

Experimental Report – MX-831

"Photolesion recognition and repair by the DNA (6-4) photolyase from *Drosophila melanogaster*"

Quality of measurement/data and status / progress of evaluation

Co-crystals from the (6-4) photolyase from *Drosophila melanogaster* in complex with a DNA double strand containing the 6(T-C)4 photolesion were obtained and diffracted X-rays to 2.9 Å spacing. Data processing statistics are shown in Table 1 and the structure was solved by molecular replacement using the coordinates of the enzyme in complex with DNA containing the 6(T-C)4 photolesion (PDB code 3CVU).

Results

The protein molecule flips-out the lesion into its active site (Fig. 1). Only minor differences to the photolyase in complex with the 6(T-T)4 lesion can be observed.

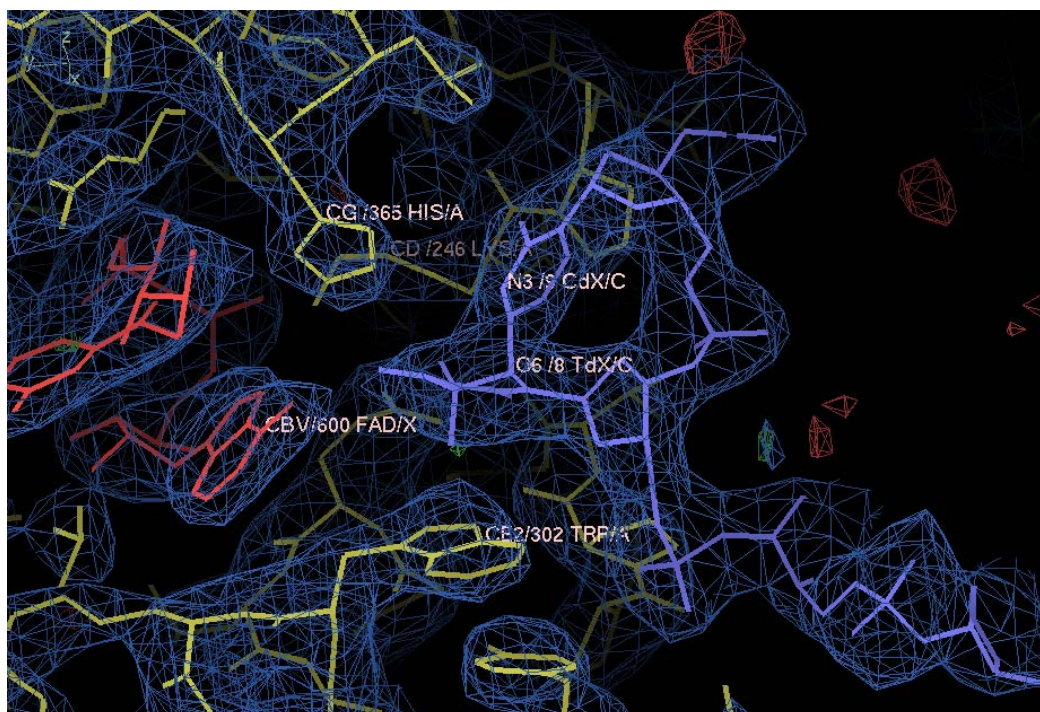


Figure 1 The flipped-out 6(T-C)4 photolesion in the active site of the enzyme. The DNA is colored in blue, the FAD cofactor in red and the protein in yellow. 2Fo-Fc electron density contoured at 1 σ level.

The preliminary structure refinement statistics are summarised in Table 1. Model building, refinement as well as crystal optimisation are currently under way.

Table 1: Data collection, processing and preliminary structure refinement statistics.

| | |
|------------------------|---|
| Data collection | |
| Spacegroup | P2 ₁ 2 ₁ 2 ₁ |
| Cell dimensions | 86.4, 88.7, 90.4 |
| Rmerge | 0.07 (0.41) |
| Number of observations | 14835 |
| Mean I/ σ I | 11.9 (3.5) |
| Completeness | 99.9 (100) |
| Multiplicity | 5.3 (5.6) |
| Refinement | |
| Resolution | 44.0 - 2.95 |
| Rwork/Rfree | 21.3 / 24.7 |
| R.m.s Bond | 0.012 |
| R.m.s. Angle | 1.28 |
