack, Best, ARP/wARP, Solve/Resolve, SHARP, SHELXC/D/E, SnB, CCP4, Phenix.

Co-author of PHENIX software.

**Synchrotron Crystallography**

Performed experiments on most crystallographic beam lines at the EMBL-Hamburg outstation.

Performed user support and experiments on NSLS beam line X9B.

Performed experiment on SERCAT 22-BM APS beam line.

Performed experiments on sector 8 ALS beam lines.

Beamline scientist responsible for 2 fixed (ALS BL5.0.1. and ALS BL5.0.3.) wavelength and 1 MAD station (ALS BL5.0.2). All three stations have ALS style sample mounters. Approximately 60% of the users are industrial crystallographers.

**Other**

Working knowledge of  $\LaTeX$ .

Refereed a number of crystallographic papers.

I co-supervise a team of 5 scientific engineering associates at the BCSB.

RESEARCH  
SUMMARY

The last two and a half years I have been working on the development of tools that allow users to validate the quality of their experimental data. The result is a program named *Xtrriage* which allows the user to obtain an overview of the presence of problems such as twinning, pseudo-translational symmetry, data anisotropy and possible data processing problems. The analysis carried out by *Xtrriage* will in the future be used to aid the decision making processes in the automated structure solution and refinement methods available in Phenix.

Other developments are in the area of refinement of twinned data, the exploration of relations between different unit cells and space groups (with the automatic generation of non-merohedral twin laws as a special case) as well as substructure solution ( $F_A$  calculation).

Current development of more experimentally oriented methods are focussed on the implementation and optimisation of (semi) automated methods for crystal screening and data collection. I am involved in the development of a new collimator/inline viewing system to be installed at the sector 5 beamlines at the ALS.