



Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

<http://193.49.43.2:8080/smis/servlet/UserUtils?start>

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.



	Experiment title:	Experiment number:
Beamline: BM14	Date of experiment: from: 10/11/2007 to: 12/11/2007	Date of report:
Shifts:	Local contact(s): Dr. Martin Walsh	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Dr. Jochen Kuper, Stefanie Wolski Rudolf Virchow Center - DFG Research Center for Experimental Biomedicine Structure Biology Unit University of Würzburg Versbacher Str. 9 D - 97078 Würzburg		

Report:

Preserving the structural integrity of DNA and hence the genetic information stored in this molecule is essential for cellular survival. It is estimated that the DNA in each human cell acquires about 10^4 damages per day. Consequently, different repair mechanisms have evolved to protect the genome. One of these DNA repair mechanisms, nucleotide excision repair (NER), is present in all organisms and is unique in its versatility to repair a broad range of damages. In humans, NER is the major repair mechanism protecting DNA from damage induced by ultraviolet light. The consequences of defective genes involved in NER are apparent in three severe diseases: xeroderma pigmentosum, Cockayne syndrome and trichothiodystrophy. The XPD protein plays a key role in NER because it verifies the presence of damage on the DNA and thereby allows the repair cascade to proceed. We have solved the crystal structure of XPD, and show how the protein has assembled several domains to form a donut shaped molecule, which is able to separate two DNA strands and scan the DNA for damage with the aid of a 4Fe-4S cluster. (Wolski and Kuper et al, PLoS Biol (2008), 6(6): e149)

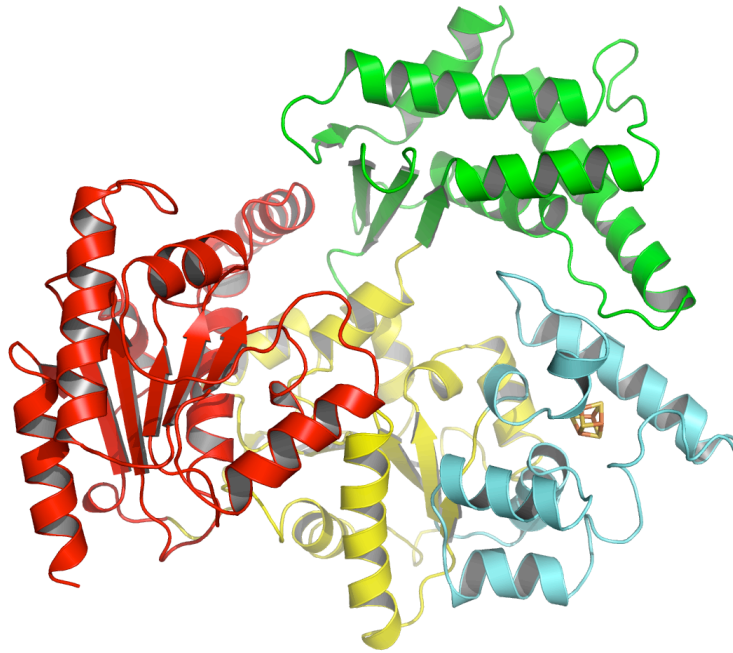


Figure 1: Overall structure of XPD. (Wolski and Kuper ; PDB:2vsf)

Table I: Crystallization, Data Collection and Refinement Statistics

Data set	Native	Fe Peak	Fe Inflection	Fe Remote
Resolution (Å)	2.9	3.6	3.6	3.6
Wavelength (Å)	1.0	1.7367	1.7419	1.7
Unique Reflections	13,622	6,963	6,967	6,909
$\langle I \rangle / \langle \sigma I \rangle$	38.3 (1.7)	23.1 (4.5)	19 (3.9)	32.6 (16.1)
Completeness (%)	99.0 (99.4)	99.9 (100)	100 (100)	99.2 (100)
Redundancy	4	14.8	12.4	14.3
R_{sym}	0.07 (0.617)	0.14 (0.52)	0.16 (0.59)	0.07 (0.17)
Phasing to 4.0 Å				
Number of sites			1	
Phasing Power				
Ano		1.505	0.758	1.915
Iso (acentric/centric)		0.303/0.288	1.236/0.987	
Mean Figure of merit				
Acetnric/centric			0.43/0.15	
$R_{cryst} (R_{free})$	0.209 (0.287)			
r.m.s. deviations bond lengths (Å)	0.007			
r.m.s. deviations bond angles (°)	0.92			
Mean B-factor (Å ²)	54.2			
Ramachandran Statistics	86.6/11.1/1.5 /0.8			

References: Wolski and Kuper et al, PLoS Biol (2008), 6(6): e149