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## Supplementary Table 1

### Summaries of interactions in pre-threaded T5FenD153K DNA complex C1

Buried area upon the complex formation (Å <sup>2</sup> )	1383.1							
Buried area upon the complex formation (%)	7.33							
Interface area (Å <sup>2</sup> )	691.6							
Interface area protein (%)	5.02							
Interface area DNA (%)	13.58							
Polar buried area upon the complex formation (Å <sup>2</sup> )	726.4							
Polar Interface (%)	52.52							
Polar Interface area (Å <sup>2</sup> )	363.2							
Non polar buried area upon the complex formation (Å <sup>2</sup> )	656.8							
Non polar Interface (%)	47.48							
Non polar Interface area (Å <sup>2</sup> )	328.4							
Protein residues at the interface	38							
Nucleotides residues at the interface	27							
<b>Hydrogen Bonding</b>								
<b>H-bond acceptor</b>				<b>H-bond donor</b>				
<b>Residue</b>	<b>Res. No.</b>	<b>Atom</b>	<b>Chain</b>	<b>Residue</b>	<b>Res. No.</b>	<b>Atom</b>	<b>Chain</b>	<b>Distance (Å)</b>
Lys	153	NZ	A	dA	2	OP1	X	2.64
<u>Arg</u>	86	NH1	A	dA	2	OP2	X	3.18
<u>Arg</u>	86	NH2	A	dA	2	OP2	X	3.34
<u>Thr</u>	170	OG1	A	dA	2	N3	X	3.13
<u>Gly</u>	154	N	A	dA	3	OP1	X	2.81
<u>Gly</u>	213	N	A	dA	9	OP1	Y	2.87
<u>Ala</u>	214	N	A	dA	9	OP2	Y	3.49
<u>Arg</u>	216	N	A	dA	9	OP1	Y	2.86
Lys	215	N	A	dA	9	OP2	Y	3.15
<u>Gly</u>	211	N	A	<u>dC</u>	10	OP1	Y	2.75
dA	2	O3'	X	<u>Thr</u>	152	O	A	3.29

\* Details of interactions between oligonucleotide 5ov4 (chains X and Y) and T5FenD153K (Chain A) determined using COCOMAPS (Vangone, A., Spinelli, R., Scarano, V., Cavallo, L. & Oliva, R. *Bioinformatics* **27**, 2915–2916, 2011) and PDBePISA (Krissinel, E. & Henrick, K. *J. Mol. Biol.* **372**, 774–797, 2007).

## Supplementary Table 2

### Summaries of interactions in fully threaded T5FenD153K DNA complex C2

Buried area upon the complex formation (Å <sup>2</sup> )	2415.2							
Buried area upon the complex formation (%)	12.57							
Interface area (Å <sup>2</sup> )	1207.6							
Interface area protein (%)	8.55							
Interface area DNA (%)	23.71							
Polar buried area upon the complex formation (Å <sup>2</sup> )	1329.6							
Polar Interface (%)	55.05							
Polar Interface area (Å <sup>2</sup> )	664.8							
Non polar buried area upon the complex formation (Å <sup>2</sup> )	1085.6							
Non polar Interface (%)	44.95							
Non polar Interface area (Å <sup>2</sup> )	542.8							
Protein residues at the interface	41							
Nucleotides residues at the interface	16							
<b>Direct hydrogen bonds between protein and DNA</b>								
<b>H-bond acceptor</b>				<b>H-bond donor</b>				
<b>Residue</b>	<b>Res. No.</b>	<b>Atom</b>	<b>Chain</b>	<b>Residue</b>	<b>Res. No.</b>	<b>Atom</b>	<b>Chain</b>	<b>Distance (Å)</b>
<u>dC</u>	12	N1	X	<u>Phe</u>	32	O	B	3.41
<u>Arg</u>	216	A	NE	<u>dA</u>	4	O3'	X	3.57
<u>Lys</u>	215	N	B	<u>dG</u>	5	OP1	X	3.27
<u>Gly</u>	213	N	B	<u>dG</u>	5	OP2	X	2.82
<u>Ala</u>	214	A	N	<u>dG</u>	5	OP1	X	3.45
<u>Arg</u>	216	N	B	<u>dG</u>	5	OP2	X	2.96
<u>Gly</u>	211	N	B	<u>dC</u>	6	OP1	X	2.7
<u>Arg</u>	86	NH1	B	<u>dA</u>	3	OP2	Y	3.23
<u>Gly</u>	70	N	B	<u>dA</u>	4	OP1	Y	3.4
<u>Gly</u>	70	N	B	<u>dA</u>	4	OP2	Y	3.08
<u>Tyr</u>	90	OH	B	<u>dA</u>	4	O3'	Y	3.58
<u>Arg</u>	86	NH1	B	<u>dA</u>	4	OP2	Y	3.03
<u>Arg</u>	86	NH2	B	<u>dG</u>	5	OP1	Y	2.88
<u>Tyr</u>	90	OH	B	<u>dG</u>	5	OP2	Y	2.56
<u>Gly</u>	154	N	B	<u>dG</u>	7	OP1	Y	2.87

\* Details of interactions between two copies of oligonucleotide 5ov4 (chains X and Y) and T5FenD153K (Chain A) that form complex 2 (see Fig. 4 and Supplementary Fig. 3) determined using COCOMAPS and PDBePISA.

### Supplementary Table 3

#### Summary of interactions in T5FenD155K–DNA pseudo-product complex C3

Buried area upon the complex formation (Å <sup>2</sup> )				3186.3				
Buried area upon the complex formation (%)				16.8				
Interface area (Å <sup>2</sup> )				1593.2				
Interface area protein (%)				11.8				
Interface area DNA (%)				29.2				
Polar buried area upon the complex formation (Å <sup>2</sup> )				1616.6				
Polar Interface (%)				50.7				
Polar Interface area (Å <sup>2</sup> )				808.3				
Non polar buried area upon the complex formation (Å <sup>2</sup> )				1569.7				
Non polar Interface (%)				49.3				
Non polar Interface area (Å <sup>2</sup> )				784.9				
Protein residues at the interface				49				
Nucleotides residues at the interface				22				
<b>Hydrogen Bonding</b>								
<b>H-bond acceptor</b>				<b>H-bond donor</b>				
Residue	Res. No.	Atom	Chain	Residue	Res. No.	Atom	Chain	Distance (Å)
Asn	29	ND2	A	dG	1	O4'	X	3.63
Arg	86	NH2	A	dG	1	O5'	X	3.37
Lys	89	NZ	A	dG	1	O6	X	3.87
Gly	154	N	A	dG	1	O3'	X	3.77
Gly	154	N	A	dA	2	OP1	X	2.96
Ile	212	N	A	dC	4	O3'	X	3.81
Gly	213	N	A	dC	4	OP1	X	2.80
Lys	215	N	A	dC	4	OP2	X	3.17
Arg	216	N	A	dC	4	OP1	X	2.83
Gly	211	N	A	dT	5	OP1	X	2.86
Ala	214	N	A	dC	4	OP2	X	3.48
Lys	241	N	A	dG	10	OP2	X	3.35
Lys	35	NZ	A	dC	11	OP2	X	3.78
Asn	37	ND2	A	dC	11	OP1	X	2.80
Arg	33	NH2	A	dA	13	O3'	X	3.15
Arg	172	NH2	A	dT	13	O3'	X	3.45
Lys	71	NZ	A	dT	14	OP2	X	2.90
Arg	125	NH1	A	dC	15	OP1	X	2.85
Gly	70	N	A	dG	16	OP1	X	2.79
Asn	29	ND2	A	dG	17	O3'	X	2.86
Arg	86	NH1	A	dG	17	OP1	X	3.33
dG	1	O3'	X	Thr	152	O	A	3.20
dG	10	N2	X	Thr	94	OG1	A	2.88
dA	13	N6	X	Asn	38	OD1	A	3.47

\* Details of interactions between oligonucleotide 3ov6 (chain X) and T5FenD155K (Chain A) determined using COCOMAPS and PDBEPIA. DNA strands X, Y and Z (Fig. 5) correspond to symmetry related copies of 3ov6 residues 13–17, 1–12 and 1–11 respectively (Supplementary Fig. 4a–c).