Poster Presentations

[MS12-P02] Radiation-induced Disorder of a Protein Crystal. Tatiana Petrova,[1,2] Vladimir Y. Lunin,[1] Stephan Ginell,[2] Andre Mitschler,[3] Youngchang Kim,[2] Grazyna Joachimiak,[2] Alexandra Cousido-Siah,[3] Isabelle Hazemann,[3] Alberto Podjarny,[3] Krzysztof Lazarski,[2] and Andrzej Joachimiak[2]

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At cryogenic temperatures, the radiation damage to protein crystals manifests itself at different levels: as local chemical changes, overall structural changes of a protein molecule, and global crystal disorder. The latter shows up mainly as the degradation of the crystal diffraction pattern. The exact mechanism of the crystal disorder at the atomic level and its interrelation with local damage are unknown. In our previous studies, multiple data sets corresponding to increasing absorbed doses were consequently collected from the same crystals of aldose and elastase ([1], [2]). The refined models obtained corresponded to an increase in crystal disorder, which was characterized by a decrease in the maximum value of resolution of diffraction data, the appearance of new conformations for protein residues, the displacements of protein atoms and water molecules, and the increase in atomic displacement parameters (ADPs) and R-Rfree values. By using these characteristics, the radiation-induced disorder of a single elastase crystal was compared with the crystal ordering in different crystals. It was found that irradiation gives rise to new conformations for some residues localized in the nearest vicinity of those residues that were damaged by x-rays (for example, in the vicinity of damaged Glu, Asp, and disulfide bridges). An analysis revealed a distinct increase in ADP values for the atoms of some side chain residues, which also can be explained by possible appearance of multiple conformations. It was also found that, along with the X-rays-induced displacement of the water network, irradiation causes changes in the length of hydrogen bonds between water molecules and between water molecules and protein atoms. These changes can be due to a decrease in occupancy values (which are masked by an increase in ADPs and cannot be detected) of either protein atoms or water molecules. The displacements of water molecules involved in crystal contacts and changes of the corresponding hydrogen bond lengths were observed. This suggests that the radiation-induced displacement of water molecules can cause a weakening of crystal contacts.

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[2]. Petrova,T., Ginell, S., Mitschler,A., Kim, Y., Lunin, V.Y., Joachimiak, G., Cousido-Siah, A., Hazemann, I, Podjarny,A., Lazarki, K. & Joachimiak, A. (2010). *Acta Cryst.* **D66**, 1075-1091.

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