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Supporting information for article:

Radiation-damage investigation of a DNA 16-mer

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Supplementary Material

Radiation damage investigation of a DNA 16-mer

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Supplementary Table 1. The non-water atoms listed in the top 25 radiation damage sites based on the D_{neg} $(atom)$ values from RIDL (Bury and Garman 2018) for datasets 7, 13, 19, 25, 31 and 37, respectively, which are 60° wedges of the same irradiated crystal volume. (Atom names are listed with nucleotide IDs in parentheses. Different building blocks of the DNA chain are colour-coded: nucleotide base: light blue, deoxyribose moiety: yellow, phosphate moieties: orange, calcium ions: grey. O3' and O5' atoms of the sugar are coloured light orange as they are also part of the phosphate groups.)

Dataset No.	**7**	**13**	**19**	**25**	**31**	**37**
Dose (MGy)	**6.2**	**12.0**	**17.7**	**23.5**	**29.2**	**35.0**
Atom name (residue id)	N4(C14)	P(A15)	P(A15)	P(A15)	O5'(G5)	P(G16)
	P(G16)	P(G5)	P(G5)	P(G5)	P(G5)	Ca^{2+} (2)
	C2(G2)	O5'(A15)	O5'(G5)	O5'(G5)	C8(G6)	C8(G6)
	O3'(G5)	O5'(G5)	C8(G6)	C8(G6)	P(G16)	P(G5)
	P(G5)	C5'(A15)	P(G6)	P(G16)	N7(G6)	P(G6)
	P(G6)	O5'(T10)	OP2(G6)	O5'(A15)	P(A15)	Ca^{2+} (1)
	Ca^{2+} (4)	C8(A7)	P(G16)	C5'(G6)	C4'(G5)	C5'(G6)
	N7(G6)	C4'(A15)	N7(G6)	C4'(G5)	O5'(G16)	O3'(A15)
	C2(C13)	O3'(A8)	OP1(G5)	N1(C17)	P(G6)	P(A7)
	O5'(A15)	C4(G2)	P(A9)	P(G6)	O5'(A15)	O3'(G16)
	O4(T12)	C5(G6)	C5'(C3)	P(A7)	P(A7)	C4'(G5)
	O5'(G2)	OP1(G5)	Ca^{2+} (4)	C5'(G5)	Ca^{2+} (2)	O5'(G16)
	P(A8)	P(C14)	O5'(A9)	N7(G6)	P(C17)	O5'(G5)
	O4'(G5)	C5'(T10)	O5'(A15)	O5'(G16)	OP1(G16)	P(A15)
	O3'(C17)	C6(G6)	O3'(C13)	O3'(A15)	N1(C17)	P(C17)
		O3'(C17)	C4(C3)	Ca^{2+} (4)	C5'(G5)	OP1(A7)
		C4(C3)	O5'(T10)	C4'(T10)	O3'(A15)	O3'(G5)
		C2(G6)	C6(C3)	C4'(A15)	Ca^{2+} (4)	OP1(C17)
		OP1(T12)	O5'(C17)	O3'(G6)	O3'(G16)	C5'(G5)
				C4'(A7)	C1'(G6)	N7(G6)
				O3'(G5)	C5'(G6)	OP2(G16)
				P(C17)	OP2(G16)	C4'(G16)
				O5'(A7)		C3'(G16)

Supplementary Table 2. Comparison of sites in proximity to calcium ions with those most affected by radiation damage. Rows for nucleotides not involved in calcium-binding are coloured grey.

Residue ID	No. of interactions*: **- directly coordinating Ca^{2+}** (in bold)**,** - water-mediated binding of Ca^{2+}				Number of atoms involved in the top 25 damage sites**			
	base	sugar	phosphate before or after	**all**	base	Sugar	phosphate before or after	**all**
2 G			1	**1**	1		2	**3**
3 C			1	**1**		1	2	**3**
4 T	1			**1**			3	**3**
5 G			1	**1**	1	3	7	**11**
6 G			**2**+1	**3**	6	2	8	**16**
7 A	1		**2**+1	**4**	3		4	**7**
8 A	1		**1**	**2**	3		2	**5**
9 A				**0**			2	**2**
10 T				**0**				**0**
11 T				**0**			2	**2**
12 T				**0**	1		2	**3**
13 C				**0**			1	**1**
14 C				**0**	1		5	**6**
15 A			**1**	**1**	0	3	9	**12**
16 G	1		**2**	**3**		3	10	**13**
17 C			**1**	**1**	1	1	5	**7**

*Detailed for **base/sugar/phosphate before or after** the residue moieties of each residue (visually inspected in *COOT*).

**Indicated by $D_{loss}{}^{\rho}$ (*atom*) for structures from datasets 7, 13, 19, 25, 31 and 37, respectively (calculated using *RIDL*).

$$D_{loss}{}^{\rho}(atom) = \frac{max_{v \in Vatom} - [\rho_{\Delta}(v)\ \rho_{\mathrm{calc}}(v)]}{max_{v \in Vatom}[\rho_{\mathrm{calc}}(v)]}$$

where $\rho_{\Delta}(v)$ is the difference density map, $F_{obs,n}$ - $F_{obs,1}$, and $\rho_{calc}(v)$ is the electron density map calculated using F_{calc} amplitudes and φ_{calc} phases of the refined model at a voxel, v, within the volume pertaining to that atom, V_{atom}.

Supplementary Figure 1

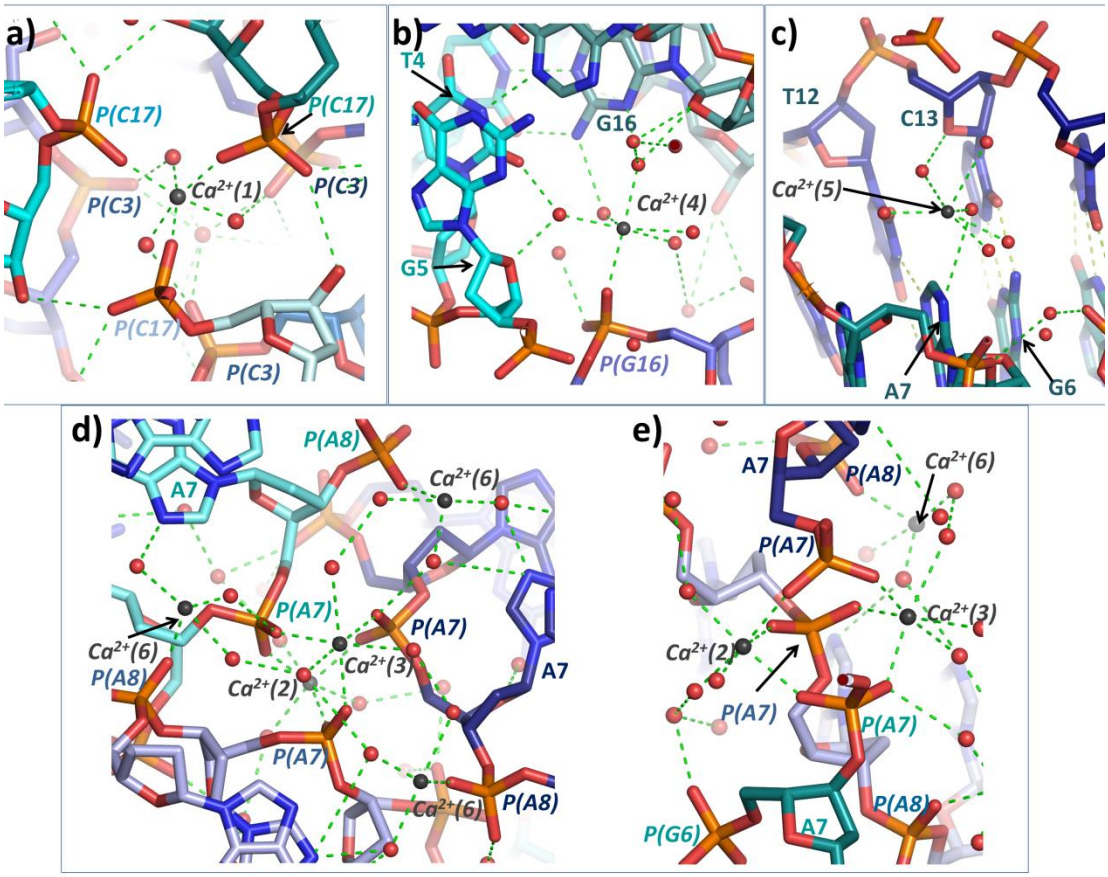

Figure 1. Coordination spheres of the calcium ions in the DNA structure. The binding environments of (a) $Ca^{2+}(1)$, (b) $Ca^{2+}(4)$, (c) $Ca^{2+}(5)$, and (d) $Ca^{2+}(2)$, $Ca^{2+}(3)$ and $Ca^{2+}(6)$ are shown. (e) A close up of three symmetry equivalent phosphates (of the A7 nucleotide) coordinating two calcium ions. $Ca^{2+}(1)$, $Ca^{2+}(2)$ and $Ca^{2+}(3)$ are positioned on a vertical crystallographic threefold axis. Atoms are shown as follows: carbon, sky blue, light blue, dark blue and teal for different DNA chains; phosphorus, orange: oxygen, red, and nitrogen, dark blue. Phosphorus atoms are labelled with the one letter code and number of the nucleotide to which they belong. Hydrogen bonds are shown in green (having donor-acceptor distance < 3.5Å).

Supplementary Figure 2.

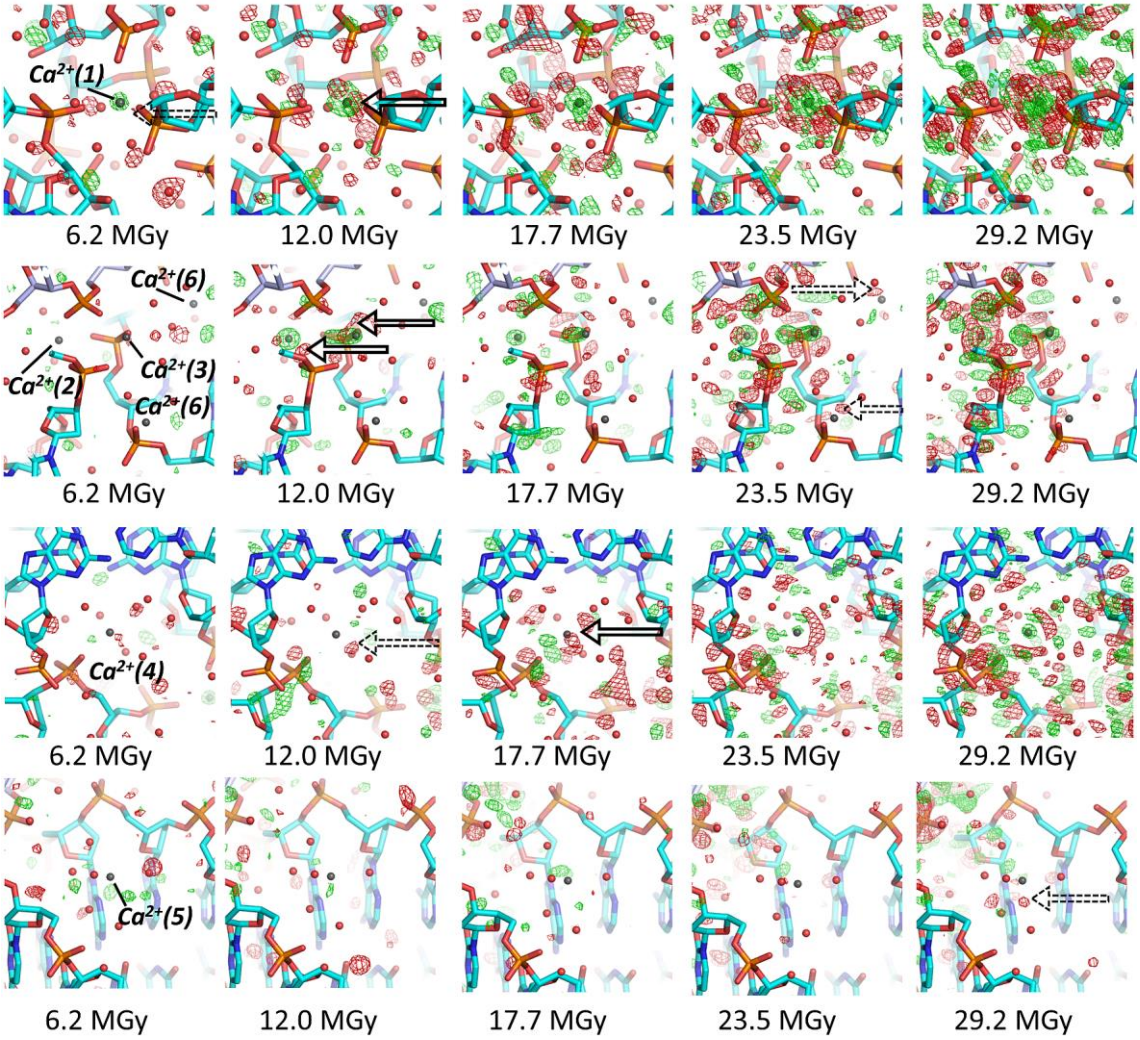

Figure 2. Electron density changes at the calcium sites. $F_{obs,n}$ - $F_{obs,1}$ difference electron density maps calculated using RIDL for datasets n = 7, 13, 19, 25 and 31 are contoured at 3.0σ and -3.0σ levels in green and red, respectively. The calcium ions are shown in grey and they are labelled in the left panels. Black arrows show electron density loss commencing around Ca^{2+} ions. The positive difference electron density contoured in green around Ca^{2+}(1) and Ca^{2+}(2) at doses of 6.2 MGy and 12.0 MGy, respectively, indicate reduction of the metal ions.

Supplementary Figure 3

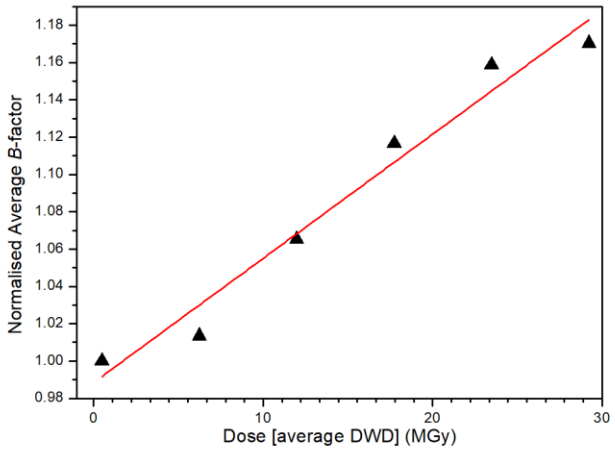

Figure 3. Average atomic *B*-factors for the structures derived from the 1st, 7th, 13th, 19th and 31st datasets against dose (MGy), normalised to that of the structure from the lowest dose dataset. A linear fit to the data is shown, giving a gradient of approximately 0.007 MGy^{-1}.

Reference

Bury, C. S. & Garman, E. F. (2018). *J. Appl. Crys* **51**, 952-962.