B-DNA Characteristics are Preserved in Double Stranded $d(A)_3 \cdot d(T)_3$ and $d(G)_3 \cdot d(C)_3$ Mini-Helixes: Conclusions from DFT/M06-2X Study

Tetiana A. Zubatiuk, Oleg V. Shishkin, Leonid Gorb, Dmytro M. Hovorun, and Jerzy Leszczynski

Electronic Supplementary Information

Table 1S. M06-2X/6-31G(d,p) optimized reference geometry for d(ApApA) duplex in Model 1.

O	-7.656433	-5.000782	4.348359
C	-6.333819	-5.182992	4.808549
H	-6.296165	-5.147733	5.909358
H	-6.014940	-6.174599	4.476963
H	-5.649310	-4.426128	4.416151
C	-8.201190	-3.738567	4.677499
H	-7.861168	-3.427951	5.678862
H	-9.289902	-3.868861	4.707987
C	-7.878264	-2.637797	3.678427
H	-8.471254	-1.749773	3.938474
O	-6.489172	-2.324463	3.743329
C	-5.934277	-2.384130	2.423263
N	-4.541344	-2.757730	2.536970
C	-3.530812	-1.946261	3.000183
N	-3.617715	-0.669883	3.399172
C	-2.424962	-0.185271	3.710756
H	-2.389547	0.862138	4.003275
N	-1.232604	-0.805883	3.692521
C	-1.170512	-2.088309	3.285576
N	0.014301	-2.713978	3.240686
H	0.860371	-2.172341	3.422982
H	0.100599	-3.523293	2.644146
C	-2.379594	-2.723671	2.931090
N	-2.651169	-3.979116	2.422707
C	-3.936664	-3.948048	2.196746
H	-4.501386	-4.750269	1.745286
H	-5.990567	-1.394940	1.951055
C	-6.796892	-3.407546	1.702011
H	-6.574407	-4.413437	2.072894
H	-6.739322	-3.358116	0.615512
C	-8.177252	-3.002742	2.212602
H	-8.922085	-3.803331	2.117355
O	-8.627369	-1.827757	1.582363
P	-9.178921	-1.972493	0.011770
O	-10.455880	-2.742838	0.035756
O	-9.508841	-0.380581	-0.221691
C	-9.043278	0.684543	0.580826
H	-8.931281	0.372616	1.623285
H	-9.811737	1.467263	0.526683
C	-7.741736	1.305304	0.105722
H	-7.630580	2.280462	0.602843
O	-6.629012	0.476519	0.443095
C	-5.744483	0.487116	-0.676785
N	-4.799948	-0.596255	-0.552995
C	-3.489990	-0.462936	-0.147124
N	-2.844685	0.652924	0.219804
C	-1.568563	0.419245	0.499944
H	-0.967632	1.272215	0.809741
N	-0.909161	-0.757275	0.453348
C	-1.577784	-1.860074	0.071347
N	-0.914581	-3.025301	-0.028832
H	0.051741	-3.099694	0.283077
H	-1.453510	-3.866641	-0.155002
C	-2.946711	-1.739598	-0.253781
N	-3.883931	-2.643521	-0.724835
C	-4.968031	-1.919446	-0.890044
H	-5.938456	-2.275632	-1.223047
H	-5.145337	1.407660	-0.685550
C	-6.703680	0.446558	-1.861204
H	-7.225170	-0.516877	-1.869863
H	-6.251190	0.665717	-2.825275
C	-7.666289	1.544840	-1.418367
O	-7.094005	2.834700	-1.600386
P	-7.140496	3.547857	-3.089775
O	-6.680256	5.049880	-2.564152
C	-5.606899	5.223865	-1.667746
H	-5.732807	4.594670	-0.778742
H	-5.647547	6.276484	-1.362444
C	-4.207724	4.966607	-2.228731
H	-3.500632	5.632591	-1.704115
O	-3.818314	3.623595	-2.008226
C	-2.786929	3.333510	-2.924579
H	-1.813590	3.677014	-2.547817
N	-2.684888	1.903922	-3.064900
C	-1.598306	1.098554	-2.833444
N	-0.356205	1.450927	-2.474293
C	0.434606	0.395858	-2.342787
H	1.463668	0.578020	-2.040624
N	0.114343	-0.901847	-2.529858
C	-1.139563	-1.233899	-2.881348
N	-1.475136	-2.534512	-3.060227
H	-0.844355	-3.217837	-2.642885
H	-2.464391	-2.724623	-2.947323
C	-2.063827	-0.192619	-3.073455
N	-3.397382	-0.194753	-3.429679
C	-3.726792	1.072713	-3.416618
H	-4.691076	1.518226	-3.654698
C	-3.194503	4.051303	-4.222815
H	-2.322053	4.363951	-4.803403
H	-3.828092	3.385113	-4.810451
C	-4.032495	5.239387	-3.733163
O	-3.385521	6.501516	-3.870096
C	-3.451157	6.985552	-5.179703
H	-2.956144	7.961071	-5.198676
H	-4.492980	7.103750	-5.515447
H	-2.940897	6.321805	-5.894909
H	-5.007506	5.257624	-4.231437
O	-8.545296	3.652169	-3.570704
O	-6.045818	2.992132	-3.960667
H	-8.646001	1.492427	-1.904095
O	-8.039226	-2.390135	-0.871441
O	6.941517	-5.750937	-3.727758
C	7.816722	-4.753176	-4.221945
C	7.626767	-3.405073	-3.538418
C	8.065471	-3.346450	-2.059278
C	6.741635	-3.274361	-1.304817
H	6.843665	-2.683760	-0.398527
H	6.431871	-4.283405	-1.021541
C	5.770609	-2.662463	-2.307843
N	4.402497	-3.148632	-2.185207
C	3.344585	-2.231110	-2.164475
N	2.090882	-2.799832	-2.147968
C	1.786041	-4.143263	-2.147731
C	2.936031	-5.046315	-2.141539
C	2.667015	-6.517971	-2.112901
H	2.082742	-6.778688	-1.225390
H	3.601342	-7.086702	-2.098011
H	2.073575	-6.823182	-2.980898
O	0.626086	-4.547009	-2.182840
H	1.295917	-2.096392	-2.222487
O	3.518041	-1.027612	-2.162127
C	4.166888	-4.501869	-2.186937
H	5.063566	-5.112790	-2.232375
H	5.716895	-1.573130	-2.221517
H	8.631816	-4.236528	-1.758909
O	8.870474	-2.198408	-1.928047
P	9.345702	-1.715371	-0.392335
O	9.073561	-2.838167	0.550442
O	8.150008	-0.585032	-0.135480
C	8.144546	0.494001	-1.056048
C	7.074663	1.505649	-0.699291
C	7.183983	2.109648	0.710016
C	6.200613	1.257086	1.496227
H	5.875742	1.780996	2.389189
H	6.670960	0.303075	1.747490
C	5.096342	1.081541	0.455228
N	4.215622	-0.061883	0.665370
C	4.763792	-1.302629	0.854667
C	4.028789	-2.424205	1.022907
C	4.610371	-3.773352	1.312187
H	4.196866	-4.162842	2.247892
H	5.698322	-3.719385	1.400109
H	4.345985	-4.489285	0.525278
C	2.580949	-2.315622	0.914355
O	1.828021	-3.292396	0.994144
N	2.092202	-1.047173	0.687551
H	1.063818	-0.914541	0.614934
H	5.851723	-1.316986	0.861111
C	2.836265	0.113744	0.546118
O	2.309545	1.194352	0.366055
H	4.448788	1.962458	0.414148
H	8.206424	2.082258	1.103631
O	6.717512	3.448501	0.625966
P	6.852627	4.460174	1.931354
O	5.917313	4.023077	3.029437
O	8.282667	4.760253	2.209600
O	6.197629	5.770820	1.169151
C	5.006013	5.667379	0.420844
C	3.720509	5.498469	1.228484
C	3.730513	6.130637	2.630483
C	2.947671	5.121436	3.484145
H	3.620185	4.639207	4.196212
H	2.115319	5.590217	4.016843
C	2.448089	4.090007	2.455922
N	2.371424	2.735066	2.964656
C	3.532511	2.136212	3.395238
C	3.583787	0.845085	3.788267
C	4.820101	0.165978	4.292458
H	4.612769	-0.334025	5.243820
H	5.629257	0.885909	4.431444
H	5.153115	-0.610235	3.594229
C	2.373348	0.046969	3.685794
O	2.336790	-1.157752	3.944254
N	1.239016	0.729095	3.289119
H	0.337336	0.218824	3.334450
H	4.409529	2.789560	3.374196
C	1.156058	2.056920	2.921177
O	0.101712	2.590806	2.630428
H	1.447716	4.335573	2.085319
H	4.759518	6.230871	2.989815
O	3.114295	7.409294	2.536273
C	3.350036	8.190265	3.671616
H	2.928340	7.736722	4.582386
H	4.426833	8.344481	3.839205
H	2.869965	9.160308	3.513198
O	3.397306	4.132240	1.411253
H	2.900369	5.983495	0.670817
H	4.923045	6.612935	-0.127309
H	5.067131	4.845976	-0.302093
O	5.789008	0.887016	-0.772196
H	7.122351	2.327258	-1.426475
H	9.127145	0.983356	-1.063113
H	7.944393	0.111457	-2.066582
O	10.650891	-1.025067	-0.571026
O	6.250932	-3.052293	-3.598158
H	8.229147	-2.660051	-4.076138
H	8.846640	-5.092194	-4.054372
H	7.671629	-4.639805	-5.306821
C	5.821999	-5.940998	-4.565953
H	5.165648	-6.667470	-4.079152
H	5.272213	-5.005959	-4.717554
H	6.131256	-6.343760	-5.543651

Table 2S. M06-2X/6-31G(d,p) optimized reference geometry for d(ApApA) duplex in Model 2.

O	0.524725	8.323298	0.934860	N	2.273777	-1.209110	-5.456030	H	-1.626816	-6.492733	-1.804886
C	1.644743	7.986395	1.719030	C	0.967647	-1.141786	-5.668013	H	-3.224049	-6.376491	-2.640106
H	1.330702	7.510307	2.660031	H	0.385449	-2.042782	-5.492159	C	-1.665232	-5.243766	-3.623563
H	2.225225	8.891094	1.965569	N	0.255424	-0.067198	-6.060892	N	-2.067316	-3.912364	-3.243105
C	2.516190	7.012516	0.949713	C	0.870815	1.104952	-6.286684	C	-3.403020	-3.604583	-3.128190
H	3.492386	6.934514	1.445208	N	0.145939	2.188042	-6.631335	C	-3.852690	-2.341253	-2.982788
O	1.881261	5.742246	0.918486	H	0.591829	3.082157	-6.477614	C	-5.292943	-1.958997	-2.840742
C	1.821726	5.281448	-0.429362	H	-0.862769	2.140117	-6.489409	H	-5.426470	-1.314084	-1.967820
N	0.709178	4.381854	-0.571259	C	2.273220	1.139322	-6.150143	H	-5.923330	-2.845117	-2.729091
C	0.720728	3.060083	-0.188910	N	3.204316	2.147222	-6.315068	H	-5.628424	-1.388611	-3.715328
N	1.748130	2.361266	0.313016	C	4.337241	1.579762	-5.987121	C	-2.879299	-1.257205	-3.004752
C	1.414906	1.093933	0.501350	H	5.326751	2.020115	-6.009297	O	-3.211135	-0.069234	-2.995233
H	2.198064	0.433409	0.866175	C	6.328702	-0.934521	-6.131915	N	-1.556412	-1.637109	-3.035326
N	0.229935	0.496616	0.278080	H	6.060948	-1.821026	-6.711057	H	-0.822463	-0.889882	-3.014565
C	-0.788992	1.222632	-0.222423	H	6.466813	-0.081116	-6.800001	H	-4.074711	-4.460153	-3.176668
N	-1.966414	0.638028	-0.460061	C	7.583830	-1.146193	-5.271142	C	-1.080442	-2.919217	-3.199598
H	-2.080506	-0.359268	-0.283128	O	7.949170	-2.498382	-5.095221	O	0.108983	-3.167872	-3.265376
H	-2.638883	1.111228	-1.043800	C	8.635798	-3.027340	-6.200501	H	-0.571380	-5.228595	-3.679176
C	-0.554163	2.590663	-0.475584	H	8.886591	-4.062467	-5.963049	H	-2.318598	-8.487015	-3.522914
N	-1.341802	3.578819	-1.031516	H	9.562355	-2.468900	-6.399581	O	-0.353321	-7.831999	-3.580705
C	-0.555916	4.619008	-1.066633	H	8.022056	-3.013502	-7.112233	P	0.200531	-8.764308	-2.385841
H	-0.833886	5.585677	-1.459856	H	8.434324	-0.574406	-5.666185	O	0.120298	-8.089613	-1.017826
H	2.731256	4.718163	-0.675067	O	9.328876	3.503181	-4.897836	O	-0.481877	-10.114934	-2.366569
C	1.712551	6.561701	-1.247004	Na	8.674788	3.593695	-6.985158	Na	-0.863882	-9.895865	-0.227945
H	0.727607	7.011099	-1.100904	O	7.402371	2.208427	-5.842850	O	1.719382	-8.935038	-2.873905
H	1.937245	6.432010	-2.303544	H	7.429968	4.981560	-3.601398	C	2.468123	-7.895093	-3.502421
C	2.731731	7.424601	-0.518074	O	4.856665	9.046942	-2.271957	C	2.875144	-6.770667	-2.574134
H	2.608589	8.501399	-0.674375	Na	3.741859	9.166063	-4.147777	C	3.389271	-7.209438	-1.188990
O	4.060893	7.029965	-0.870386	O	3.895022	7.076627	-3.475102	C	2.849781	-6.110720	-0.255609
P	4.694648	7.541342	-2.262974	C	-0.389807	9.130495	1.632200	H	2.065888	-6.505051	0.395975
O	6.121626	6.807617	-2.205146	H	-0.775707	8.616939	2.523770	H	3.637273	-5.661990	0.354458
C	6.490079	5.783305	-1.280361	H	0.070691	10.078117	1.948791	C	2.240038	-5.094013	-1.232230
H	5.962051	5.914633	-0.333909	H	-1.220419	9.345409	0.958070	N	1.124919	-4.339050	-0.709164
H	7.565361	5.899648	-1.117002	O	-7.744155	-2.817773	-7.764099	C	-0.050712	-4.992966	-0.430643
C	6.221476	4.401538	-1.837874	C	-8.763693	-2.087625	-8.403134	C	-1.182546	-4.342653	-0.090737
H	6.728775	3.663843	-1.200713	H	-9.108777	-1.324749	-7.703280	C	-2.485880	-5.007243	0.227203
O	4.822485	4.147493	-1.861624	H	-9.609423	-2.735318	-8.674287	H	-2.884224	-4.627395	1.172152
C	4.549875	3.435477	-3.072597	H	-8.391278	-1.599675	-9.314315	H	-2.363614	-6.091449	0.299672
H	4.864924	2.386607	-2.982956	C	-7.217062	-3.834619	-8.587215	H	-3.231923	-4.785654	-0.545389
N	3.139200	3.402172	-3.314418	C	-6.027605	-4.480899	-7.901206	C	-1.159254	-2.885079	-0.077676
C	2.343588	2.295492	-3.109307	C	-6.297703	-4.905069	-6.450040	O	-2.167695	-2.204760	0.107288
N	2.728773	1.084425	-2.692561	C	-5.810820	-3.699585	-5.666037	N	0.077839	-2.305014	-0.271517
C	1.711084	0.233139	-2.663073	H	-5.566990	-3.955605	-4.639701	H	0.161892	-1.274393	-0.107058
H	1.930356	-0.784056	-2.346420	H	-6.566716	-2.912268	-5.698952	H	0.007382	-6.076820	-0.527627
N	0.425324	0.474742	-2.982822	C	-4.578784	-3.318088	-6.481800	C	1.248054	-2.954503	-0.595665
C	0.064418	1.698932	-3.411618	H	-3.713683	-3.928175	-6.205474	O	2.308231	-2.374961	-0.737379
N	-1.206291	1.914034	-3.777476	N	-4.162466	-1.939569	-6.354241	H	2.981027	-4.359789	-1.562550
H	-1.920026	1.220422	-3.556559	C	-2.815013	-1.678439	-6.096351	H	2.974804	-8.190777	-0.921113
H	-1.498912	2.862897	-3.948734	O	-2.000090	-2.563687	-5.896590	O	4.795244	-7.280968	-1.265907
C	1.069246	2.689665	-3.498692	N	-2.482849	-0.349002	-6.075893	C	5.369265	-7.937126	-0.164261
N	1.069227	3.995600	-3.959389	H	-1.441278	-0.171298	-5.991061	H	5.161425	-7.413320	0.779635
C	2.316840	4.374786	-3.838394	C	-3.312812	0.720487	-6.339989	H	4.997378	-8.968608	-0.076520
H	2.717335	5.349485	-4.087793	O	-2.883140	1.870829	-6.355381	H	6.448525	-7.958398	-0.323394
C	5.417736	4.182042	-4.080787	C	-4.705317	0.379122	-6.639188	O	1.799973	-5.883649	-2.328383
H	5.033140	5.199146	-4.204470	C	-5.642497	1.499616	-6.965026	H	3.700388	-6.223356	-3.059249
H	5.524642	3.682550	-5.040204	H	-5.727221	2.186664	-6.118245	H	3.376934	-8.380149	-3.866561
C	6.718967	4.210265	-3.289463	H	-6.636735	1.119130	-7.212146	H	1.906755	-7.489615	-4.349060
O	7.353827	2.926510	-3.329972	H	-5.264698	2.083472	-7.809134	O	-2.242154	-5.572910	-4.892620
P	8.244470	2.490104	-4.602536	C	-5.044044	-0.923482	-6.664127	H	-1.082805	-7.096891	-5.682599
O	8.898722	1.148226	-4.010758	H	-6.033137	-1.263718	-6.960879	H	-2.845972	-8.586600	-6.182110
C	8.197121	0.231270	-3.170248	O	-5.442885	-6.025841	-6.199593	H	-3.434960	-6.980579	-6.687757
H	7.724899	0.768409	-2.342783	P	-5.558804	-6.868428	-4.825778	H	-7.343448	-5.181577	-6.274497
H	8.965675	-0.438781	-2.777551	O	-5.449928	-5.979035	-3.589871	O	-4.953672	-3.554410	-7.841288
C	7.158413	-0.605279	-3.889367	O	-6.827249	-7.691607	-4.781664	H	-5.723872	-5.360577	-8.481624
H	6.940232	-1.483158	-3.259949	Na	-7.339385	-6.821442	-2.841576	H	-7.987663	-4.595068	-8.794775
O	5.969513	0.135374	-4.095911	O	-4.278652	-7.819530	-4.979450	H	-6.879823	-3.414525	-9.546483
C	5.256202	-0.571322	-5.096643	C	-3.152449	-7.597027	-5.831860				
H	4.770747	-1.462104	-4.675953	C	-1.997911	-6.958775	-5.089408				
N	4.204594	0.267416	-5.599963	C	-1.755883	-7.562946	-3.685176				
C	2.870579	-0.037964	-5.706262	C	-2.135848	-6.413583	-2.761329				

Table 3S. M06-2X/6-31G(d,p) optimized reference geometry for d(ApApA) duplex in Model 3.

O	0.232910	8.052580	1.021370
C	-0.455750	8.935300	1.886070
H	-0.551470	8.505310	2.891140
H	0.065760	9.897690	1.964460
H	-1.449230	9.096360	1.466160
C	1.543210	7.787020	1.475520
H	1.517380	7.340050	2.480030
H	2.130230	8.715510	1.529190
C	2.212540	6.828470	0.514350
H	3.262850	6.709300	0.801520
O	1.546940	5.557810	0.581500
C	1.215370	5.140190	-0.738230
N	0.087910	4.242410	-0.664480
C	0.186900	2.919870	-0.308500
N	1.307280	2.220360	-0.062520
C	1.033370	0.949050	0.194530
H	1.880140	0.290550	0.373220
N	-0.170310	0.356280	0.252940
C	-1.284430	1.080780	0.028110
N	-2.484510	0.490750	0.144210
H	-2.520110	-0.528280	0.150620
H	-3.287790	0.983450	-0.218640
C	-1.118660	2.448100	-0.277910
N	-2.011770	3.449350	-0.606010
C	-1.254320	4.495970	-0.820690
H	-1.616670	5.472600	-1.106490
H	2.046170	4.561830	-1.161610
C	0.990720	6.431080	-1.510210
H	0.041960	6.888300	-1.223830
H	1.046360	6.303550	-2.590600
C	2.137570	7.266520	-0.958880
H	1.983540	8.345350	-1.054680
O	3.355830	6.870800	-1.599580
P	3.891620	7.815230	-2.829090
O	4.342200	9.133330	-2.267280
O	5.157270	6.890910	-3.261990
C	6.152120	6.556630	-2.291470
H	5.779820	6.736410	-1.279020
C	6.509300	5.090830	-2.438770
H	7.302020	4.854610	-1.721570
O	5.359110	4.280330	-2.149370
C	5.021730	3.479320	-3.276930
H	5.392470	2.454900	-3.147730
N	3.580730	3.369380	-3.369410
C	2.832530	2.241710	-3.119340
N	3.256560	1.026590	-2.734250
C	2.252890	0.158960	-2.656310
H	2.508710	-0.857570	-2.364640
N	0.946130	0.369770	-2.888680
C	0.537160	1.602990	-3.254040
N	-0.759530	1.821710	-3.500000
H	-1.451850	1.109510	-3.268900
H	-1.071880	2.761750	-3.692170
C	1.521530	2.605850	-3.398910
N	1.449800	3.920510	-3.814400
C	2.694070	4.334370	-3.783420
H	3.014990	5.338330	-4.034070
C	5.678340	4.163850	-4.468700
H	5.076960	5.012360	-4.798930
H	5.852170	3.502040	-5.311680
C	6.963340	4.692480	-3.849870
O	7.956500	3.674560	-3.676670
P	8.582360	2.851540	-4.948030
O	10.028270	2.618520	-4.625480
O	7.764120	1.433440	-4.829630
C	7.975500	0.660380	-3.645890
H	7.535960	1.179420	-2.786230
H	9.048050	0.528210	-3.469620
C	7.329440	-0.699160	-3.799270
H	7.569660	-1.289940	-2.908970
O	5.906070	-0.557290	-3.887920
C	5.424150	-1.064670	-5.123690
H	4.922260	-2.024280	-4.970950
N	4.412870	-0.151460	-5.617300
C	3.066640	-0.378970	-5.728570
N	2.406420	-1.533070	-5.543340
C	1.104080	-1.382960	-5.738190
H	0.482850	-2.268720	-5.635610
N	0.440710	-0.258370	-6.048370
C	1.113930	0.895900	-6.213720
N	0.425950	2.014620	-6.509330
H	-0.579350	1.995370	-6.347460
H	0.895120	2.900300	-6.376880
C	2.517600	0.851300	-6.084540
N	3.499170	1.819830	-6.183500
C	4.604330	1.178050	-5.893230
H	5.600910	1.599230	-5.860980
C	6.640900	-1.186810	-6.038420
H	6.828960	-0.235370	-6.540580
H	6.510800	-1.966710	-6.789350
C	7.764850	-1.475710	-5.047980
O	7.818690	-2.846370	-4.687720
C	8.454720	-3.652110	-5.663470
H	8.492740	-4.667150	-5.266490
H	9.475640	-3.298030	-5.854120
H	7.903740	-3.661470	-6.610900
H	8.744940	-1.144070	-5.414690
O	8.158310	3.469880	-6.245020
H	7.389550	5.531940	-4.405430
H	7.043040	7.170500	-2.456250
O	2.927720	7.776800	-3.980300
O	-7.884040	-2.196450	-7.117300
C	-8.864520	-1.216930	-7.405080
H	-8.944020	-0.569360	-6.530970
H	-9.838050	-1.682310	-7.603170
H	-8.574750	-0.617680	-8.277220
C	-7.682590	-3.083270	-8.198780
C	-6.534410	-4.021910	-7.885470
C	-6.608780	-4.663550	-6.494740
C	-5.731820	-3.740630	-5.660670
H	-5.312710	-4.226770	-4.783910
H	-6.327150	-2.883250	-5.340840
C	-4.659280	-3.309490	-6.651670
N	-4.119690	-1.974060	-6.403370
C	-2.758030	-1.805840	-6.247000
N	-2.351420	-0.508860	-6.075890
H	-1.313250	-0.373780	-6.018830
C	-3.141450	0.618090	-6.096760
O	-2.630930	1.739940	-5.993300
C	-4.566210	0.384490	-6.267820
C	-5.486520	1.565540	-6.303920
H	-5.442330	2.120530	-5.362140
H	-6.516710	1.246530	-6.472520
H	-5.198480	2.256450	-7.101860
O	-1.951830	-2.735100	-6.259760
C	-4.974830	-0.890920	-6.432790
H	-6.014670	-1.145390	-6.622880
H	-3.803260	-3.987400	-6.642580
H	-7.632930	-4.723440	-6.117810
O	-6.066610	-5.984410	-6.616130
P	-5.795160	-6.897000	-5.281200
O	-6.540090	-6.345160	-4.103840
O	-4.207410	-6.583510	-5.003170
C	-3.279170	-7.017690	-6.000380
C	-1.875970	-6.948310	-5.442090
C	-1.709610	-7.678540	-4.100040
C	-1.738430	-6.542400	-3.087190
H	-1.187330	-6.777640	-2.180650
H	-2.777640	-6.332470	-2.828070
C	-1.112270	-5.390230	-3.862770
N	-1.531810	-4.052990	-3.453640
C	-0.571200	-3.073630	-3.272030
N	-1.059930	-1.803230	-3.085590
H	-0.339540	-1.063390	-2.977490
C	-2.384530	-1.438630	-2.997170
O	-2.705000	-0.253150	-2.850160
C	-3.348150	-2.522710	-3.090060
C	-4.790150	-2.185930	-2.871040
H	-4.905070	-1.675180	-1.909600
H	-5.406810	-3.085270	-2.861240
H	-5.159730	-1.508920	-3.649420
O	0.636530	-3.295460	-3.279580
C	-2.875920	-3.757840	-3.358870
H	-3.540150	-4.603260	-3.510830
H	-0.023510	-5.405830	-3.778530
H	-2.506620	-8.406540	-3.930010
O	-0.448930	-8.356020	-4.134620
P	0.066760	-9.193400	-2.821040
O	-1.053380	-9.380660	-1.844040
O	1.089390	-8.107510	-2.136270
C	2.237590	-7.748860	-2.908570
C	3.037590	-6.710090	-2.158890
C	3.501060	-7.129290	-0.751100
C	2.572600	-6.345200	0.175580
H	3.027630	-6.103020	1.136610
H	1.664550	-6.924260	0.352580
C	2.286560	-5.096300	-0.652360
N	1.035690	-4.415250	-0.353830
C	1.034120	-3.034900	-0.255670
N	-0.202220	-2.468270	-0.088690
H	-0.203320	-1.430910	0.034220
C	-1.414930	-3.117710	-0.065910
O	-2.467810	-2.477800	0.048800
C	-1.359020	-4.565670	-0.178390
C	-2.645550	-5.328230	-0.102150
H	-3.144570	-5.135350	0.852570
H	-2.471930	-6.401420	-0.195560
H	-3.330060	-5.010590	-0.896220
O	2.054750	-2.352360	-0.294750
C	-0.143960	-5.129930	-0.336730
H	-0.028190	-6.201900	-0.451960
H	3.075140	-4.353200	-0.530960
H	3.420590	-8.213250	-0.600290
O	4.854130	-6.724890	-0.621360
C	5.493650	-7.284400	0.511850
H	5.034800	-6.948850	1.449110
H	6.533050	-6.955340	0.489430
H	5.457940	-8.380470	0.476330
O	2.226170	-5.543840	-1.998810
H	3.925260	-6.463770	-2.752680
H	2.860440	-8.629860	-3.093500
H	1.916100	-7.333430	-3.870740
O	0.858890	-10.351550	-3.350310
O	-1.517540	-5.578910	-5.212990
H	-1.189720	-7.379080	-6.178510
H	-3.496560	-8.050190	-6.291770
H	-3.359630	-6.375560	-6.884970
O	-5.953040	-8.323780	-5.713940
O	-5.286580	-3.310080	-7.926460
H	-6.509630	-4.803250	-8.651450
H	-8.592400	-3.672570	-8.383270
H	-7.445090	-2.522860	-9.114150

Table 4S. M06-2X/6-31G(d,p) optimized reference geometry for d(ApApA) duplex in Model 4.

O	-0.386750	8.234430	0.224020
C	0.628940	8.566310	1.146440
H	0.345800	8.240470	2.157840
H	0.788620	9.654290	1.170590
C	1.924830	7.880490	0.761700
H	2.704610	8.219940	1.450030
O	1.800750	6.455720	0.893000
C	1.813230	5.827080	-0.381330
N	0.729860	4.866820	-0.469870
C	0.865670	3.508040	-0.325360
N	1.988960	2.816570	-0.072900
C	1.760050	1.510300	-0.047290
H	2.618040	0.866090	0.132330
N	0.594670	0.869840	-0.224190
C	-0.526130	1.579940	-0.473650
N	-1.673810	0.926360	-0.677850
H	-1.716460	-0.082850	-0.550050
H	-2.523580	1.441780	-0.847030
C	-0.407320	2.987140	-0.524810
N	-1.317250	3.995990	-0.775640
C	-0.600980	5.092890	-0.728720
H	-0.986190	6.095590	-0.851810
H	2.732360	5.240520	-0.492340
C	1.729620	6.945960	-1.413940
H	0.691950	7.205350	-1.621430
H	2.221010	6.698110	-2.350840
C	2.373010	8.113610	-0.682840
O	3.812040	8.048770	-0.662970
P	4.706030	7.811640	-1.996580
O	6.027660	8.501580	-1.768360
Na	5.781020	9.649410	-3.827470
O	4.909710	6.196020	-2.013190
C	5.675850	5.618210	-0.947180
H	5.082600	5.637150	-0.026060
H	6.594360	6.193030	-0.793100
C	6.041080	4.186680	-1.277760
H	6.662500	3.814110	-0.457400
O	4.866670	3.369600	-1.364970
C	4.692460	2.874150	-2.687490
H	4.917640	1.802580	-2.721420
N	3.298940	2.990930	-3.054390
C	2.407530	1.954660	-3.130950
N	2.664680	0.649370	-2.975770
C	1.579750	-0.083260	-3.172520
H	1.696340	-1.162710	-3.129580
N	0.335240	0.346110	-3.427460
C	0.082460	1.664610	-3.535660
N	-1.180880	2.059900	-3.751980
H	-1.921030	1.372290	-3.627240
H	-1.411260	3.037700	-3.653390
C	1.183300	2.541740	-3.433270
N	1.310670	3.916260	-3.533210
C	2.583100	4.134420	-3.302950
H	3.072660	5.099280	-3.305030
C	5.639010	3.681100	-3.566390
H	5.177020	4.625830	-3.858320
H	5.950410	3.148460	-4.462390
C	6.778580	3.987980	-2.607460
O	7.659460	2.870650	-2.391610
P	8.344150	2.008230	-3.584780
O	9.692230	1.556970	-3.079450
Na	10.728660	2.573430	-4.955760
O	7.339650	0.736180	-3.728310
C	7.194520	-0.124410	-2.588150
H	6.583900	0.382850	-1.832710
H	8.177540	-0.348080	-2.161740
C	6.523520	-1.417930	-2.997840
H	6.471820	-2.056470	-2.109560
O	5.191310	-1.160930	-3.455490
C	5.042350	-1.543740	-4.817780
H	4.461790	-2.469010	-4.879520
C	6.453950	-1.719980	-5.368510
H	6.853700	-0.764800	-5.715370
H	6.481650	-2.435510	-6.190970
N	4.246280	-0.533940	-5.488040
C	4.518040	0.811160	-5.568890
H	5.493300	1.192040	-5.291580
N	3.505560	1.527560	-5.991070
C	2.494160	0.601920	-6.184130
C	1.123010	0.721320	-6.496610
N	0.397940	-0.413420	-6.562870
C	0.975590	-1.591630	-6.288210
N	2.230350	-1.817820	-5.924120
H	0.315850	-2.452660	-6.353420
N	0.500330	1.890980	-6.741070
H	0.965810	2.741770	-6.457120
H	-0.516740	1.883930	-6.697590
C	2.940670	-0.681950	-5.877250
C	7.213830	-2.188690	-4.129320
O	6.986820	-3.566140	-3.868870
C	7.744390	-4.432960	-4.694160
H	7.476820	-5.452010	-4.410390
H	8.819400	-4.278910	-4.537800
H	7.519140	-4.290310	-5.756910
H	8.290180	-1.980410	-4.180090
O	8.331310	2.740810	-4.900950
H	7.367850	4.859260	-2.901900
O	3.963100	8.176540	-3.254880
H	2.065780	9.086260	-1.073730
C	-1.637820	8.784130	0.592080
H	-1.952010	8.418300	1.577670
H	-1.592790	9.880020	0.621190
H	-2.365030	8.470820	-0.158100
O	-8.067580	-2.237010	-6.958670
C	-9.029830	-1.244360	-7.262910
H	-9.058240	-0.550390	-6.421960
H	-10.022720	-1.689690	-7.401020
H	-8.755790	-0.699940	-8.175210
C	-7.950540	-3.200920	-7.985270
C	-6.810390	-4.145650	-7.660440
C	-6.845650	-4.676150	-6.223290
C	-5.901560	-3.734260	-5.495120
H	-5.448790	-4.187070	-4.617520
H	-6.458520	-2.846360	-5.192220
C	-4.866770	-3.396610	-6.561330
N	-4.274370	-2.065640	-6.434120
C	-2.898010	-1.935070	-6.432220
N	-2.438490	-0.643960	-6.416940
C	-3.195200	0.506650	-6.446470
C	-4.636660	0.311380	-6.438950
C	-5.520760	1.519760	-6.461340
H	-5.352070	2.137020	-5.573650
H	-6.572070	1.227980	-6.488990
H	-5.305060	2.141450	-7.335220
O	-2.643070	1.611200	-6.495090
H	-1.402760	-0.527670	-6.468260
O	-2.127620	-2.893190	-6.442920
C	-5.096750	-0.956690	-6.457650
H	-6.157720	-1.184670	-6.521140
H	-4.030820	-4.099220	-6.542960
H	-7.854060	-4.673400	-5.803820
O	-6.355460	-6.028650	-6.258060
P	-6.103480	-6.852040	-4.877820
O	-6.772530	-6.190670	-3.700990
O	-4.497020	-6.702280	-4.663150
C	-3.659600	-7.256540	-5.687360
C	-2.209860	-7.051620	-5.315310
C	-1.778210	-7.670370	-3.975920
C	-1.760240	-6.477140	-3.031500
H	-1.058820	-6.598900	-2.209110
H	-2.762480	-6.340370	-2.619250
C	-1.368520	-5.332960	-3.955870
N	-1.837340	-4.010320	-3.563750
C	-3.171940	-3.791740	-3.287450
C	-3.697050	-2.566400	-3.067610
C	-5.113040	-2.301400	-2.658980
H	-5.130260	-1.792310	-1.690030
H	-5.684460	-3.227360	-2.575130
H	-5.607670	-1.643120	-3.380650
C	-2.818580	-1.418630	-3.234610
O	-3.197530	-0.241760	-3.168860
N	-1.499240	-1.709860	-3.477150
H	-0.824160	-0.900030	-3.516370
H	-3.783190	-4.688370	-3.242410
C	-0.945820	-2.951580	-3.623130
O	0.262300	-3.099550	-3.793590
H	-0.282290	-5.254430	-4.039290
H	-2.450530	-8.464720	-3.643640
O	-0.471080	-8.227940	-4.199500
P	0.444860	-8.800190	-2.984790
O	-0.347630	-8.982640	-1.716680
O	1.492620	-7.580410	-2.734220
C	2.347340	-7.233550	-3.835270
C	3.287060	-6.127000	-3.416540
C	4.200280	-6.442980	-2.220310
C	3.493600	-5.744890	-1.059970
H	4.157410	-5.476110	-0.237850
H	2.697030	-6.389160	-0.680560
C	2.921910	-4.520320	-1.762540
N	1.766370	-3.898800	-1.131510
C	0.624320	-4.638220	-0.896160
C	-0.541050	-4.091080	-0.490720
C	-1.767780	-4.867400	-0.122950
H	-2.098990	-4.584600	0.880700
H	-1.571510	-5.940420	-0.133260
H	-2.592950	-4.650480	-0.809550
C	-0.608620	-2.640330	-0.404370
O	-1.648430	-2.016570	-0.159630
N	0.577620	-1.971030	-0.605510
H	0.585530	-0.935750	-0.463390
H	0.730910	-5.707940	-1.049910
C	1.788450	-2.530920	-0.923860
O	2.806690	-1.851320	-1.021090
H	3.672860	-3.735210	-1.861960
H	4.320070	-7.522150	-2.061660
O	5.455290	-5.848480	-2.513780
C	6.478910	-6.192830	-1.598270
H	6.256880	-5.844670	-0.583480
H	6.632060	-7.278910	-1.573660
H	7.390380	-5.703900	-1.946430
O	2.516780	-4.979720	-3.047140
H	3.919230	-5.879880	-4.276940
H	2.924070	-8.108310	-4.150450
H	1.730370	-6.888160	-4.672050
O	1.172230	-10.014510	-3.506990
Na	0.346730	-11.278150	-1.677050
O	-1.944910	-5.649120	-5.218610
H	-1.598800	-7.482650	-6.115410
H	-3.863520	-8.325800	-5.801640
H	-3.864280	-6.747880	-6.635620
O	-6.465840	-8.292180	-5.141410
Na	-7.947070	-8.226210	-3.269100
O	-5.553580	-3.465240	-7.803520
H	-6.836170	-4.980820	-8.367280
H	-8.883800	-3.774590	-8.079480
H	-7.747470	-2.713020	-8.949100

Table 5S. M06-2X/6-31G(d,p) optimized reference geometry for d(CpCpC) duplex in Model 1.

O	4.615020	6.162820	-2.678750
C	3.567390	5.688510	-1.860520
H	3.922970	5.516220	-0.832120
H	2.801890	6.469310	-1.840410
H	3.137510	4.754900	-2.234330
C	5.726330	5.286750	-2.748060
H	5.899170	4.818530	-1.765980
H	6.596630	5.900920	-3.005840
C	5.587110	4.211760	-3.809790
O	4.528800	3.322110	-3.451710
C	3.740190	3.099800	-4.619720
N	2.442770	2.583290	-4.227380
C	2.398740	1.248720	-3.744410
N	1.196510	0.766340	-3.319350
C	0.073540	1.432600	-3.559460
N	-1.088640	0.909820	-3.150700
H	-1.107940	0.000440	-2.679980
H	-1.951320	1.282130	-3.518540
C	0.075870	2.707870	-4.223130
H	-0.840810	3.187460	-4.535610
O	3.431910	0.590420	-3.717650
C	1.279980	3.230480	-4.530880
H	1.373800	4.172390	-5.054580
H	4.234820	2.347270	-5.243220
C	3.743230	4.470820	-5.288610
H	3.195670	5.187950	-4.666710
H	3.372380	4.477960	-6.313140
H	6.531840	3.657440	-3.885080
C	5.235720	4.769500	-5.208780
H	5.487590	5.830680	-5.298620
O	5.866000	3.997400	-6.199220
P	7.083010	4.622010	-7.140000
O	7.864350	5.563020	-6.280870
O	7.877960	3.177580	-7.326480
C	8.395180	2.579660	-6.155870
H	8.098200	3.149960	-5.269380
C	7.928730	1.139590	-6.007460
H	8.361950	0.736940	-5.082690
O	6.507240	1.076330	-5.907980
C	5.950590	0.315120	-6.966390
H	5.615950	-0.662750	-6.607850
N	4.725730	0.995330	-7.422020
C	3.463540	0.461800	-7.061580
O	3.388650	-0.693970	-6.650400
N	2.363200	1.260420	-7.196910
C	2.445670	2.430290	-7.819570
N	1.348080	3.215980	-7.850380
H	0.433470	2.837420	-7.579260
H	1.318500	3.929090	-8.561780
C	3.683700	2.908230	-8.360580
H	3.792940	3.882940	-8.819660
C	4.797690	2.192430	-8.059660
H	5.785470	2.572030	-8.297780
C	7.058490	0.189960	-8.011270
H	7.008770	-0.706790	-8.625180
H	7.087280	1.074710	-8.653590
C	8.323630	0.200220	-7.157740
O	8.642090	-1.045780	-6.558310
P	8.799860	-2.439530	-7.441080
O	9.752300	-3.313140	-6.701360
O	7.254890	-3.035320	-7.190820
C	6.895910	-3.291460	-5.847060
H	7.729520	-3.780080	-5.325710
H	6.658330	-2.353060	-5.328550
C	5.681350	-4.196550	-5.843410
H	5.428430	-4.486850	-4.816750
O	4.570620	-3.499860	-6.406260
C	4.080860	-4.142690	-7.571060
H	3.139730	-4.651150	-7.353940
C	5.185940	-5.109150	-8.007000
H	4.773020	-5.978130	-8.524380
H	5.901560	-4.607170	-8.661630
N	3.766070	-3.116260	-8.554470
C	2.415220	-2.875740	-8.894480
O	1.564570	-3.710170	-8.589840
N	2.122410	-1.715950	-9.545350
C	3.083970	-0.868730	-9.887510
C	4.471610	-1.172500	-9.691330
H	5.248200	-0.491430	-10.012660
N	2.735570	0.304450	-10.442500
H	1.755810	0.617210	-10.333930
H	3.437940	1.029640	-10.455360
C	4.754500	-2.266210	-8.952110
H	5.761540	-2.512080	-8.620190
C	5.879580	-5.459510	-6.691750
O	5.249760	-6.537040	-6.014310
C	5.560140	-7.787110	-6.560580
H	5.077150	-8.543540	-5.937470
H	6.647180	-7.965300	-6.564740
H	5.194100	-7.901770	-7.591190
H	6.948930	-5.674780	-6.832530
O	8.868890	-2.123660	-8.895990
H	9.183380	0.571250	-7.727050
H	9.494160	2.586490	-6.197960
O	6.538740	4.947370	-8.490020
O	-6.696310	2.320150	-11.334640
C	-7.673860	1.305770	-11.449430
C	-7.561120	0.220290	-10.379130
C	-7.965680	0.641670	-8.956140
C	-6.625400	1.054840	-8.362370
H	-6.620010	1.015690	-7.277020
H	-6.432500	2.082190	-8.677800
C	-5.636670	0.105330	-9.029980
H	-5.467710	-0.813830	-8.454960
N	-4.331840	0.700790	-9.257440
C	-3.142220	0.020670	-9.340330
N	-2.962790	-1.292320	-9.104930
C	-1.700100	-1.657740	-9.189470
N	-1.343760	-2.945630	-8.964330
H	-1.963640	-3.432480	-8.325810
H	-0.356000	-3.144750	-8.804970
N	-0.683740	-0.793190	-9.530840
H	0.286830	-1.148100	-9.507260
C	-0.828370	0.574880	-9.766850
O	0.162840	1.278810	-10.012600
C	-2.192170	0.982080	-9.677510
N	-2.769020	2.231240	-9.798560
C	-4.026020	2.021430	-9.535320
H	-4.794380	2.779770	-9.546680
O	-8.569880	-0.492080	-8.381090
P	-8.763180	-0.688190	-6.731250
O	-8.481690	0.605720	-6.042260
O	-7.438870	-1.650320	-6.463350
C	-7.400430	-2.869940	-7.188680
C	-6.191550	-3.699960	-6.802470
C	-6.119900	-4.136590	-5.332890
C	-5.385380	-2.962800	-4.695720
H	-4.883870	-3.239180	-3.766060
H	-6.075140	-2.129730	-4.544660
C	-4.372180	-2.627000	-5.790090
H	-3.451910	-3.210100	-5.682150
N	-3.946800	-1.238040	-5.801270
C	-4.724830	-0.093020	-5.810450
H	-5.799030	-0.146270	-5.665770
N	-4.033290	0.996960	-6.019170
C	-2.727440	0.557090	-6.156300
C	-1.528110	1.251710	-6.523270
N	-0.437660	0.372860	-6.574520
C	-0.490540	-0.990690	-6.419740
N	-1.590730	-1.645840	-6.114340
N	0.646500	-1.653350	-6.697080
H	0.642050	-2.646340	-6.501200
H	1.553640	-1.185350	-6.678040
H	0.478150	0.765920	-6.824600
O	-1.352380	2.447220	-6.779200
C	-2.662380	-0.830290	-6.022700
H	-7.114140	-4.323810	-4.912540
O	-5.264570	-5.256360	-5.155400
P	-5.578620	-6.792330	-5.694210
O	-5.628380	-7.726260	-4.538780
O	-4.071700	-7.016860	-6.383330
C	-3.826450	-6.315780	-7.584390
H	-4.178120	-5.276440	-7.526080
C	-2.328720	-6.272180	-7.839760
O	-1.734400	-5.237910	-7.052110
C	-0.840930	-5.762020	-6.085780
N	-1.066980	-5.087470	-4.829780
C	-2.289580	-4.997970	-4.175500
N	-2.293810	-4.101500	-3.231160
C	-1.023940	-3.556130	-3.264640
C	-0.506860	-2.389150	-2.629490
O	-1.055180	-1.629930	-1.824790
N	0.794150	-2.098460	-3.068980
H	1.122810	-1.153130	-2.831340
C	1.496200	-2.786710	-4.025760
N	2.734680	-2.329330	-4.297880
H	2.978550	-1.369370	-4.050410
H	3.178570	-2.678970	-5.141490
N	1.011650	-3.851790	-4.645550
H	-3.141760	-5.591680	-4.488480
C	-0.252350	-4.143040	-4.260650
C	-1.130070	-7.265060	-6.032810
H	-1.948630	-7.460080	-5.336770
H	-0.247810	-7.836130	-5.734150
H	0.192420	-5.540570	-6.374800
C	-1.610270	-7.568450	-7.449530
H	-2.293150	-8.428760	-7.481180
O	-0.533820	-7.761380	-8.358580
C	0.063860	-9.019100	-8.241540
H	0.535800	-9.176150	-7.260670
H	-0.667530	-9.829020	-8.397230
H	0.837420	-9.086680	-9.010690
H	-2.132710	-6.045290	-8.894620
H	-4.339740	-6.810030	-8.420650
O	-6.607120	-6.732780	-6.778090
O	-4.985110	-2.958240	-7.029130
H	-6.190260	-4.590090	-7.437370
H	-8.316990	-3.447100	-7.011010
H	-7.335270	-2.645500	-8.262340
O	-10.007000	-1.488450	-6.564360
H	-8.672290	1.483660	-8.958050
O	-6.219950	-0.241090	-10.296000
H	-8.209800	-0.615700	-10.671870
H	-8.661770	1.779870	-11.374140
H	-7.603460	0.839220	-12.444300
C	-5.589610	2.095490	-12.185370
H	-5.124380	1.124500	-11.987110
H	-4.858140	2.882540	-11.994530
H	-5.902570	2.140950	-13.241870

Table 6S. M06-2X/6-31G(d,p) optimized reference geometry for d(CpCpC) duplex in Model 2.

O	1.953300	4.485810	-5.451270	O	2.362550	-3.403750	-8.571130	C	-4.485980	-0.293740	-4.983220
C	2.937100	5.449440	-5.201530	N	2.994240	-1.614720	-9.846890	H	-5.520790	-0.321660	-4.680170
C	4.057690	4.797410	-4.411910	C	3.994040	-0.942640	-10.408720	N	-3.699300	0.745010	-4.940400
O	3.586390	4.402540	-3.122930	C	5.358740	-1.350700	-10.245600	C	-2.505770	0.297700	-5.482790
C	3.330390	3.019920	-3.074920	H	6.182710	-0.872380	-10.758640	C	-1.278000	0.973540	-5.773190
H	3.856340	2.588470	-2.220020	N	3.679820	0.132780	-11.146760	O	-1.003510	2.176960	-5.698340
N	1.887590	2.779560	-2.846910	H	2.745740	0.545230	-11.009700	N	-0.309640	0.074440	-6.225400
C	1.517170	1.434660	-2.722860	H	4.425280	0.731870	-11.459230	H	0.632190	0.454080	-6.431320
N	0.201580	1.129190	-2.639240	C	5.596560	-2.310800	-9.318040	C	-0.497790	-1.256330	-6.477830
C	-0.727380	2.080920	-2.732650	H	6.596940	-2.622230	-9.043390	N	-1.655810	-1.865920	-6.337310
N	-2.009230	1.711700	-2.667820	C	6.381760	-5.517810	-8.055170	N	0.580250	-1.928350	-6.943600
H	-2.229580	0.710900	-2.616930	O	6.819090	-6.830590	-7.824860	H	1.507510	-1.536980	-6.792200
H	-2.706590	2.291310	-3.110990	C	6.471170	-7.714840	-8.864850	H	0.519410	-2.932570	-6.844070
C	-0.368720	3.465900	-2.844550	H	6.906960	-8.685280	-8.623340	C	-2.599440	-1.041300	-5.843450
H	-1.123710	4.238410	-2.889960	H	5.382530	-7.825410	-8.956040	H	-3.636570	-3.339460	-6.122550
O	2.416510	0.585490	-2.717980	H	6.870200	-7.370800	-9.829440	H	-7.086790	-4.606380	-6.315630
C	0.950570	3.759770	-2.901130	H	6.770480	-5.145360	-9.017690	O	-5.132290	-5.339160	-6.364630
H	1.339360	4.766530	-2.981440	H	8.966470	-5.083480	-7.033400	P	-5.587920	-6.807120	-5.889200
C	3.787540	2.415190	-4.411890	O	8.776010	-1.382930	-9.624050	O	-5.825520	-6.900790	-4.397030
H	4.367610	1.502330	-4.290510	O	6.604210	3.802230	-7.178890	Na	-7.812110	-7.735620	-4.804030
H	2.909670	2.201870	-5.025830	H	4.506330	3.532070	-6.150680	O	-4.220450	-7.601670	-6.208630
H	4.868230	5.519570	-4.259550	H	2.526440	6.283550	-4.608020	C	-3.550490	-7.453330	-7.460300
C	4.601100	3.520990	-5.061700	H	3.333210	5.870750	-6.143490	C	-2.071480	-7.236090	-7.195890
O	5.984280	3.372690	-4.702440	C	0.704630	5.032970	-5.817490	C	-1.453810	-8.286340	-6.256450
P	7.133370	3.786610	-5.746780	H	0.386060	5.787040	-5.080380	C	-1.445260	-7.565840	-4.912250
O	7.778020	5.109010	-5.387300	H	-0.014790	4.213640	-5.831920	H	-0.672010	-7.922770	-4.229420
Na	7.361730	5.867880	-7.381250	H	0.757170	5.510160	-6.806310	H	-2.422970	-7.670410	-4.435600
O	8.211670	2.598370	-5.556640	O	-5.851210	3.644180	-9.167820	C	-1.217410	-6.112880	-5.328320
C	8.017830	1.436180	-4.754740	C	-5.787790	5.036070	-9.361700	N	-1.741950	-5.151600	-4.399180
H	7.384390	1.663510	-3.893940	H	-5.160090	5.448210	-8.570020	C	-3.036890	-5.102950	-3.904970
H	9.010380	1.135390	-4.406920	H	-6.786500	5.492670	-9.305060	N	-3.293990	-3.998820	-3.265400
C	7.395620	0.312090	-5.557420	H	-5.346240	5.281960	-10.337730	C	-2.121820	-3.273820	-3.335750
H	7.440360	-0.619950	-4.977920	C	-6.636620	3.000380	-10.145080	C	-1.830720	-1.935670	-2.918910
O	6.046090	0.654000	-5.839220	C	-6.570830	1.496720	-9.945720	O	-2.590510	-1.107870	-2.417540
C	5.770800	0.234790	-7.172020	C	-6.759150	1.058940	-8.488890	N	-0.495890	-1.606510	-3.185870
H	5.621290	-0.849280	-7.181760	H	-7.369810	1.766870	-7.917910	H	-0.211670	-0.644040	-2.917070
N	4.524290	0.841010	-7.587110	C	-5.331460	0.942080	-7.978610	C	0.411150	-2.401900	-3.837980
C	3.338870	0.256510	-7.074420	H	-5.254090	0.209960	-7.178660	N	1.636180	-1.874930	-4.004930
O	3.389380	-0.859410	-6.558110	H	-4.972670	1.911620	-7.626880	H	1.923100	-1.000080	-3.562750
N	2.192210	0.975480	-7.172690	C	-4.569990	0.502170	-9.225610	H	2.297670	-2.383430	-4.566620
C	2.125450	2.093390	-7.889280	H	-4.481960	-0.587940	-9.277600	N	0.125800	-3.604730	-4.312000
N	0.976130	2.774600	-7.900320	N	-3.217210	1.010030	-9.310340	H	-3.740300	-5.913190	-4.048880
H	0.197170	2.453050	-7.325510	C	-2.826440	2.328660	-9.439400	C	-1.145470	-3.966250	-4.038190
H	0.733450	3.320840	-8.715390	H	-3.556630	3.121130	-9.343120	H	-0.153110	-5.881500	-5.445650
C	3.280960	2.600130	-8.579160	N	-1.553100	2.469250	-9.688610	H	-2.043910	-9.214610	-6.235030
H	3.221590	3.488940	-9.191630	C	-1.072030	1.173060	-9.728090	O	-0.147740	-8.548620	-6.734070
C	4.457060	1.979060	-8.340700	C	0.220710	0.659020	-10.039820	C	0.459120	-9.657810	-6.120070
H	5.400240	2.364290	-8.703960	N	0.265950	-0.726600	-9.903660	H	0.607510	-9.511950	-5.041750
C	7.044720	0.624400	-7.912310	C	-0.799930	-1.536240	-9.611470	H	-0.138760	-10.569600	-6.265610
H	7.146390	1.713700	-7.934250	N	-2.023740	-1.087710	-9.434510	H	1.434360	-9.793170	-6.590270
H	7.153820	0.182730	-8.901440	N	-0.546750	-2.873280	-9.552030	O	-1.886800	-5.970670	-6.577630
C	8.068220	0.065920	-6.928900	H	-1.260080	-3.361390	-9.023860	H	-1.531230	-7.265490	-8.150860
H	9.055510	0.535260	-6.997350	H	0.406080	-3.120290	-9.283520	H	-3.946230	-6.595100	-8.010680
O	8.181670	-1.353030	-7.087010	H	1.215520	-1.137770	-9.955560	H	-3.701870	-8.364470	-8.049850
P	9.096200	-1.974500	-8.263430	O	1.227250	1.289170	-10.398430	O	-6.774930	-7.288870	-6.700860
O	10.567120	-1.887280	-7.919850	C	-2.090230	0.255110	-9.491100	O	-4.998430	-2.355830	-7.351830
Na	10.937230	-1.010170	-9.901030	O	-7.395110	-0.224040	-8.536900	H	-5.250130	-4.134460	-8.386260
O	8.531420	-3.485900	-8.250740	P	-8.091990	-0.824960	-7.207420	H	-7.572990	-3.883700	-8.823010
C	8.331830	-4.192240	-7.025280	O	-7.325190	-0.410300	-5.961440	H	-6.801280	-2.323730	-9.213410
H	8.595880	-3.565880	-6.169000	Na	-9.173250	0.396270	-5.105840	O	-5.302030	0.998500	-10.342950
C	6.887170	-4.631950	-6.918990	O	-9.551910	-0.438790	-7.100370	H	-7.342420	1.030130	-10.568850
H	6.774930	-5.197830	-5.980700	O	-7.990020	-2.401870	-7.510260	H	-7.683820	3.338810	-10.072920
O	6.024360	-3.501970	-6.923450	C	-7.059430	-3.012280	-8.405330	H	-6.266270	3.236950	-11.154100
C	4.789260	-3.824730	-7.524450	C	-5.801030	-3.473210	-7.702000				
H	3.963960	-3.622000	-6.839760	C	-6.056620	-4.243840	-6.387300				
C	4.870020	-5.294830	-7.948530	C	-5.648200	-3.238500	-5.316460				
H	4.484020	-5.936580	-7.149490	H	-5.379250	-3.703860	-4.368140				
H	4.294100	-5.475940	-8.856490	H	-6.432450	-2.483950	-5.197180				
N	4.574470	-2.914730	-8.663500	C	-4.461930	-2.619030	-6.043290				
C	3.237520	-2.664630	-9.022070	N	-3.886660	-1.409610	-5.538270				

Table 7S. M06-2X/6-31G(d,p) optimized reference geometry for d(CpCpC) duplex in Model 3.

O	4.636290	5.979850	-2.161310
C	4.697970	6.893040	-1.082900
H	4.478130	6.393280	-0.130820
H	5.690350	7.356470	-1.014130
H	3.950480	7.666130	-1.264270
C	5.568480	4.928420	-2.016860
H	5.369560	4.362580	-1.095170
H	6.594280	5.322640	-1.964670
C	5.465520	4.009540	-3.213730
H	6.259160	3.257790	-3.147820
O	4.185790	3.359830	-3.207940
C	3.609320	3.477210	-4.505750
N	2.170140	3.305300	-4.384100
C	1.709930	1.996620	-4.175320
N	0.389100	1.786560	-3.983920
C	-0.474240	2.810180	-3.997970
N	-1.756760	2.543050	-3.769370
H	-2.057470	1.585740	-3.575310
H	-2.442930	3.281510	-3.793840
C	-0.037350	4.152940	-4.245870
H	-0.735790	4.977000	-4.282850
O	2.541210	1.072740	-4.160000
C	1.288070	4.346490	-4.420400
H	1.701030	5.327970	-4.604790
C	4.111560	4.819450	-5.013040
H	3.644710	5.643060	-4.470770
H	3.996670	4.954220	-6.087960
H	3.967720	2.663160	-5.144310
C	5.564280	4.741670	-4.567840
H	6.026650	5.726380	-4.466310
O	6.279880	3.937710	-5.510640
P	7.893130	4.191710	-5.678390
O	8.452660	4.605500	-4.346620
O	8.343750	2.671320	-6.056730
C	8.382930	1.687750	-5.021020
H	7.870880	2.045260	-4.122750
H	9.426550	1.481800	-4.764480
C	7.717820	0.416960	-5.501270
H	7.853090	-0.356600	-4.737680
O	6.319640	0.664560	-5.693750
C	5.931370	0.237090	-6.998390
H	5.589090	-0.799920	-6.976000
N	4.778050	1.035200	-7.391230
C	3.488860	0.512250	-7.174910
O	3.360930	-0.681790	-6.855830
N	2.421460	1.332030	-7.318740
C	2.579850	2.606890	-7.693380
N	1.499960	3.383400	-7.732120
H	0.587300	2.998760	-7.481400
H	1.574580	4.344880	-8.026420
C	3.871290	3.135550	-8.021590
H	3.998930	4.153770	-8.361990
C	4.931910	2.325770	-7.809210
H	5.947390	2.673480	-7.945800
C	7.195330	0.360830	-7.840420
H	7.408220	1.395900	-8.112130
H	7.184700	-0.255890	-8.736110
C	8.251970	-0.105260	-6.846270
O	8.285670	-1.531950	-6.749260
P	9.066230	-2.431890	-7.878270
O	10.209210	-3.132000	-7.201940
O	7.884860	-3.518320	-8.203090
C	7.473910	-4.361300	-7.124070
H	7.315690	-3.762340	-6.220740
H	8.240990	-5.115560	-6.920570
C	6.174760	-5.037290	-7.497090
H	5.881850	-5.698990	-6.674420
O	5.170180	-4.031140	-7.680300
C	4.525270	-4.214500	-8.932760
H	3.604910	-4.785460	-8.811160
N	4.133920	-2.901110	-9.429550
C	5.094190	-1.945180	-9.597670
H	6.107800	-2.248470	-9.348270
C	4.777190	-0.705530	-10.028090
H	5.525800	0.061400	-10.167860
C	3.383620	-0.418220	-10.198230
N	2.448060	-1.360230	-10.050610
N	2.988270	0.817390	-10.514820
H	2.000010	1.057590	-10.415580
H	3.662890	1.568820	-10.501510
C	2.791570	-2.626800	-9.707730
O	1.954760	-3.541620	-9.634390
C	5.534690	-4.948150	-9.808510
H	6.260470	-4.245140	-10.225350
H	5.054310	-5.488820	-10.624880
C	6.221110	-5.860760	-8.796170
O	5.478850	-7.047360	-8.563830
C	5.652110	-8.017070	-9.581500
H	5.078010	-8.896580	-9.288420
H	6.710150	-8.290360	-9.682130
H	5.287640	-7.662050	-10.552040
H	7.249870	-6.113060	-9.083590
O	9.279250	-1.637760	-9.131260
H	9.248000	0.283650	-7.073190
O	8.147740	5.011390	-6.908670
O	-7.123610	2.596090	-9.824180
C	-7.219980	4.005280	-9.915880
H	-6.806960	4.421540	-8.996360
H	-8.265370	4.321500	-10.021410
H	-6.649390	4.380730	-10.774580
C	-7.634620	1.956230	-10.975120
C	-7.408840	0.460090	-10.883100
C	-7.811710	-0.156380	-9.542670
C	-6.505010	-0.146050	-8.756570
H	-6.458000	-0.928120	-7.998420
H	-6.363840	0.830160	-8.288720
C	-5.459870	-0.365940	-9.846790
N	-4.198870	0.314400	-9.614860
C	-4.027170	1.680770	-9.498470
H	-4.882860	2.335810	-9.395750
N	-2.775430	2.047730	-9.561460
C	-2.082640	0.865580	-9.747500
C	-0.686640	0.621870	-9.877880
O	0.230070	1.459500	-9.863650
N	-0.408230	-0.730330	-10.032450
C	-1.340270	-1.736470	-10.014460
N	-2.643580	-1.527280	-9.914980
N	-0.862570	-2.990430	-10.138880
H	-1.518420	-3.728810	-9.929270
H	0.126250	-3.172110	-9.954390
H	0.598110	-0.983800	-10.072800
C	-2.947590	-0.219680	-9.782640
H	-5.210820	-1.424430	-9.967970
H	-8.612750	0.398400	-9.049630
O	-8.249260	-1.491120	-9.823870
P	-8.978950	-2.370180	-8.651990
O	-9.712390	-1.467960	-7.706580
O	-7.698710	-2.943270	-7.810010
C	-6.831830	-3.871320	-8.461520
C	-5.625590	-4.110690	-7.581490
C	-5.994180	-4.301470	-6.094250
C	-5.590120	-2.972940	-5.474020
H	-5.404000	-3.037960	-4.404450
H	-6.361010	-2.228710	-5.687790
C	-4.343780	-2.676500	-6.291580
H	-3.512270	-3.330260	-5.994020
N	-3.836280	-1.328680	-6.242160
C	-4.510510	-0.141290	-6.037960
H	-5.564020	-0.124310	-5.799790
N	-3.742800	0.910740	-6.149740
C	-2.490970	0.394790	-6.434000
C	-1.255060	1.044820	-6.731430
O	-1.047750	2.262360	-6.841560
N	-0.223920	0.130640	-6.923880
C	-0.375100	-1.231470	-6.973750
N	-1.529080	-1.848440	-6.777440
N	0.723320	-1.941920	-7.302210
H	0.663970	-2.934930	-7.123270
H	1.640690	-1.509930	-7.176030
H	0.712400	0.536460	-7.115720
C	-2.532220	-0.989750	-6.503080
O	-5.185110	-5.328840	-5.511530
P	-5.802780	-6.850340	-5.515160
O	-6.576070	-7.087770	-4.251720
O	-4.405550	-7.666610	-5.348210
C	-3.494020	-7.727290	-6.448240
C	-2.097050	-7.419360	-5.955360
C	-1.689240	-8.205570	-4.695060
C	-1.834840	-7.168520	-3.581350
H	-1.197220	-7.363610	-2.718670
H	-2.877910	-7.123220	-3.260630
C	-1.448910	-5.894470	-4.317680
N	-1.934140	-4.664720	-3.742160
C	-3.208880	-4.399940	-3.284500
N	-3.410820	-3.134460	-3.036270
C	-2.213460	-2.524170	-3.361930
C	-1.848650	-1.146240	-3.383420
O	-2.577010	-0.173210	-3.130000
N	-0.521600	-0.968810	-3.755870
H	-0.182590	0.012950	-3.805940
C	0.351120	-1.979550	-4.082560
N	-0.000690	-3.255920	-4.156320
N	1.621350	-1.620770	-4.314820
H	1.908280	-0.639960	-4.343200
H	2.231950	-2.319720	-4.709790
H	-3.940490	-5.186840	-3.168380
C	-1.283010	-3.457210	-3.795160
H	-0.361860	-5.791700	-4.394790
H	-2.328560	-9.083310	-4.537040
O	-0.342280	-8.613240	-4.869170
C	0.076080	-9.565980	-3.908160
H	0.058760	-9.157310	-2.891310
H	-0.563240	-10.457060	-3.938980
H	1.099750	-9.846480	-4.158590
O	-2.023330	-6.029830	-5.613000
H	-1.381860	-7.639250	-6.756200
H	-3.521700	-8.734050	-6.875870
H	-3.771560	-7.008450	-7.225830
O	-6.431440	-7.109580	-6.855590
H	-7.056070	-4.522850	-5.961170
O	-4.743970	-2.975660	-7.629510
H	-5.095110	-4.998500	-7.942320
H	-7.352150	-4.823150	-8.611810
H	-6.514880	-3.477910	-9.434630
O	-9.660150	-3.499300	-9.364770
O	-6.021020	0.140210	-11.052440
H	-7.968370	-0.017970	-11.692970
H	-8.712780	2.151710	-11.072210
H	-7.135600	2.337130	-11.877990

Table 8S. M06-2X/6-31G(d,p) optimized reference geometry for d(CpCpC) duplex in Model 4.

O	4.194780	6.552070	-2.612220
C	4.993930	5.939940	-1.620560
H	4.389570	5.691420	-0.736690
H	5.796610	6.622900	-1.306370
C	5.612720	4.669190	-2.168500
H	6.379500	4.331420	-1.464620
O	4.626790	3.632880	-2.289270
C	4.430990	3.252490	-3.646020
H	4.853570	2.263790	-3.833190
N	2.987050	3.130830	-3.870450
C	2.202240	4.219500	-3.609830
H	2.733550	5.129130	-3.346570
C	0.855810	4.141030	-3.641910
H	0.233260	4.997870	-3.425290
C	0.287430	2.849210	-3.896210
N	-1.033320	2.689120	-3.838540
H	-1.618110	3.471660	-3.588150
H	-1.458810	1.762580	-3.881460
N	1.051800	1.785640	-4.174550
C	2.407190	1.887150	-4.154500
O	3.139560	0.907870	-4.377990
C	5.118050	4.331790	-4.481120
H	4.433930	5.156570	-4.691800
H	5.502380	3.947900	-5.421940
C	6.224940	4.830750	-3.562560
O	7.393300	3.991650	-3.593910
P	8.236650	3.764920	-4.963680
O	9.695560	3.692600	-4.586810
Na	10.152290	5.444090	-6.132160
O	7.705880	2.307540	-5.456590
C	7.937950	1.207190	-4.564950
H	7.355070	1.354940	-3.649720
H	9.000940	1.153890	-4.309930
C	7.517450	-0.081550	-5.230480
H	7.777970	-0.902850	-4.554700
O	6.102420	-0.079720	-5.440640
C	5.784800	-0.263480	-6.816120
H	5.440860	-1.283190	-6.998490
N	4.658800	0.612540	-7.127170
C	4.836490	1.964350	-7.069050
H	5.848410	2.304400	-6.877970
C	3.804090	2.819740	-7.219740
H	3.942320	3.891450	-7.179290
C	2.499690	2.242370	-7.353860
N	2.321280	0.917240	-7.409110
N	1.433280	3.035290	-7.414090
H	1.551480	4.032100	-7.312900
H	0.489660	2.643410	-7.375280
C	3.377310	0.072600	-7.303770
O	3.242020	-1.161260	-7.362450
C	7.067760	0.041710	-7.586030
H	7.157280	1.105630	-7.813510
H	7.131700	-0.509460	-8.522010
C	8.165820	-0.336080	-6.599880
O	8.502810	-1.732650	-6.626450
P	9.057260	-2.465560	-7.965950
O	10.136580	-3.430020	-7.540010
Na	11.634610	-2.391510	-9.069530
O	7.740950	-3.276510	-8.472070
C	7.213620	-4.263400	-7.570680
H	6.918060	-3.776130	-6.635340
H	7.976690	-5.018730	-7.359640
C	6.008640	-4.918150	-8.203110
H	5.647400	-5.695890	-7.520990
O	4.988880	-3.930830	-8.387900
C	4.530180	-3.957190	-9.734740
H	3.639590	-4.578610	-9.821290
N	4.124930	-2.603120	-10.085150
C	5.051630	-1.602210	-10.038030
H	6.068060	-1.911650	-9.818880
C	4.706740	-0.311730	-10.233370
H	5.437490	0.484520	-10.186900
C	3.309820	-0.039160	-10.409500
N	2.401270	-1.018040	-10.442650
N	2.880740	1.217510	-10.550290
H	3.528000	1.974590	-10.385020
H	1.882630	1.404650	-10.437630
C	2.771660	-2.313220	-10.294880
O	1.951590	-3.244110	-10.342750
C	5.685340	-4.525790	-10.549910
H	6.433060	-3.758450	-10.764120
H	5.347440	-4.964000	-11.489800
C	6.267320	-5.552710	-9.580570
O	5.556790	-6.779000	-9.614660
C	5.918760	-7.597000	-10.713080
H	5.351040	-8.523870	-10.624640
H	6.991900	-7.824300	-10.690840
H	5.680250	-7.123640	-11.672550
H	7.335960	-5.735920	-9.752250
O	9.424950	-1.476650	-9.040610
H	9.076290	0.250660	-6.743220
O	7.863880	4.763540	-6.027770
H	6.519080	5.860600	-3.775480
C	3.531020	7.703540	-2.123690
H	2.867910	7.448200	-1.287980
H	4.253080	8.456420	-1.784130
H	2.939870	8.111690	-2.944080
O	-7.323150	2.438830	-9.565960
C	-7.485150	3.840510	-9.451030
H	-7.045070	4.142940	-8.500000
H	-8.547320	4.114970	-9.465610
H	-6.974710	4.361960	-10.270240
C	-7.857110	1.942040	-10.775640
H	-8.945690	2.096270	-10.803290
C	-7.563300	0.460120	-10.904240
C	-7.888820	-0.355890	-9.651850
C	-6.560580	-0.384840	-8.906780
H	-6.450240	-1.255260	-8.258200
H	-6.454330	0.528200	-8.317570
C	-5.543280	-0.400020	-10.046650
N	-4.309210	0.308530	-9.760860
C	-4.192970	1.653950	-9.466780
H	-5.074050	2.247470	-9.257680
N	-2.959330	2.081490	-9.501790
C	-2.220960	0.966960	-9.857200
C	-0.815880	0.797590	-10.015440
O	0.067480	1.659540	-9.880060
N	-0.484860	-0.511340	-10.346660
H	0.530440	-0.714400	-10.423500
C	-1.379500	-1.543560	-10.479680
N	-2.687700	-1.403880	-10.335380
N	-0.860270	-2.742270	-10.809600
H	0.135770	-2.913410	-10.656140
H	-1.487200	-3.528590	-10.721120
C	-3.041060	-0.140290	-10.021670
H	-5.248480	-1.418400	-10.317370
H	-8.706890	0.073560	-9.069760
O	-8.258660	-1.667350	-10.109990
P	-9.018770	-2.708440	-9.124500
O	-9.889210	-1.967570	-8.138300
Na	-9.160980	-2.710690	-6.146360
O	-7.808330	-3.290650	-8.180430
C	-6.880330	-4.198980	-8.787320
C	-5.699040	-4.415660	-7.867600
C	-6.087270	-4.604800	-6.388180
C	-5.716190	-3.267020	-5.764120
H	-5.556370	-3.327400	-4.689040
H	-6.477330	-2.519300	-5.999120
C	-4.459080	-2.963170	-6.563140
H	-3.628180	-3.610450	-6.251990
N	-3.969830	-1.612180	-6.512110
C	-4.627560	-0.439290	-6.199100
H	-5.671260	-0.433360	-5.919970
N	-3.857250	0.613570	-6.273820
C	-2.624410	0.111380	-6.649440
C	-1.378220	0.763860	-6.884370
O	-1.154320	1.983450	-6.856950
N	-0.366300	-0.139020	-7.188390
H	0.586240	0.253150	-7.334940
C	-0.533220	-1.491670	-7.339600
N	-1.688090	-2.111860	-7.154760
N	0.546410	-2.184660	-7.751670
H	1.480830	-1.781350	-7.645350
H	0.471500	-3.189610	-7.681210
C	-2.675370	-1.263850	-6.801440
O	-5.238190	-5.622350	-5.837340
P	-5.848290	-6.597840	-4.691420
O	-6.188870	-5.839320	-3.430670
O	-4.532970	-7.478110	-4.384440
C	-3.792770	-8.081180	-5.458180
C	-2.329920	-7.716060	-5.305160
C	-1.705800	-8.136600	-3.962830
C	-1.681940	-6.832470	-3.172130
H	-0.901100	-6.795990	-2.411810
H	-2.652700	-6.667700	-2.698680
C	-1.458780	-5.807560	-4.277290
N	-1.924280	-4.476380	-3.960770
C	-3.189590	-4.120400	-3.541270
N	-3.328230	-2.831540	-3.373470
C	-2.089370	-2.308490	-3.694810
C	-1.631730	-0.957850	-3.723490
O	-2.281680	0.066240	-3.464050
N	-0.296430	-0.875310	-4.101150
H	0.127790	0.067190	-4.147250
C	0.506530	-1.941690	-4.426160
N	0.085810	-3.199030	-4.435980
N	1.772750	-1.648680	-4.746670
H	2.156360	-0.703710	-4.690620
H	2.369080	-2.401260	-5.053650
H	-3.964920	-4.860280	-3.385000
C	-1.205850	-3.313110	-4.066190
H	-0.398610	-5.708700	-4.530070
H	-2.290470	-8.921220	-3.465980
O	-0.399860	-8.612930	-4.243320
C	0.198000	-9.270090	-3.139990
H	0.347950	-8.592480	-2.291870
H	-0.418820	-10.115390	-2.810260
H	1.168120	-9.639550	-3.473860
O	-2.192660	-6.292360	-5.395430
H	-1.769170	-8.192720	-6.117010
H	-3.916280	-9.165680	-5.404510
H	-4.161770	-7.725340	-6.423280
O	-6.979910	-7.418710	-5.266430
Na	-8.381600	-6.735660	-3.489550
H	-7.137850	-4.883910	-6.270530
O	-4.834810	-3.270810	-7.905400
H	-5.150600	-5.299850	-8.210670
H	-7.377930	-5.155320	-8.971170
H	-6.526260	-3.788630	-9.739530
O	-9.562780	-3.796520	-9.993560
O	-6.170070	0.232900	-11.155460
H	-8.130620	0.074110	-11.756590
H	-7.415590	2.468010	-11.634440

Table 9S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyadenosine diphosphate d(A)$_3$ in Model 1.

O	-7.501830	-5.070790	4.327100
C	-6.189240	-5.137670	4.840600
H	-6.198980	-5.117500	5.941820
H	-5.766150	-6.089840	4.510260
H	-5.563920	-4.312660	4.485650
C	-8.176270	-3.870550	4.650130
H	-7.884890	-3.529580	5.656250
H	-9.246860	-4.106240	4.663390
C	-7.944990	-2.745120	3.654190
H	-8.605700	-1.906890	3.912210
O	-6.582270	-2.315840	3.720800
C	-6.027410	-2.349680	2.406040
N	-4.599830	-2.586160	2.528380
C	-3.682250	-1.675300	2.996960
N	-3.893370	-0.423660	3.412530
C	-2.756000	0.186860	3.713580
H	-2.844040	1.216350	4.053240
N	-1.498330	-0.285350	3.639250
C	-1.327400	-1.538260	3.217490
N	-0.050740	-2.034980	3.094280
H	0.614040	-1.301800	2.883690
H	-0.007080	-2.807070	2.441520
C	-2.449550	-2.320520	2.906660
N	-2.589180	-3.593670	2.385060
C	-3.877680	-3.697870	2.174630
H	-4.360070	-4.551000	1.720180
H	-6.167840	-1.380960	1.910300
C	-6.789490	-3.458110	1.699710
H	-6.498970	-4.433630	2.102990
H	-6.724850	-3.431280	0.613040
C	-8.200070	-3.126390	2.184900
H	-8.905810	-3.959080	2.073460
O	-8.680900	-1.966560	1.550130
P	-9.185810	-2.097790	-0.039070
O	-10.447080	-2.886710	-0.065750
O	-9.516750	-0.506030	-0.266280
C	-9.105340	0.550870	0.573790
H	-9.006410	0.217340	1.610440
H	-9.894090	1.312860	0.523910
C	-7.813760	1.221090	0.141430
H	-7.725450	2.170380	0.688360
O	-6.679020	0.401260	0.447330
C	-5.820730	0.424180	-0.687870
N	-4.881990	-0.673650	-0.600720
C	-3.562370	-0.536320	-0.249530
N	-2.907280	0.577310	0.087540
C	-1.616150	0.351750	0.290880
H	-1.012480	1.217310	0.552080
N	-0.950730	-0.815800	0.221810
C	-1.639400	-1.910820	-0.105950
N	-0.954640	-3.112890	-0.207120
H	-0.000100	-3.011840	0.113630
H	-1.455200	-3.877190	0.234710
C	-3.010480	-1.814600	-0.380580
N	-3.962560	-2.718880	-0.814670
C	-5.054430	-1.994640	-0.940760
H	-6.036320	-2.350910	-1.243360
H	-5.204930	1.333450	-0.689640
C	-6.790260	0.429490	-1.861260
H	-7.329970	-0.523640	-1.892780
H	-6.341070	0.672900	-2.822330
C	-7.721790	1.535250	-1.366030
O	-7.098730	2.810180	-1.464070
P	-7.024900	3.587670	-2.921710
O	-6.485100	5.026760	-2.308770
C	-5.391530	5.079430	-1.422410
H	-5.508360	4.349840	-0.612330
H	-5.412250	6.087320	-0.992000
C	-4.004950	4.868230	-2.042920
H	-3.287970	5.519730	-1.514800
O	-3.590600	3.520200	-1.883670
C	-2.639600	3.239480	-2.882620
H	-1.629290	3.538920	-2.567650
N	-2.593540	1.809870	-3.074880
C	-1.523260	0.960470	-2.958000
N	-0.241660	1.239730	-2.680340
C	0.493010	0.132280	-2.630500
H	1.549550	0.278980	-2.410220
N	0.121330	-1.144930	-2.800910
C	-1.170910	-1.389030	-3.062470
N	-1.600170	-2.680410	-3.197370
H	-1.046630	-3.317180	-2.636180
H	-2.597010	-2.783950	-3.030640
C	-2.057260	-0.308760	-3.185130
N	-3.415130	-0.253270	-3.418980
C	-3.694080	1.024520	-3.348900
H	-4.658370	1.511020	-3.492270
C	-3.110760	4.013050	-4.123690
H	-2.270260	4.325840	-4.749450
H	-3.800320	3.387030	-4.691140
C	-3.877690	5.205890	-3.539310
O	-3.175520	6.440610	-3.642120
C	-3.303660	7.013840	-4.913010
H	-2.756680	7.960760	-4.905680
H	-4.356930	7.208420	-5.162730
H	-2.882200	6.372550	-5.702490
H	-4.868520	5.292850	-3.996160
O	-8.390630	3.802910	-3.464450
O	-5.918950	2.991320	-3.752170
H	-8.697410	1.545960	-1.862150
O	-8.008280	-2.484280	-0.888190

Table 10S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxythymidine diphosphate d(T)$_3$ in Model 1.

O	6.889590	-5.596850	-4.165620
C	7.698850	-4.519240	-4.605950
C	7.498420	-3.259130	-3.773820
C	8.030710	-3.331530	-2.326240
C	6.760250	-3.531400	-1.516950
H	6.875260	-3.128640	-0.517680
H	6.545820	-4.600840	-1.442000
C	5.706160	-2.812410	-2.340880
N	4.362250	-3.364710	-2.173930
C	3.310360	-2.505360	-1.877060
N	2.095860	-3.151880	-1.705960
C	1.808530	-4.508800	-1.823560
C	2.969380	-5.328580	-2.161590
C	2.754030	-6.802440	-2.306900
H	2.336750	-7.215910	-1.384260
H	3.693950	-7.314760	-2.527770
H	2.034850	-7.015730	-3.104280
O	0.673430	-4.928860	-1.679780
H	1.333140	-2.542760	-1.438460
O	3.418090	-1.302450	-1.775730
C	4.160130	-4.718100	-2.319510
H	5.054650	-5.271180	-2.587230
H	5.633140	-1.750320	-2.084850
H	8.727260	-4.167510	-2.184890
O	8.673240	-2.107230	-2.067460
P	9.213480	-1.749200	-0.513990
O	8.906220	-2.910810	0.373640
O	8.076530	-0.594020	-0.150820
C	8.057950	0.536660	-1.003580
C	6.954100	1.484120	-0.579120
C	7.081500	2.067760	0.835480
C	6.186240	1.148930	1.655230
H	5.813820	1.658750	2.543920
H	6.737670	0.248090	1.934820
C	5.078850	0.831190	0.649190
N	4.424700	-0.454330	0.891150
C	5.196710	-1.592800	0.996220
C	4.693610	-2.822440	1.249380
C	5.532120	-4.046340	1.465760
H	5.293250	-4.486070	2.439440
H	6.599500	-3.810930	1.426920
H	5.304940	-4.810910	0.714040
C	3.246600	-2.969760	1.358920
O	2.654890	-4.019370	1.559650
N	2.544200	-1.776820	1.200050
H	1.556020	-1.801270	1.419040
H	6.265520	-1.431180	0.858620
C	3.041900	-0.510700	0.940020
O	2.299770	0.446050	0.811980
H	4.287260	1.585780	0.665600
H	8.116590	2.103370	1.191550
O	6.530000	3.375740	0.800680
P	6.766800	4.342870	2.125320
O	5.703690	4.056000	3.155150
O	8.207880	4.375450	2.484360
O	6.394610	5.760900	1.363730
C	5.275030	5.869650	0.517330
C	3.915780	5.835580	1.210070
C	3.885420	6.429200	2.631520
C	3.007870	5.445600	3.417670
H	3.634200	4.860850	4.092100
H	2.215140	5.953200	3.974780
C	2.431980	4.545110	2.315080
N	2.128980	3.190340	2.738410
C	3.140230	2.410220	3.275130
C	2.939180	1.145300	3.701800
C	4.012960	0.271090	4.276170
H	3.668090	-0.187840	5.207630
H	4.917670	0.848940	4.474690
H	4.265370	-0.549330	3.593680
C	1.614670	0.558610	3.536060
O	1.308880	-0.597930	3.788550
N	0.647180	1.448760	3.073330
H	-0.262720	1.053280	2.880490
H	4.116020	2.908200	3.302290
C	0.835490	2.722960	2.580970
O	-0.082270	3.371170	2.106570
H	1.494840	4.953090	1.921660
H	4.897010	6.469520	3.048080
O	3.335130	7.737780	2.537330
C	3.573250	8.493970	3.691500
H	3.107830	8.046970	4.583510
H	4.650120	8.599020	3.889080
H	3.140070	9.485360	3.533160
O	3.418020	4.511730	1.309280
H	3.209030	6.433560	0.607950
H	5.367480	6.847500	0.030370
H	5.287630	5.089460	-0.252530
O	5.705010	0.790010	-0.619430
H	6.920810	2.321250	-1.288220
H	9.028730	1.047650	-0.976620
H	7.864540	0.211650	-2.034710
O	10.542480	-1.107350	-0.675380
O	6.098570	-2.983970	-3.701590
H	8.015140	-2.426690	-4.268260
H	8.748190	-4.830730	-4.538810
H	7.479730	-4.300550	-5.660900
C	5.756150	-5.782040	-4.983780
H	5.172670	-6.602300	-4.556000
H	5.137180	-4.878170	-5.018850
H	6.051060	-6.058650	-6.007540

Table 11S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyadenosine diphosphate d(A)$_3$ in Model 2.

O	-7.177616	0.098901	-0.285579
C	-6.941537	-0.697253	-1.422647
H	-7.219259	-0.157296	-2.340159
H	-7.537825	-1.623555	-1.372758
C	-5.467012	-1.043213	-1.488584
H	-5.315812	-1.840235	-2.227460
O	-4.731613	0.115993	-1.860641
C	-3.651169	0.277806	-0.943168
N	-3.212901	1.645719	-0.946781
C	-2.299582	2.152553	-1.844711
N	-1.630683	1.489441	-2.790721
C	-0.814203	2.297546	-3.455867
H	-0.225744	1.837263	-4.245876
N	-0.606735	3.612318	-3.280706
C	-1.289844	4.240990	-2.319572
N	-1.086564	5.573974	-2.129133
H	-0.231861	5.920332	-2.541092
H	-1.277167	5.902044	-1.193201
C	-2.208463	3.507576	-1.544758
N	-3.040913	3.843637	-0.491331
C	-3.620443	2.714753	-0.180488
H	-4.343587	2.587910	0.613075
H	-2.789391	-0.319711	-1.260187
C	-4.223300	-0.230296	0.371431
H	-5.001197	0.449522	0.728633
H	-3.480699	-0.421840	1.139693
C	-4.892183	-1.500473	-0.133031
H	-5.658762	-1.909521	0.533225
O	-3.905328	-2.498661	-0.422242
P	-3.233466	-3.363162	0.764351
O	-2.028818	-4.062665	-0.037006
C	-1.581013	-3.723387	-1.348896
H	-2.392427	-3.279872	-1.929563
H	-1.272202	-4.662907	-1.816633
C	-0.400185	-2.775655	-1.313093
H	0.038809	-2.730488	-2.319113
O	-0.832258	-1.480285	-0.912490
C	0.161430	-0.956175	-0.030398
H	1.029989	-0.597262	-0.599333
N	-0.352715	0.186861	0.664599
C	-0.006001	1.490700	0.386287
N	0.843194	1.936771	-0.541079
C	0.972264	3.258387	-0.486411
H	1.652145	3.702504	-1.209014
N	0.362360	4.124959	0.341916
C	-0.475498	3.640533	1.260480
N	-1.066676	4.503524	2.145451
H	-1.013331	5.470612	1.857308
H	-1.978899	4.207699	2.465132
C	-0.687840	2.253592	1.329630
N	-1.420464	1.452004	2.187526
C	-1.179678	0.236485	1.762485
H	-1.590065	-0.677179	2.174784
C	0.514261	-2.177529	0.812770
H	-0.358903	-2.461785	1.409999
H	1.398357	-2.062552	1.435758
C	0.708683	-3.183251	-0.316044
O	1.952550	-2.941727	-0.986771
P	3.348812	-3.460548	-0.365224
O	4.362280	-2.961351	-1.505836
C	4.102782	-1.964992	-2.494565
H	3.038103	-1.932798	-2.736100
H	4.665814	-2.271088	-3.380739
C	4.575084	-0.592153	-2.064346
H	4.618969	0.054813	-2.952051
O	3.666535	-0.045497	-1.116462
C	4.431609	0.756593	-0.228578
H	4.690626	1.721254	-0.684746
N	3.638878	1.048748	0.932331
C	3.327642	2.285396	1.447965
N	3.771098	3.485776	1.062365
C	3.238837	4.455894	1.802380
H	3.558470	5.466738	1.559805
N	2.345651	4.362682	2.796855
C	1.900155	3.147317	3.135152
N	0.941720	3.031538	4.096414
H	0.386248	3.871546	4.196507
H	0.400875	2.176416	4.047292
C	2.429460	2.021388	2.480055
N	2.179342	0.666956	2.598793
C	2.924510	0.130467	1.666645
H	3.040390	-0.925694	1.451711
C	5.670767	-0.102020	0.014948
H	5.379788	-0.955662	0.637270
H	6.492458	0.445821	0.480194
C	5.977022	-0.573410	-1.407961
O	6.758727	0.357046	-2.130630
C	8.129011	0.289303	-1.822356
H	8.639011	1.013111	-2.459635
H	8.531933	-0.714066	-2.022952
H	8.333013	0.539842	-0.772607
H	6.449238	-1.565191	-1.431159
O	3.383394	-4.968000	-0.246667
Na	3.980129	-4.787773	1.857535
O	3.663710	-2.802186	0.973629
H	0.646304	-4.233706	-0.015129
O	-4.189395	-4.404216	1.303775
Na	-3.874211	-3.664243	3.334780
O	-2.695412	-2.486129	1.889783
C	-8.506467	0.552480	-0.220205
H	-8.760248	1.169818	-1.092825
H	-9.215525	-0.286839	-0.169719
H	-8.603712	1.155988	0.683613

Table 12S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxythymidine diphosphate d(T)$_3$ in Model 2.

O	-6.921104	-1.982261	-0.694664
C	-8.313169	-2.195815	-0.715295
H	-8.741176	-1.650563	0.127520
H	-8.553732	-3.263121	-0.612661
H	-8.757839	-1.824704	-1.648741
C	-6.260009	-2.644264	-1.750708
C	-4.791643	-2.265466	-1.723953
C	-4.154866	-2.405914	-0.331823
C	-4.195563	-0.983168	0.200447
H	-3.413740	-0.796372	0.936535
H	-5.180610	-0.780471	0.629057
C	-4.000559	-0.164058	-1.076647
H	-2.943696	-0.022785	-1.318319
N	-4.594437	1.157653	-0.994806
C	-3.772389	2.272456	-1.106805
O	-2.600792	2.211856	-1.427954
N	-4.399467	3.458797	-0.792718
H	-3.774343	4.251276	-0.681880
C	-5.745913	3.664994	-0.486384
O	-6.168741	4.772756	-0.222489
C	-6.564320	2.448223	-0.524497
C	-8.032819	2.603412	-0.280827
H	-8.211139	3.057687	0.697833
H	-8.541612	1.637582	-0.325267
H	-8.477082	3.272529	-1.023080
C	-5.953359	1.273804	-0.760051
H	-6.489128	0.328182	-0.800531
O	-2.798716	-2.822986	-0.517563
P	-2.004363	-3.384663	0.774595
O	-1.718060	-2.292564	1.801208
O	-2.756667	-4.534364	1.409971
Na	-2.676243	-3.538084	3.351795
O	-0.651279	-3.896411	0.086031
C	-0.206530	-3.577643	-1.233161
C	0.721969	-2.383722	-1.233817
C	1.799981	-2.428670	-0.122026
C	1.395545	-1.270148	0.783548
H	2.249068	-0.866156	1.325639
H	0.598121	-1.586841	1.463917
C	0.837949	-0.323552	-0.276475
N	0.095873	0.825736	0.171596
C	-0.965744	0.686713	1.047516
C	-1.728142	1.722690	1.447749
C	-2.912297	1.595296	2.355915
H	-2.852481	2.326914	3.165890
H	-2.966822	0.589345	2.781466
H	-3.845045	1.798602	1.814040
C	-1.454407	3.048527	0.891802
O	-2.143304	4.037320	1.075147
N	-0.317522	3.110083	0.094474
H	-0.140184	3.995894	-0.361901
H	-1.156471	-0.335080	1.372741
C	0.431376	2.060246	-0.385632
O	1.328127	2.215988	-1.191343
H	1.651039	0.061080	-0.902326
O	3.050455	-2.142813	-0.755751
P	4.437644	-2.402326	0.025637
O	4.733460	-1.342911	1.084214
O	4.488608	-3.792914	0.619333
Na	5.104833	-2.952028	2.542419
O	5.456437	-2.293488	-1.210859
C	5.248821	-1.437543	-2.333135
C	5.474031	0.029786	-2.037589
C	6.745224	0.344229	-1.219991
C	6.272471	1.438403	-0.248969
H	6.949260	2.295369	-0.221202
H	6.154223	1.029416	0.757706
C	4.893394	1.811807	-0.806013
N	3.971842	2.351222	0.167551
C	3.524460	1.541606	1.188421
C	2.624046	1.942271	2.109702
C	2.120924	1.082667	3.228459
H	2.182980	1.622511	4.177163
H	2.703365	0.160302	3.301330
H	1.065899	0.824215	3.077201
C	2.087313	3.298685	2.022929
O	1.269991	3.777503	2.787527
N	2.605308	4.046874	0.964143
H	2.266620	4.996416	0.873991
H	3.955517	0.540221	1.181909
C	3.507504	3.652116	-0.006990
O	3.886751	4.394569	-0.887061
H	4.970510	2.557463	-1.603410
H	7.085601	-0.547963	-0.676884
O	7.734379	0.761897	-2.134310
C	9.022124	0.793071	-1.571577
H	9.087622	1.501896	-0.734106
H	9.322384	-0.200533	-1.208354
H	9.711836	1.111343	-2.354762
O	4.388337	0.586857	-1.317022
H	5.582684	0.552350	-3.002055
H	5.988314	-1.751625	-3.074071
H	4.243573	-1.586494	-2.736482
H	1.855510	-3.400491	0.376734
O	-0.016897	-1.187819	-1.028400
H	1.239278	-2.343341	-2.203220
H	0.339840	-4.456999	-1.585148
H	-1.058103	-3.389806	-1.890219
H	-4.681161	-3.137018	0.290865
O	-4.660657	-0.899944	-2.096436
H	-4.244082	-2.895440	-2.435149
H	-6.368339	-3.735631	-1.645347
H	-6.686417	-2.344035	-2.719301

Table 13S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyadenosine diphosphate $d(A)_3$ in Model 3.

O	0.350450	7.939437	0.948869
C	-0.298351	8.849009	1.816725
H	-0.376747	8.436310	2.830564
H	0.244442	9.801459	1.866785
H	-1.298777	9.023901	1.419476
C	1.667649	7.657665	1.372074
H	1.662036	7.231091	2.385739
H	2.273337	8.575369	1.390443
C	2.292134	6.669578	0.411397
H	3.350406	6.542015	0.664625
O	1.611708	5.410291	0.528030
C	1.284170	4.951799	-0.778589
N	0.187040	4.019818	-0.673426
C	0.322534	2.739992	-0.192695
N	1.448195	2.129359	0.204262
C	1.209209	0.877750	0.585850
H	2.073574	0.307077	0.918074
N	0.042216	0.217554	0.609825
C	-1.070030	0.856571	0.203458
N	-2.246903	0.204410	0.236407
H	-2.236687	-0.793962	0.383394
H	-3.047679	0.604857	-0.227786
C	-0.956979	2.199763	-0.214414
N	-1.870571	3.119721	-0.694888
C	-1.149896	4.183783	-0.949023
H	-1.534420	5.111288	-1.348734
H	2.133696	4.394876	-1.195847
C	1.017283	6.222094	-1.570427
H	0.073263	6.671317	-1.254924
H	1.039174	6.075459	-2.649567
C	2.174336	7.077391	-1.069821
H	2.013068	8.152748	-1.185649
O	3.374495	6.671604	-1.735103
P	3.940584	7.613280	-2.952206
O	4.287444	8.964781	-2.396867
O	5.278737	6.741165	-3.273815
C	6.211116	6.507197	-2.214411
H	5.785288	6.811028	-1.253971
C	6.551124	5.030074	-2.165428
H	7.237221	4.863597	-1.327787
O	5.351178	4.276072	-1.953376
C	5.175627	3.313415	-2.984776
H	5.479343	2.321399	-2.634473
N	3.761690	3.209564	-3.289343
C	2.940571	2.141777	-3.007279
N	3.271092	0.947331	-2.492727
C	2.209717	0.157652	-2.368627
H	2.395441	-0.834686	-1.963147
N	0.926963	0.421597	-2.667259
C	0.621383	1.628762	-3.170929
N	-0.661894	1.906109	-3.484490
H	-1.373678	1.302085	-3.097202
H	-0.917601	2.871638	-3.633473
C	1.666203	2.552111	-3.385212
N	1.690433	3.834143	-3.895283
C	2.951737	4.186391	-3.816204
H	3.342773	5.150006	-4.118172
C	6.033524	3.787883	-4.152391
H	5.485089	4.513133	-4.757930
H	6.360833	2.956369	-4.775519
C	7.192248	4.481682	-3.448832
O	8.206434	3.553521	-3.046068
P	9.163052	2.861294	-4.183717
O	10.401715	2.427696	-3.459462
O	8.286292	1.541242	-4.602255
C	8.085468	0.551666	-3.593704
H	7.694730	1.017159	-2.681244
H	9.033096	0.054970	-3.360819
C	7.101367	-0.472247	-4.102923
H	7.049780	-1.300183	-3.384964
O	5.811024	0.137578	-4.225929
C	5.180027	-0.455329	-5.351955
H	4.773262	-1.439426	-5.091067
N	4.051934	0.351961	-5.746253
C	2.734683	-0.044897	-5.743019
N	2.222755	-1.233988	-5.392930
C	0.899357	-1.253114	-5.525258
H	0.406614	-2.185166	-5.258507
N	0.083330	-0.271655	-5.939730
C	0.624234	0.908549	-6.287473
N	-0.177645	1.901087	-6.730046
H	-1.165625	1.812035	-6.538522
H	0.197329	2.839070	-6.737899
C	2.022660	1.055271	-6.207302
N	2.867049	2.113105	-6.482836
C	4.058066	1.650722	-6.196317
H	4.978469	2.207593	-6.299756
C	6.301437	-0.578022	-6.374858
H	6.533966	0.407985	-6.786488
H	6.063026	-1.264815	-7.187841
C	7.451716	-1.061281	-5.489202
O	7.473457	-2.471979	-5.353912
C	8.073123	-3.122304	-6.460195
H	8.060232	-4.192333	-6.250105
H	9.110462	-2.789703	-6.591624
H	7.524925	-2.934984	-7.390772
H	8.426759	-0.707911	-5.845893
O	9.213988	3.721476	-5.409097
H	7.643359	5.269689	-4.056339
H	7.119705	7.089049	-2.396003
O	3.061226	7.498113	-4.164645

Table 14S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxythymidine diphosphate $d(T)_3$ in Model 3.

O	-7.725433	-2.115478	-6.666543
C	-8.720397	-1.111060	-6.738147
H	-8.678317	-0.543792	-5.807588
H	-9.717332	-1.554844	-6.849766
H	-8.536642	-0.437015	-7.584265
C	-7.699660	-2.925746	-7.824163
C	-6.553830	-3.912246	-7.727187
C	-6.479528	-4.648451	-6.384381
C	-5.450559	-3.835878	-5.610098
H	-4.935136	-4.420410	-4.850195
H	-5.946929	-2.985964	-5.136788
C	-4.505341	-3.357672	-6.708784
N	-3.888055	-2.058717	-6.439121
C	-2.515528	-1.955539	-6.376212
N	-2.053342	-0.678367	-6.155103
H	-1.044858	-0.590893	-6.084011
C	-2.800264	0.471155	-5.947034
O	-2.240663	1.538830	-5.712789
C	-4.239688	0.288272	-6.047446
C	-5.119141	1.487531	-5.870925
H	-4.971300	1.930203	-4.881186
H	-6.170574	1.214386	-5.976885
H	-4.880591	2.257794	-6.610330
O	-1.746941	-2.903419	-6.498681
C	-4.703414	-0.952849	-6.298894
H	-5.763815	-1.163991	-6.414593
H	-3.684200	-4.058698	-6.871105
H	-7.447985	-4.688600	-5.880727
O	-6.026425	-5.978862	-6.657272
P	-5.840191	-7.036996	-5.417270
O	-6.576430	-6.549064	-4.207074
O	-4.245503	-6.862368	-5.075602
C	-3.318032	-7.296377	-6.072012
C	-1.914356	-7.129877	-5.535939
C	-1.698424	-7.792765	-4.162961
C	-1.691268	-6.611030	-3.201932
H	-1.097086	-6.804581	-2.313166
H	-2.719250	-6.390822	-2.909568
C	-1.097951	-5.510976	-4.070420
N	-1.398867	-4.142092	-3.675130
C	-0.424419	-3.177568	-3.876795
N	-0.824872	-1.893887	-3.588823
H	-0.103239	-1.185922	-3.675927
C	-2.084334	-1.462766	-3.208443
O	-2.289678	-0.273144	-2.977798
C	-3.087031	-2.513091	-3.117695
C	-4.477180	-2.123183	-2.722501
H	-4.466141	-1.624434	-1.748507
H	-5.123644	-3.000389	-2.661027
H	-4.901793	-1.420683	-3.448379
O	0.713106	-3.421122	-4.257211
C	-2.693219	-3.780874	-3.356340
H	-3.395489	-4.603229	-3.291220
H	-0.009051	-5.587973	-4.095324
H	-2.486633	-8.511508	-3.929253
O	-0.437140	-8.471716	-4.193152
P	0.065167	-9.266678	-2.846850
O	-1.090864	-9.495180	-1.920695
O	0.999539	-8.129386	-2.122181
C	2.229077	-7.804621	-2.770251
C	2.797044	-6.543426	-2.166974
C	3.032531	-6.562927	-0.658712
C	2.950395	-5.072534	-0.301537
H	3.951540	-4.641898	-0.392594
H	2.565472	-4.872028	0.698765
C	2.037378	-4.479096	-1.387781
N	0.694308	-4.120018	-0.914517
C	0.342150	-2.788366	-0.862803
N	-0.957324	-2.560219	-0.470836
H	-1.241534	-1.585616	-0.453193
C	-1.923855	-3.501384	-0.146287
O	-3.058879	-3.144416	0.160705
C	-1.472061	-4.882167	-0.201042
C	-2.452340	-5.964244	0.130787
H	-2.792991	-5.879776	1.167107
H	-2.004646	-6.949787	-0.013445
H	-3.336637	-5.886513	-0.510213
O	1.104843	-1.869823	-1.141641
C	-0.197945	-5.114808	-0.578535
H	0.189303	-6.124942	-0.669152
H	2.446696	-3.567506	-1.821301
H	2.237073	-7.133410	-0.157387
O	4.281710	-7.161138	-0.408668
C	4.524694	-7.358760	0.973818
H	4.584707	-6.403607	1.508996
H	5.479053	-7.878661	1.062890
H	3.733635	-7.969320	1.426570
O	1.881158	-5.473908	-2.384445
H	3.756673	-6.329740	-2.659729
H	2.952596	-8.616505	-2.643020
H	2.057762	-7.647037	-3.841430
O	0.936425	-10.387315	-3.328586
O	-1.648073	-5.731865	-5.365130
H	-1.208368	-7.554081	-6.258037
H	-3.492534	-8.349429	-6.314460
H	-3.441903	-6.696610	-6.981395
O	-6.078059	-8.398248	-5.998227
O	-5.298964	-3.229568	-7.877874
H	-6.652330	-4.637607	-8.540353
H	-8.645080	-3.478287	-7.922994
H	-7.568086	-2.306958	-8.723351

Table 15S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyadenosine diphosphate d(A)$_3$ in Model 4.

O	-0.299050	7.775606	-1.285674
C	0.188682	8.384375	-0.108220
H	-0.512695	8.224368	0.722878
H	0.306139	9.468069	-0.255240
C	1.531837	7.781336	0.251092
H	1.951068	8.340096	1.093591
O	1.367209	6.412769	0.647971
C	2.009251	5.537289	-0.268050
N	1.127651	4.416271	-0.539193
C	1.283190	3.135627	-0.064485
N	2.344181	2.606419	0.562278
C	2.134755	1.333777	0.886281
H	2.950995	0.831476	1.399836
N	1.047447	0.581130	0.664112
C	-0.000211	1.134790	0.027863
N	-1.112689	0.393155	-0.163980
H	-1.022500	-0.606642	-0.049169
H	-1.780613	0.708863	-0.852378
C	0.093064	2.483163	-0.372819
N	-0.791176	3.340720	-1.002586
C	-0.139622	4.474912	-1.073109
H	-0.523881	5.402841	-1.479048
H	2.902385	5.102357	0.189883
C	2.353060	6.373718	-1.495689
H	1.521960	6.376346	-2.202951
H	3.252041	6.001854	-1.984020
C	2.528073	7.766667	-0.911467
O	3.842180	7.940380	-0.348246
P	5.122538	8.121920	-1.332685
O	6.212047	8.757953	-0.507515
Na	6.357640	10.509497	-2.112572
O	5.524738	6.596802	-1.730860
C	5.953332	5.731095	-0.672775
H	5.277508	5.824288	0.184484
H	6.966280	6.004029	-0.361539
C	5.947816	4.300909	-1.159099
H	6.397095	3.679634	-0.376586
O	4.598597	3.874791	-1.389832
C	4.538922	3.180418	-2.631721
H	4.765986	2.115767	-2.488474
N	3.190151	3.234434	-3.138503
C	2.271125	2.216856	-3.032359
N	2.451350	0.997792	-2.505844
C	1.364664	0.243666	-2.644221
H	1.434996	-0.770397	-2.255198
N	0.184502	0.567260	-3.195024
C	0.027502	1.803214	-3.701949
N	-1.147680	2.132928	-4.270081
H	-1.932429	1.512046	-4.137172
H	-1.343316	3.101446	-4.473481
C	1.122991	2.690343	-3.653808
N	1.325781	3.962248	-4.158141
C	2.566274	4.237590	-3.839847
H	3.079378	5.152960	-4.097069
C	5.591607	3.860401	-3.488339
H	5.240749	4.848760	-3.796810
H	5.880359	3.290979	-4.369014
C	6.714878	4.058276	-2.477995
O	7.513240	2.885889	-2.249960
P	8.187702	1.983250	-3.416498
O	9.526664	1.518008	-2.899175
Na	10.579784	2.462360	-4.804856
O	7.154875	0.730407	-3.515328
C	6.982632	-0.077025	-2.340981
H	6.417764	0.490386	-1.593548
H	7.959269	-0.344969	-1.925390
C	6.227598	-1.337699	-2.700482
H	6.165157	-1.957959	-1.800422
O	4.900118	-1.007611	-3.125906
C	4.687667	-1.403041	-4.473942
H	4.030076	-2.276215	-4.507011
C	6.067127	-1.696462	-5.060637
H	6.508679	-0.783340	-5.464611
H	6.020040	-2.447204	-5.850155
N	3.974736	-0.341311	-5.156735
C	4.415823	0.944440	-5.355344
H	5.417032	1.235615	-5.061063
N	3.521641	1.725800	-5.910142
C	2.419947	0.907443	-6.076262
C	1.119062	1.142842	-6.562635
N	0.249906	0.118508	-6.589928
C	0.648602	-1.074846	-6.123116
N	1.826560	-1.413179	-5.607911
H	-0.098271	-1.864086	-6.167642
N	0.725249	2.356022	-7.015357
H	1.252439	3.157807	-6.694322
H	-0.272793	2.495780	-7.099625
C	2.678672	-0.377473	-5.607127
C	6.852736	-2.156743	-3.835937
O	6.617578	-3.523710	-3.540632
C	7.371083	-4.404550	-4.355002
H	7.132755	-5.419813	-4.036238
H	8.446300	-4.226485	-4.228017
H	7.120877	-4.297851	-5.416768
H	7.930606	-1.971061	-3.930214
O	8.191099	2.672722	-4.755656
H	7.375219	4.888324	-2.738889
O	4.738708	8.818317	-2.611851
H	2.339273	8.563624	-1.633600
C	-1.585234	8.252292	-1.635430
H	-2.308226	8.052324	-0.834809
H	-1.564293	9.331910	-1.829576
H	-1.892620	7.726723	-2.540230

Table 16S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxythymidine diphosphate d(T)$_3$ in Model 4.

O	-8.181508	-2.380579	-6.157725
C	-9.230993	-1.430080	-6.163710
H	-9.106504	-0.801840	-5.280719
H	-10.208644	-1.926166	-6.123002
H	-9.188624	-0.805349	-7.064574
C	-8.246455	-3.253881	-7.266766
C	-7.030550	-4.158388	-7.272988
C	-6.727379	-4.790160	-5.910725
C	-5.659220	-3.868777	-5.338359
H	-5.002011	-4.361623	-4.623735
H	-6.150594	-3.027023	-4.846239
C	-4.909505	-3.398881	-6.581885
N	-4.376230	-2.040420	-6.472282
C	-3.025423	-1.818965	-6.637832
N	-2.651239	-0.499200	-6.529538
C	-3.455515	0.589478	-6.226045
C	-4.872853	0.284578	-6.104852
C	-5.817811	1.413673	-5.831234
H	-5.571493	1.899197	-4.882025
H	-6.846445	1.052425	-5.781430
H	-5.749969	2.175569	-6.613188
O	-2.962063	1.706110	-6.096516
H	-1.655201	-0.325481	-6.615681
O	-2.204873	-2.703293	-6.859326
C	-5.256994	-1.000050	-6.245553
H	-6.300797	-1.300218	-6.196882
H	-4.058814	-4.042600	-6.813508
H	-7.614366	-4.852405	-5.276972
O	-6.237711	-6.118502	-6.164141
P	-5.728016	-7.042814	-4.927777
O	-6.284587	-6.565576	-3.612299
O	-4.127739	-6.756069	-4.901182
C	-3.371512	-7.180285	-6.044129
C	-1.910673	-6.901997	-5.783559
C	-1.391953	-7.502743	-4.464090
C	-1.210466	-6.289979	-3.561160
H	-0.402278	-6.419563	-2.844619
H	-2.139892	-6.103646	-3.018812
C	-0.912525	-5.184239	-4.566238
N	-1.233629	-3.831131	-4.135661
C	-2.494526	-3.555384	-3.641812
C	-2.939656	-2.312445	-3.367590
C	-4.280515	-2.007775	-2.776277
H	-4.159733	-1.461626	-1.836172
H	-4.835272	-2.926476	-2.577535
H	-4.868985	-1.377633	-3.451983
C	-2.041327	-1.196853	-3.627462
O	-2.302929	-0.018194	-3.398564
N	-0.817586	-1.547492	-4.174616
H	-0.160914	-0.794991	-4.353382
H	-3.118352	-4.426395	-3.474691
C	-0.353341	-2.810913	-4.457388
O	0.756791	-2.991868	-4.940808
H	0.143731	-5.177031	-4.839100
H	-2.087039	-8.233744	-4.047298
O	-0.145230	-8.160958	-4.748391
P	0.619160	-8.948553	-3.545889
O	-0.346622	-9.357255	-2.464158
O	1.586771	-7.808708	-2.909785
C	2.669830	-7.336528	-3.721228
C	3.201175	-6.050329	-3.139595
C	3.627135	-6.099117	-1.673862
C	3.492341	-4.630011	-1.250006
H	4.455799	-4.135941	-1.401083
H	3.183764	-4.494847	-0.212880
C	2.454652	-4.048389	-2.228505
N	1.177048	-3.688306	-1.609915
C	0.368974	-4.681720	-1.099579
C	-0.863524	-4.462459	-0.598289
C	-1.761308	-5.546879	-0.088136
H	-1.968822	-5.416584	0.978206
H	-1.307865	-6.528281	-0.241931
H	-2.722436	-5.520448	-0.612245
C	-1.352270	-3.093062	-0.569635
O	-2.448697	-2.747383	-0.136403
N	-0.470063	-2.150995	-1.076956
H	-0.779340	-1.184033	-1.077872
H	0.788874	-5.681171	-1.150055
C	0.778628	-2.367549	-1.613604
O	1.460377	-1.449211	-2.053605
H	2.809722	-3.142308	-2.718015
H	2.944137	-6.740542	-1.099004
O	4.935556	-6.613205	-1.604962
C	5.367939	-6.818221	-0.270732
H	5.424012	-5.871149	0.279019
H	4.688388	-7.495999	0.260995
H	6.361391	-7.265155	-0.318121
O	2.183281	-5.056703	-3.191525
H	4.070638	-5.741068	-3.737656
H	3.470844	-8.081479	-3.739589
H	2.320584	-7.157730	-4.744068
O	1.437051	-10.041586	-4.184857
Na	0.331134	-11.630636	-2.795652
O	-1.722570	-5.487204	-5.696369
H	-1.324668	-7.305503	-6.616824
H	-3.516795	-8.251745	-6.210675
H	-3.704666	-6.626202	-6.928450
O	-6.000103	-8.477779	-5.302845
Na	-7.173284	-8.773254	-3.260090
O	-5.856827	-3.416639	-7.638227
H	-7.188042	-4.942788	-8.018927
H	-9.155058	-3.870502	-7.213343
H	-8.272818	-2.682210	-8.205207

Table 17S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyguanosine diphosphate d(G)$_3$ in Model 1.

O	-7.894865	-0.175015	-0.496409
C	-7.451149	-1.254807	-1.293262
C	-5.960154	-1.523450	-1.182129
C	-5.437886	-1.701772	0.260268
C	-4.851336	-0.321301	0.550933
H	-4.160524	-0.330105	1.390548
H	-5.665915	0.387804	0.737030
C	-4.218873	-0.045427	-0.798053
H	-3.316699	-0.654173	-0.925668
N	-3.813516	1.312213	-1.076350
C	-2.598725	1.636380	-1.605078
N	-1.619293	0.745639	-1.858919
C	-0.494894	1.315828	-2.198267
N	0.631906	0.558864	-2.380534
H	0.479586	-0.344931	-1.927318
H	1.477886	0.981895	-2.001740
N	-0.381236	2.671214	-2.399717
H	0.544054	3.056699	-2.557677
C	-1.352680	3.652451	-2.089164
O	-1.031734	4.838174	-2.140467
C	-2.580097	3.026135	-1.693574
N	-3.765824	3.555222	-1.222247
C	-4.460463	2.512961	-0.859927
H	-5.446207	2.542957	-0.417478
O	-4.451068	-2.708647	0.171606
P	-3.559912	-3.183854	1.505641
O	-3.900187	-2.284316	2.647622
O	-2.068495	-2.672733	0.991048
C	-1.447923	-3.341901	-0.086159
C	-0.001285	-2.887422	-0.215877
C	0.930413	-3.195520	0.961195
C	0.624480	-2.046648	1.915699
H	1.435886	-1.886444	2.627776
H	-0.327591	-2.206311	2.421836
C	0.527036	-0.896009	0.914306
H	1.509224	-0.443838	0.729525
N	-0.334909	0.199677	1.328052
C	-1.594051	0.171891	1.903830
H	-2.064558	-0.755750	2.215922
N	-2.129415	1.362851	2.008405
C	-1.196310	2.215936	1.465760
C	-1.247401	3.636411	1.239698
N	-0.067480	4.063047	0.525100
C	0.934504	3.234080	0.094342
N	1.019135	1.971274	0.382021
N	1.888943	3.774947	-0.757833
H	2.777990	3.291035	-0.651414
H	1.947450	4.782914	-0.779515
H	-0.228343	4.928239	0.014307
O	-2.078361	4.466814	1.536701
C	-0.086256	1.507104	1.033027
H	0.771733	-4.194544	1.378531
O	2.283250	-2.980764	0.588311
P	3.181479	-3.976235	-0.379458
O	4.344797	-4.480482	0.396979
O	3.838360	-2.742367	-1.302720
C	2.981574	-2.058174	-2.180911
H	2.004366	-1.871112	-1.716203
C	3.610554	-0.716050	-2.518125
O	3.426241	0.221367	-1.446264
C	4.618295	0.402435	-0.708249
N	4.374396	0.201352	0.706333
C	4.254497	-0.987515	1.416863
N	3.827169	-0.801291	2.635564
C	3.617024	0.553101	2.733362
C	3.104685	1.331142	3.830801
O	2.795257	1.022160	4.961786
N	2.984067	2.694594	3.422814
H	2.642086	3.311410	4.148063
C	3.353936	3.217351	2.219534
N	3.176135	4.592319	2.093440
H	2.249929	4.893681	2.379818
H	3.355895	4.869550	1.137487
N	3.875981	2.523856	1.250065
H	4.475854	-1.953960	0.978700
C	3.949535	1.192408	1.550668
C	5.663635	-0.547074	-1.303576
H	5.690955	-1.492048	-0.760824
H	6.656860	-0.091159	-1.302875
H	4.923492	1.450492	-0.801790
C	5.125251	-0.795021	-2.714081
H	5.430430	-1.773663	-3.107939
O	5.498925	0.242053	-3.611856
C	6.808964	0.103542	-4.088849
H	7.558946	0.163679	-3.286597
H	6.946900	-0.856431	-4.608922
H	6.988771	0.917968	-4.794401
H	3.132817	-0.287203	-3.405610
H	2.824507	-2.639138	-3.100762
O	2.262294	-4.790724	-1.225594
O	0.057637	-1.450995	-0.310071
H	0.424263	-3.316721	-1.128169
H	-1.490578	-4.428657	0.059049
H	-1.972963	-3.095241	-1.019951
O	-3.582188	-4.669628	1.534966
H	-6.227179	-1.976561	0.969192
O	-5.223179	-0.430541	-1.742295
H	-5.731510	-2.442349	-1.737885
H	-7.986495	-2.147806	-0.948856
H	-7.716064	-1.084110	-2.348780
C	-7.871933	1.059237	-1.176681
H	-6.904550	1.240163	-1.654906
H	-8.069879	1.839965	-0.437078
H	-8.658036	1.098046	-1.948200

Table 18S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxycytidine diphosphate d(C)$_3$ in Model 1.

O	-7.323244	-2.582948	-0.199419
C	-8.150875	-1.501097	-0.559271
H	-8.668162	-1.700188	-1.510777
H	-8.899794	-1.398302	0.230699
H	-7.590363	-0.566779	-0.665178
C	-6.361984	-2.926771	-1.179549
H	-6.777090	-2.779371	-2.188484
H	-6.144231	-3.992013	-1.044433
C	-5.067512	-2.147846	-1.040243
O	-5.333624	-0.772912	-1.344070
C	-4.639204	0.000570	-0.381799
N	-5.180249	1.362439	-0.379203
C	-4.923912	2.160184	-1.547610
N	-5.380251	3.464588	-1.526099
C	-5.959157	3.946431	-0.458775
N	-6.412915	5.242239	-0.520721
H	-6.037855	5.761971	-1.301323
H	-6.483390	5.746921	0.348663
C	-6.163175	3.199227	0.745632
H	-6.627557	3.625861	1.623899
O	-4.320512	1.671505	-2.472134
C	-5.754157	1.902556	0.717006
H	-5.854859	1.251497	1.576544
H	-3.581814	0.077854	-0.656439
C	-4.820732	-0.784585	0.907361
H	-5.876191	-0.770629	1.205702
H	-4.156384	-0.514544	1.731320
H	-4.315406	-2.546018	-1.734040
C	-4.480243	-2.183378	0.388854
H	-4.923632	-2.979544	0.998716
O	-3.082921	-2.340374	0.310850
P	-2.355469	-2.712363	1.783049
O	-2.893953	-4.030295	2.219560
O	-0.825090	-2.813127	1.206357
C	-0.507719	-3.672081	0.127278
H	-1.394222	-3.840648	-0.493835
C	0.572223	-3.030166	-0.733312
H	0.787920	-3.701323	-1.574549
O	0.090283	-1.787509	-1.245558
C	0.902082	-0.719466	-0.773303
H	1.594419	-0.385695	-1.547115
N	0.028092	0.421128	-0.491504
C	0.164571	1.616505	-1.250324
O	1.087508	1.737431	-2.041301
N	-0.766423	2.603373	-1.030101
C	-1.664293	2.467367	-0.082823
N	-2.557397	3.500820	0.080028
H	-2.663079	4.072955	-0.746919
H	-3.417706	3.283664	0.562198
C	-1.739240	1.335088	0.783689
H	-2.467236	1.225657	1.578548
C	-0.891495	0.310197	0.491320
H	-0.928536	-0.625441	1.039148
C	1.651182	-1.267972	0.435951
H	2.568952	-0.727518	0.658149
H	1.008730	-1.291399	1.319001
C	1.898223	-2.696840	-0.032777
O	2.890165	-2.758542	-1.052146
P	4.399828	-2.162643	-0.743091
O	5.296959	-2.645368	-1.834283
O	4.115196	-0.529651	-0.999720
C	4.567398	0.093376	-2.182042
H	4.842077	-0.657905	-2.931085
H	3.757952	0.726752	-2.569077
C	5.782344	0.957857	-1.877127
H	6.213192	1.341791	-2.808580
O	5.433752	2.100128	-1.081395
C	5.718036	1.872509	0.271310
H	6.316845	2.704311	0.655734
C	6.463849	0.533541	0.382119
H	7.333965	0.632665	1.032657
H	5.810663	-0.244929	0.785301
N	4.462430	1.890415	1.058554
C	4.626722	1.850945	2.465254
O	5.766589	1.859880	2.914901
N	3.495544	1.792472	3.234491
C	2.318795	1.905345	2.657761
C	2.133818	2.122064	1.262424
H	1.153975	2.300013	0.844845
N	1.206975	1.833739	3.461140
H	1.390639	1.409721	4.359095
H	0.355101	1.527079	3.009737
C	3.249153	2.054578	0.486776
H	3.221207	2.130257	-0.594439
C	6.846220	0.219455	-1.067773
O	8.111550	0.782156	-1.419526
C	9.180200	0.006760	-0.952842
H	10.105564	0.493417	-1.274785
H	9.147447	-1.012536	-1.365996
H	9.191819	-0.075329	0.143518
H	6.834293	-0.856814	-1.289551
O	4.680948	-2.292765	0.716066
H	2.149069	-3.376152	0.788350
H	-0.155602	-4.639560	0.509115
O	-2.376540	-1.476266	2.630722

Table 19S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyguanosine diphosphate $d(G)_3$ in Model 2.

O	6.647381	-1.180255	-0.861175
C	7.733873	-2.073906	-0.830506
H	7.396148	-2.981818	-0.329170
H	8.583645	-1.650416	-0.275898
H	8.070388	-2.325163	-1.846065
C	6.968828	0.034028	-1.493679
C	5.731783	0.908895	-1.579403
C	5.001834	1.126968	-0.245090
H	5.676067	1.118594	0.617348
C	3.978618	0.004341	-0.252135
H	3.142726	0.193866	0.418683
H	4.471957	-0.939099	-0.006829
C	3.584691	0.014606	-1.726138
H	2.823171	0.774597	-1.918371
N	3.027257	-1.221631	-2.218445
C	3.660924	-2.433677	-2.398343
H	4.720972	-2.527389	-2.202891
N	2.858395	-3.372482	-2.820195
C	1.628535	-2.756515	-2.912950
C	0.341749	-3.271255	-3.303490
N	-0.650412	-2.252473	-3.134446
C	-0.434370	-0.957180	-2.731088
N	0.743556	-0.477770	-2.467778
N	-1.552760	-0.159706	-2.637257
H	-1.336033	0.704605	-2.148896
H	-2.350680	-0.608274	-2.193954
H	-1.566572	-2.507453	-3.482509
O	-0.004106	-4.363463	-3.704895
C	1.718524	-1.419605	-2.548471
O	4.359964	2.406237	-0.374184
P	3.638356	3.152939	0.867702
O	3.181160	2.152705	1.913754
Na	4.333585	3.238757	3.434452
O	4.516023	4.226032	1.471517
O	2.403836	3.872842	0.106451
C	1.854556	3.428206	-1.128171
C	0.725838	2.434050	-0.930713
C	-0.443006	2.950804	-0.060903
C	-0.277234	2.165302	1.233420
H	-1.188615	2.097258	1.825507
H	0.545404	2.603789	1.809431
C	0.209733	0.850840	0.637091
N	0.736492	-0.137772	1.529456
C	1.442739	0.019405	2.711414
H	1.657553	1.003635	3.090841
N	1.817917	-1.107212	3.239997
C	1.341429	-2.068956	2.374497
C	1.309270	-3.499146	2.503973
O	1.674591	-4.232502	3.405451
N	0.677504	-4.070076	1.366064
H	0.676585	-5.081741	1.356553
C	0.024376	-3.392584	0.371271
N	-0.020468	-2.086525	0.299163
N	-0.574308	-4.161432	-0.578753
H	-0.938051	-5.054628	-0.284154
H	-1.153350	-3.643177	-1.222407
C	0.666416	-1.490046	1.308478
H	-0.591298	0.349523	0.073880
H	-0.413856	4.037706	0.066231
O	-1.669428	2.562707	-0.721612
P	-3.004116	3.433779	-0.416400
O	-3.142546	3.738167	1.057918
Na	-3.331941	5.877704	0.552230
O	-4.146445	2.355545	-0.802579
C	-4.233867	1.842273	-2.128894
C	-4.864260	0.462402	-2.056284
C	-6.257259	0.416262	-1.417253
C	-5.949045	0.108991	0.046154
H	-6.764214	-0.405960	0.557306
H	-5.724234	1.034528	0.577791
C	-4.698718	-0.770361	-0.048403
N	-3.806397	-0.619496	1.075921
C	-3.442503	0.547179	1.730245
N	-2.612611	0.338856	2.713832
C	-2.406237	-1.019230	2.714557
C	-1.603473	-1.823523	3.601868
O	-0.938494	-1.511449	4.560598
N	-1.680330	-3.195365	3.195523
H	-1.034776	-3.802371	3.693887
C	-2.432375	-3.684643	2.166669
N	-2.328273	-5.045626	1.922671
H	-2.192968	-5.619874	2.744749
H	-3.097291	-5.366607	1.348233
N	-3.194370	-2.958064	1.395662
H	-3.808385	1.520280	1.433106
C	-3.124544	-1.633510	1.704761
H	-4.941795	-1.835725	-0.099841
H	-6.799816	1.364833	-1.544793
O	-6.952791	-0.640820	-2.044152
C	-8.330196	-0.658545	-1.753649
H	-8.530449	-0.810645	-0.684699
H	-8.812849	0.277882	-2.067271
H	-8.765057	-1.488437	-2.311820
O	-4.049465	-0.396294	-1.259104
H	-4.927885	0.048116	-3.068867
H	-3.239974	1.761185	-2.580133
H	-4.844097	2.511275	-2.746103
O	-3.068674	4.665006	-1.291720
O	1.224708	1.290519	-0.261873
H	0.342954	2.150604	-1.922824
H	1.464208	4.316868	-1.634774
H	2.636248	2.987581	-1.751835
O	4.778934	0.296447	-2.442999
H	6.020532	1.881921	-1.994177
H	7.760546	0.563577	-0.937244
H	7.336149	-0.150481	-2.515143

Table 20S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxycytidine diphosphate $d(C)_3$ in Model 2.

O	3.327917	-1.379700	1.062081
C	3.761543	-0.498575	2.068508
C	4.098380	0.837227	1.428910
O	5.285330	0.730939	0.644637
C	4.985631	0.697546	-0.731903
H	5.510775	1.509255	-1.239519
N	5.504483	-0.552757	-1.319272
C	5.515749	-0.595368	-2.741127
N	5.951064	-1.750507	-3.330162
C	6.311948	-2.770206	-2.585957
N	6.759900	-3.883204	-3.238705
H	6.571701	-3.897582	-4.229765
H	6.743146	-4.766302	-2.756311
C	6.301299	-2.759751	-1.154714
H	6.626469	-3.607472	-0.567161
O	5.133215	0.393280	-3.344661
C	5.882978	-1.606914	-0.570269
H	5.845344	-1.456563	0.501203
C	3.461763	0.811974	-0.880227
H	3.179856	1.481358	-1.690596
H	3.017896	-0.168279	-1.067114
H	4.284115	1.578695	2.214470
C	3.004548	1.321019	0.476962
O	2.977791	2.760467	0.460802
P	1.870238	3.563291	1.307142
O	2.497304	4.735396	2.025445
Na	1.714265	3.995564	3.914626
O	0.838200	4.122517	0.191696
C	0.905097	3.835741	-1.200011
H	1.928857	3.592859	-1.496156
H	0.583542	4.740223	-1.725166
C	-0.014507	2.683627	-1.546899
H	-0.082001	2.580594	-2.638034
O	0.524845	1.499139	-0.970601
C	-0.560147	0.745821	-0.441336
H	-1.069829	0.220542	-1.255034
N	-0.102680	-0.294433	0.454079
C	0.288978	-1.534658	-0.153023
O	0.511525	-1.557211	-1.344136
N	0.312901	-2.639373	0.665245
C	0.228762	-2.494559	1.965767
N	0.252052	-3.622302	2.742947
H	0.009995	-4.451462	2.212347
H	-0.298327	-3.548498	3.591487
C	0.133410	-1.217031	2.612717
H	0.126535	-1.122374	3.690707
C	-0.080167	-0.148681	1.806973
H	-0.212597	0.855910	2.189400
C	-1.443905	1.828451	0.165952
H	-0.927807	2.294321	1.011577
H	-2.441947	1.507421	0.459350
C	-1.444324	2.836779	-0.974081
H	-1.659386	3.853774	-0.636753
O	-2.354408	2.493767	-2.031716
P	-3.922804	2.235113	-1.730262
O	-4.718276	2.589973	-2.962502
Na	-5.925459	3.942690	-1.709775
O	-3.974678	0.629389	-1.462238
C	-3.636980	-0.205909	-2.573726
H	-2.688943	0.128924	-3.010945
C	-3.498800	-1.632163	-2.100617
H	-3.187161	-2.242593	-2.961503
O	-2.525331	-1.698971	-1.066878
C	-2.802563	-2.770319	-0.194335
H	-1.955271	-3.456571	-0.149444
C	-4.102244	-3.417184	-0.687763
H	-3.874826	-4.240743	-1.372377
H	-4.694817	-3.802272	0.143054
N	-2.944042	-2.221417	1.171150
C	-2.711750	-3.124750	2.236659
O	-2.523121	-4.302212	1.971124
N	-2.684046	-2.607108	3.504983
C	-3.008829	-1.346700	3.700455
C	-3.394196	-0.451943	2.655317
H	-3.675017	0.576243	2.841773
N	-2.912943	-0.878202	4.980064
H	-2.845261	-1.589530	5.692602
H	-3.413629	-0.038993	5.222809
C	-3.316568	-0.941981	1.389305
H	-3.524507	-0.350084	0.502351
C	-4.740667	-2.282191	-1.498409
O	-5.586771	-2.684219	-2.540754
C	-6.798732	-3.238240	-2.086257
H	-7.402086	-3.461694	-2.966945
H	-6.634660	-4.166249	-1.522443
H	-7.344659	-2.531196	-1.445171
H	-5.255554	-1.563235	-0.838265
H	-4.422321	-0.149997	-3.334973
O	-4.379766	2.931088	-0.467907
O	1.133302	2.633030	2.268125
H	2.028895	0.938910	0.762280
H	4.664582	-0.889145	2.566971
H	2.973995	-0.365040	2.828538
C	3.373517	-2.734437	1.454844
H	4.414705	-3.058517	1.608532
H	2.914873	-3.315199	0.654052
H	2.808192	-2.904329	2.380880

Table 21S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyguanosine diphosphate $d(G)_3$ in Model 3.

O	-6.783944	2.677053	-9.534764
C	-6.860626	4.088015	-9.453973
H	-6.304902	4.395026	-8.567416
H	-7.902829	4.419357	-9.364442
H	-6.417534	4.557065	-10.341625
C	-7.454389	2.177295	-10.673003
C	-7.328924	0.668016	-10.725218
C	-7.748216	-0.049193	-9.439757
C	-6.432230	-0.179374	-8.685269
H	-6.426020	-1.002070	-7.971348
H	-6.204816	0.758925	-8.175459
C	-5.450470	-0.418900	-9.825236
N	-4.097618	0.038400	-9.576924
C	-3.695773	1.339054	-9.350979
H	-4.426403	2.119037	-9.178037
N	-2.397777	1.489800	-9.404154
C	-1.917813	0.225776	-9.696050
C	-0.582399	-0.238061	-9.901234
O	0.475809	0.387542	-9.822820
N	-0.571243	-1.601588	-10.228286
C	-1.664193	-2.424283	-10.291211
N	-2.896704	-2.002371	-10.099176
N	-1.439990	-3.718085	-10.627988
H	-2.213099	-4.343573	-10.448557
H	-0.522915	-4.108951	-10.463401
H	0.350339	-2.002042	-10.365303
C	-2.958983	-0.681934	-9.819045
H	-5.361400	-1.482880	-10.064959
H	-8.518172	0.492903	-8.886492
O	-8.245761	-1.335568	-9.832910
P	-9.009499	-2.281791	-8.736393
O	-9.737095	-1.430329	-7.740617
O	-7.761295	-2.947505	-7.913877
C	-6.908080	-3.864443	-8.597417
C	-5.697879	-4.152351	-7.734842
C	-6.050948	-4.409588	-6.255635
C	-5.699971	-3.086369	-5.593841
H	-5.533797	-3.174818	-4.522551
H	-6.483693	-2.355512	-5.804521
C	-4.444521	-2.745802	-6.379874
H	-3.605418	-3.388389	-6.081182
N	-3.966293	-1.389595	-6.281877
C	-4.645008	-0.236877	-5.947107
H	-5.695206	-0.252020	-5.694628
N	-3.885832	0.827335	-5.962363
C	-2.638215	0.353707	-6.319061
C	-1.390865	1.039335	-6.461536
O	-1.149108	2.236571	-6.318972
N	-0.364401	0.143755	-6.796644
C	-0.502010	-1.209153	-6.976972
N	-1.650575	-1.843061	-6.851244
N	0.607406	-1.893455	-7.344934
H	0.547047	-2.896751	-7.238223
H	1.513505	-1.487503	-7.159958
H	0.546071	0.565451	-6.948663
C	-2.668370	-1.015086	-6.521188
O	-5.177534	-5.399670	-5.702342
P	-5.662399	-6.966067	-5.758107
O	-6.480723	-7.290170	-4.543797
O	-4.204181	-7.651340	-5.522100
C	-3.231092	-7.586628	-6.567850
C	-1.897567	-7.167396	-5.988170
C	-1.497756	-7.935226	-4.712331
C	-1.748285	-6.913385	-3.602399
H	-1.133633	-7.072980	-2.716209
H	-2.804010	-6.931325	-3.322283
C	-1.415760	-5.616909	-4.325276
N	-1.972780	-4.414721	-3.755777
C	-3.268640	-4.215861	-3.329211
N	-3.534068	-2.963903	-3.065959
C	-2.358950	-2.297100	-3.348404
C	-2.057635	-0.900410	-3.308464
O	-2.796849	0.037531	-3.013797
N	-0.725252	-0.668126	-3.679082
H	-0.436564	0.305162	-3.661537
C	0.187956	-1.624977	-4.042540
N	-0.099069	-2.908527	-4.120046
N	1.453974	-1.202412	-4.284722
H	1.595870	-0.245332	-4.578897
H	2.044420	-1.882528	-4.743131
H	-3.966822	-5.036040	-3.240018
C	-1.378196	-3.178101	-3.773809
H	-0.333677	-5.459931	-4.383807
H	-2.092274	-8.848202	-4.583118
O	-0.124090	-8.266357	-4.830986
C	0.304325	-9.205702	-3.861033
H	0.225261	-8.808482	-2.842659
H	-0.286459	-10.127992	-3.924920
H	1.350104	-9.431304	-4.072470
O	-1.964247	-5.781256	-5.627576
H	-1.119758	-7.313303	-6.746410
H	-3.138531	-8.575436	-7.026324
H	-3.533831	-6.869585	-7.338091
O	-6.189370	-7.263379	-7.133597
H	-7.098730	-4.692302	-6.122040
O	-4.806923	-3.022310	-7.732341
H	-5.176217	-5.023273	-8.145015
H	-7.441664	-4.803622	-8.779580
H	-6.586864	-3.444941	-9.558155
O	-9.704532	-3.340147	-9.538782
O	-5.961440	0.291757	-10.946603
H	-7.930683	0.303143	-11.563581
H	-8.519673	2.449211	-10.641564
H	-7.020840	2.605567	-11.588639

Table 22S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxycytidine diphosphate $d(C)_3$ in Model 3.

O	4.505057	5.683259	-1.878107
C	4.511890	6.590782	-0.793057
H	4.185530	6.100383	0.132971
H	5.514438	7.007914	-0.634319
H	3.819831	7.397876	-1.036179
C	5.367405	4.587519	-1.654378
H	5.039148	4.012300	-0.776459
H	6.394744	4.934835	-1.470681
C	5.360853	3.698169	-2.877788
H	6.116734	2.913983	-2.755061
O	4.062387	3.105440	-3.021498
C	3.684952	3.208681	-4.392719
N	2.254375	2.994832	-4.505585
C	1.808398	1.661092	-4.366253
N	0.490950	1.391538	-4.537973
C	-0.364649	2.378594	-4.789106
N	-1.654539	2.058946	-4.948669
H	-1.936559	1.091839	-4.895869
H	-2.346155	2.759447	-5.162242
C	0.044825	3.749025	-4.892742
H	-0.661969	4.542415	-5.090606
O	2.636181	0.784754	-4.093977
C	1.366269	3.999263	-4.750167
H	1.773636	4.997113	-4.838054
C	4.241709	4.560163	-4.815007
H	3.706982	5.375874	-4.323930
H	4.275054	4.710745	-5.893565
H	4.161969	2.404766	-4.965512
C	5.631040	4.450835	-4.196572
H	6.113754	5.416622	-4.024966
O	6.453002	3.618010	-5.019191
P	7.551089	4.319777	-6.013063
O	8.504534	5.133074	-5.185911
O	8.249411	2.940341	-6.536379
C	8.833386	2.068537	-5.563667
H	8.585310	2.405242	-4.553251
H	9.921477	2.080854	-5.676195
C	8.318027	0.651681	-5.747582
H	8.735741	0.040683	-4.939835
O	6.887029	0.639113	-5.653810
C	6.305796	0.134429	-6.855304
H	5.980482	-0.898146	-6.712721
N	5.097078	0.896132	-7.151593
C	3.830187	0.299166	-6.976897
O	3.749872	-0.873172	-6.594949
N	2.722607	1.041789	-7.240088
C	2.834184	2.291224	-7.673661
N	1.699591	2.964194	-7.930743
H	0.825203	2.558654	-7.626884
H	1.724901	3.959077	-8.094323
C	4.103186	2.917665	-7.893274
H	4.193574	3.935668	-8.246903
C	5.196665	2.180833	-7.594168
H	6.195572	2.587619	-7.682593
C	7.403196	0.224390	-7.910680
H	7.459562	1.223049	-8.346892
H	7.284539	-0.501232	-8.712187
C	8.662612	-0.006759	-7.090447
O	8.898116	-1.391536	-6.807298
P	9.147377	-2.475468	-8.010733
O	10.129382	-3.476132	-7.478301
O	7.663774	-3.173317	-8.108753
C	7.229281	-3.896958	-6.953758
H	7.104801	-3.204134	-6.113458
H	7.973575	-4.652681	-6.683052
C	5.912007	-4.575513	-7.248100
H	5.634737	-5.176476	-6.375078
O	4.911796	-3.577184	-7.473828
C	4.245664	-3.818345	-8.708089
H	3.314862	-4.359803	-8.541592
N	3.879109	-2.530061	-9.277673
C	4.869623	-1.628649	-9.528388
H	5.875293	-1.971338	-9.305281
C	4.595882	-0.392246	-9.999602
H	5.378763	0.329372	-10.192530
C	3.208510	-0.073217	-10.172099
N	2.234460	-0.933023	-9.895101
N	2.860432	1.133830	-10.649772
H	1.887079	1.400539	-10.610377
H	3.545717	1.873097	-10.695666
C	2.525974	-2.178663	-9.433661
O	1.644710	-3.001738	-9.162875
C	5.229203	-4.628141	-9.547821
H	5.961799	-3.970940	-10.022784
H	4.726743	-5.214030	-10.318435
C	5.920528	-5.483663	-8.489473
O	5.167650	-6.641849	-8.166253
C	5.308513	-7.677664	-9.121924
H	4.740262	-8.533271	-8.755230
H	6.362400	-7.962297	-9.234060
H	4.917439	-7.386259	-10.103513
H	6.940056	-5.769525	-8.778507
O	9.371475	-1.775071	-9.315951
H	9.552938	0.425756	-7.554421
O	6.875207	4.930658	-7.207434

Table 23S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxyguanosine diphosphate d(G)$_3$ in Model 4.

O	-7.476082	2.573318	-10.149864
C	-7.472081	3.982839	-10.284184
H	-6.998455	4.394227	-9.392055
H	-8.494204	4.372580	-10.366991
H	-6.904789	4.288686	-11.171975
C	-8.073025	1.937400	-11.261381
H	-9.138997	2.199685	-11.325404
C	-7.935040	0.434693	-11.122518
C	-8.356040	-0.099614	-9.750351
C	-7.037361	-0.187410	-8.996189
H	-7.040205	-0.959844	-8.228090
H	-6.810126	0.780748	-8.545200
C	-6.030438	-0.502291	-10.103010
N	-4.717154	0.074674	-9.872317
C	-4.437894	1.412385	-9.697692
H	-5.232572	2.147176	-9.726023
N	-3.162043	1.652746	-9.535516
C	-2.569366	0.409164	-9.613656
C	-1.199757	0.028822	-9.461478
O	-0.223360	0.742996	-9.232494
N	-1.045469	-1.358094	-9.593409
H	-0.094241	-1.698896	-9.494518
C	-2.054125	-2.261284	-9.811798
N	-3.316995	-1.917152	-9.941143
N	-1.689027	-3.564213	-9.948042
H	-0.843084	-3.864310	-9.480252
H	-2.458185	-4.216883	-9.873583
C	-3.516378	-0.582603	-9.824590
H	-5.871210	-1.578278	-10.218140
H	-9.086668	0.547304	-9.260954
O	-8.936468	-1.398422	-9.959818
P	-9.661695	-2.177581	-8.728870
O	-10.145388	-1.189642	-7.696058
Na	-8.854026	-1.640448	-5.913577
O	-8.408273	-2.923891	-7.968500
C	-7.719875	-3.936418	-8.710582
C	-6.403494	-4.260202	-8.050543
C	-6.468911	-4.722668	-6.567433
C	-5.648640	-3.655244	-5.847280
H	-5.141703	-4.002625	-4.951209
H	-6.303830	-2.823870	-5.576022
C	-4.709281	-3.200967	-6.952033
H	-3.918872	-3.939523	-7.124407
N	-4.040846	-1.945729	-6.732840
C	-4.587844	-0.696728	-6.535382
H	-5.657435	-0.543755	-6.523663
N	-3.685096	0.235453	-6.366997
C	-2.480740	-0.435463	-6.452671
C	-1.139253	0.045627	-6.345811
O	-0.745378	1.190272	-6.127776
N	-0.219736	-1.001448	-6.514708
H	0.756115	-0.727295	-6.450249
C	-0.526989	-2.322255	-6.710949
N	-1.763199	-2.770458	-6.792815
N	0.509374	-3.185573	-6.892897
H	1.404507	-2.896770	-6.518067
H	0.261570	-4.141821	-6.645966
C	-2.682274	-1.787740	-6.676197
O	-5.916926	-6.053979	-6.529804
P	-4.925063	-6.634022	-5.386926
O	-5.331028	-6.195621	-3.999290
O	-3.512819	-5.899247	-5.698498
C	-2.578836	-6.434088	-6.642729
C	-1.261604	-6.715229	-5.945804
C	-1.361429	-7.610538	-4.708770
C	-1.545498	-6.607166	-3.567689
H	-1.142664	-6.968104	-2.621000
H	-2.607357	-6.397830	-3.436972
C	-0.784567	-5.374116	-4.060433
N	-1.419075	-4.110525	-3.722359
C	-2.764172	-3.821466	-3.614766
N	-3.005632	-2.546622	-3.449078
C	-1.756168	-1.958110	-3.456559
C	-1.383051	-0.582459	-3.349344
O	-2.107048	0.403792	-3.218645
N	0.009714	-0.434763	-3.433315
H	0.341877	0.523979	-3.425788
C	0.911718	-1.446305	-3.641841
N	0.572370	-2.715401	-3.729378
N	2.206603	-1.082508	-3.827825
H	2.518455	-0.204235	-3.436617
H	2.871390	-1.840327	-3.752722
H	-3.514834	-4.598169	-3.656389
C	-0.763811	-2.908275	-3.636445
H	0.225822	-5.320329	-3.649786
H	-2.198388	-8.317713	-4.780011
O	-0.133267	-8.310305	-4.608195
C	-0.160682	-9.348163	-3.644727
H	-0.307188	-8.962093	-2.629519
H	-0.960608	-10.065417	-3.867922
H	0.803065	-9.856165	-3.693336
O	-0.679371	-5.492277	-5.475869
H	-0.573441	-7.159078	-6.671539
H	-2.963641	-7.351899	-7.094504
H	-2.421394	-5.682650	-7.422350
O	-4.832258	-8.120829	-5.618618
Na	-5.450495	-8.476489	-3.329849
H	-7.492134	-4.786612	-6.192229
O	-5.560473	-3.105010	-8.082942
H	-5.933995	-5.070687	-8.621853
H	-8.331132	-4.842226	-8.757752
H	-7.531330	-3.578782	-9.728874
O	-10.568548	-3.197132	-9.338162
O	-6.564369	0.046650	-11.297382
H	-8.531318	-0.041363	-11.906833
H	-7.584034	2.256041	-12.192980

Table 24S. M06-2X/6-31G(d,p) optimized reference geometry for trideoxycytidine diphosphate d(C)$_3$ in Model 4.

O	4.190069	6.613881	-2.773145
C	5.055234	6.145123	-1.758935
H	4.497247	5.968382	-0.828318
H	5.839319	6.888348	-1.553818
C	5.703704	4.849582	-2.203228
H	6.479655	4.586061	-1.477758
O	4.732933	3.793911	-2.238938
C	4.579605	3.283855	-3.559006
H	5.072702	2.315026	-3.658841
N	3.160335	3.044207	-3.796866
C	2.297991	4.100423	-3.736443
H	2.742342	5.055956	-3.471282
C	0.976959	3.942825	-3.973403
H	0.287755	4.774468	-3.928641
C	0.537113	2.609257	-4.267459
N	-0.749763	2.383561	-4.563050
H	-1.433577	3.122929	-4.528752
H	-1.060184	1.437763	-4.727795
N	1.361268	1.566630	-4.265760
C	2.686643	1.738221	-4.024098
O	3.477686	0.786466	-4.006343
C	5.204028	4.332163	-4.477408
H	4.486975	5.123496	-4.704980
H	5.573929	3.913515	-5.410781
C	6.309465	4.913406	-3.608958
O	7.485859	4.084947	-3.583398
P	8.314122	3.759204	-4.942831
O	9.771956	3.669776	-4.566790
Na	10.270951	5.319702	-6.209386
O	7.745837	2.291742	-5.360104
C	8.023137	1.212584	-4.454110
H	7.467061	1.368565	-3.523476
H	9.094236	1.182155	-4.232667
C	7.604969	-0.096720	-5.081816
H	7.919598	-0.903395	-4.411357
O	6.181402	-0.130957	-5.224357
C	5.813252	-0.384921	-6.577066
H	5.551482	-1.435553	-6.718286
N	4.609486	0.381081	-6.863482
C	4.673348	1.740898	-6.826017
H	5.649716	2.159283	-6.604226
C	3.580642	2.508061	-7.039903
H	3.629811	3.588414	-7.012555
C	2.348775	1.808064	-7.261533
N	2.266761	0.482938	-7.250625
N	1.225012	2.500872	-7.506701
H	1.200734	3.499904	-7.370315
H	0.346207	2.003401	-7.517885
C	3.376371	-0.274859	-7.046817
O	3.330496	-1.510169	-7.027634
C	7.034926	0.001238	-7.406036
H	7.056871	1.075774	-7.600647
H	7.082150	-0.520626	-8.359272
C	8.191837	-0.345724	-6.479532
O	8.556470	-1.736284	-6.524958
P	9.017081	-2.450258	-7.910312
O	10.053317	-3.487162	-7.555747
Na	11.537620	-2.502933	-9.138500
O	7.643411	-3.169072	-8.406965
C	7.107112	-4.188936	-7.548897
H	6.813922	-3.738389	-6.594260
H	7.865508	-4.956625	-7.367969
C	5.899948	-4.813269	-8.208825
H	5.544970	-5.624780	-7.563069
O	4.876720	-3.822966	-8.340399
C	4.401924	-3.783043	-9.682081
H	3.501857	-4.388441	-9.786927
N	4.013507	-2.411572	-9.973485
C	4.957094	-1.434139	-9.862779
H	5.958585	-1.778065	-9.625660
C	4.644521	-0.129625	-10.018809
H	5.388211	0.650171	-9.923663
C	3.261450	0.166325	-10.258385
N	2.329180	-0.776912	-10.334613
N	2.877741	1.441287	-10.425814
H	3.517856	2.196129	-10.231257
H	1.890448	1.651237	-10.452475
C	2.660366	-2.086661	-10.184889
O	1.816968	-2.987995	-10.239205
C	5.546663	-4.322873	-10.533788
H	6.284998	-3.542682	-10.734955
H	5.195046	-4.728329	-11.483317
C	6.154401	-5.381100	-9.615998
O	5.466468	-6.618011	-9.699879
C	5.840111	-7.379784	-10.834053
H	5.286240	-8.317989	-10.788310
H	6.916606	-7.591809	-10.822072
H	5.594675	-6.866717	-11.771116
H	7.224645	-5.536624	-9.804637
O	9.402246	-1.442501	-8.961479
H	9.081261	0.258968	-6.671427
O	7.959627	4.711189	-6.054838
H	6.591163	5.928412	-3.897418
C	3.530580	7.810311	-2.400879
H	2.921943	7.659649	-1.500693
H	4.254233	8.611962	-2.208124
H	2.884579	8.097700	-3.230971

Table 25S. Base-pair step and helical parameters (for two steps RR/YY) for duplex structures obtained from M06-2X/6-31G(d,p) and 3DNA (ideal structure) and MD averaged parameters along with their standard deviations (within parenthesis).

Parameter	Gas models				PCM models				Ideal structure		MD
	Model 1		Model 2		Model 3		Model 4		A-DNA	B-DNA	
Local base-pair step parameters											
	1GG/CC	2GG/CC	1GG/CC	2GG/CC	1GG/CC	2GG/CC	1GG/CC	2GG/CC	**Average**		
Shift (Å)	-0.54	-	0.02	0.05	0.7	-0.93	-0.29	-0.85	0.0	0.0	-0.05 (0.76)
Slide (Å)	0.56	-	2.42	1.87	2.13	0.6	0.89	0.45	-1.40	0.45	-0.44 (0.68)
Rise (Å))	3.63	-	3.44	4.01	3.15	3.38	3.2	3.05	3.3	3.36	3.32 (0.37)
Tilt (deg.)	-7.17	-	16.22	-9.25	1.1	-8.79	-1.21	-4.13	-0.02	0.0	-0.3 (4.6)
Roll (deg.)	-2.67	-	-10.34	-12.06	-7.58	2.86	-7.29	0.22	12.43	1.71	3.6 (7.2)
Twist (deg.)	44.58	-	51.28	50.09	48.29	37.2	43.44	34.58	30.30	35.96	32.6 (7.3)
	1AA/TT	2AA/TT	1AA/TT	2AA/TT	1AA/TT	2AA/TT	1AA/TT	2AA/TT	**Average**		
Shift (Å)	0.3	0.47	0.37	0.66	-0.67	0.51	0.44	-0.15	0.0	0.0	-0.05 (0.76)
Slide (Å)	0.51	-0.07	0.66	0.02	0.83	-0.3	-0.01	0.02	-1.40	0.45	-0.44 (0.68)
Rise (Å))	2.98	2.91	3.07	2.86	3.1	3.1	3.32	3.07	3.3	3.36	3.32 (0.37)
Tilt (deg.)	-1.64	-2.19	0.24	-3.08	-1.98	-2.62	1.14	-5.28	-0.02	0.0	-0.3 (4.6)
Roll (deg.)	0.2	-0.54	-2.22	-6.5	-2.83	-2.8	-2.19	-6.49	12.43	1.71	3.6 (7.2)
Twist (deg.)	35.12	38.44	39.07	39.66	40.69	43.94	44.08	44.02	30.30	35.96	32.6 (7.3)
Local base-pair helical parameters											
	1GG/CC	2GG/CC	1GG/CC	2GG/CC	1GG/CC	2GG/CC	1GG/CC	2GG/CC	**Average**		
X-disp. (Å)	0.99	-	3.26	-0.77	3.1	0.53	1.84	0.72	-4.48	0.49	-1.44 (0.89)
Y-disp. (Å)	-0.01	-	0.96	3.45	-0.01	0.23	0.27	0.83	0.0	0.01	0.02 (0.55)
Incl. (deg.)	-3.49	-	-11.49	10.64	-9.19	4.4	-9.77	0.37	22.63	2.76	6.8 (5.4)
Tip (deg.)	9.37	-	-18.03	52.2	-1.33	13.52	1.61	6.92	0.03	0.0	0.3 (5)
	1AA/TT	2AA/TT	1AA/TT	2AA/TT	1AA/TT	2AA/TT	1AA/TT	2AA/TT	**Average**		
X-disp. (Å)	0.81	-0.05	1.23	0.66	1.49	-0.15	0.19	0.58	-4.48	0.49	-1.44 (0.89)
Y-disp. (Å)	-0.71	-0.95	-0.53	-1.27	0.75	-0.91	-0.48	-0.25	0.0	0.01	0.02 (0.55)
Incl. (deg.)	0.33	-0.82	-3.32	-9.49	-4.05	-3.74	-2.92	-8.56	22.63	2.76	6.8 (5.4)
Tip (deg.)	2.72	3.33	-0.37	4.49	2.84	3.49	-1.52	6.97	0.03	0.0	0.3 (5)

Table 26S. d(ApApA) duplex's backbone torsions in both strands (R/Y), and mean values for the torsion angles taken from MD sequence-averaged and experimental studies along with their standard deviations (within parenthesis).

Angle	Gas models		PCM models		Ideal structure [a]		Molecular Dynamics [b]	Experiment [c]	
	Model 1	Model 2	Model 3	Model 4	A-DNA	B-DNA		BI	BII
α	15.8/ -61.4	11.8/ 19.7	-56.3/ -64.5	-65.5/ -61.5	-51.7	-29.9	-72.6 (15.7)	-62 (15)	-
β	92.1/ -176.9	92.3/ 96.9	136.7/ -166.7	-166.8/ -179.0	174.8	136.3	169.6 (16.2)	176 (9)	146 (8)
γ	43.8/ 57.8	46.6/ 42.4	55.4/ 52.5	55.2/ 58.5	41.7	31.2	54.8 (14.1)	48 (11)	-
δ	136.9/ 146.7	136.4/ 132	145.7/ 139.7	147.6/ 139.8	79.1	143.3	125.4 (19.1)	128 (13)	144 (7)
ε	-167.7/ -173.1	-168.3/ -166.3	172.9/ 177.6	162.1/ 171.3	-147.8	-140.8	-162.6 (33.3)	-176 (11)	-114 (15)
ζ	167.8/ 178.6	170.2/ 170.9	-102.3/ -98.7	-96.6/ -100.9	-75.1	-160.5	-102.8 (47.6)	-95 (10)	174 (14)
χ	-102.5/ -109.3	-104.2/ -112.4	-109.3/ -108.8	-105.6/ -107.0	-157.2	-98.0	-116 (19.5)	-102 (14) / -119 (8)	-89 (8)
Phase angle	144.1/ 159.8	140.0/ 135.0	166.4/ 159.0	177.2/ 159.9	8.0	153.9	136.7 (33.6)	144 (30)	-

[a] Obtained using comprehensive software package 3DNA.

[b] The conformational parameters averaged over the 39 oligomers and corresponds to a total of 19.5 million data points for each parameter. Simulations were run with 150 mM KCl using the AMBER suite of programs with the parmbsc0 modifications to the parm99 force field.

[c] The sample of 34 B-DNAs with reported resolutions between 0.7 and 3.3 Å taken from the Nucleic Acid Database was interrogated using the NDBQuery interface program. The mean values for the torsion angles were calculated in ranges determined from the scattergrams.

Table 27S. d(GpGpG) duplex's backbone torsions in both strands (R/Y), and mean values for the torsion angles taken from MD sequence-averaged and experimental studies along with their standard deviations (within parenthesis).

Angle	Gas models		PCM models		Ideal structure [a]		Molecular Dynamics [b]	Experiment [c]	
	Model 1	Model 2	Model 3	Model 4	A-DNA	B-DNA		BI	BII
α	-58.5/ -63.3	22.3/ 6.5	-66.4/ -74.9	-72.5/ -60.8	-51.7	-29.9	-72.6 (15.7)	-62 (15)	-
β	-176.6/ 127.1	93.3/ 90.1	172.0/ 134.0	169.0/ -174.2	174.8	136.3	169.6 (16.2)	176 (9)	146 (8)
γ	61.4/ 59.6	46.2/ 47.3	43.7/ 52.0	43.0/ 54.4	41.7	31.2	54.8 (14.1)	48 (11)	-
δ	159.3/ 142.1	138.9/ 137.4	140.5/ 142.0	140.7/ 138.8	79.1	143.3	125.4 (19.1)	128 (13)	144 (7)
ε	-69.1/ 166.3	-137.6/ -167.8	-93.1/ -168.2	-146.7/ 172.7	-147.8	-140.8	-162.6 (33.3)	-176 (11)	-114 (15)
ζ	132.1/ -96.8	174.8/ -164.3	158.8/ -130.5	-177.9/ -103.3	-75.1	-160.5	-102.8 (47.6)	-95 (10)	174 (14)
χ	-100.5/ -104.7	-85.2/ -76.8	-86.8/ -95.3	-84.6/ -105.8	-157.2	-98.0	-116 (19.5)	-102 (14) / -119 (8)	-89 (8)
Phase angle	182.9/ 172.2	141.8/ 139.4	145.3/ 154.3	145.2/ 164.9	8.0	153.9	136.7 (33.6)	144 (30)	-

[a] Obtained using comprehensive software package 3DNA.

[b] The conformational parameters averaged over the 39 oligomers and corresponds to a total of 19.5 million data points for each parameter. Simulations were run with 150 mM KCl using the AMBER suite of programs with the parmbsc0 modifications to the parm99 force field.

[c] The sample of 34 B-DNAs with reported resolutions between 0.7 and 3.3 Å taken from the Nucleic Acid Database was interrogated using the NDBQuery interface program. The mean values for the torsion angles were calculated in ranges determined from the scattergrams.

Table 28S. The angle of pseudorotation of sugar ring (P) and the main chain torsion angles (in the 5′→3′ direction) obtained in different models for optimized reference structures of trideoxyribonucleotide diphosphates [a].

Angles	$d(A)_3$			
	Gas models		PCM models	
	Model 1	Model 2	Model 3	Model 4
α	+sp	+sp	-sc	-sc
β	+ac	+ac	+ac	+ac
γ	+sc	+sc	+sc	+sc
δ	+ac	+ac	+ac	+ac
ε	-ap	-ap	+ap	+ap
ζ	-sc	+ap	-sc	-ac
χ	-ac	-ac	-ac	-ac
P	C2′-endo	C2′-endo	C2′-endo	C2′-endo
form	B-DNA	B-DNA	B-DNA	B-DNA
	$d(G)_3$			
α	-sc	+sp	-sc	-sc
β	-ap	+ac	+ap	-ap
γ	+sc	+sc	+sc	-ap
δ	+ap	+ac	+ac	+ap
ε	-sc	-ap	+ac	-ap
ζ	+ac	-ap	-sc	-sc
χ	-ac	-ac	-ac	-ac
P	C2′-endo	C2′-endo	C2′-endo	C2′-endo
form	B-DNA	B-DNA	B-DNA	B-DNA

$d(T)_3$			
Gas models		PCM models	
Model 1	Model 2	Model 3	Model 4
-sc	+sp	+sp	+sc
+ap	+ac	+ac	+sc
+sc	+sc	+sc	+sc
+ac	+ac	+ac	+ac
-ap	-ap	-ap	+ap
+ap	+ap	+ap	-sc
-ac	-ac	-ac	-ac
C2′-endo	C2′-endo	C2′-endo	C2′-endo
B-DNA	B-DNA	B-DNA	B-DNA
$d(C)_3$			
-sc	+sp	-sc	-sc
+ac	+ac	-ap	+ac
+sc	+sc	+sc	+sc
+ap	+ac	+ac	+ac
+ap	+ap	+ap	+ap
-sc	-ac	-ac	-ac
-ac	-sc	-ac	-ac
C2′-endo	C2′-endo	C2′-endo	C2′-endo
B-DNA	B-DNA	B-DNA	B-DNA

[a] For reference, in practice, torsion angles are often not known exactly, but can be assigned to particular conformational regions. The Klyne-Prelog notation of torsion angle ranges characterize the B-DNA conformational forms of polynucleotides obtained from fiber diffraction measurements are the followings: α (-sc),β (+ac to -ap), γ (+sc),δ (+sc to +ap), ε (+ap to -ac), ζ (-ac to –sc and +ap to -ap), χ (-ac to -sc). For the majority of angles, we can assume that the conformational ranges obtained for trideoxyribonucleotide diphosphates fit B-DNA conformational form of polynucleotide.