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Supporting Information

Accommodation of a 1S (–)-Benzo[c]phenanthrenyl-N⁶-dA Adduct in a Y Family Dpo4 DNA Polymerase Active Site: Structural Insights through Molecular Dynamics Simulations

Lihua Wang¹, Min Wu^{2,4}, S. Frank Yan^{2,5}, Dinshaw J. Patel³, Nicholas E. Geacintov^{*,2}, Suse Broyde^{*,1,2}

¹Department of Biololgy and ²Department of Chemistry, New York University, New York, NY 10003 ³Cellular Biochemistry & Biophysics Program, Memorial Sloan-Kettering Cancer Center, New York, NY 10021

⁴Current address: Pfizer Global Research and Development, La Jolla Laboratories, San Diego, CA 92121

⁵Current address: Genomics Institute of the Novartis Research Foundation, San Diego, CA 92121

*Corresponding authors: (212) 998-8231, Fax (212) 995-4015, broyde@nyu.edu; (212) 998-8407, Fax (212) 998-8421, ng1@nyu.edu

Running Title: Benzo[c]phenanthrenyl- N^6 -dA adduct in Dpo4

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Tables

Table S1. Torsion angles in modeled Dpo4 ternary complexes from Type I and Type II crystal structures. a

Model	Residue	α (°)	β (°)	γ(°)	δ (°)	€ (°)	ζ (°)	χ (°)
Control and Major	tG_1	N/A	N/A	36.4	156.4	155.0	-94.6	116.0
Groove Type I	tG_2	139.8	-132.8	116.1	146.1	-103.2	127.8	-139.1
	tG_1	N/A	N/A	36.3	156.4	155.0	-95.2	-97.8
	tG_2	-46.8	-146.0	36.4	156.4	-62.3	-129.9	-97.8
	tA ₃	-112.9	-150.7	-47.0	138.5	-177.0	-110.3	-114.0
Intercalation	tC_4	-87.2	-94.3	36.3	156.4	107.0	-80.0	148.9
	tA*5	-114.3	125.7	132.6	135.4	-151.3	-89.1	-35.5
	tA ₆	-79.2	-175.4	52.6	146.1	-161.0	-112.1	-99.3
	tG ₇	-65.0	171.2	47.6	119.8	-179.1	-120.7	-111.1
	tG_1	N/A	N/A	36.4	156.4	154.9	-95.2	-97.8
-1 Deletion	tG_2	-46.8	-146.1	36.4	156.4	-62.3	-108.8	-97.7
	tA ₃	-135.2	-172.2	-5.2	-138.5	-143.3	-150.4	-114.1

^{*a*} N/A denotes values not applicable to the terminal residue. Italicized numbers denote crystal values.

Model	Hydrogen Bond ^{<i>a</i>}	Occupancy ^b	
	$(Arg51)N\eta1-H\eta12O2\gamma(dTTP)$	100%	
	$(Arg51)N\eta2-H\eta22O3\beta(dTTP)$	99.70%	
	$(Arg51)N\eta2-H\eta22O2\gamma(dTTP)$	90.90%	
	$(Thr 45)O\gamma 1 - H\gamma 1O1\beta(dTTP)$	99.5%	
	$(Tyr10)N-HO2\gamma(dTTP)$	95.60%	
	$(Tyr10)N-HO1\gamma(dTTP)$	61.40%	
	$(Tyr10)N-HO3\beta(dTTP)$	33.20%	
Control	$(Phe11)N-HO2\beta(dTTP)$	95.30%	
	(Tyr12)N–HO3′(dTTP)	81.75%	
	(Lys159)Nζ–Ηζ1Ο3γ(dTTP)	44.65%	
	(Lys159)Nζ–Hζ3O3γ(dTTP)	32.50%	
	(Lys159)Nζ–Ηζ2Ο3γ(dTTP)	21.70%	
	$(Lys159)N\zeta - H\zeta 1O2\gamma(dTTP)$	6.60%	
	$(Lvs159)N\zeta - H\zeta 3O2\gamma(dTTP)$	4.65%	
	$(Lvs159)N\zeta - H\zeta 2O2\gamma(dTTP)$	4.10%	
	(Arg51)Nn1-Hn12O1v(dTTP)	98.75%	
	(Arg51)Nn2-Hn22O3v(dTTP)	95.94%	
	(Arg51)Nn2-Hn22O1v(dTTP)	40.62%	
	(Arg51)Nn1-Hn12O3v(dTTP)	36.27%	
	(Arg51)Nn1-Hn12 O1B(dTTP)	12.06%	
	(Thr 45)Ov1-Hv1 O3v(dTTP)	36 51%	
	$(\text{Tyr}10)$ N-HO1 γ (dTTP)	16.41%	
	(Tyr 12)On-Hn O3'(dTTP)	14.71%	
	$(Tyr12)On_Hn = 375O4'(dTTP)$	7 15%	
	(1 y 12) O (1 m 1 3750 + (a T T T)) (I v 159) N(-H(1 O 1B(dTTP))	42.47%	
	$(Lys159)N\zeta H\zeta 1 Oly(dTTP)$	18 51%	
	$(Lys159)N\zeta H\zeta 2 O1B(dTTP)$	12.06%	
	$(Lys159)N\zeta -\Pi \zeta 2O1p(d111)$ $(Lys159)N\zeta H\zeta 2O1p(d111)$	12.00%	
	$(Lys159)N\zeta = H\zeta 2 \dots O1p(dTTT)$	10.86%	
	$(Lys159)N\zeta -\Pi \zeta 2OT \gamma(dTTT)$	9.65%	
	$\frac{(Lys139)N\zeta - H\zeta 3OT}{(UTTP)}$	40.10%	
	$(\text{Alg}_{J})[\text{NI}]_{Z} = \text{HI}_{ZZ} \dots \text{OI}_{\gamma}(\text{dCIP})$ $(\text{The}_{45})[\text{Out}_{J}][\text{He}_{J}] = O_{Z}^{2} (\text{dCTP})$	40.10%	
Intercalation	$(1 \Pi f 45) O \gamma I - \Pi \gamma I \dots O 5 \gamma (d C I P)$ $(T_{M} r 10) N H = O 1 u (d C T P)$	99.9% 20.10%	
	$(Tyr10)N = H \dots OT\gamma(dCTP)$	30.10% 10.75%	
	$(Tyr10)N = H = O2\beta(dCTP)$	19.75%	
	(Tyr12)On Hn = 275O2(dCTD)	99.05%	
	$(1y_{112})0y_{111} = 111(,37502(dCTT))$	10 35%	
	$(Lys159)N\zeta - H\zeta 2 \dots O1\beta(dCTP)$	12.80%	
	$(Lys159)N\zeta = H\zeta 5O1p(dC1P)$	1 25%	
	$\frac{(Lys159)N\zeta - H\zeta IOIp(dCIP)}{(T_{curr}12)Op Hp O2/(dATP)}$	08.60%	
	(1yf12)O[-H[1O3(dA1P)]	98.00%	
	$(\text{Args1})\text{Nr}[1-\text{Hr}[1201\gamma(syn-dATP)]$	99.30%	
	$(\text{Args1})\text{N}\eta 2 - \text{H}\eta 22\text{O}3\gamma(\text{syn-dATP})$	92.55%	
	(Argo1)N η 2-H η 22O γ (syn-dA1P) (The 45)Oct 1 Hel - O2 (14TD)	18.33%	
	$(1 \text{ Inr45}) \text{Uy1} - \text{Hy1} \dots \text{U3y}(\text{syn-dA1P})$	37.03% 27.00%	
	$(1y_{110})N = \Pi \dots O1\gamma(Syn-dA1P)$	27.00%	
	$(1y_{110})N = \Pi \dots O_2\gamma(syn - OATP)$ (Tyr10)N H O3B(syn - OATP)	1.23%	
	$(1y_{110}) = 110y_{(3y_{1}-uA1F)}$ $(Ty_{12}) = 02'(y_{1}-uA1F)$	33.20% 88 700/	
	$(1y_{112})\cup_{ -\Pi \cup 3}(sy_{l-}(AIP))$	65 000/	
	$(Ly_{S1},S)_{IV} = \Pi_{S} \dots \cup Ip(Syn-uAIP)$ $(Ly_{S1},S)_{IV} = \Pi_{S} \dots \cup Ip(Syn-uAIP)$	10 200/0	
	(Lysisy)ing-mg2Oip(syn-dAIP)	18.20%	

Table S2. Hydrogen bonding interactions of > 10% occupancy or bifurcated hydrogen bonds between polymerase residues and the sugar-triphosphate backbone of the incoming dNTP.

	(Lys159)Nζ–Hζ1O1β(<i>syn</i> -dATP)	15.25%
	(Arg51)Nη2–Hη22O3γ(dGTP)	89.40%
	(Arg51)Nη1–Hη12Ο1γ(dGTP)	72.90%
Intercalation	(Arg51)Nη2–Hη22Ο1γ(dGTP)	22.60%
(Cont'd)	(Arg51)Nη1–Hη12O3γ(dGTP)	16.15%
	$(Thr45)O\gamma 1-H\gamma 1O3\gamma (dGTP)$	16.05%
	(Tvr12)On–Hn375O4'(dGTP)	10.65%
	$(Lvs159)N\zeta - H\zeta 2O1\beta(dGTP)$	32.55%
	(Lvs159)N(-H(1 O1B(dGTP)))	32.00%
	$(I_{vs159})N\zeta - H\zeta_3 = O1\beta(dGTP)$	28.30%
	(Lys159) N ζ -H ζ 2 Ω 1 ω (dGTP)	9 350%
	$(Lys159)N\zeta -H\zeta 1 - \Omega_{10}(dGTP)$	6 30%
	$(Lys159)N\zeta H\zeta 3 Oly(dGTP)$	4 70%
	(dGTP)O3' HO3' O82(Asp105)	4.70%
	$(4011)05 - 1105 \dots 002(Asp105)$	09.10%
	(ArgS1) N η 1- Π η 1201 γ (syn-dO1P) (ArgS1)N η 2. H η 2202 (syn-dO1P)	99.40% 00.00%
	$(\text{Arg51})\text{NH}_2 - \text{HH}_22 \dots \text{O5}\gamma(\text{syn-dGTP})$	99.00% 70.00%
	(Algo 1) Γ [22 U [γ (Syn-dU IP) (Thr 45) Ω (1.1. Ω (2 10TP)	70.00%
	$(1\Pi F45)U\gamma I - H\gamma I \dots U5\gamma(syn-dU1P)$	20.20%
	$(1y_{110})N = H \dots O1\gamma(syn-dO1P)$	J/.8U%
	$(1yf10)N-HO2\gamma(syn-dG1P)$	9.30%
	(Pho11)N + O2q(syn-dOTP)	5 25%
	(FileT1) N-HOS $\gamma(\text{syn-dOTF})$ (Tyr12)N-H. O2'(syn-dCTP)	J.2.3% 11.30%
	$(1y_{112})N = 1105 (syn-dOTT)$ (Lyg_150)NZ $HZ_1 = O1B(syn-dOTT)$	11.30%
	$(Lys159)N\zeta -H\zeta 1OIp(syn-dOIP)$	48.20%
	$(Lys159)N\zeta -H\zeta 2OIP(syn-dOIP)$	20.75%
	$(Lys139)N\zeta = H\zeta 5OIP(syn-dOIP)$	21.03%
	$(Aig_{31})Ni[1-Hi][1205\gamma(011P)]$	99.00%
	$(Arg_{51})N\eta_{2}-H\eta_{22}O_{3p}(d_{11P})$	03.00% 10.20%
	$(\text{ArgS1})N\eta 2 - H\eta 22O3\gamma(\text{d11P})$	19.30%
	$(\text{Arg}51)$ N η 1–H η 12O3 β (dTTP)	17.95%
	$(\text{Arg}51)$ N η 2–H η 22OI β (dTTP)	12.40%
	$(Tyr10)N-HO2\gamma(dTTP)$	100%
	$(PneII)N-HOI\beta(dIIP)$	27.45%
	(1yr12)N-H03(d11P)	91./5%
	$(1yr12)O\eta - H\eta 3/5O2(d11P)$	7.90%
Major	$(Tyr48)O\eta -H\eta O3\gamma(dTTP)$	93.35%
Groove	$(Lys159)N\zeta - H\zeta 3O1\gamma(dTTP)$	51.20%
I ype I	$(Lys159)N\zeta - H\zeta 1O1\gamma (dTTP)$	44.40%
	$(Arg51)N\eta 2-H\eta 22O3\beta(dCTP)$	87.25%
	(Arg51)Nη1–Hη12O2γ(dCTP)	85.40%
	(Arg51)Nη2–Hη22O2γ(dCTP)	34.80%
	$(Arg51)N\eta2-H\eta22O1\beta(dCTP)$	22.10%
	$(Arg51)N\eta1-H\eta12O3\beta(dCTP)$	15.35%
	$(Thr 45)O\gamma 1-H\gamma 1O1\beta(dCTP)$	100%
	$(Tyr10)N-HO2\gamma(dCTP)$	88.20%
	$(Tyr10)N-HO3\beta(dCTP)$	57.20%
	(Tyr10)N–HO1γ(dCTP)	37.65%
	$(Phe11)N-HO2\beta(dCTP)$	22.25%
	(Tyr12)Oη–Hη375O2(dCTP)	88.85%
	(Tyr12)N–HO3′(dCTP)	83.45%
	$(Tyr48)O\eta-H\etaO2\gamma(dCTP)$	37.75%
	(Lys159)Nζ-Ηζ1O3γ(dCTP)	45.95%
	(Lys159)Nζ-Ηζ3O3γ(dCTP)	36.95%
	(Lys159)Nζ-Ηζ2Ο3γ(dCTP)	14.55%

		(Lys159)Nζ–Hζ1O2γ(dCTP)	13.75%
$ \begin{array}{c} (Uys159)N_{4}^{2}-H_{2}^{2}O_{2}^{\gamma}(dCTP) & 4.50\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{2}^{\gamma}(dATP) & 72.95\% \\ (Arg51)N\eta^{1}-H\eta^{1}2O_{2}^{\gamma}(dATP) & 70.05\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(dATP) & 56.35\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(dATP) & 15.50\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(dATP) & 13.45\% \\ (Tr45)O\gamma^{1}-H\gamma^{1}O_{3}^{\gamma}(dATP) & 7.25\% \\ (Tyr10)N-HO_{3}^{\gamma}(dATP) & 86.30\% \\ (Tr45)O\gamma^{1}-H\gamma^{1}O_{3}^{\gamma}(dATP) & 98.65\% \\ (Tyr10)N-HO_{3}^{\gamma}(dATP) & 88.65\% \\ (Tyr10)N-HO_{3}^{\gamma}(dATP) & 98.65\% \\ (Tyr10)N-HO_{3}^{\gamma}(dATP) & 8.10\% \\ (Lys159)N_{5}^{2}-H_{2}^{2}O_{3}^{\gamma}(dATP) & 19.75\% \\ (Uys159)N_{5}^{2}-H_{2}^{2}O_{3}^{\gamma}(dATP) & 19.90\% \\ (Lys159)N_{5}^{2}-H_{2}^{2}O_{3}^{\gamma}(dATP) & 14.0\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 99.90\% \\ (Lys159)N_{5}^{2}-H_{2}^{2}O_{3}^{\gamma}(syn-dATP) & 99.90\% \\ (Lys159)N_{5}^{2}-H_{2}^{2}O_{3}^{\gamma}(syn-dATP) & 11.65\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 11.65\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 8.30\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 8.30\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 13.35\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 13.35\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 13.35\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 13.35\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Lys159)N_{5}^{2}-H_{5}^{2}O_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Tyr10)N-HO_{3}^{\gamma}(syn-dATP) & 14.00\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(syn-dATP) & 14.09\% \\ (Tyr10)N-HO_{3}^{\gamma}(dGTP) & 14.00\% \\ (Arg51)N\eta^{2}-H\eta^{2}O_{3}^{\gamma}(dGTP) & 14.00\% \\ (Arg51)N\eta^{2}-H\eta^{2}$		$(Lys159)N\zeta - H\zeta 3O2\gamma(dCTP)$	9.10%
$ \begin{array}{c} (Arg51)Nn2-Hn22O3\beta(dATP) 72.95\% \\ (Arg51)Nn1-Hn12O3p(dATP) 70.05\% \\ (Arg51)Nn2-Hn22O3p(dATP) 70.05\% \\ (Arg51)Nn2-Hn22O1p(dATP) 70.05\% \\ (Arg51)Nn2-Hn22O1p(dATP) 70.05\% \\ (Arg51)Nn2-Hn22O3p(dATP) 70.05\% \\ (Arg51)Nn2-Hn22O3p(dATP) 70.05\% \\ (Arg51)Nn1-Hn12O3p(dATP) 70.05\% \\ (Thr45)Op1-Hp1O3p(dATP) 70.05\% \\ (Thr45)Op1-Hp1O3p(dATP) 70.05\% \\ (Tyr10)N-HO3p(dATP) 70.05\% \\ (Tyr10)N-HO3p(dATP) 70.05\% \\ (Tyr48)On-HnO3p(dATP) 70.05\% \\ (Tyr48)On-HnO3p(dATP) 70.05\% \\ (Tyr48)On-HnO3p(dATP) 70.05\% \\ (Tyr48)On-Hn2O3p(dATP) 70.05\% \\ (Tyr51)Nn2-Hn22O3p(syn-dATP) 70.05\% \\ (Tyr51)Nn2-Hn22O3p(syn-dATP) 70.05\% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) 70.05\% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) 70.05\% \\ (Thr45)Op1-Hp1O3p(syn-dATP) 70.05\% \\ (Thr45)Op1-Hp1O3p(syn-dATP) 70.05\% \\ (Thr45)Op1-Hp1O3p(syn-dATP) 70.05\% \\ (Tyr10)N-HO3p(syn-dATP) 70.05\% \\ (Tyr10$		$(Lvs159)N\zeta - H\zeta 2O2\gamma(dCTP)$	4.50%
$ \begin{array}{c} (Arg51)N\eta 1-H\eta 12O2y(dATP) & 70.05\% \\ (Arg51)N\eta 1-H\eta 12O2y(dATP) & 56.35\% \\ (Arg51)N\eta 2-H\eta 22O2y(dATP) & 55.30\% \\ (Arg51)N\eta 1-H\eta 12O3y(dATP) & 13.45\% \\ (Thr45)Oy1-Hy1O3y(dATP) & 13.45\% \\ (Thr45)Oy1-Hy1O3y(dATP) & 7.25\% \\ (Tyr10)N-HO2y(dATP) & 98.65\% \\ (Tyr10)N-HO2y(dATP) & 98.65\% \\ (Tyr10)N-HO2y(dATP) & 98.65\% \\ (Tyr10)N-HO2y(dATP) & 98.65\% \\ (Tyr48)O\eta-H\etaO2y(dATP) & 8.10\% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 8.10\% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 1.00\% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 1.00\% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 99.90\% \\ (Lys159)N\zeta-H\zeta2O1y(dATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta2O1y(dATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta2O1y(dATP) & 1.40\% \\ (Arg51)N\eta 1-H\eta 12O2y(syn-dATP) & 99.90\% \\ (Arg51)N\eta 2-H\eta 22O3y(syn-dATP) & 99.50\% \\ (Arg51)N\eta 2-H\eta 22O3y(syn-dATP) & 99.50\% \\ (Arg51)N\eta 2-H\eta 22O3y(syn-dATP) & 8.30\% \\ (Arg51)N\eta 2-H\eta 22O3y(syn-dATP) & 11.65\% \\ (Arg51)N\eta 2-H\eta 22O3y(syn-dATP) & 11.65\% \\ (Arg51)N\eta 2-H\eta 22O3y(syn-dATP) & 13.35\% \\ (Thr45)Oy1-Hy1O3y(syn-dATP) & 13.35\% \\ (Thr45)Oy1-Hy1O3y(syn-dATP) & 13.35\% \\ (Thr45)Oy1-Hy1O3y(syn-dATP) & 13.35\% \\ (Tyr10)N-HO2y(syn-dATP) & 14.95\% \\ (Lys159)N\zeta-H\zeta1O1y(syn-dATP) & 14.95\% \\ (Lys159)N\zeta-H\zeta1O3y(syn-dATP) & 14.55\% \\ (Lys159)N\zeta-H\zeta1O3y(syn-dATP) & 14.05\% \\ (Tyr10)N-HO2y(syn-dATP) & 14.05\% \\ (Tyr10)N-HO2y(dGTP) & 32.70\% \\ (Arg51)N\eta 2-H\eta 22O3\beta(dGTP) & 100\% \\ (Tyr10)N-HO2y(dGTP) & 32.70\% \\ (Arg51)N\eta 2-H\eta 22O3\beta(dGTP) & 14.00\% \\ (Arg51)N\eta 2-H\eta 22O3\beta(dGTP) & 14.00\% \\ (Arg51)N\eta 2-H\eta 22O3\beta(dGTP) & 14.00\% \\ (Tyr10)N-HO2\beta(dGTP) & 99.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 99.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 99.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 14.25\% \\ (Tyr48)O\eta-H\etaO2\gamma(dGTP) & 14.25\% \\ (Tyr48)O\eta-H\etaO2\gamma(dGTP) & 14.05\% \\ (Tyr48)O\eta-H\etaO2\gamma(dGTP) & 14.05\% \\ (Tyr48)O\eta-H\etaO2\gamma$		$(\text{Arg51})\text{Nn2}-\text{Hn22}$ O3 β (dATP)	72.95%
$ \begin{array}{c} (Arg51)N\eta 1-H\eta 12O3\beta(dATP) & 56.33% \\ (Arg51)N\eta 2-H\eta 22O3\beta(dATP) & 55.33% \\ (Arg51)N\eta 2-H\eta 22O3\gamma(dATP) & 15.50% \\ (Arg51)N\eta 1-H\eta 12O3\gamma(dATP) & 13.45% \\ (Thr45)Oy 1-H\gamma 1O3(dATP) & 86.30% \\ (Thr45)Oy 1-H\gamma 1O3(dATP) & 86.30% \\ (Thr45)Oy 1-H\gamma 1O3(dATP) & 86.5% \\ (Tyr10)N-HO3\beta(dATP) & 38.65% \\ (Tyr10)N-HO3\gamma(dATP) & 97.50% \\ (Tyr48)O\eta -H\etaO3\gamma(dATP) & 97.50% \\ (Tyr48)O\eta -H\etaO3\gamma(dATP) & 10.0% \\ (Lys159)N\zeta -H\zeta 2O3\gamma(dATP) & 46.60% \\ (Lys159)N\zeta -H\zeta 2O3\gamma(dATP) & 19.90% \\ (Lys159)N\zeta -H\zeta 2O3\gamma(dATP) & 19.90% \\ (Lys159)N\zeta -H\zeta 2O3\gamma(dATP) & 19.90% \\ (Lys159)N\zeta -H\zeta 2O3\beta(sym-dATP) & 99.50% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 99.50% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 99.50% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 11.65% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 11.65% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 11.65% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 8.30% \\ (Arg51)N\eta 2-H\eta 22O3\beta(sym-dATP) & 13.35% \\ (Thr45)O\gamma 1-H\gamma 1O3\beta(sym-dATP) & 13.35% \\ (Thr45)O\gamma 1-H\gamma 1O3\beta(sym-dATP) & 100% \\ (Tyr10)N-HO3\beta(sym-dATP) & 10.0% \\ (Tyr10)N-HO3\beta(sym-dATP) & 10.0% \\ (Tyr10)N-HO3\beta(sym-dATP) & 10.35% \\ (Lys159)N\zeta -H\zeta 1O1\gamma(sym-dATP) & 10.50% \\ (Lys159)N\zeta -H\zeta 1O3\gamma(sym-dATP) & 10.50% \\ (Lys159)N\zeta -H\zeta 1O3\gamma(sym-dATP) & 15.00% \\ (Lys159)N\zeta -H\zeta 1O3\gamma(sfP) & 32.70% \\ (Arg51)N\eta 1-H\eta 12O3\gamma(dGTP) & 32.70% \\ (Arg51)N\eta 1-H\eta 12O3\gamma(dGTP) & 33.00% \\ (Lys159)N\zeta -H\zeta 2O3\gamma(dGTP) & 33.00% \\ (Lys159)N\zeta -H\zeta 2O3\gamma(dGTP) & 40.15\% \\ \end{array}$		(Arg51)Nn1-Hn12 O2y(dATP)	70.05%
$ \begin{array}{c} (Arg51)N\eta^2-H\eta^22Olf(dATP) & 53.30\% \\ (Arg51)N\eta^2-H\eta^22Olf(dATP) & 13.45\% \\ (Arg51)N\eta^2-H\eta^22O37(dATP) & 13.45\% \\ (Thr45)OY1-HY1O37(dATP) & 86.30\% \\ (Thr45)OY1-HY1O1f(dATP) & 7.25\% \\ (Tyr10)N-HO27(dATP) & 98.65\% \\ (Tyr10)N-HO27(dATP) & 98.65\% \\ (Tyr10)N-HO27(dATP) & 7.50\% \\ (Tyr48)O\eta-H\etaO27(dATP) & 7.50\% \\ (Tyr48)O\eta-H\etaO37(dATP) & 8.10\% \\ (Lys159)N\zeta-H\zeta2O37(dATP) & 46.60\% \\ (Lys159)N\zeta-H\zeta2O37(dATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta2O37(dATP) & 9.90\% \\ (Lys159)N\zeta-H\zeta2O37(syn-dATP) & 9.90\% \\ (Arg51)N\eta^2-H\eta^22O27(syn-dATP) & 99.50\% \\ (Arg51)N\eta^2-H\eta^22O37(syn-dATP) & 11.65\% \\ (Arg51)N\eta^2-H\eta^22O37(syn-dATP) & 11.65\% \\ (Arg51)N\eta^2-H\eta^22O37(syn-dATP) & 8.30\% \\ (Arg51)N\eta^2-H\eta^22O37(syn-dATP) & 8.30\% \\ (Arg51)N\eta^2-H\eta^22O37(syn-dATP) & 8.30\% \\ (Thr45)OY1-HY1O37(syn-dATP) & 98.25\% \\ (Thr45)OY1-HY1O37(syn-dATP) & 98.25\% \\ (Thr45)OY1-HY1O37(syn-dATP) & 13.35\% \\ (Tyr10)N-HO27(syn-dATP) & 13.35\% \\ (Tyr10)N-HO37(syn-dATP) & 14.05\% \\ (Lys159)N\zeta-H\zeta1O37(syn-dATP) & 14.05\% \\ (Lys159)N\zeta-H\zeta1O37(syn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O37(syn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O37(dGTP) & 32.70\% \\ (Arg51)N\eta^1-H\eta^2O37(dGTP) & 32.00\% \\ (Tyr10)N-HO27(dGTP) & 32.00\% \\ (Lys159)N\zeta-H\zeta2O37(dGTP) & 33.00\% \\ (Lys159)N\zeta-H\zeta2O37(dGTP) & 40.15\% \\ \end{array}$		(Arg51)Nn1-Hn12 O3B(dATP)	56 35%
$ \begin{array}{c} (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}2O2\gamma(\operatorname{dATP}) & 15.50\% \\ (\operatorname{Arg}51)\operatorname{N\eta}1-\operatorname{H\eta}1O3\gamma(\operatorname{dATP}) & 13.45\% \\ (\operatorname{Thr}45)O\gamma1-\operatorname{H\eta}1O3\gamma(\operatorname{dATP}) & 86.30\% \\ (\operatorname{Thr}45)O\gamma1-\operatorname{H\eta}1O3\gamma(\operatorname{dATP}) & 86.65\% \\ (\operatorname{Tyr}10)\operatorname{N-HO2\gamma}(\operatorname{dATP}) & 98.65\% \\ (\operatorname{Tyr}10)\operatorname{N-HO2\gamma}(\operatorname{dATP}) & 98.65\% \\ (\operatorname{Tyr}10)\operatorname{N-HO2\gamma}(\operatorname{dATP}) & 98.65\% \\ (\operatorname{Tyr}48)O\eta-\operatorname{H\eta}O2\gamma(\operatorname{dATP}) & 97.50\% \\ (\operatorname{Tyr}48)O\eta-\operatorname{H\eta}O3\gamma(\operatorname{dATP}) & 8.10\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(\operatorname{dATP}) & 46.60\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}1O3\gamma(\operatorname{dATP}) & 19.90\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}1O3\gamma(\operatorname{dATP}) & 19.90\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(\operatorname{dATP}) & 19.90\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O1\gamma(\operatorname{dATP}) & 1.40\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O23\beta(syn-\operatorname{dATP}) & 99.90\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O2\gamma(syn-\operatorname{dATP}) & 99.50\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O2\gamma(syn-\operatorname{dATP}) & 99.50\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O2\gamma(syn-\operatorname{dATP}) & 99.50\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O2\gamma(syn-\operatorname{dATP}) & 11.65\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O2\gamma(syn-\operatorname{dATP}) & 11.65\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O2\gamma(syn-\operatorname{dATP}) & 11.65\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O3\gamma(syn-\operatorname{dATP}) & 6.80\% \\ (\operatorname{Thr}45)\operatorname{Oy}1-\operatorname{H\gamma}1O3\beta(syn-\operatorname{dATP}) & 5.80\% \\ (\operatorname{Thr}45)\operatorname{Oy}1-\operatorname{H\gamma}1O3\gamma(syn-\operatorname{dATP}) & 5.80\% \\ (\operatorname{Thr}45)\operatorname{Oy}1-\operatorname{H\gamma}1O3\gamma(syn-\operatorname{dATP}) & 5.80\% \\ (\operatorname{Thr}45)\operatorname{Oy}1-\operatorname{H\gamma}1O3\gamma(syn-\operatorname{dATP}) & 5.80\% \\ (\operatorname{Thr}45)\operatorname{Oy}1-\operatorname{H\gamma}1O3\gamma(syn-\operatorname{dATP}) & 13.35\% \\ (\operatorname{Tyr}10)\operatorname{N-HO3\beta(syn-\operatorname{dATP}) & 13.35\% \\ (\operatorname{Tyr}10)\operatorname{N-HO3\beta(syn-\operatorname{dATP}) & 13.47\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}1O3\gamma(syn-\operatorname{dATP}) & 20.55\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(syn-\operatorname{dATP}) & 20.55\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(syn-\operatorname{dATP}) & 20.55\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(syn-\operatorname{dATP}) & 25.50\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(sm-\operatorname{dATP}) & 15.00\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(sm-\operatorname{dATP}) & 10.0\% \\ (\operatorname{Arg}51)\operatorname{N\eta}1-\operatorname{Hn}12O3\gamma(sm-\operatorname{dATP}) & 15.00\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(sm-\operatorname{dATP}) & 10.0\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O3\gamma(sm-\operatorname{dATP}) & 10.0\% \\ (\operatorname{Arg}51)\operatorname{N\eta}2-\operatorname{H\eta}22O3\gamma(sm-\operatorname{dATP}) & 10.0\% \\ (\operatorname{Lys}159)\operatorname{N\zeta}-\operatorname{H\zeta}2O3\gamma(sm-\operatorname{dATP}) & 10$		$(\Delta rg51)Nn2-Hn22 O1B(d\Delta TP)$	53 30%
$ \begin{array}{c} (Arg 51)N1[-H1]2037(dATP) & 13.45\% \\ (Thr45)Oy1-Hy1O37(dATP) & 86.30\% \\ (Thr45)Oy1-Hy1O37(dATP) & 86.53\% \\ (Tyr10)N-HO27(dATP) & 98.65\% \\ (Tyr10)N-HO27(dATP) & 98.65\% \\ (Tyr10)N-HO37(dATP) & 98.65\% \\ (Tyr10)N-HO37(dATP) & 98.65\% \\ (Tyr48)On-HnO37(dATP) & 97.50\% \\ (Tyr48)On-HnO37(dATP) & 10\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dATP) & 46.60\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dATP) & 19.90\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dATP) & 19.90\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dATP) & 19.90\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dATP) & 19.90\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dATP) & 14.0\% \\ (Arg 51)Nn1-Hn12O27(syn-dATP) & 99.90\% \\ (Lys159)N\zeta-H\zeta_{2O37}(syn-dATP) & 99.90\% \\ (Arg 51)Nn1-Hn12O27(syn-dATP) & 99.50\% \\ (Arg 51)Nn1-Hn12O27(syn-dATP) & 11.65\% \\ (Arg 51)Nn1-Hn12O37(syn-dATP) & 8.30\% \\ (Arg 51)Nn1-Hn12O37(syn-dATP) & 10.05\% \\ (Thr45)Oy1-HY1O1β(syn-dATP) & 10.05\% \\ (Tyr10)N-HO38(syn-dATP) & 10.05\% \\ (Tyr10)N-HO38(syn-dATP) & 10.05\% \\ (Lys159)N\zeta-H\zeta_{1O37}(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{1O37}(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{1O37}(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{1O37}(syn-dATP) & 10.05\% \\ (Arg 51)Nn2-Hn22O37(syn-dATP) & 10.05\% \\ (Arg 51)Nn1-Hn12O37(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{1O37}(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{2O37}(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{2O37}(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{2O37}(sym-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta_{2O37}(sym-dATP) & 20.55\% \\ (Arg 51)Nn1-Hn12O27(dGTP) & 7.60\% \\ (Arg 51)Nn1-Hn12O37(dGTP) & 7.95\% \\ (Arg 51)Nn1-Hn12O37(dGTP) & 7.95\% \\ (Arg 51)Nn1-Hn12O37(dGTP) & 8.25\% \\ (Tyr10)N-HO27(dGTP) & 9.95\% \\ (Tyr10)N-HO27(dGTP) & 9.95\% \\ (Tyr10)N-HO27(dGTP) & 9.25\% \\ (Tyr48)On-HnO27(dGTP) & 42.25\% \\ (Tyr48)On-HnO27(dGTP) & 43.20\% \\ (Lys159)N\zeta-H\zeta_{2O37}(dGTP) & 40.15\% \\ \end{array}$		(Arg51)Nn2 Hn22 O2y(dATP)	15 50%
$\begin{array}{c} (Aug51)Au[1-m]12O3y(dATP) & 15.45.76 \\ (Thr45)Oy[1-Hy]O3y(dATP) & 86.33% \\ (Thr45)Oy[1-Hy]O3y(dATP) & 98.65% \\ (Tyr10)N-HO3p(dATP) & 98.65% \\ (Tyr10)N-HO3p(dATP) & 98.65% \\ (Tyr10)N-HO3p(dATP) & 27.55% \\ (Tyr48)On-HnO3y(dATP) & 97.50% \\ (Tyr48)On-HnO3y(dATP) & 10.0% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 19.90% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 19.90% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 19.90% \\ (Lys159)N\zeta-H\zeta2O3y(dATP) & 19.90% \\ (Lys159)N\zeta-H\zeta2O3p(dATP) & 19.90% \\ (Lys159)N\zeta-H\zeta2O3p(syn-dATP) & 99.90% \\ (Lys159)N\zeta-H\zeta2O3p(syn-dATP) & 99.90% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) & 99.50% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) & 99.50% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) & 11.65% \\ (Arg51)Nn1-Hn12O3p(syn-dATP) & 11.65% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) & 18.30% \\ (Arg51)Nn2-Hn22O3p(syn-dATP) & 8.30% \\ (Thr45)Oy[1-Hy]O3p(syn-dATP) & 8.30% \\ (Thr45)Oy[1-Hy]O3p(syn-dATP) & 13.35% \\ (Thr45)Oy[1-Hy]O3p(syn-dATP) & 13.35% \\ (Thr45)Oy[1-Hy]O3p(syn-dATP) & 13.35% \\ (Thr45)Oy[1-Hy]O3p(syn-dATP) & 19.45% \\ (Lys159)N\zeta-H\zeta2O3y(syn-dATP) & 14.00% \\ (Tyr10)N-HO2p(syn-dATP) & 15.00% \\ (Lys159)N\zeta-H\zeta2O3y(syn-dATP) & 16.50% \\ (Lys159)N\zeta-H\zeta2O3y(dGTP) & 14.00% \\ (Arg51)Nn1-Hn12O3p(dGTP) & 18.40% \\ (Thr45)Oy[1-Hy]O3p(dGTP) & 18.40% \\ (Thr45)Oy[1-Hy]O3p(dGTP) & 18.40% \\ (Thr45)Oy[1-Hy]O3p(dGTP) & 18.25% \\ (Tyr10)N-HO2p(dGTP) & 9.95% \\ (Tyr10)N-HO2p(dGTP) & 9.95% \\ (Tyr10)N-HO2p(dGTP) & 9.95% \\ (Tyr10)N-HO2p(dGTP) & 18.25% \\ (Tyr48)On-HnO2p(dGTP) & 13.20% \\ (Lys159)N\zeta-HZ2O3y(dGTP) & 14.05% \\ (Lys159)N\zeta-HZ2O3y(dGTP) & 14.05% \\ (Lys159)N\zeta-HZ2O3y(dGTP) & 14.05% \\ (Lys159)N\zeta-HZ2O3y(dGTP) & 14.05\% \\ (Lys159)N\zeta-HZ2O3y(dGTP) & 14.05\% \\ (Lys159)N\zeta-HZ2O3y(dGTP) & 14.$		(Arg51)Nn1 Hn12 O2v(dATD)	13.30%
$ \begin{array}{c} (1114-3)071-H7103 (JA1P) & 30.3070 \\ (Thr45)071-H7103 (JA1P) & 7.25% \\ (Tyr10)N-H027(JATP) & 98.65% \\ (Tyr10)N-H027(JATP) & 38.65% \\ (Tyr10)N-H027(JATP) & 7.50% \\ (Tyr48)07-H71027(JATP) & 7.50% \\ (Tyr48)07-H71027(JATP) & 7.50% \\ (Lys159)N\zeta-Hζ2037(JATP) & 46.60% \\ (Lys159)N\zeta-Hζ2037(JATP) & 7.30% \\ (Lys159)N\zeta-Hζ1017(JATP) & 7.30% \\ (Lys159)N\zeta-Hζ2017(JATP) & 7.30% \\ (Lys159)N\zeta-Hζ2017(JATP) & 7.30% \\ (Lys159)N\zeta-Hζ2017(JATP) & 9.90% \\ \hline Major & (Arg51)N12-H722023g(syn-dATP) & 99.90% \\ \hline Major & (Arg51)N12-H72203g(syn-dATP) & 99.90% \\ \hline (Arg51)N12-H72203g(syn-dATP) & 99.50% \\ (Arg51)N12-H72203g(syn-dATP) & 99.50% \\ (Arg51)N12-H72203g(syn-dATP) & 8.30% \\ (Arg51)N12-H72203g(syn-dATP) & 11.65% \\ (Arg51)N11-H71203g(syn-dATP) & 11.65% \\ (Thr45)O71-H7103g(syn-dATP) & 13.35% \\ (Thr45)O71-H7103g(syn-dATP) & 13.35% \\ (Thr45)O71-H7103g(syn-dATP) & 13.35% \\ (Tyr10)N-H03g(syn-dATP) & 13.35% \\ (Tyr10)N-H03g(syn-dATP) & 13.55% \\ (Lys159)N\zeta-Hζ1017(syn-dATP) & 14.05% \\ (Lys159)N\zeta-Hζ1037(syn-dATP) & 15.00% \\ (Lys159)N\zeta-Hζ3037(syn-dATP) & 15.00% \\ (Lys159)N\zeta-Hζ3037(syn-dATP) & 15.00% \\ (Lys159)N\zeta-Hζ203g(syn-dATP) & 15.00% \\ (Lys159)N\zeta-Hζ203g(syn-dATP) & 10.0% \\ (Tyr10)N-H027(dGTP) & 32.70% \\ (Arg51)N71-H712O27(dGTP) & 32.70% \\ (Arg51)N71-H712O27(dGTP) & 7.95% \\ (Arg51)N71-H712O27(dGTP) & 7.95% \\ (Arg51)N71-H712O27(dGTP) & 7.95% \\ (Tyr10)N-H027(dGTP) & 7.95% \\ (Tyr12)N-H03(dGTP) & 7.25% \\ (Tyr48)On-H71O27(dGTP) & 7.25% \\ (Tyr48)On-H71027(dGTP) & 7.25% \\ (Tyr48)On-H71037(dGTP) & 7.25% \\ (Tyr48)On-H71037(dGTP) & 7.25% \\ (Tyr48)On-H71037(dGTP) & 7.25% \\ (Tyr48)On-H71037(dGTP) & 7.25\% \\ \end{array}$		$(\text{Alg}_{J})(\textbf{u}_{I}) = (11)(1205)(\textbf{u}_{A})(\textbf{u}_{A})$	15. 1 570 86 30%
$\begin{array}{cccc} (11143)071-H71071ptdATP) & 7.25\% \\ (Tyr10)N-H02ptdATP) & 98.65\% \\ (Tyr10)N-H02ptdATP) & 38.65\% \\ (Tyr148)0\eta-H\eta02ptdATP) & 7.50\% \\ (Tyr48)0\eta-H\eta02ptdATP) & 97.50\% \\ (Tyr48)0\eta-H\eta02ptdATP) & 8.10\% \\ (Lys159)N\zeta-H\zeta203ptdATP) & 46.60\% \\ (Lys159)N\zeta-H\zeta103ptdATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta103ptdATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta101ptdATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta101ptdATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta203ptdATP) & 9.90\% \\ (Lys159)N\zeta-H\zeta203ptdATP) & 9.90\% \\ (Lys159)N\zeta-HZ203ptdATP) & 9.90\% \\ (Lys159)N\chi-HZ203ptdATP) & 9.90\% \\ (Arg51)Nn2-Hn2202ptsyn-dATP) & 9.50\% \\ (Arg51)Nn2-Hn2202ptsyn-dATP) & 8.05\% \\ (Arg51)Nn2-Hn2202ptsyn-dATP) & 8.05\% \\ (Arg51)Nn1-Hn1203ptsyn-dATP) & 11.65\% \\ (Arg51)Nn1-Hn1203ptsyn-dATP) & 8.30\% \\ (Arg51)Nn2-Hn2203ptsyn-dATP) & 8.30\% \\ (Arg51)Nn2-Hn2203ptsyn-dATP) & 8.30\% \\ (Thr45)Opt-Hp1O3ptsyn-dATP) & 13.35\% \\ (Tyr10)N-H02ptsyn-dATP) & 13.35\% \\ (Tyr10)N-H03ptsyn-dATP) & 10.0\% \\ (Tyr10)N-H03ptsyn-dATP) & 10.0\% \\ (Tyr10)N-H03ptsyn-dATP) & 14.05\% \\ (Lys159)N\zeta-H\zeta103ptsyn-dATP) & 15.05\% \\ (Lys159)N\zeta-H\zeta103ptsyn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O3pttsyn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O3pttsyn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O3pttsyn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O3pttsyn-dATP) & 10.0\% \\ (Arg51)Nn1-Hn12O3pttsyn-dATP) & 15.00\% \\ (Lys159)N\zeta-HZ2O3pttsyn-dATP) & 10.00\% \\ (Arg51)Nn1-Hn12O3pttsyn-dATP) & 10.00\% \\ (Arg$		$(11143)Oy1-\Pi y1OS(dATP)$	7 25%
$ \begin{array}{c} (1y10)N-H02y(UATP) & 30.05\% \\ (Tyr10)N-H02y(UATP) & 36.05\% \\ (Tyr10)N-H01y(UATP) & 27.50\% \\ (Tyr48)O\eta-H\etaO2y(UATP) & 97.50\% \\ (Tyr48)O\eta-H\etaO3y(UATP) & 97.50\% \\ (Lys159)N\zeta-H\zetaO3y(UATP) & 46.60\% \\ (Lys159)N\zeta-H\zetaO3y(UATP) & 27.55\% \\ (Lys159)N\zeta-H\zetaO3y(UATP) & 19.90\% \\ (Lys159)N\zeta-H\zetaO1y(UATP) & 7.30\% \\ (Lys159)N\zeta-H\zetaO1y(UATP) & 7.30\% \\ (Lys159)N\zeta-H\zetaO1y(UATP) & 7.30\% \\ (Lys159)N\zeta-H\zetaO1y(UATP) & 99.90\% \\ (Lys159)N\zeta-H\zetaO3y(UATP) & 99.90\% \\ (Lys159)N\zeta-H\zetaO3y(UATP) & 99.90\% \\ (Arg51)N\eta2-H\eta2O3\beta(syn-dATP) & 99.50\% \\ (Arg51)N\eta2-H\eta2O3y(syn-dATP) & 48.05\% \\ (Yr10)N-HO3y(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta2O3y(syn-dATP) & 8.30\% \\ (Arg51)N\eta2-H\eta2O3y(syn-dATP) & 8.30\% \\ (Arg51)N\eta2-H\eta2O3y(syn-dATP) & 8.30\% \\ (Thr45)Oy1-Hy1O3(syn-dATP) & 13.35\% \\ (Tyr10)N-HO2y(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3y(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3y(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3y(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3y(syn-dATP) & 14.00\% \\ (Tyr12)N-HO3y(syn-dATP) & 14.05\% \\ (Lys159)N\zeta-H\zeta1O1y(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H\zeta1O1y(syn-dATP) & 16.50\% \\ (Lys159)N\zeta-H\zeta2O3y(syn-dATP) & 16.50\% \\ (Lys159)N\zeta-H\zeta2$		(11143)Oy1-Hy1O1p(dA1P) (Tyr10)NH O2r(dATD)	1.2.5%
$ \begin{array}{c} (1y10)N-H01y(dATP) & 36.05\% \\ (Tyr48)O\eta-H\etaO2y(dATP) & 97.50\% \\ (Tyr48)O\eta-H\etaO2y(dATP) & 8.10\% \\ (Lys159)N\zeta-H22O3y(dATP) & 46.60\% \\ (Lys159)N\zeta-H22O3y(dATP) & 27.55\% \\ (Lys159)N\zeta-H23O3y(dATP) & 19.90\% \\ (Lys159)N\zeta-H23O3y(dATP) & 7.30\% \\ (Lys159)N\zeta-H22O3y(dATP) & 7.30\% \\ (Lys159)N\zeta-H22O1y(dATP) & 7.30\% \\ (Lys159)N\zeta-H22O1y(dATP) & 1.40\% \\ \hline (Arg51)N\eta2-H\eta22O2y(syn-dATP) & 99.90\% \\ (Arg51)N\eta2-H\eta22O2y(syn-dATP) & 99.90\% \\ (Arg51)N\eta2-H\eta22O2y(syn-dATP) & 99.50\% \\ (Arg51)N\eta2-H\eta22O2y(syn-dATP) & 48.05\% \\ (Arg51)N\eta2-H\eta22O2y(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ (Thr45)O\gamma1-H\gamma1O3\beta(syn-dATP) & 13.35\% \\ (Tyr10)N-HO2y(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3(syn-dATP) & 14.47\% \\ (Lys159)N\zeta-H21O1y(syn-dATP) & 14.47\% \\ (Lys159)N\zeta-H21O1y(syn-dATP) & 14.47\% \\ (Lys159)N\zeta-H22O3y(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H21O1y(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H22O3y(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H22O3y(syn-dATP) & 15.00\% \\ (Arg51)N\eta2-H\eta22O3y(syn-dATP) & 16.50\% \\ (Arg51)N\eta2-H\eta22O3y(dGTP) & 100\% \\ (Arg51)N\eta2-H\eta22O3y(dGTP) & 100\% \\ (Arg51)N\eta2-H\eta22O3y(dGTP) & 27.95\% \\ (Arg51)N\eta1-H\eta12O3y(dGTP) & 27.95\% \\ (Arg51)N\eta1-H\eta12O3y(dGTP) & 27.95\% \\ (Tr45)O\gamma1-Hy1O2y(dGTP) & 99.95\% \\ (Tyr10)N-HO2y(dGTP) & 81.25\% \\ (Tyr48)O\eta-H\etaO2y(dGTP) & 81.25\% \\ (Tyr48)O\eta-H\etaO2y(dGTP) & 43.20\% \\ (Lys159)N\zeta-H22O3y(dGTP) & 40.15\% \\ \end{array}$		$(1y_110)N = \Pi \dots O2\gamma(dATP)$	90.03% 28.65%
$(1y10)N-H02y(dATP) 27.50\% (Tyr48)O\eta-H\etaO2y(dATP) 97.50\% (Tyr48)O\eta-H\etaO3y(dATP) 8.10\% (Lys159)N\zeta-H\zeta2O3y(dATP) 46.60\% (Lys159)N\zeta-Hζ1O3y(dATP) 7.30\% (Lys159)N\zeta-Hζ1O1y(dATP) 7.30\% (Lys159)N\zeta-Hζ1O1y(dATP) 7.30\% (Lys159)N\zeta-Hζ2O1y(dATP) 7.30\% (Lys159)N\zeta-Hζ2O1y(dATP) 7.30\% (Lys159)N\zeta-Hζ2O1y(dATP) 99.90\% (Arg51)N\eta2-H\eta22O2y(syn-dATP) 99.50\% (Arg51)N\eta2-H\eta22O2y(syn-dATP) 99.50\% (Arg51)N\eta2-H\eta22O2y(syn-dATP) 99.50\% (Arg51)N\eta2-H\eta22O3j(syn-dATP) 11.65\% (Arg51)N\eta2-H\eta22O1jb(syn-dATP) 11.05\% (Arg51)N\eta2-H\eta22O2y(syn-dATP) 8.30\% (Arg51)N\eta2-H\eta22O3j(syn-dATP) 8.30\% (Thr45)Oy1-Hy1O3j(syn-dATP) 8.30\% (Thr45)Oy1-Hy1O3j(syn-dATP) 13.35\% (Tyr10)N-HO2y(syn-dATP) 10.00\% (Tyr10)N-HO2y(syn-dATP) 10.00\% (Tyr10)N-HO3j(syn-dATP) 10.00\% (Tyr10)N-HO3j(syn-dATP) 10.00\% (Tyr10)N-HO3j(syn-dATP) 19.45\% (Lys159)N\zeta-Hζ1O1y(syn-dATP) 19.45\% (Lys159)N\zeta-Hζ1O1y(syn-dATP) 15.00\% (Lys159)N\zeta-Hζ2O1y(syn-dATP) 15.00\% (Lys159)N\zeta-Hζ2O1y(syn-dATP) 15.00\% (Lys159)N\zeta-Hζ2O3y(syn-dATP) 15.00\% (Lys159)N\zeta-Hζ2O3y(syn-dATP) 15.00\% (Arg51)N\eta2-H\eta22O2j(dGTP) 10.00\% (Arg51)N\eta2-H\eta22O3j(syn-dATP) 15.00\% (Arg51)N\eta2-H\eta22O3j(dGTP) 10.00\% (Thr45)Oy1-Hy1O2j(dGTP) 10.00\% (Tyr10)N-HO2j(dGTP) 25.90\% (Arg51)N\eta2-H\eta22O3j(dGTP) 18.40\% (Thr45)Oy1-Hy1O1jb(dGTP) 25.90\% (Arg51)N\eta2-H\eta22O3j(dGTP) 18.40\% (Thr45)Oy1-Hy1O3j(dGTP) 12.50\% (Lys159)N\zeta-Hζ2O1j(dGTP) 15.00\% (Arg51)N\eta2-H\eta22O3j(dGTP) 18.40\% (Thr45)Oy1-Hy1O3j(dGTP) 12.50\% (Tyr10)N-HO2j(dGTP) 12.50\% (Tyr10)N-HO2j(dGTP) 12.00\% (Tyr10)N-HO2j(dGTP) 12.50\% (Tyr10)N-HO2j(dGTP) 12.50\% (Tyr10)N-HO2j(dGTP) 13.30\% (Tyr10)N-HO2j(dGTP) 13.00\% (Tyr10)N-HO2j(dGTP) 14.20\% (Thr45)Oy1-Hy1O1jk(dGTP) 14.20\% (Thr45)Oy1-Hy1O1jk(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 13.00\% (Lys159)N\zeta-Hζ2O3y(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr10)N-HO2j(dGTP) 14.20\% (Tyr1$		$(Tyr10)N = \Pi \dots OSp(dATP)$	58.05% 27.50%
$(1y43)0\eta-H\eta02y(dATP) = 930\%(Tyr43)0\eta-H\eta03y(dATP) = 8.10\%(Lys159)N\zeta-H\zeta03y(dATP) = 46.60\%(Lys159)N\zeta-H\zeta03y(dATP) = 27.55\%(Lys159)N\zeta-H\zeta03y(dATP) = 19.90\%(Lys159)N\zeta-Hζ01y(dATP) = 7.30\%(Lys159)N\zeta-Hζ01y(dATP) = 7.30\%(Lys159)N\zeta-Hζ01y(dATP) = 7.30\%(Lys159)N\zeta-Hζ01y(dATP) = 9.90%(Arg51)N\eta2-H\eta203β(syn-dATP) = 99.50\%(Arg51)N\eta2-H\eta203β(syn-dATP) = 99.50\%(Arg51)N\eta2-H\eta203β(syn-dATP) = 99.50\%(Arg51)N\eta2-H\eta203β(syn-dATP) = 21.00%(Arg51)N\eta2-Hη203β(syn-dATP) = 11.65%(Arg51)N\eta2-Hη203β(syn-dATP) = 8.30%(Arg51)N\eta2-Hη203β(syn-dATP) = 8.30%(Arg51)N\eta2-Hη203β(syn-dATP) = 8.30%(Thr45)Oy1-Hy1O3β(syn-dATP) = 13.35%(Thr45)Oy1-Hy1O3β(syn-dATP) = 13.35%(Tyr10)N-H03β(syn-dATP) = 13.35%(Tyr10)N-H03β(syn-dATP) = 13.35%(Tyr10)N-H03β(syn-dATP) = 14.00%(Tyr10)N-H03β(syn-dATP) = 20.55%(Lys159)Nζ-Hζ1O1γ(syn-dATP) = 20.55%(Lys159)Nζ-Hζ1O1γ(syn-dATP) = 16.50%(Lys159)Nζ-Hζ2O3γ(syn-dATP) = 16.50%(Lys159)Nζ-Hζ2O1γ(syn-dATP) = 16.50%(Lys159)Nζ-Hζ2O3γ(syn-dATP) = 16.50%(Lys159)Nζ-Hζ2O3β(dGTP) = 7.95%(Arg51)Nη-Hη12O3β(dGTP) = 7.95%(Arg51)Nη-Hη12O3β(dGTP) = 7.95%(Arg51)Nη-Hη12O3β(dGTP) = 7.95%(Arg51)Nη-Hη12O3β(dGTP) = 7.95%(Arg51)Nη-Hη12O3β(dGTP) = 7.95%(Tyr10)N-HO2γ(dGTP) = 8.25%(Tyr10)N-HO2γ(dGTP) = 8.25%(Tyr10)N-HO2γ(dGTP) = 8.25%(Tyr10)N-HO2γ(dGTP) = 8.25%(Tyr12)N-HO3(dGTP) = 8.25%(Tyr12)N-HO3(dGTP) = 8.25%(Tyr12)N-HO3(dGTP) = 43.20%(Lys159)Nζ-Hζ2O3γ(dGTP) = 43.20%(Lys159)Nζ-Hζ2O3γ(dGTP) = 43.20%(Lys159)Nζ-Hζ2O3γ(dGTP) = 43.20%$		$(TyTO)N = \Pi \dots OTy(dATF)$	27.30%
(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)		$(1\text{y}\text{f}48)\text{O}\text{f}-\text{H}\text{f}\dots\text{O}2\gamma(\text{dATP})$	97.30%
$(Ly_{3}159)N\zeta - H\zeta_{2}O3\gamma(dATP) 46.60\% \\(Ly_{3}159)N\zeta - H\zeta_{1}O3\gamma(dATP) 27.55\% \\(Ly_{3}159)N\zeta - H\zeta_{1}O3\gamma(dATP) 19.90\% \\(Ly_{3}159)N\zeta - H\zeta_{2}O1\gamma(dATP) 7.30\% \\(Ly_{3}159)N\zeta - H\zeta_{2}O1\gamma(dATP) 6.90\% \\(Ly_{3}159)N\zeta - H\zeta_{2}O1\gamma(dATP) 99.90\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\beta(syn-dATP) 99.90\% \\(Arg_{5}1)N\eta - H\eta_{2}O2\gamma(syn-dATP) 99.50\% \\(Arg_{5}1)N\eta - H\eta_{2}O2\gamma(syn-dATP) 99.50\% \\(Arg_{5}1)N\eta - H\eta_{2}O2\gamma(syn-dATP) 99.50\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\beta(syn-dATP) 99.50\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(syn-dATP) 11.65\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(syn-dATP) 11.65\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\beta(syn-dATP) 11.65\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\beta(syn-dATP) 8.30\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\beta(syn-dATP) 8.30\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(syn-dATP) 98.25\% \\(Thr45)O\gamma - H\eta_{2}O3\gamma(syn-dATP) 98.25\% \\(Thr45)O\gamma - H\eta_{1}O3(syn-dATP) 13.35\% \\(Tyr 10)N - HO3(syn-dATP) 100\% \\(Tyr 10)N - HO3(syn-dATP) 100\% \\(Tyr 10)N - HO3(syn-dATP) 100\% \\(Tyr 10)N - HLO3\gamma(syn-dATP) 100\% \\(Tyr 10)N - HL,O3\gamma(syn-dATP) 26.95\% \\(Ly_{3}159)N\zeta - H\zeta_{1}O1\gamma(syn-dATP) 16.50\% \\(Ly_{3}159)N\zeta - H\zeta_{3}O1\gamma(syn-dATP) 16.50\% \\(Ly_{3}159)N\zeta - H\zeta_{3}O3\gamma(syn-dATP) 16.50\% \\(Ly_{3}159)N\zeta - H\zeta_{2}O3\gamma(dGTP) 100\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(dGTP) 12.00\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(dGTP) 18.40\% \\(Thr45)O\gamma - H\eta_{2}O3\beta(dGTP) 19.95\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(dGTP) 18.40\% \\(Thr45)O\gamma - H\eta_{2}O3\beta(dGTP) 19.95\% \\(Arg_{5}1)N\eta - H\eta_{2}O3\gamma(dGTP) 18.40\% \\(Thr45)O\gamma - H\eta_{2}O3\beta(dGTP) 19.90\% \\(Tyr 10)N - HO2\gamma(dGTP) 18.25\% \\(Tyr 10)N - HO2\gamma(dGTP) 18.20\% \\(Ly_{3}159)N\zeta - H\zeta_{2}O3\gamma(dGTP) 18.20\% \\(Ly_{3}159)N\zeta - H\zeta_{2}O3\gamma(dGTP) 19.95\% \\(Tyr 10)N - HO2\gamma(dGTP) 19.95\% \\(Tyr 10)N - HO2\gamma(dGTP) 19.95\% \\(Tyr 10)N - HO2\gamma(dGTP) 19.95\% \\(Tyr 10)N - HO2\gamma(d$		$(1\text{yr}48)\text{O}\eta-\text{H}\eta\text{O}3\gamma(\text{dATP})$	8.10%
$ \begin{array}{ccccc} (L_{ys}159)N\zeta-H\zeta1O3\gamma(dATP) & 27.55\% \\ (L_{ys}159)N\zeta-H\zeta3O3\gamma(dATP) & 19.90\% \\ (L_{ys}159)N\zeta-H\zeta2O1\gamma(dATP) & 7.30\% \\ (L_{ys}159)N\zeta-H\zeta2O1\gamma(dATP) & 6.90\% \\ (L_{ys}159)N\zeta-H\zeta2O1\gamma(dATP) & 99.90\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 99.50\% \\ \hline (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 99.50\% \\ (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 48.05\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 8.30\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 8.30\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 8.30\% \\ (Thr45)O\gamma1-H\gamma1O3\beta(syn-dATP) & 8.30\% \\ (Thr45)O\gamma1-H\gamma1O3(syn-dATP) & 98.25\% \\ (Thr45)O\gamma1-H\gamma1O3(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3(syn-dATP) & 13.35\% \\ (Tyr10)N-HO3(syn-dATP) & 10.0\% \\ (Tyr12)N-HO3(syn-dATP) & 19.45\% \\ (L_{ys}159)N\zeta-H\zeta1O1\gamma(syn-dATP) & 34.95\% \\ (L_{ys}159)N\zeta-H\zeta1O1\gamma(syn-dATP) & 26.95\% \\ (L_{ys}159)N\zeta-H\zeta1O3\gamma(syn-dATP) & 16.50\% \\ (L_{ys}159)N\zeta-H\zeta1O3\gamma(syn-dATP) & 16.50\% \\ (L_{ys}159)N\zeta-H\zeta2O3\gamma(syn-dATP) & 16.50\% \\ (L_{ys}159)N\zeta-H\zeta2O3\gamma(dGTP) & 10.0\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 10.0\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 10.0\% \\ (Tyr10)N-HO3\beta(dGTP) & 25.90\% \\ (Arg51)N\eta2-H\eta22O3\gamma(dGTP) & 18.40\% \\ (Thr45)O\gamma1-H\gamma1O1\beta(dGTP) & 99.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 99.10\% \\ (Tyr10)N-HO2\gamma(dGTP) & 98.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 98.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 98.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 98.95\% \\ (Tyr12)N-HO3(dGTP) & 43.20\% \\ (L_{ys159})N\zeta-H\zeta2O3\gamma(dGTP) & 43.20\% $		$(Lys159)N\zeta -H\zeta 2O3\gamma(dATP)$	46.60%
$ \begin{array}{c} (Lys159)N\zeta-H\zeta3O3\gamma(dATP) & 19.90\% \\ (Lys159)N\zeta-H\zeta1O1\gamma(dATP) & 7.30\% \\ (Lys159)N\zeta-H\zeta2O1\gamma(dATP) & 6.90\% \\ (Lys159)N\zeta-H\zeta3O1\gamma(dATP) & 1.40\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 99.90\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 99.50\% \\ (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 48.05\% \\ (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 48.05\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 11.65\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ (Thr45)O\gamma1-H\gamma1O3\beta(syn-dATP) & 6.80\% \\ (Thr45)O\gamma1-H\gamma2O3\gamma(syn-dATP) & 6.80\% \\ (Thr45)O\gamma1-H\gamma1O3\beta(syn-dATP) & 13.35\% \\ (Tyr10)N-HO2\gamma(syn-dATP) & 100\% \\ (Tyr10)N-HO3\gamma(syn-dATP) & 100\% \\ (Tyr12)N-HO3'(syn-dATP) & 19.45\% \\ (Lys159)N\zeta-H\zeta1O1\gamma(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H\zeta2O1\gamma(syn-dATP) & 16.50\% \\ (Lys159)N\zeta-H\zeta2O1\gamma(syn-dATP) & 16.50\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) & 16.50\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 100\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 100\% \\ (Tr10)N-HO2\gamma(dGTP) & 7.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 7.95\% \\ (Tyr12)N-HO2\gamma(dGTP) & 7.95\% \\ (Tyr15)NYC-HZ2O3\gamma(dGTP) & 7.95\% \\ (Tyr15)N$		(Lys159)Nζ–Ηζ1O3γ(dATP)	27.55%
$ \begin{array}{c} (Lys159)N\zeta -H\zeta1O1\gamma(dATP) & 7.30\% \\ (Lys159)N\zeta -H\zeta2O1\gamma(dATP) & 6.90\% \\ (Lys159)N\zeta -H\zeta2O3\beta(syn-dATP) & 99.90\% \\ (Arg51)N\eta2 -H\eta22O3\beta(syn-dATP) & 99.50\% \\ (Arg51)N\eta2 -H\eta22O2\gamma(syn-dATP) & 99.50\% \\ (Arg51)N\eta2 -H\eta22O2\gamma(syn-dATP) & 48.05\% \\ (Arg51)N\eta2 -H\eta22O1\beta(syn-dATP) & 11.65\% \\ (Arg51)N\eta2 -H\eta22O1\beta(syn-dATP) & 11.65\% \\ (Arg51)N\eta2 -H\eta22O3\beta(syn-dATP) & 8.30\% \\ (Arg51)N\eta2 -H\eta22O3\beta(syn-dATP) & 8.30\% \\ (Arg51)N\eta2 -H\eta22O3\gamma(syn-dATP) & 8.30\% \\ (Arg51)N\eta2 -H\eta22O3\gamma(syn-dATP) & 98.25\% \\ (Thr45)O\gamma1 -H\gamma1O3\beta(syn-dATP) & 98.25\% \\ (Thr45)O\gamma1 -H\gamma1O3\beta(syn-dATP) & 13.35\% \\ (Tyr10)N -HO3\beta(syn-dATP) & 10.0\% \\ (Tyr10)N -HO3\beta(syn-dATP) & 19.45\% \\ (Lys159)N\zeta -H\zeta1O1\gamma(syn-dATP) & 34.95\% \\ (Lys159)N\zeta -H\zeta1O1\gamma(syn-dATP) & 26.95\% \\ (Lys159)N\zeta -H\zeta3O1\gamma(syn-dATP) & 15.00\% \\ (Lys159)N\zeta -H\zeta2O3\gamma(syn-dATP) & 16.50\% \\ (Lys159)N\zeta -H\zeta2O3\beta(dGTP) & 100\% \\ (Arg51)N\eta1 -H\eta12O3\beta(dGTP) & 10.0\% \\ (Arg51)N\eta1 -H\eta12O3\beta(dGTP) & 27.95\% \\ (Arg51)N\eta1 -H\eta12O3\beta(dGTP) & 18.40\% \\ (Thr45)O\gamma1 -H\gamma1O1\beta(dGTP) & 99.95\% \\ (Tyr10)N -HO3\beta(dGTP) & 18.40\% \\ (Thr45)O\gamma1 -H\gamma1O1\beta(dGTP) & 99.95\% \\ (Tyr10)N -HO2\gamma(dGTP) & 91.0\% \\ (Arg51)N\eta1 -H\eta12O3\gamma(dGTP) & 18.40\% \\ (Thr45)O\gamma1 -H\gamma1O1\beta(dGTP) & 99.95\% \\ (Tyr10)N -HO2\beta(dGTP) & 99.95\% \\ (Tyr10)N -HO2\beta(dGTP) & 99.95\% \\ (Tyr10)N -HO2\gamma(dGTP) & 91.0\% \\ (Lys159)N\zeta -H\zeta2O3\gamma(dGTP) & 18.40\% \\ (Thr45)O\gamma1 -H\gamma1O1\beta(dGTP) & 99.95\% \\ (Tyr10)N -HO2\gamma(dGTP) & 91.0\% \\ (Lys159)N\zeta -H\zeta2O3\gamma(dGTP) & 81.25\% \\ (Tyr12)N -HO3\beta(dGTP) & 81.25\% \\ (Tyr12)N -HO2\gamma(dGTP) & 33.00\% \\ (Lys159)N\zeta -H\zeta2O3\gamma(dGTP) & 33.00\% \\ (Lys159)N\zeta -H\zeta2O3\gamma(dGTP) & 40.15\% \\ \end{array}$		(Lys159)Nζ–Hζ3O3γ(dATP)	19.90%
$ \begin{array}{c} (Lys159)N\zeta-H\zeta2O1\gamma(dATP) & 6.90\% \\ (Lys159)N\zeta-H\zeta3O1\gamma(dATP) & 1.40\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 99.90\% \\ \hline (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 99.90\% \\ \hline (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 48.05\% \\ \hline (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) & 48.05\% \\ \hline (Arg51)N\eta2-H\eta22O1\beta(syn-dATP) & 11.65\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ \hline (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) & 8.30\% \\ \hline (Arg51)N\eta2-H\eta22O3\beta(syn-dATP) & 8.30\% \\ \hline (Thr45)O\gamma1-H\gamma1O3\beta(syn-dATP) & 98.25\% \\ \hline (Thr45)O\gamma1-H\gamma1O3\beta(syn-dATP) & 13.35\% \\ \hline (Tyr10)N-HO2\gamma(syn-dATP) & 100\% \\ \hline (Tyr10)N-HO3\beta(syn-dATP) & 34.70\% \\ \hline (Tyr12)N-HO3(syn-dATP) & 19.45\% \\ \hline (Lys159)N\zeta-H\zeta1O3\gamma(syn-dATP) & 26.95\% \\ \hline (Lys159)N\zeta-H\zeta1O3\gamma(syn-dATP) & 26.95\% \\ \hline (Lys159)N\zeta-H\zeta3O1\gamma(syn-dATP) & 15.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\beta(syn-dATP) & 15.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\beta(syn-dATP) & 15.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\beta(syn-dATP) & 15.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\beta(dGTP) & 100\% \\ \hline (Arg51)N\eta1-H\eta12O3\beta(dGTP) & 27.95\% \\ \hline (Arg51)N\eta1-H\eta12O3\beta(dGTP) & 27.95\% \\ \hline (Tyr10)N-HO3\beta(dGTP) & 27.95\% \\ \hline (Tyr10)N-HO3\beta(dGTP) & 18.40\% \\ \hline (Thr45)O\gamma1-H\gamma1O1\beta(dGTP) & 99.95\% \\ \hline (Tyr10)N-HO2\beta(dGTP) & 10.0\% \\ \hline (Tyr10)N-HO2\beta(dGTP) & 10.0\% \\ \hline (Tyr10)N-HO2\beta(dGTP) & 10.0\% \\ \hline (Tyr10)N-HO2\beta(dGTP) & 18.40\% \\ \hline (Thr45)O\gamma1-H\gamma1O3\beta(dGTP) & 18.40\% \\ \hline (Tyr10)N-HO2\beta(dGTP) & 10.0\% \\ \hline (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 13.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 13.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 33.00\% \\ \hline (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 40.15\% \\ \hline \right$		(Lys159)Nζ–Ηζ1Ο1γ(dATP)	7.30%
$ \begin{array}{c} \frac{(Lys159)N\zeta-H\zeta3O1\gamma(dATP)}{(Arg51)N\eta2-H\eta22O3\beta(syn-dATP)} 99.90\% \\ (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) 99.50\% \\ (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) 48.05\% \\ (Arg51)N\eta2-H\eta22O2\gamma(syn-dATP) 48.05\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) 11.65\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) 8.30\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) 8.30\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) 8.30\% \\ (Arg51)N\eta2-H\eta22O3\gamma(syn-dATP) 8.25\% \\ (Thr45)O\gamma1-H\gamma1O1\beta(syn-dATP) 98.25\% \\ (Thr45)O\gamma1-H\gamma1O3'(syn-dATP) 100\% \\ (Tyr10)N-HO2\gamma(syn-dATP) 100\% \\ (Tyr10)N-HO3\beta(syn-dATP) 100\% \\ (Tyr12)N-HO3'(syn-dATP) 100\% \\ (Tyr12)N-HO3'(syn-dATP) 100\% \\ (Lys159)N\zeta-H\zeta1O1\gamma(syn-dATP) 26.95\% \\ (Lys159)N\zeta-H\zeta1O1\gamma(syn-dATP) 26.95\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) 16.50\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) 16.50\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) 16.00\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) 100\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) 100\% \\ (Arg51)N\eta1-H\eta12O3\beta(dGTP) 27.95\% \\ (Arg51)N\eta1-H\eta12O3\beta(dGTP) 27.95\% \\ (Arg51)N\eta1-H\eta12O3\beta(dGTP) 18.40\% \\ (Thr45)O\gamma1-H\gamma1O1\beta(dGTP) 99.95\% \\ (Tyr10)N-HO3\beta(dGTP) 18.40\% \\ (Thr45)O\gamma1-H\gamma1O3\beta(dGTP) 18.25\% \\ (Tyr18)N\zeta-H\zeta2O3\gamma(dGTP) 18.25\% \\ (Tyr18)N\zeta-H\zeta2O3\gamma(dGTP) 18.20\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) 14.0.5\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) 14.0.5\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) 14.0.5\% \\ (Lys$		(Lys159)Nζ-Hζ2Ο1γ(dATP)	6.90%
$ \begin{array}{llllllllllllllllllllllllllllllllllll$		(Lys159)Nζ–Ηζ3Ο1γ(dATP)	1.40%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Arg51)Nη2–Hη22O3β(<i>syn</i> -dATP)	99.90%
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Major	$(Arg51)N\eta 1-H\eta 12O2\gamma(syn-dATP)$	99.50%
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Groove	$(Arg51)N\eta2-H\eta22O2\gamma(syn-dATP)$	48.05%
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Type I	(Arg51) Nn1–Hn12O3 γ (syn-dATP)	21.00%
$\begin{array}{c} (\operatorname{Arg51}) \operatorname{N\eta} 1-\operatorname{H\eta} 12O3\beta(syn-\operatorname{AATP}) & 8.30\% \\ (\operatorname{Arg51}) \operatorname{N\eta} 2-\operatorname{H\eta} 22O3\gamma(syn-\operatorname{AATP}) & 6.80\% \\ (\operatorname{Thr45}) O\gamma 1-\operatorname{H\gamma} 1O1\beta(syn-\operatorname{AATP}) & 98.25\% \\ (\operatorname{Thr45}) O\gamma 1-\operatorname{H\gamma} 1O3(syn-\operatorname{AATP}) & 13.35\% \\ (\operatorname{Tyr10}) \operatorname{N-HO2\gamma(syn-\operatorname{AATP})} & 100\% \\ (\operatorname{Tyr10}) \operatorname{N-HO3\beta(syn-\operatorname{AATP})} & 100\% \\ (\operatorname{Tyr12}) \operatorname{N-HO3}(syn-\operatorname{AATP}) & 19.45\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 1O1\gamma(syn-\operatorname{AATP}) & 26.95\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 1O3\gamma(syn-\operatorname{AATP}) & 26.95\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 1O3\gamma(syn-\operatorname{AATP}) & 26.95\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 2O1\gamma(syn-\operatorname{AATP}) & 26.95\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 2O3\gamma(syn-\operatorname{AATP}) & 16.50\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 2O3\gamma(\operatorname{GTP}) & 14.00\% \\ (\operatorname{Arg51}) \operatorname{N\eta} 2-\operatorname{H\eta} 22O3\beta(\operatorname{GTP}) & 100\% \\ (\operatorname{Arg51}) \operatorname{N\eta} 2-\operatorname{H\eta} 22O3\beta(\operatorname{GTP}) & 27.95\% \\ (\operatorname{Arg51}) \operatorname{N\eta} 2-\operatorname{H\eta} 22O3\gamma(\operatorname{GTP}) & 25.90\% \\ (\operatorname{Arg51}) \operatorname{N\eta} 2-\operatorname{H\eta} 22O3\gamma(\operatorname{GTP}) & 25.90\% \\ (\operatorname{Arg51}) \operatorname{N\eta} 2-\operatorname{H\eta} 22O3\gamma(\operatorname{GTP}) & 18.40\% \\ (\operatorname{Thr45}) O\gamma 1-\operatorname{H\gamma} 1O1\beta(\operatorname{GTP}) & 99.95\% \\ (\operatorname{Tyr10}) \operatorname{N-HO3\beta(\operatorname{dGTP}) & 79.10\% \\ (\operatorname{Tyr10}) \operatorname{N-HO3\beta(\operatorname{dGTP}) & 79.10\% \\ (\operatorname{Tyr10}) \operatorname{N-HO3\beta(\operatorname{dGTP}) & 99.95\% \\ (\operatorname{Tyr10}) \operatorname{N-HO3\beta(\operatorname{dGTP}) & 98.95\% \\ (\operatorname{Tyr12}) \operatorname{N-HO3\beta(\operatorname{dGTP}) & 81.25\% \\ (\operatorname{Tyr48}) \operatorname{O\eta} -\operatorname{H\eta}O2\gamma(\operatorname{dGTP}) & 33.00\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 2O3\gamma(\operatorname{dGTP}) & 43.20\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 2O3\gamma(\operatorname{dGTP}) & 43.20\% \\ (\operatorname{Lys159}) \operatorname{N\zeta} -\operatorname{H\zeta} 2O3\gamma(\operatorname{dGTP}) & 40.15\% \\ \end{array}$	(Cont d)	$(Arg51)Nn2-Hn22O1\beta(svn-dATP)$	11.65%
$\begin{array}{c} (\mathrm{Arg}51)\mathrm{N\eta}_2-\mathrm{H\eta}22O3\gamma(syn-\mathrm{dATP}) & 6.80\% \\ (\mathrm{Thr}45)\mathrm{Oy}1-\mathrm{Hy}1O1\beta(syn-\mathrm{dATP}) & 98.25\% \\ (\mathrm{Thr}45)\mathrm{Oy}1-\mathrm{Hy}1O3(syn-\mathrm{dATP}) & 13.35\% \\ (\mathrm{Tyr}10)\mathrm{N-H}O2\gamma(syn-\mathrm{dATP}) & 100\% \\ (\mathrm{Tyr}10)\mathrm{N-H}O3\beta(syn-\mathrm{dATP}) & 34.70\% \\ (\mathrm{Tyr}12)\mathrm{N-H}O3(syn-\mathrm{dATP}) & 94.5\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}1O1\gamma(syn-\mathrm{dATP}) & 34.95\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}1O3\gamma(syn-\mathrm{dATP}) & 26.95\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}3O1\gamma(syn-\mathrm{dATP}) & 20.55\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}3O3\gamma(syn-\mathrm{dATP}) & 16.50\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}2O3\gamma(syn-\mathrm{dATP}) & 15.00\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}2O3\gamma(syn-\mathrm{dATP}) & 15.00\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}2O3\gamma(\mathrm{dGTP}) & 100\% \\ (\mathrm{Arg}51)\mathrm{N\eta}2-\mathrm{H\eta}22O3\beta(\mathrm{dGTP}) & 100\% \\ (\mathrm{Arg}51)\mathrm{N\eta}2-\mathrm{H\eta}22O3\beta(\mathrm{dGTP}) & 27.95\% \\ (\mathrm{Arg}51)\mathrm{N\eta}2-\mathrm{H\eta}22O3\gamma(\mathrm{dGTP}) & 25.90\% \\ (\mathrm{Arg}51)\mathrm{N\eta}1-\mathrm{H\eta}12O3\gamma(\mathrm{dGTP}) & 18.40\% \\ (\mathrm{Thr}45)\mathrm{Oy}1-\mathrm{Hy}1O1\beta(\mathrm{dGTP}) & 99.95\% \\ (\mathrm{Tyr}10)\mathrm{N-H}O2\gamma(\mathrm{dGTP}) & 99.95\% \\ (\mathrm{Tyr}10)\mathrm{N-H}O3\beta(\mathrm{dGTP}) & 99.95\% \\ (\mathrm{Tyr}10)\mathrm{N-H}O3\beta(\mathrm{dGTP}) & 99.95\% \\ (\mathrm{Tyr}10)\mathrm{N-H}O3\beta(\mathrm{dGTP}) & 98.95\% \\ (\mathrm{Tyr}12)\mathrm{N-H}O3\beta(\mathrm{dGTP}) & 81.25\% \\ (\mathrm{Tyr}48)\mathrm{O\eta}-\mathrm{H\eta}O2\gamma(\mathrm{dGTP}) & 33.00\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}2O3\gamma(\mathrm{dGTP}) & 43.20\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}2O3\gamma(\mathrm{dGTP}) & 43.20\% \\ (\mathrm{Lys}159)\mathrm{N\zeta}-\mathrm{H\zeta}2O3\gamma(\mathrm{dGTP}) & 40.15\% \\ \end{array}$		(Arg51)Nn1-Hn12O3B(syn-dATP)	8.30%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Arg51)Nn2-Hn22O3v(svn-dATP)	6.80%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Thr 45)Ov1-Hv1 O1B(svn-dATP)	98.25%
$\begin{array}{cccc} (\mathrm{TH}4.5) \mathcal{O}[1-\mathrm{H}11\mathrm{OO}(S) \mathrm{H}\mathrm{d}\mathrm{A}\mathrm{H}1) & 10.05 \mathrm{H}\mathrm{d}\mathrm{H}1) \\ (\mathrm{Tyr10})\mathrm{N-H}\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 100\% \\ (\mathrm{Tyr10})\mathrm{N-H}\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 34.70\% \\ (\mathrm{Tyr12})\mathrm{N-H}\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 19.45\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta1\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 34.95\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta1\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 26.95\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta3\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 26.95\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta3\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 20.55\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 16.50\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 15.00\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(syn-\mathrm{d}\mathrm{A}\mathrm{TP}) & 15.00\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 14.00\% \\ (\mathrm{Arg51})\mathrm{N}\eta2-\mathrm{H}\eta22\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 100\% \\ (\mathrm{Arg51})\mathrm{N}\eta2-\mathrm{H}\eta22\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 32.70\% \\ (\mathrm{Arg51})\mathrm{N}\eta2-\mathrm{H}\eta22\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 25.90\% \\ (\mathrm{Arg51})\mathrm{N}\eta2-\mathrm{H}\eta22\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 25.90\% \\ (\mathrm{Arg51})\mathrm{N}\eta2-\mathrm{H}\eta22\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 25.90\% \\ (\mathrm{Arg51})\mathrm{N}\eta2-\mathrm{H}\eta22\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 18.40\% \\ (\mathrm{Thr45})\mathrm{O}(\mathrm{I}-\mathrm{H}\gamma1\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 99.95\% \\ (\mathrm{Tyr10})\mathrm{N-H}\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 99.95\% \\ (\mathrm{Tyr10})\mathrm{N-H}\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 99.95\% \\ (\mathrm{Tyr10})\mathrm{N-H}\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 98.95\% \\ (\mathrm{Tyr12})\mathrm{N-H}\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 81.25\% \\ (\mathrm{Tyr48})\mathrm{O}-\mathrm{H}\eta\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 33.00\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 43.20\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 43.20\% \\ (\mathrm{Lys159})\mathrm{N}\zeta-\mathrm{H}\zeta2\mathrm{OO}(\mathrm{d}\mathrm{G}\mathrm{TP}) & 40.15\% \end{array}$		(Thr 45)Oy1 Hy1 O3'(syn dATP)	13 35%
$\begin{array}{c} (1y110)N + HO3\beta(syn-dATP) & 34.70\% \\ (Tyr10)N-HO3'(syn-dATP) & 19.45\% \\ (Lys159)N\zeta-H\zeta1O1\gamma(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H\zeta1O3\gamma(syn-dATP) & 26.95\% \\ (Lys159)N\zeta-H\zeta3O1\gamma(syn-dATP) & 20.55\% \\ (Lys159)N\zeta-H\zeta3O3\gamma(syn-dATP) & 16.50\% \\ (Lys159)N\zeta-H\zeta2O1\gamma(syn-dATP) & 15.00\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) & 14.00\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 100\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 32.70\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 32.70\% \\ (Arg51)N\eta2-H\eta22O3\beta(dGTP) & 25.90\% \\ (Arg51)N\eta2-H\eta22O1\beta(dGTP) & 25.90\% \\ (Arg51)N\eta1-H\eta12O3\beta(dGTP) & 18.40\% \\ (Thr45)O\gamma1-H\gamma1O1\beta(dGTP) & 99.95\% \\ (Tyr10)N-HO2\gamma(dGTP) & 99.95\% \\ (Tyr10)N-HO2\beta(dGTP) & 42.25\% \\ (Phe11)N-HO3(dGTP) & 81.25\% \\ (Tyr48)O\eta-H\etaO2\gamma(dGTP) & 33.00\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 43.20\% \\ (Lys159)N\zeta-H\zeta2O3\gamma(dGTP) & 40.15\% \\ \end{array}$		$(Tur 10)N-H = O^2 (syn-dATP)$	100%
$(Tyr12)N-HO3'(syn-dATP) = 19.45\%$ $(Lys159)N\zeta-H\zeta1O1\gamma(syn-dATP) = 34.95\%$ $(Lys159)N\zeta-H\zeta1O3\gamma(syn-dATP) = 26.95\%$ $(Lys159)N\zeta-H\zeta3O1\gamma(syn-dATP) = 20.55\%$ $(Lys159)N\zeta-H\zeta3O3\gamma(syn-dATP) = 16.50\%$ $(Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) = 15.00\%$ $(Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) = 15.00\%$ $(Lys159)N\zeta-H\zeta2O3\gamma(syn-dATP) = 14.00\%$ $(Arg51)N\eta2-H\eta22O3\beta(dGTP) = 100\%$ $(Arg51)N\eta2-H\eta22O2\gamma(dGTP) = 97.60\%$ $(Arg51)N\eta2-H\eta22O3\beta(dGTP) = 27.95\%$ $(Arg51)N\eta2-H\eta22O1\beta(dGTP) = 25.90\%$ $(Arg51)N\eta1-H\eta12O3\gamma(dGTP) = 18.40\%$ $(Thr45)O\gamma1-H\gamma1O1\beta(dGTP) = 99.95\%$ $(Tyr10)N-HO2\gamma(dGTP) = 79.10\%$ $(Tyr10)N-HO3\beta(dGTP) = 42.25\%$ $(Phe11)N-HO2\beta(dGTP) = 81.25\%$ $(Tyr48)O\eta-H\etaO2\gamma(dGTP) = 33.00\%$ $(Lys159)N\zeta-H\zeta3O3\gamma(dGTP) = 43.20\%$		$(Tyr10)N-H O3\beta(syn-dATP)$	34 70%
$(1y_{11}) (1y_{11}) (1y_$		(Tyr12)N-H O3'(syn-dATP)	19.45%
$(Lys159)N\zeta-H\zeta1O3\gamma(syn-dATP) 26.95\% (Lys159)N\zeta-H\zeta3O1\gamma(syn-dATP) 26.95\% (Lys159)N\zeta-Hζ3O3\gamma(syn-dATP) 20.55\% (Lys159)N\zeta-Hζ3O3\gamma(syn-dATP) 16.50\% (Lys159)N\zeta-Hζ2O3\gamma(syn-dATP) 15.00\% (Lys159)N\zeta-Hζ2O3\gamma(syn-dATP) 14.00\% (Arg51)Nη2-Hη22O3β(dGTP) 100% (Arg51)Nη2-Hη22O3β(dGTP) 97.60% (Arg51)Nη2-Hη22O2\gamma(dGTP) 32.70% (Arg51)Nη2-Hη22O1β(dGTP) 25.90% (Arg51)Nη2-Hη22O1β(dGTP) 25.90% (Arg51)Nη2-Hη22O1β(dGTP) 18.40% (Thr45)Oγ1-Hγ1O1β(dGTP) 99.95% (Tyr10)N-HO2\gamma(dGTP) 79.10% (Tyr10)N-HO3β(dGTP) 42.25% (Phe11)N-HO3β(dGTP) 81.25% (Tyr48)Oη-HηO2γ(dGTP) 33.00% (Lys159)Nζ-Hζ3O3γ(dGTP) 43.20% (Lys159)Nζ-Hζ2O3γ(dGTP) 40.15%$		$(I_{ye12})N'_{H'_1} O_{1}(syn_dATP)$	34 95%
(Lys159)N\zeta-Hζ1O3 γ (Syn-dATP)20.93%(Lys159)Nζ-Hζ3O1 γ (syn-dATP)20.55%(Lys159)Nζ-Hζ2O3 γ (syn-dATP)16.50%(Lys159)Nζ-Hζ2O1 γ (syn-dATP)15.00%(Lys159)Nζ-Hζ2O3 γ (syn-dATP)14.00%(Arg51)Nη2-Hη22O3 β (dGTP)100%(Arg51)Nη2-Hη22O2 γ (dGTP)97.60%(Arg51)Nη2-Hη22O2 γ (dGTP)32.70%(Arg51)Nη2-Hη22O2 γ (dGTP)25.90%(Arg51)Nη2-Hη22O3 β (dGTP)25.90%(Arg51)Nη2-Hη22O3 γ (dGTP)18.40%(Thr45)O γ 1-H γ 1O1 β (dGTP)99.95%(Tyr10)N-HO2 γ (dGTP)98.95%(Tyr10)N-HO2 β (dGTP)81.25%(Tyr48)O\eta-H η 1O2 γ (dGTP)33.00%(Lys159)Nζ-Hζ3O3 γ (dGTP)43.20%(Lys159)Nζ-Hζ2O3 γ (dGTP)40.15%		$(Lys159)N\zeta -\Pi\zeta 1O1\gamma(syn-dATD)$	26.05%
(Lys159)N ζ -H ζ 3O γ (syn-dATP)20.33%(Lys159)N ζ -H ζ 3O γ (syn-dATP)16.50%(Lys159)N ζ -H ζ 2O γ (syn-dATP)15.00%(Lys159)N ζ -H ζ 2O γ (syn-dATP)14.00%(Arg51)N η 2-H η 22O γ (dGTP)97.60%(Arg51)N η 2-H η 22O γ (dGTP)97.60%(Arg51)N η 2-H η 22O γ (dGTP)32.70%(Arg51)N η 2-H η 22O γ (dGTP)25.90%(Arg51)N η 2-H η 22O β (dGTP)25.90%(Arg51)N η 2-H η 22O β (dGTP)18.40%(Thr45)O γ 1-H γ 1O β (dGTP)99.95%(Tyr10)N-HO γ (dGTP)79.10%(Tyr10)N-HO β (dGTP)81.25%(Tyr48)O η -H η 1O γ (dGTP)33.00%(Lys159)N ζ -H ζ 2O γ (dGTP)43.20%(Lys159)N ζ -H ζ 2O γ (dGTP)43.20%		$(Lys159)N\zeta - H\zeta I \dots O5\gamma(syn-uATF)$	20.95%
(Lys159)N ζ -H ζ 3O3 γ (syn-dA1P)16.50%(Lys159)N ζ -H ζ 2O1 γ (syn-dATP)15.00%(Lys159)N ζ -H ζ 2O3 γ (syn-dATP)14.00%(Arg51)N η 2-H η 22O3 β (dGTP)100%(Arg51)N η 2-H η 22O2 γ (dGTP)97.60%(Arg51)N η 2-H η 22O2 γ (dGTP)32.70%(Arg51)N η 2-H η 22O2 γ (dGTP)27.95%(Arg51)N η 2-H η 22O1 β (dGTP)25.90%(Arg51)N η 2-H η 22O1 β (dGTP)18.40%(Thr45)O γ 1-H γ 1O1 β (dGTP)99.95%(Tyr10)N-HO2 γ (dGTP)79.10%(Tyr10)N-HO2 β (dGTP)81.25%(Tyr12)N-HO3'(dGTP)33.00%(Lys159)N ζ -H ζ 2O3 γ (dGTP)43.20%(Lys159)N ζ -H ζ 2O3 γ (dGTP)40.15%		$(Lys159)N\zeta - H\zeta 5OI\gamma(syn-dAIP)$	20.33%
(Lys159)N ζ -H ζ 2O1 γ (syn-dATP)15.00%(Lys159)N ζ -H ζ 2O3 γ (syn-dATP)14.00%(Arg51)N η 2-H η 22O3 β (dGTP)100%(Arg51)N η 1-H η 12O2 γ (dGTP)97.60%(Arg51)N η 2-H η 22O2 γ (dGTP)32.70%(Arg51)N η 2-H η 22O3 β (dGTP)27.95%(Arg51)N η 2-H η 22O1 β (dGTP)25.90%(Arg51)N η 2-H η 22O3 γ (dGTP)18.40%(Thr45)O γ 1-H γ 1O3 β (dGTP)99.95%(Tyr10)N-HO2 γ (dGTP)79.10%(Tyr10)N-HO3 β (dGTP)42.25%(Phe11)N-HO2 β (dGTP)81.25%(Tyr48)O η -H η O2 γ (dGTP)33.00%(Lys159)N ζ -H ζ 3O3 γ (dGTP)43.20%(Lys159)N ζ -H ζ 2O3 γ (dGTP)40.15%		$(Lys159)N\zeta -H\zeta 3O3\gamma(syn-dA1P)$	16.50%
(Lys159)N ζ -H ζ 2O3 γ (syn-dATP)14.00%(Arg51)N η 2-H η 22O3 β (dGTP)100%(Arg51)N η 1-H η 12O2 γ (dGTP)97.60%(Arg51)N η 2-H η 22O2 γ (dGTP)32.70%(Arg51)N η 2-H η 22O3 β (dGTP)27.95%(Arg51)N η 2-H η 22O1 β (dGTP)25.90%(Arg51)N η 2-H η 22O1 β (dGTP)18.40%(Thr45)O γ 1-H γ 1O1 β (dGTP)99.95%(Tyr10)N-HO2 γ (dGTP)79.10%(Tyr10)N-HO2 β (dGTP)98.95%(Tyr12)N-HO3'(dGTP)81.25%(Tyr48)O η -H η O2 γ (dGTP)33.00%(Lys159)N ζ -H ζ 2O3 γ (dGTP)43.20%(Lys159)N ζ -H ζ 2O3 γ (dGTP)40.15%		$(Lys159)N\zeta - H\zeta 2O1\gamma(syn-dATP)$	15.00%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$(Lys159)N\zeta - H\zeta 2O3\gamma(syn-dATP)$	14.00%
$(Arg51)N\eta 1-H\eta 12O2\gamma(dGTP)$ 97.60% $(Arg51)N\eta 2-H\eta 22O2\gamma(dGTP)$ 32.70% $(Arg51)N\eta 1-H\eta 12O3\beta(dGTP)$ 27.95% $(Arg51)N\eta 2-H\eta 22O1\beta(dGTP)$ 25.90% $(Arg51)N\eta 1-H\eta 12O3\gamma(dGTP)$ 18.40% $(Thr45)O\gamma 1-H\gamma 1O1\beta(dGTP)$ 99.95% $(Tyr10)N-HO2\gamma(dGTP)$ 79.10% $(Tyr10)N-HO3\beta(dGTP)$ 42.25% $(Phe11)N-HO2\beta(dGTP)$ 98.95% $(Tyr12)N-HO3'(dGTP)$ 81.25% $(Tyr48)O\eta-H\etaO2\gamma(dGTP)$ 33.00% $(Lys159)N\zeta-H\zeta 3O3\gamma(dGTP)$ 40.15%		(Arg51)Nη2–Hη22O3β(dGTP)	100%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Arg51)Nη1–Hη12O2γ(dGTP)	97.60%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$(Arg51)N\eta2-H\eta22O2\gamma(dGTP)$	32.70%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$(Arg51)N\eta1-H\eta12O3\beta(dGTP)$	27.95%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Arg51)Nη2–Hη22O1β(dGTP)	25.90%
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Arg51)Nη1–Hη12O3γ(dGTP)	18.40%
$(Tyr10)N-HO2\gamma(dGTP)$ 79.10% $(Tyr10)N-HO3\beta(dGTP)$ 42.25% $(Phe11)N-HO2\beta(dGTP)$ 98.95% $(Tyr12)N-HO3'(dGTP)$ 81.25% $(Tyr48)O\eta-H\etaO2\gamma(dGTP)$ 33.00% $(Lys159)N\zeta-H\zeta3O3\gamma(dGTP)$ 43.20% $(Lvs159)N\zeta-H\zeta2O3\gamma(dGTP)$ 40.15%		$(Thr 45)O\gamma 1-H\gamma 1O1\beta(dGTP)$	99.95%
$(Tyr10)N-HO3\beta(dGTP)$ 42.25% $(Phe11)N-HO2\beta(dGTP)$ 98.95% $(Tyr12)N-HO3'(dGTP)$ 81.25% $(Tyr48)O\eta-H\etaO2\gamma(dGTP)$ 33.00% $(Lys159)N\zeta-H\zeta3O3\gamma(dGTP)$ 43.20% $(Lys159)N\zeta-H\zeta2O3\gamma(dGTP)$ 40.15%		$(Tyr10)N-HO2\gamma(dGTP)$	79.10%
(Phe11)N-HO2 β (dGTP)98.95%(Tyr12)N-HO3'(dGTP)81.25%(Tyr48)O\eta-H\etaO2 γ (dGTP)33.00%(Lys159)N\zeta-H\zeta3O3 γ (dGTP)43.20%(Lvs159)N\zeta-Hζ2O3 γ (dGTP)40.15%		$(Tyr10)N-HO3\beta(dGTP)$	42.25%
$(Tyr12)N-HO3'(dGTP)$ 81.25% $(Tyr48)O\eta-H\etaO2\gamma(dGTP)$ 33.00% $(Lys159)N\zeta-H\zeta3O3\gamma(dGTP)$ 43.20% $(Lvs159)N\zeta-H\zeta2O3\gamma(dGTP)$ 40.15%		(Phe11)N–HO2 β (dGTP)	98.95%
$(Tyr48)O\eta-H\etaO2\gamma(dGTP)$ 33.00% $(Lys159)N\zeta-H\zeta3O3\gamma(dGTP)$ 43.20% $(Lvs159)N\zeta-H\zeta2O3\gamma(dGTP)$ 40.15%		(Tyr12)N–HO3′(dGTP)	81.25%
(Lys159)Nζ–Hζ3O3γ(dGTP) 43.20% (Lys159)Nζ–Hζ2O3γ(dGTP) 40.15%		$(Tyr48)O\eta - H\eta \dots O2\gamma(dGTP)$	33.00%
$(Lvs159)N\zeta - H\zeta 2O3\gamma(dGTP)$ 40.15%		(Lys159)Nζ-Hζ3O3v(dGTP)	43.20%
		(Lys159)Νζ–Ηζ2Ο3γ(dGTP)	40.15%

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$(I_{\rm MC}150)N\ell$ $H\ell 1$ $\Omega_{\rm M}(d\rm CTD)$	15.05%
(Lys139)(15-1151057(00117))	10.0070
(Lys159)Nζ-Hζ2O2γ(dGTP)	14.45%
(Lys159)Nζ-Hζ3O2γ(dGTP)	11.60%
(Lys159)Nζ–Hζ1O2γ(dGTP)	4.60%
$\begin{array}{c} \text{Major} \\ \text{Groove} \end{array} (\text{Arg51}) \text{N}\eta 2 - \text{H}\eta 22O3\beta(syn\text{-dGTP}) \end{array}$	99.95%
Type I (Arg51)N η 1–H η 12O3 γ (syn-dGTP)	99.10%
$(Cont'd)$ (Arg51)N η 1–H η 12O2 γ (syn-dGTP)	33.65%
(Arg51) N η 2–H η 22O3 γ (syn-dGTP)	19.65%
$(Arg51)N\eta1-H\eta12O3\beta(syn-dGTP)$	12.15%
$(Arg51)N\eta2-H\eta22O1\beta(syn-dGTP)$	11.55%
$(Thr 45)O\gamma 1-H\gamma 1O1\beta(syn-dGTP)$	100%
$(Tyr10)N-HO2\gamma(syn-dGTP)$	99.95%
$(Tyr10)N-HO3\beta(syn-dGTP)$	43.90%
(Phe11)N–HO2 β (syn-dGTP)	85.00%
(Phe11)N–HO1 β (syn-dGTP)	6.40%
(Tyr12)N–HO3'(syn-dGTP)	51.10%
$(Tyr48)O\eta-H\etaO2\gamma(syn-dGTP)$	100%
(Lys159)Nζ–Ηζ1O3γ(syn-dGTP)	41.90%
(Lys159)Nζ–Ηζ3O3γ(syn-dGTP)	40.70%
(Lys159)Nζ–Ηζ2O3γ(syn-dGTP)	16.80%
(Lys159)Nζ–Hζ3…O2γ(syn-dGTP)	3.90%
(Lys159)Nζ–Hζ1O2 γ (syn-dGTP)	3.80%
(Lys159)Nζ–Hζ2O2 γ (syn-dGTP)	1.15%
(Tyr10)N–HΟ1γ(dGTP)	47.45%
-1 Deletion (Tyr10)N-HO2 γ (dGTP)	19.40%
(Phe11)N–HO 3γ (dGTP)	12.50%
(Phe11)N–HO2y(dGTP)	9.80%

^{*a*} Hydrogen bonds are specified in the format (A)B–C...D(E), where A is the residue name of the donor atom, B is the name of the donor atom, C is the name of the hydrogen atom, D is the name of the acceptor atom, and E is the residue name of the acceptor atom. * denotes 1S (–)-B[c]Ph-dA modification.

^b Criterion for hydrogen bond occupancy is: heavy-to-heavy distance ≤ 3.4 Å and bond angle $\leq 135^{\circ}$.

Table S3. Hydrogen bonding interactions of >10% occupancy between the adducted adenine and neighboring bases or protein residues other than the incoming dNTP.

Model	dNTP	Hydrogen Bond ^{<i>a</i>}	Distance (Å) b	Angle (°) ^b	Occupancy ^c
		$(tA_3)N6-H61O4Z(tA_5)$	3.08 ± 0.16	160.5 ± 10.3	71.59%
	ATTD	$(tA*_5)O2Z-HO2ZO4(pT_{13})$	2.86 ± 0.18	158.0 ± 8.4	63.48%
	uiir	$(tC_4)N4-H42O3Z(tA*_5)$	3.06 ± 0.17	150.2 ± 10.1	35.22%
		$(tA_3)N6-H61O3Z(tA_5)$	3.07 ± 0.18	150.0 ± 10.6	16.66%
		$(tA*_5)O4Z-HO4ZO(Gly58)$	2.81 ± 0.17	166.6 ± 9.1	56.10%
		$(tA_{5})O2Z-HO2ZO4(pT_{13})$	2.91 ± 0.19	154.9 ± 8.5	52.20%
		(tA*5)O3Z-HO3ZN3(tC4)	2.94 ± 0.18	165.1 ± 8.3	49.35%
		$(tA_3)N6-H61O3Z(tA_5)$	3.06 ± 0.17	155.8 ± 12.7	42.50%
	ACTD	$(tA_6)N6-H61O2Z(tA_5)$	3.00 ± 0.16	151.1 ± 9.9	33.75%
	uerr	(tA*5)N6-H6O(Gly58)	3.18 ± 0.15	164.7 ± 7.8	29.65%
		$(tA_3)N6-H61O4Z(tA_5)$	3.12 ± 0.16	158.2 ± 10.0	27.45%
		$(tA_{5})O4Z-HO4ZN1(tA_{3})$	2.95 ± 0.17	161.5 ± 11.3	25.70%
		$(tA_{5})O3Z-HO3ZN1(tA_{3})$	2.90 ± 0.16	162.8 ± 10.8	20.75%
		$(tC_4)N4-H41O3Z(tA_5)$	3.16 ± 0.18	155.3 ± 10.9	12.85%
		(tA* ₅)O2Z–HO2ZO4(pT ₁₃)	2.82 ± 0.16	153.6 ± 8.2	78.35%
		$(tA_3)N6-H61O4Z(tA_{5})$	3.03 ± 0.16	162.9 ± 10.2	73.75%
T / 1 /		$(tA_6)N6-H61O2Z(tA_5)$	2.96 ± 0.14	150.5 ± 9.7	61.65%
Intercalation	14.555	$(tA_{5})O4Z-HO4ZN1(tA_{3})$	2.86 ± 0.14	165.8 ± 8.6	24.25%
	dATP	$(tA_3)N6-H61O3Z(tA_5)$	3.11 ± 0.16	152.4 ± 11.4	14.60%
		$(tA_{5})O2Z-HO2ZN1(tA_{6})$	2.91 ± 0.21	165.9 ± 9.7	12.75%
		$(tC_4)N4-H42O3Z(tA*_5)$	3.03 ± 0.17	144.8 ± 7.6	7.60%
		$(tC_4)N4-H41O3Z(tA*_5)$	2.99 ± 0.16	154.2 ± 11.8	5.85%
		$(tA_{5})O2Z-HO2ZO4(pT_{13})$	2.81 ± 0.15	158.4 ± 8.1	95.75%
	14 575	$(tA_3)N6-H61O4Z(tA_5)$	3.02 ± 0.16	158.1 ± 10.7	74.95%
	syn-dATP	$(tA_6)N6-H61O2Z(tA_{5})$	2.92 ± 0.14	159.3 ± 9.9	66.75%
		$(tC_4)N4-H42O3Z(tA_5)$	3.02 ± 0.16	149.2 ± 9.4	29.25%
		$(tA_{5})O2Z-HO2ZO4(pT_{13})$	2.81 ± 0.17	158.5 ± 8.1	76.00%
	dGTP	$(tA_6)N6-H61O2Z(tA_{5})$	2.95 ± 0.15	155.1 ± 10.3	57.20%
		$(tC_4)N4-H41O3Z(tA_5)$	2.99 ± 0.16	156.7 ± 10.9	18.45%
		$(tA_{5})O2Z-HO2ZO4(pT_{13})$	2.93 ± 0.20	157.8 ± 9.6	55.25%
		$(tC_4)N4-H42O3Z(tA_5)$	3.01 ± 0.17	154.4 ± 10.6	34.60%
	svn-dGTP	$(tC_4)N4-H41O3Z(tA_5)$	3.00 ± 0.16	159.1 ± 11.8	20.60%
	~)	$(tA_6)N6-H62N7(tA_{5})$	3.18 ± 0.13	155.1 ± 10.3	17.40%
		$(tA_3)N6-H61O4Z(tA_{5})$	3.11 ± 0.17	162.8 ± 10.3	14.00%
-		$(tA_{5})O3Z-HO3ZO(Val43)$	2.66 ± 0.10	169.4 ± 6.2	99.85%
	dTTP	(Glv58)N–HO3Z(tA*5)	2.90 ± 0.12	164.8 ± 8.8	96.00%
	10770	$(tA*_5)O3Z-HO3ZO(Val43)$	2.66 ± 0.10	169.4 ± 6.0	92.55%
	dCTP	(Gly58)N–HO3Z(tA*5)	2.95 ± 0.15	157.9 ± 10.4	85.70%
	1455	(tA* ₅)O3Z–HO3ZO(Ala57)	2.77 ± 0.16	167.7 ± 7.9	67.30%
	dATP	$(tA_{5})O3Z-HO3ZO(Val43)$	2.84 ± 0.19	165.5 ± 10.2	31.45%
Major Groove		$(tA*_5)O3Z-HO3ZO(Val43)$	2.67 ± 0.10	169.6 ± 5.9	100%
Type I _	syn-dATP	(Glv58)N–HO3Z(tA*5)	2.92 ± 0.12	164.6 ± 8.1	98.95%
		$(tA_{5})O3Z-HO3ZO(Val43)$	2.69 ± 0.11	168.8 ± 6.9	99.40%
	dGTP	$(Glv58)N-HO3Z(tA*_{5})$	2.90 ± 0.12	163.3 ± 8.3	97.70%
		$(tA_{5})O2Z-HO2ZO(Glv58)$	3.02 ± 0.20	152.0 ± 9.5	12.15%
	syn-dGTP	$(tA*_5)O3Z-HO3ZO(Val43)$	2.68 ± 0.11	169.5 ± 6.3	99.85%
		(Gly58)N–HO3Z(tA* ₅)	2.93 ± 0.13	161.3 ± 10.4	84.00%
		$(tC_4)N4-H42O3Z(tA*_5)$	3.00 ± 0.15	163.8 ± 7.9	79.35%
-1 Deletion	dGTP	$(tA_{5})O2Z-HO2ZN7(tA_{3})$	3.12 ± 0.16	151.6 ± 8.3	31.70%

a-c See footnotes of Table 1.

Figure Legends

Figure S1. RMSDs for the Dpo4 ternary complexes over the 1 ns MD simulations. (A) RMSDs for the unmodified control with incoming dTTP and 1S (–)-B[c]Ph-dA intercalation models with varying incoming dNTPs. Color code: control, black; dTTP, green; dCTP, orange; dATP, red; *syn*-dATP, cyan; dGTP, blue; *syn*-dGTP, magenta. (B) RMSDs for the major groove Type I models with varying dNTPs and –1 deletion model with incoming dGTP. Color code: same as in (A) except that *black* represents the –1 deletion case.

Figure S2. Time dependence of the linkage site torsional angles α' , β' and χ over 1 ns time frame for unmodified control and 1*S* (–)-B[*c*]Ph-dA intercalation structures in the Dpo4 DNA polymerase. See Figure 1 for definition of the torsion angles. Color code: same as in Figure S1A.

Figure S3. Time dependence of the linkage site torsional angles α' , β' and χ over 1 ns time frame for 1*S* (–)-B[*c*]Ph-dA major groove Type I structures and –1 deletion model in the Dpo4 DNA polymerase. See Figure 1 for definition of the torsion angles. Color code: same as in Figure S1B.

Figure S4. Time dependence of distances and angles of significantly occupied hydrogen bonds (> 50% occupancy) between the templating residue and incoming dNTP in unmodified control and 1*S* (–)-B[c]Ph-dA intercalation structures in the Dpo4 DNA polymerase. Refer to Table 1 for complete specifications of these hydrogen bonds. Color code: the same as in Figure S1A.

Figure S5. Stacking interactions in the unmodified control and in the 1*S* (–)-B[*c*]Ph-dA intercalation structures of the Dpo4 ternary complexes after 1 ns of MD. (A)–(G) are the same as in Figure 2. Color code: unmodified or modified adenine, green; incoming dNTP, purple; B[*c*]Ph, red; tA₆, magenta; pT₁₃, cyan. The view is along the DNA helix axis from 5' to 3' end of the template strand. All stereo images are constructed for viewing with a stereoviewer.

Figure S6. Time dependence of the distances between C1's of the nascent base pair and distances between P α of dNTP and O3' of the primer terminus, in the unmodified control and 1*S* (–)-B[c]Ph-dA intercalation structures in the Dpo4 DNA polymerase. Color code: the same as in Figure S1A.

Figure S7. Time dependence of the distances between C1's of the nascent base pair and distances between P α of dNTP and O3' of the primer terminus, in the 1*S* (–)-B[*c*]Ph-dA major groove and –1 deletion models of the Dpo4 ternary complexes. Color code: the same as in Figure S1B.

Figure S8. Time dependence of distances and angles of significantly occupied hydrogen bonds (> 50% occupancy) between the templating residue and incoming dNTP in the 1S (–)-B[c]Ph-dA major groove and –1 deletion models of the Dpo4 ternary complexes. Refer to Table 1 for complete specifications of these hydrogen bonds. Color code: the same as in Figure S1B.

Figure S9. Stacking interactions in the unmodified control and in the 1S (–)-B[*c*]Ph-dA major groove and –1 deletion models of the Dpo4 ternary complexes after 1 ns of MD. (A)–(G) are the same as in Figure 5. Color code: the same as in Figure S5 except that tC₄ is shown in orange in (G). All stereo images are constructed for viewing with a stereoviewer.





























(G) syn-dGTP















(G) -1 Deletion









