

Supplementary Materials

Structural and Energetic Properties of the Potential HIV-1 Reverse Transcriptase Inhibitors d4A and d4G: a Comprehensive Theoretical Investigation

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Methodological details

Conformational analysis

To obtain full conformational families for d4A and d4G, initial structures were generated and optimized by combining three possible values (gauche⁺, gauche⁻ and trans) for each of the β and γ torsion angles and four values for the χ angle (syn, anti, high-syn, high-anti). The detailed procedure is as follows:

(a) First, d4A and d4G structures corresponding to X-ray crystallographic data (Hutcheon & James 1974; van Roey & Chu 1992) were created and optimized with Gaussian at the B3LYP/6-31G(d,p) level of theory.

(b) The optimized structures were multiplied by changing a single torsion angle – β and γ in 120° steps and χ between syn, anti, high-syn and high-anti regions. The resulting structures were subsequently optimized by the same method.

(c) The newly-obtained equilibrium structures were checked for uniqueness; any new conformers were subjected to the procedure described in step (b).

Steps (b) and (c) were repeated continuously until no new conformers were obtained. After this, the conformational family of molecule was assumed to be complete. This procedure is implemented in an in-house software program.

To confirm the stationary points as local minima on the d4A and d4G energy landscapes and to calculate Gibbs free energies, harmonic vibrational frequencies were computed at the same level of theory (using Gaussian's OPT and FREQ keywords). The absence of imaginary frequencies confirmed the optimized conformations to be true minima on the potential energy surface. Relative Gibbs free energies (ΔG) were obtained as sums of the MP2/6-311++G(d,p) electronic energies and the zero-point energies, thermal corrections, and entropy contributions calculated at the B3LYP/6-31G(d,p) level of theory.

Identification and characterization of non-covalent intramolecular interactions

Specific closed-shell intramolecular interactions were identified using analysis based on Bader's quantum theory of atoms in molecules (QTAIM) (Bader 1990), implemented in the AIMAll program package (Keith 2011). The QTAIM analysis employed the equilibrium geometry wavefunctions calculated at the B3LYP/6-31G(d,p) level. The presence of a bond critical point (BCP, the so-called (3,-1) type) as well as a positive value of the Laplacian of the density at the BCP, were considered as indicators of a closed-shell interaction (Matta, Castillo & Boyd 2006). Moreover, potential H-bond contacts were verified by additional geometric and QTAIM criteria (Koch & Popelier 1995). The energies of the closed-shell interactions were subsequently evaluated by two methods: the Espinosa-Molins-Lecomte (EML) method (Espinosa, Molins & Lecomte 1998) and the compliance constants formalism (Grunenberg 2004; Brandhorst & Grunenberg 2008; Brandhorst & Grunenberg 2010). The EML method is based on the electron density distribution at the BCP:

$$E_{HB} = 0.5 V(r), \quad [1]$$

where $V(r)$ is the value of the local potential energy at the critical point. Compliance constants measure the displacement of an internal coordinate resulting from a unit force acting on it. The

physical meaning of compliance constants comes from their definition as partial second derivatives of the potential energy due to an external force:

$$C_{ij} = \partial^2 E / \partial f_i \partial f_j . \quad [2]$$

The H...B distances (where B is the H-bond acceptor) were used as internal coordinates for the calculation of the C_{ij} constants. For the hydrogen-hydrogen bonds, the distance between the two hydrogen atoms, H...H, were used as the internal coordinates. In contrast to force constants, the numerical values of compliance constants do not depend on the coordinate system. As follows from equation [2], a lower numerical value of compliance constant implies a stronger bond. The compliance constants were calculated using the Compliance 3.0.2 program (Brandhorst & Grunenberg 2008; Brandhorst & Grunenberg 2010). The energies of the OH...N and NH...O H-bonds were also evaluated by Iogansen's empirical formula (Iogansen 1981) (which can only be applied to conventional H-bonds):

$$E_{HB} = 0.33 (\Delta\nu - 40)^{1/2} , \quad [3]$$

where E_{HB} is the H-bond energy change in kcal/mol and $\Delta\nu$ is the frequency red shift of the $\nu(\text{OH})$ stretching mode (in cm^{-1}). Structurally close conformers without H-bonds (d4A: conformer 21; d4G: conformers 11 and 20) were taken as reference molecules.

The electronic nature of the specific intramolecular interactions (including H-bonds) was analyzed with Natural Bond Orbital (NBO) analysis, which interprets the electronic wavefunction in terms of occupied Lewis and unoccupied non-Lewis localized orbitals (Weinhold & Landis 2005). A second-order Fock matrix analysis was carried out to evaluate the interaction between donor (i) and acceptor (j) bonds. Such a donor-acceptor interaction results in a migration of the electron density from the idealized Lewis structure into an empty non-Lewis orbital σ^* . The stabilization energy of a donor-acceptor pair is:

$$E^{(2)} = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\varepsilon_j - \varepsilon_i} , \quad [4]$$

where q_i is the occupancy of the donor orbital, ε_j and ε_i are diagonal elements and $F(i,j)$ is the off-diagonal element of the NBO Fock matrix.

Natural Bond Order (NBO) results

The NBO results of the specific intramolecular interactions in d4A and d4G are listed in Tables SIII and SIV, respectively. For the NH...O, OH...N and CH...O H-bonds hyperconjugative interactions between the oxygen lone pair and the antibonding orbital of the donor group ($\text{BD}^*(\text{XH})$; where $\text{X}=\text{O}, \text{N}$ or C), were observed (denoted $\text{LP}(\text{O})\text{-BD}^*(\text{XH})$ in Tables SIII and SIV). Similar hyperconjugative interactions were observed for the OH...N and CH...O H-bonds in d4T, d4U and d4C (Ponomareva, Yurenko, Zhurakivsky, van Mourik & Hovorun 2012; Ponomareva, Yurenko, Zhurakivsky, van Mourik & Hovorun 2013). The strengths of these interactions are described by the stabilization energy $E(2)$ (Eq. [4]), which ranges from 0.06 to 20.8 kcal/mol for d4A and from 0.05 to 29.2 kcal/mol for d4G. NBO analysis shows completely different donor-acceptor interactions for the $\text{C8H}\cdots\text{H2C5'}/\text{H1C5'}$ dihydrogen contacts: the electron density migrates from the antibonding

orbital BD(1)*C5'H2 or BD(1)*C5'H1 to the bonding orbital BD(1)C8H. Similar donor-acceptor interactions between antibonding and bonding orbitals are observed for the O5'H...C8 contacts.

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Table SI. Geometric, energetic and electron-topological characteristics of the specific intramolecular contacts in the d4A conformers

conf.	$\chi/\beta/\gamma$	H-bond	d(A...B) ^a	d(H...B) ^b	$\angle AHB^c$	ρ^d	$\nabla^2 \rho^e$	100· ϵ^f	d(BCP-RCP) ^g	E _{HB} ^h	C _{ij} ⁱ
1	syn/g ⁺ /g ⁺	O5'H...N3	2.848	1.867	174.9	0.036	0.087	4	1.149	7.38	4.211
2	anti/g ⁺ /g ⁺	C8H...O5'	3.294	2.586	122.3	0.008	0.031	83	0.986	1.60	19.582
3	syn/g ⁻ /t	C5'H1...N3	3.571	2.614	145.1	0.009	0.025	1	0.973	1.58	21.479
4	anti/g ⁻ /t	C8H...H1C5'	3.341	2.641	121.9	0.003	0.010	8	0.567	0.37	52.226
5	anti/t/g ⁺	C8H...O5'	3.305	2.326	149.7	0.013	0.039	5	0.988	3.05	13.071
6	anti/g ⁺ /g ⁺	O5'H...C8	3.790	2.849	164.6	0.004	0.016	89	0.256	0.63	39.617
		C2'H...N3	3.141	2.613	109.3	0.010	0.033	36	0.604	1.71	12.062
7	anti/t/g ⁻	C8H...H2C5'	3.413	2.711	122.3	0.003	0.009	12	0.494	0.32	40.394
8	syn/t/g ⁻	C5'H2...N3	3.541	2.586	145.0	0.010	0.027	2	0.990	1.69	19.740
9	anti/g ⁻ /g ⁺	C8H...O5'	3.306	2.301	153.7	0.014	0.040	5	0.943	3.27	10.992
10	anti/g ⁻ /g ⁻	C8H...H2C5'	3.463	2.744	123.8	0.002	0.008	21	0.422	0.29	55.736
11	anti/t/g ⁻	C2'H...N3	3.218	2.723	107.5	0.008	0.027	58	0.457	1.37	23.869
12	syn/g ⁻ /g ⁻	C5'H2...N3	3.522	2.586	143.2	0.009	0.027	1	0.979	1.67	20.096
13	syn/g ⁺ (90)/g ⁻	C5'H2...N3	3.531	2.560	147.2	0.010	0.028	3	1.007	1.79	18.636
14	anti/t/t	C2'H...N3	3.269	2.818	105.0	0.007	0.024	131	0.279	1.17	21.464
15	anti/g ⁻ /g ⁻	C2'H...N3	3.229	2.737	107.4	0.008	0.027	62	0.432	1.33	29.722
16	anti/t/t	C8H...H1C5'	3.350	2.674	120.1	0.003	0.009	11	0.496	0.35	59.655
17	anti/g ⁺ /g ⁻	C8H...H2C5'	3.408	2.699	122.7	0.003	0.009	10	0.506	0.33	51.726
18	anti/g ⁺ /t	no closed-shell intramolecular interactions									
19	anti/g ⁺ /g ⁻	C2'H...N3	3.188	2.689	107.6	0.008	0.029	50	0.507	1.47	23.467
20	anti/g ⁺ /t	C8H...H1C5'	3.490	2.743	126.0	0.002	0.008	29	0.397	0.28	59.654

^a Distance between the donor (A) and acceptor (B) atoms, Å; ^b Distance between the hydrogen (H) and B atoms, Å (for putative H-bonds); ^c H-bond angle (for putative H-bonds), degree; ^d Electron density value at the BCP, a.u.; ^e Laplacian of the electron density value at the BCP, a.u.; ^f Ellipticity at the BCP; ^g Distance from the BCP to the nearest ring critical point (RCP, the so-called (3,+1) point). ^h Interaction energy, calculated by Eq. [1], kcal/mol. ⁱ Compliance constant, Å/mDyn.

Table SII. Geometric, energetic and electron-topological characteristics of the specific intramolecular contacts in the d4G conformers

conf.	$\chi/\beta/\gamma$	H-bond	d(A...B) ^a	d(H...B) ^b	$\angle AHB^c$	ρ^d	$\nabla^2 \rho^e$	100· ϵ^f	d(BCP-RCP) ^g	E _{HB} ^h	C _{ij} ⁱ
1	syn/g ⁺ /g ⁺	N2H1...O5'	3.234	2.398	139.1	0.010	0.036	57	0.490	2.21	10.743
		O5'H...N3	2.738	1.766	167.5	0.045	0.109	5	1.064	10.11	3.047
2	anti/g ⁺ /g ⁺	C8H...O5'	3.319	2.634	120.7	0.008	0.030	132	0.964	1.42	20.806
3	anti/g ⁻ /t	C8H...H1C5'	3.327	2.672	118.6	0.003	0.010	7	0.530	0.36	47.055
4	anti/t/g ⁺	C8H...O5'	3.295	2.345	145.7	0.013	0.038	7	1.045	2.93	12.750
5	anti/t/g ⁻	C8H...H2C5'	3.335	2.713	116.2	0.003	0.009	5	0.494	0.34	31.394
6	syn/g ⁻ /t	C5'H1...N3	3.614	2.673	143.3	0.008	0.024	1	0.947	1.41	23.013
7	anti/g ⁺ /g ⁺	O5'H...C8	3.657	2.727	161.4	0.006	0.019	26	0.536	0.81	31.130
		C2'H...N3	3.161	2.660	107.6	0.009	0.031	43	0.548	1.56	15.750
8	anti/g ⁻ /g ⁻	C8H...H2C5'	3.448	2.786	119.4	0.002	0.008	24	0.360	0.28	30.211
9	syn/t/g ⁻	C5'H2...N3	3.684	2.751	142.5	0.007	0.020	3	0.898	1.16	31.485
10	anti/t/t	C8H...H1C5'	3.286	2.696	113.9	0.003	0.010	10	0.499	0.36	59.723
11	syn/g ⁻ /g ⁻	C5'H2...N3	3.548	2.606	144.0	0.009	0.026	1	0.956	1.62	21.880
12	anti/g ⁺ /g ⁻	C8H...H2C5'	3.369	2.747	116.4	0.003	0.008	5	0.481	0.32	64.317
13	anti/g ⁻ /g ⁺	C8H...O5'	3.318	2.312	154.0	0.014	0.039	5	0.951	3.19	10.818
14	syn/g ⁻ /t	O5'H...N3	2.826	2.000	140.8	0.028	0.074	8	0.872	6.31	9.620
		N2H1...O5'	3.284	2.414	143.2	0.010	0.034	30	0.574	2.31	10.598
15	anti/t/t	C8H...H1C5'	3.055	2.611	103.8	0.004	0.016	41	0.223	0.58	34.348
		C2'H...N3	3.281	2.854	103.5	0.006	0.024	464	0.100	1.14	19.707
16	anti/g ⁺ /g ⁻	no closed-shell intramolecular interactions									
17	syn/g ⁺ /g ⁻	C5'H2...N3	3.608	2.658	144.5	0.008	0.024	2	0.967	1.45	25.643
18	anti/g ⁺ /t	C8H...H1C5'	3.605	2.747	144.5	0.002	0.008	17	0.423	0.29	60.997
19	anti/g ⁺ /t	C8H...H1C5'	3.130	2.635	107.3	0.004	0.015	441	0.045	0.55	35.720
		C8H...O5'	3.856	2.911	146.3	0.004	0.016	183	0.109	0.66	75.497
20	syn/g ⁺ /t	C5'H1...N3	3.580	2.628	145.2	0.009	0.025	2	0.958	1.52	22.077
21	syn/g ⁺ /g ⁺	N2H1...O5'	3.234	2.398	139.1	0.010	0.036	57	0.490	2.21	10.743

^a See footnote, Table SI.

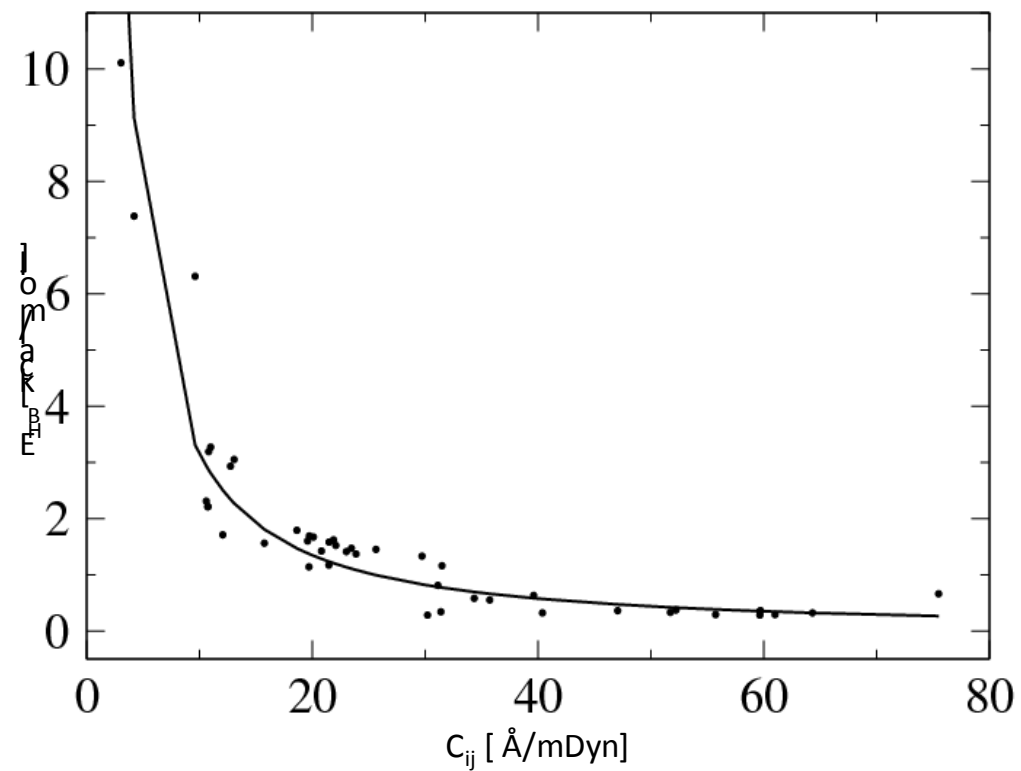


Figure S1: Correlation between the energy E_{HB} (in kcal/mol) of the specific intramolecular interactions, calculated using formula (2) and the compliance constant values C_{ij} (in Å/mDyn).

Table SIII. NBO analysis of donor-acceptor interactions in d4A through specific intramolecular contacts^a

conf.	$\chi/\gamma/\beta$	H-interaction	acceptor-donor NBOs	E(2)	Occupancy of donor NBO	Energy of donor NBO	Occupancy of acceptor NBO	Energy of acceptor NBO
1	syn/g ⁺ /g ⁺	O5'H...N3	LP(1) _{N3} – BD(1)* _{O5'H}	20.81	1.88176	-0.36057	0.05311	0.49916
2	anti/g ⁺ /g ⁺	C8H...O5'	LP(2) _{O5'} – BD(1)* _{C8H}	0.57	1.95036	-0.29583	0.02213	0.48064
3	syn/g ⁻ /t	C5'H1...N3	LP(1) _{N3} – BD(1)* _{C5'H1}	1.48	1.91046	-0.34887	0.02994	0.47730
4	anti/g ⁻ /t	C8H...H1C5'	BD(1) _{C8H} – BD(1)* _{C5'H1}	0.09	1.98458	-0.56764	0.03090	0.43261
5	anti/t/g ⁺	C8H...O5'	LP(1) _{O5'} – BD(1)* _{C8H}	1.30	1.97820	-0.58952	0.02611	0.50592
			LP(2) _{O5'} – BD(1)* _{C8H}	2.38	1.95606	-0.32759		
6	anti/g ⁺ /g ⁺	O5'H...C8	BD(1) _{C8H} – BD(1)* _{O5'H}	0.09	1.98470	-0.56407	0.01311	0.46703
		C2'H...N3	LP(1) _{N3} – BD(1)* _{C2'H}	0.83	1.91263	-0.35151	0.01549	0.49309
7	anti/t/g ⁻	C8H...H2C5'	BD(1) _{C8H} – BD(1)* _{C5'H2}	0.07	1.98462	-0.56293	0.02822	0.43515
8	syn/t/g ⁻	C5'H2...N3	LP(1) _{N3} – BD(1)* _{C5'H2}	1.69	1.91012	-0.34635	0.02687	0.47911
9	anti/g ⁻ /g ⁺	C8H...O5'	LP(1) _{O5'} – BD(1)* _{C8H}	1.27	1.97779	-0.60287	0.02760	0.50539
			LP(2) _{O5'} – BD(1)* _{C8H}	2.76	1.94927	-0.30889		
10	anti/g ⁻ /g ⁻	C8H...H2C5'	BD(1) _{C8H} – BD(1)* _{C5'H2}	0.06	1.98462	-0.56322	0.01932	0.45150
11	anti/t/g ⁻	C2'H...N3	LP(1) _{N3} – BD(1)* _{C2'H}	0.48	1.91337	-0.34794	0.01495	0.49348
12	syn/g ⁻ /g ⁻	C5'H2...N3	LP(1) _{N3} – BD(1)* _{C5'H2}	1.68	1.91016	-0.34492	0.02159	0.49450
13	syn/g ⁺ g ⁻ ^b	C5'H2...N3	LP(1) _{N3} – BD(1)* _{C5'H2}	1.69	1.91049	-0.34977	0.02460	0.47956
14	anti/t/t	C2'H...N3	LP(1) _{N3} – BD(1)* _{C2'H}	0.31	1.91371	-0.34748	0.01432	0.48832
15	anti/g ⁻ /g ⁻	C2'H...N3	LP(1) _{N3} – BD(1)* _{C2'H}	0.45	1.91344	-0.34835	0.01481	0.49165
16	anti/t/t	C8H...H1C5'	BD(1) _{C8H} – BD(1)* _{C5'H1}	0.08	1.98467	-0.56354	0.02613	0.43449
17	anti/g ⁺ /g ⁻	C8H...H2C5'	BD(1) _{C8H} – BD(1)* _{C5'H2}	0.07	1.98468	-0.56624	0.02474	0.43402
18	anti/g ⁺ /t	no closed-shell interactions						
19	anti/g ⁺ /g ⁻	C2'H...N3	LP(1) _{N3} – BD(1)* _{C2'H}	0.58	1.91326	-0.35068	0.01507	0.48834
20	anti/g ⁺ /t	C8H...H1C5'	BD(1) _{C8H} – BD(1)* _{C5'H1}	0.06	1.98469	-0.56275	0.01958	0.45162

^a LP: orbital that corresponds to the electron lone pair; BD: bonding orbital; BD^{*}: antibonding orbital; E⁽²⁾: stabilization energy, defined by formula (3), in kcal/mol. ^b The γ angle is 90°.

Table SIV. NBO analysis of donor-acceptor interactions in d4G through specific intramolecular contacts^a

conf.	$\chi/\gamma/\beta$	H-interaction	acceptor-donor NBOs	E(2)	Occupancy of donor NBO	Energy of donor NBO	Occupancy of acceptor NBO	Energy of acceptor NBO
1	syn/g ⁺ /g ⁺	N2H1...O5'	LP(1) _{O5'} – BD*(1) _{N2-H1}	0.51	1.97267	-0.54052	0.01348	0.46190
			LP(2) _{O5'} – BD*(1) _{N2-H1}	1.21	1.94486	-0.28179	0.01348	0.46190
2	anti/g ⁺ /g ⁺	O5'H...N3	LP(1) _{N3} – BD*(1) _{O5'-H'}	29.18	1.85352	-0.36455	0.06971	0.47136
		C8H...O5'	LP(1) _{O5'} – BD*(1) _{C8-H}	0.21	1.98029	-0.59347	0.02203	0.48739
			LP(2) _{O5'} – BD*(1) _{C8-H}	0.46	1.95017	-0.29287	0.02203	0.48739
3	anti/g ⁻ /t	C8H...H1C5'	BD(1) _{C5'-H1'} – BD*(1) _{C8-H}	0.08	1.98756	-0.51302	0.02110	0.47605
			BD(1) _{C8-H} – BD*(1) _{C5'-H1'}	0.08	1.98448	-0.55910	0.03025	0.43701
4	anti/t/g ⁺	C8H...O5'	LP(1) _{O5'} – BD*(1) _{C8-H}	1.17	1.97894	-0.58642	0.02566	0.51193
			LP(2) _{O5'} – BD*(1) _{C8-H}	2.10	1.95492	-0.32143	0.02566	0.51193
5	anti/t/g ⁻	C8H...H2C5'	no donor-acceptor interactions					
6	syn/g ⁻ /t	C5'H1...N3	LP(1) _{N3} – BD*(1) _{C5'-H1'}	1.22	1.89271	-0.35908	0.03150	0.45790
7	anti/g ⁺ /g ⁺	O5'H...C8	BD(2) _{C8-N7} – BD*(1) _{O5'-H'}	0.40	0.33342	0.01451	0.01302	0.46878
		C2'H...N3	LP(1) _{N3} – BD*(1) _{C2'-H'}	0.62	1.89612	-0.36243	0.01533	0.48400
8	anti/g ⁻ /g ⁻	C8H...H2C5'	BD(1) _{C8-H} – BD*(1) _{C5'-H2'}	0.05	1.98449	-0.55477	0.01911	0.45555
9	syn/t/g ⁻	C5'H2...N3	LP(1) _{N3} – BD*(1) _{C5'-H2'}	0.87	1.89272	-0.35544	0.02901	0.45762
10	anti/t/t	C8H...H1C5'	BD(1) _{C8-H} – BD*(1) _{C5'-H1'}	0.08	1.98455	-0.55543	0.02491	0.43933
11	syn/g ⁻ /g ⁻	C5'H2...N3	LP(1) _{N3} – BD*(1) _{C5'-H2'}	1.45	1.89217	-0.35485	0.02233	0.47721
12	anti/g ⁺ /g ⁻	C8H...H2C5'	BD(1) _{C8-H} – BD*(1) _{C5'-H2'}	0.07	1.98454	-0.55793	0.02382	0.43861
13	anti/g ⁻ /g ⁺	C8H...O5'	LP(1) _{O5'} – BD*(1) _{C8-H}	1.24	1.97782	-0.60043	0.02747	0.51340
			LP(2) _{O5'} – BD*(1) _{C8-H}	2.61	1.94902	-0.30535	0.02747	0.51340
14	syn/g ⁻ /t	O5'H...N3	LP(1) _{N3} – BD*(1) _{O5'-H'}	10.79	1.87684	-0.36219	0.03902	0.46263
		N2H1...O5'	LP(1) _{O5'} – BD*(1) _{N2-H1}	0.06	1.97936	-0.56712	0.01670	0.46120
			LP(2) _{O5'} – BD*(1) _{N2-H1}	2.39	1.93701	-0.29552	0.01670	0.46120
15	anti/t/t	C8H...H1C5'	BD(1) _{C8-H} – BD*(1) _{C5'-H1'}	0.06	1.98451	-0.54501	0.02665	0.43689
		C2'H...N3	LP(1) _{N3} – BD*(1) _{C2'-H'}	0.24	1.89697	-0.35861	0.01440	0.48014
16	anti/g ⁺ /g ⁻	no closed-shell interactions						
17	syn/g ⁺ /g ⁻	C5'H2...N3	LP(1) _{N3} – BD*(1) _{C5'-H2'}	1.26	1.89276	-0.35936	0.02684	0.45964

Table SIV. Continued

18	anti/g ⁺ /t	C8H...H1C5'	BD(1) _{C8-H} – BD*(1) _{C5'-H1'}	0.06	1.98457	-0.55459	0.01926	0.45605
19	anti/g ⁺ /t	C8H...H1C5'	BD(1) _{C8-H} – BD*(1) _{C5'-H1'}	0.05	1.98441	-0.54204	0.01890	0.45308
		C8H...O5' ^b	LP(1) _{O5'} – BD*(1) _{C8-H}	0.13	1.97947	-0.59458	0.02076	0.50428
			LP(2) _{O5'} – BD*(1) _{C8-H}	0.14	1.95229	-0.29835	0.02076	0.50428
20	syn/g ⁺ /t	C5'H1...N3	LP(1) _{N3} – BD*(1) _{C5'-H1'}	1.36	1.89267	-0.35549	0.02261	0.47609

^a LP: orbital that corresponds to the electron lone pair; BD: bonding orbital; BD* : antibonding orbital; E⁽²⁾: stabilization energy, defined by formula (3), in kcal/mol. ^b Bifurcated contacts.

Table SV. QTAIM atomic characteristics (charge q, dipolar polarization M, volume V, energy E and radius r) of the hydrogen atoms involved in C8H...1H/2C5' non-covalent interactions in d4A. Wavefunctions were calculated at the B3LYP/6-31G(d,p) level of theory.

conf.	$\chi / \beta / \gamma$	q(C8H)	q(C5'H1/2)	M(C8H)	M(C5'H1/2)	V(C8H)	V(C5'H1/2)	E(C8H)	E(C5'H1/2)	r(C8H)	r(C5'H1/2)
4	anti/g ⁻ /t	0.062	-0.019	0.127	0.149	46.9	51.8	-0.605	-0.641	2.508	2.514
7	anti/t/g ⁻	0.067	-0.014	0.130	0.152	46.9	51.6	-0.602	-0.639	2.575	2.579
10	anti/g ⁻ /g ⁻	0.064	0.014	0.127	0.143	47.2	49.4	-0.603	-0.630	2.617	2.608
16	anti/t/t	0.054	-0.018	0.125	0.143	47.4	51.4	-0.608	-0.642	2.554	2.531
17	anti/g ⁺ /g ⁻	0.057	-0.017	0.127	0.146	47.6	51.5	-0.607	-0.641	2.564	2.565
20	anti/g ⁺ /t	0.064	0.014	0.128	0.139	47.5	49.2	-0.604	-0.631	2.609	2.612
	MIN	0.054	-0.019	0.125	0.139	46.9	49.2	-0.608	-0.642	2.508	2.514
	MAX	0.067	0.014	0.13	0.152	47.6	51.8	-0.602	-0.630	2.617	2.612

^a MIN and MAX: minimal and maximal values for different parameters. All quantities are in atomic units.

Table SVI. QTAIM atomic characteristics (charge q, dipolar polarization M, volume V, energy E and radius r) of the hydrogen atoms involved in C8H...1H/2C5' non-covalent interactions in d4G. Wavefunctions were calculated at the B3LYP/6-31G(d,p) level of theory.

conf.	$\chi / \beta / \gamma$	q(C8H)	q(C5'H1/2)	M(C8H)	M(C5'H1/2)	V(C8H)	V(C5'H1/2)	-E(C8H)	-E(C5'H1/2)	r(C8H)	r(C5'H1/2)
3	(anti/g ⁻ /t	0.057	-0.018	0.126	0.147	47.1	51.4	-0.607	-0.641	2.561	2.528
5	(anti/t/g ⁻	0.056	-0.011	0.126	0.149	47.0	51.1	-0.607	-0.638	2.618	2.553
8	(anti/g-/g-	0.060	0.017	0.127	0.141	46.9	49.1	-0.605	-0.629	2.688	2.631
10	anti/t/t	0.054	-0.003	0.127	0.147	47.1	50.3	-0.608	-0.635	2.622	2.522
12	anti/g ⁺ /g ⁻	0.054	-0.010	0.127	0.146	47.2	50.8	-0.608	-0.638	2.650	2.583
15	anti/t/t	0.086	-0.007	0.113	0.142	42.6	49.3	-0.598	-0.638	2.576	2.440
18	anti/g ⁺ /t	0.054	0.023	0.126	0.140	47.3	48.8	-0.608	-0.627	2.649	2.589
19	anti/g ⁺ /t	0.102	0.015	0.113	0.132	41.5	47.6	-0.590	-0.632	2.521	2.544
	MIN	0.054	-0.018	0.113	0.132	41.5	47.6	-0.608	-0.641	2.521	2.440
	MAX	0.102	0.023	0.127	0.149	47.3	51.4	-0.59	-0.627	2.688	2.631

^a MIN and MAX: minimal and maximal values for different parameters. All quantities are in atomic units.

Table SVII. Cartesian coordinates (in Å) of the 21 d4A conformers located in this work (listed in decreasing order of stability)

d4A 1	X	Y	Z	d4A 2	X	Y	Z
C	-1.357874	-1.543755	-0.029753	C	-1.219659	-1.101088	0.278673
C	-2.021959	-1.203744	1.282321	C	-2.124135	-0.969168	1.477032
C	-3.050889	-0.393676	1.056409	C	-3.343219	-0.614800	1.083675
C	-3.160213	-0.083366	-0.410882	C	-3.398978	-0.513982	-0.415754
O	-2.015624	-0.755390	-0.996630	O	-2.047584	-0.780152	-0.842200
H	-1.460301	-2.614421	-0.271447	H	-0.798244	-2.104606	0.145557
H	-1.682507	-1.604095	2.229832	H	-1.774794	-1.139809	2.488014
H	-3.724949	0.021838	1.795356	H	-4.203664	-0.437490	1.718623
H	-4.065993	-0.530350	-0.852169	H	-4.060854	-1.291977	-0.830514
C	-3.143569	1.415207	-0.742226	C	-3.838850	0.841119	-0.985229
H	-4.164176	1.798483	-0.613807	H	-4.821202	1.107166	-0.580316
H	-2.893991	1.512080	-1.812503	H	-3.943087	0.746250	-2.076173
O	-2.309914	2.175569	0.090178	O	-2.946743	1.883964	-0.641872
H	-1.406216	1.788261	0.073912	H	-2.100555	1.656136	-1.052952
N	2.651771	1.818718	0.171745	N	3.865452	-0.671522	-0.455834
C	0.792487	-0.121038	0.038251	C	1.239815	-0.563983	0.027625
C	2.139065	-0.489378	-0.057269	C	1.978703	0.608991	0.202896
C	3.085933	0.553793	0.020312	C	3.361641	0.511228	-0.058891
N	4.416782	0.322286	-0.037788	N	4.203345	1.562177	0.096871
H	4.751056	-0.599425	-0.267004	H	3.819172	2.481156	0.245395
H	5.039675	1.112250	-0.087882	H	5.148130	1.465808	-0.239282
N	2.281756	-1.854063	-0.231447	N	1.170278	1.658294	0.608196
N	0.090059	-1.307845	-0.071956	N	-0.061625	-0.218927	0.345969
C	1.048676	-2.293001	-0.240674	C	-0.026575	1.128136	0.681478
H	0.756996	-3.328005	-0.364602	H	-0.930409	1.652486	0.960642
C	1.331533	2.029497	0.242171	C	3.026578	-1.713721	-0.574425
N	0.338375	1.134099	0.185672	N	1.708469	-1.758003	-0.354413
H	1.024380	3.066341	0.356396	H	3.486754	-2.646134	-0.894415

d4A 3	X	Y	Z
C	1.173821	-1.098715	-0.278980
C	2.032393	-1.185102	-1.516026
C	3.260927	-0.749841	-1.247311
C	3.359446	-0.332743	0.192203
O	2.040164	-0.575181	0.727571
H	0.775018	-2.064601	0.052887
H	1.653307	-1.556864	-2.460342
H	4.093668	-0.697580	-1.939398
H	4.068469	-0.958672	0.753844
C	3.721439	1.135639	0.432606
H	3.045553	1.772930	-0.160709
H	4.746244	1.326505	0.095257
O	3.671457	1.452320	1.807994
H	2.788685	1.194443	2.111943
N	-3.855462	-0.561652	0.702048
C	-1.272049	-0.535662	0.023192
C	-2.039045	0.583820	-0.308636
C	-3.397708	0.533903	0.068776
N	-4.252817	1.556992	-0.168586
H	-3.958636	2.325335	-0.748720
H	-5.232076	1.414474	0.018742
N	-1.280138	1.536355	-0.969948
N	-0.003804	-0.258091	-0.457492
C	-0.086327	1.000614	-1.032630
H	0.779020	1.460791	-1.488949
C	-2.993388	-1.560589	0.951625
N	-1.692537	-1.639380	0.652073
H	-3.415967	-2.421392	1.465353

d4A 4	X	Y	Z
C	1.336490	1.509889	0.174962
C	1.847695	1.145625	1.545914
C	2.853917	0.284857	1.433109
C	3.098152	-0.046459	-0.010251
O	2.125965	0.753793	-0.728856
H	1.462254	2.581186	-0.043258
H	1.424069	1.558238	2.453173
H	3.422157	-0.153068	2.245462
H	4.095507	0.269263	-0.349840
C	2.897745	-1.517946	-0.381890
H	1.911444	-1.839218	-0.021699
H	3.666807	-2.126301	0.107295
O	3.049045	-1.710400	-1.778189
H	2.379818	-1.150633	-2.196957
N	-2.751493	-1.736695	0.494884
C	-0.839473	0.125714	0.224980
C	-2.131898	0.444831	-0.205882
C	-3.109904	-0.560128	-0.049143
N	-4.392738	-0.383869	-0.443068
H	-4.698736	0.523295	-0.753894
H	-5.067458	-1.096689	-0.218108
N	-2.198300	1.730394	-0.715783
N	-0.091552	1.267996	-0.025386
C	-0.972971	2.172380	-0.596294
H	-0.632063	3.154401	-0.898863
C	-1.469180	-1.901977	0.855250
N	-0.451348	-1.040049	0.761453
H	-1.229301	-2.872774	1.283809

d4A 5	X	Y	Z
C	-1.164731	-1.132296	0.055617
C	-1.998946	-1.167160	1.312299
C	-3.252340	-0.827289	1.031567
C	-3.390265	-0.547772	-0.441481
O	-2.066854	-0.730923	-0.969755
H	-0.716271	-2.102165	-0.193331
H	-1.582137	-1.430324	2.276729
H	-4.078657	-0.749620	1.728174
H	-4.055783	-1.282457	-0.923958
C	-3.933233	0.835295	-0.793736
H	-5.019465	0.837215	-0.607353
H	-3.774547	0.994893	-1.868915
O	-3.279064	1.824232	-0.010432
H	-3.432243	2.685144	-0.418480
N	3.959915	-0.625740	-0.252785
C	1.298266	-0.551344	-0.024574
C	1.993373	0.654275	0.108451
C	3.395145	0.571951	-0.013091
N	4.199119	1.657481	0.128584
H	3.778705	2.572932	0.125569
H	5.165839	1.560034	-0.138580
N	1.127116	1.713137	0.329417
N	-0.032652	-0.214893	0.134801
C	-0.060913	1.155935	0.338229
H	-1.005888	1.668345	0.457580
C	3.157739	-1.698305	-0.353409
N	1.826251	-1.761234	-0.249914
H	3.664972	-2.641457	-0.545880

d4A 6	X	Y	Z
C	1.296881	0.715430	-1.006395
C	1.685508	1.704197	0.062487
C	2.903271	1.408095	0.505226
C	3.454144	0.206875	-0.210273
O	2.385536	-0.180629	-1.113113
H	1.115587	1.189873	-1.981462
H	1.018304	2.494750	0.377815
H	3.453851	1.931087	1.278318
H	4.333643	0.464135	-0.821249
C	3.822829	-0.981690	0.681392
H	4.696537	-0.712396	1.285252
H	4.116954	-1.820265	0.030474
O	2.800342	-1.342900	1.584356
H	2.004027	-1.520640	1.064325
N	-3.659269	0.874171	0.527524
C	-1.131446	0.455012	-0.245634
C	-1.979867	-0.655055	-0.165487
C	-3.302342	-0.393420	0.253023
N	-4.219647	-1.378357	0.401122
H	-4.004961	-2.307483	0.078081
H	-5.175392	-1.117711	0.582966
N	-1.328932	-1.816054	-0.536997
N	0.082291	-0.053893	-0.663617
C	-0.114834	-1.414121	-0.835751
H	0.686253	-2.044367	-1.192921
C	-2.733051	1.838054	0.399833
N	-1.454888	1.729401	0.024092
H	-3.075270	2.844123	0.633065

d4A 7	X	Y	Z
C	-1.054152	-1.049344	0.333298
C	-1.967931	-0.886058	1.522428
C	-3.190512	-0.561189	1.110322
C	-3.222910	-0.493855	-0.390966
O	-1.873527	-0.763814	-0.799213
H	-0.627684	-2.054907	0.234999
H	-1.624437	-1.023035	2.540710
H	-4.063915	-0.371816	1.721615
H	-3.885335	-1.269800	-0.803314
C	-3.669395	0.853317	-0.962342
H	-3.530505	0.834066	-2.052862
H	-3.028556	1.649636	-0.554007
O	-5.031790	1.021660	-0.596167
H	-5.350880	1.845570	-0.983811
N	4.018459	-0.612285	-0.488614
C	1.401827	-0.508422	0.043615
C	2.132912	0.677588	0.153895
C	3.510992	0.581070	-0.130546
N	4.346948	1.644886	-0.033362
H	3.954698	2.566428	0.072238
H	5.282040	1.542893	-0.394367
N	1.321588	1.735978	0.530868
N	0.104016	-0.163024	0.376141
C	0.133657	1.194983	0.647283
H	-0.764822	1.722682	0.935518
C	3.187416	-1.665980	-0.547267
N	1.874779	-1.712782	-0.298365
H	3.649982	-2.606562	-0.838681

d4A 8	X	Y	Z
C	-1.165092	-1.634555	0.155044
C	-1.799156	-1.145469	1.432781
C	-2.842520	-0.375344	1.143220
C	-2.995177	-0.252671	-0.345746
O	-1.927044	-1.053139	-0.888037
H	-1.199039	-2.730936	0.064454
H	-1.416565	-1.410755	2.410637
H	-3.498358	0.134071	1.837573
H	-3.953306	-0.670699	-0.688286
C	-2.881403	1.180694	-0.867291
H	-2.826398	1.150238	-1.965863
H	-1.954248	1.620718	-0.480352
O	-4.045975	1.866751	-0.413970
H	-3.915561	2.809112	-0.572867
N	2.659714	1.937497	0.279893
C	0.902394	-0.088146	0.150157
C	2.246158	-0.363724	-0.128723
C	3.138606	0.726039	-0.053459
N	4.459403	0.595058	-0.325513
H	4.849838	-0.325403	-0.444330
H	5.065499	1.376061	-0.132865
N	2.442321	-1.700626	-0.429092
N	0.257177	-1.309621	0.021260
C	1.242554	-2.214728	-0.335939
H	0.995514	-3.254386	-0.509467
C	1.342814	2.052472	0.513963
N	0.395247	1.110875	0.473281
H	1.004674	3.053394	0.774566

d4A 9	X	Y	Z
C	-1.162834	-1.093543	-0.138358
C	-1.914458	-1.286789	1.157892
C	-3.196919	-0.981073	0.982608
C	-3.427116	-0.520722	-0.434247
O	-2.131855	-0.598250	-1.050870
H	-0.725715	-2.031232	-0.505777
H	-1.432397	-1.648852	2.057969
H	-3.987305	-1.044236	1.723155
H	-4.107866	-1.201702	-0.970487
C	-4.005067	0.895731	-0.551957
H	-5.067498	0.861615	-0.261008
H	-3.955461	1.209380	-1.597850
O	-3.294478	1.874968	0.188593
H	-3.322119	1.624098	1.122186
N	3.967218	-0.653308	-0.090593
C	1.298809	-0.533025	-0.074260
C	2.000539	0.669665	0.046862
C	3.406191	0.563484	0.037326
N	4.214708	1.644996	0.178049
H	3.811062	2.563844	0.089467
H	5.197211	1.520450	-0.008317
N	1.137172	1.748649	0.139071
N	-0.034412	-0.172180	-0.042405
C	-0.057960	1.209174	0.083792
H	-0.999206	1.743174	0.095096
C	3.158040	-1.719927	-0.194139
N	1.821266	-1.760966	-0.190508
H	3.662940	-2.678472	-0.294619

d4A 10	X	Y	Z
C	-1.050824	-1.038715	0.341577
C	-1.962225	-0.872162	1.532317
C	-3.186257	-0.550450	1.122083
C	-3.221795	-0.483581	-0.378690
O	-1.873121	-0.751216	-0.789746
H	-0.627957	-2.045921	0.243341
H	-1.615382	-1.001788	2.550398
H	-4.056869	-0.354705	1.735556
H	-3.876376	-1.272274	-0.788212
C	-3.684555	0.866891	-0.946050
H	-3.507437	0.879878	-2.030384
H	-3.090507	1.671983	-0.503383
O	-5.040534	1.129047	-0.614127
H	-5.598154	0.570924	-1.171746
N	4.019440	-0.622955	-0.492217
C	1.404820	-0.507732	0.045924
C	2.139824	0.676240	0.148955
C	3.516862	0.574017	-0.138807
N	4.356084	1.635533	-0.049687
H	3.967630	2.558775	0.055145
H	5.290814	1.528742	-0.410163
N	1.332930	1.739008	0.523082
N	0.108725	-0.156276	0.379623
C	0.143314	1.203405	0.644237
H	-0.752574	1.736292	0.931152
C	3.184884	-1.674043	-0.543866
N	1.872547	-1.715331	-0.291557
H	3.643683	-2.617625	-0.831518

d4A 11	X	Y	Z
C	-1.111501	0.759949	0.991978
C	-1.550232	1.669814	-0.127618
C	-2.783825	1.340324	-0.499547
C	-3.285795	0.189653	0.324827
O	-2.209542	-0.092398	1.244722
H	-0.849034	1.302205	1.910411
H	-0.899147	2.435860	-0.527272
H	-3.375880	1.789666	-1.286789
H	-4.175675	0.462156	0.909184
C	-3.616804	-1.067854	-0.482626
H	-3.822588	-1.892297	0.216503
H	-2.742962	-1.343107	-1.091369
O	-4.748324	-0.748746	-1.279900
H	-4.960482	-1.515035	-1.826512
N	3.829720	0.789840	-0.543627
C	1.294502	0.424503	0.224127
C	2.095473	-0.712423	0.068085
C	3.424217	-0.477139	-0.342571
N	4.302571	-1.487599	-0.562163
H	4.063189	-2.415722	-0.252493
H	5.271602	-1.246247	-0.696440
N	1.395873	-1.865720	0.371930
N	0.065414	-0.057062	0.624019
C	0.200890	-1.430609	0.702301
H	-0.628656	-2.045912	1.015568
C	2.942963	1.780534	-0.353563
N	1.663568	1.699508	0.025536
H	3.323220	2.784298	-0.531595

d4A 12	X	Y	Z
C	-1.157374	-1.639291	0.147855
C	-1.789870	-1.161041	1.430735
C	-2.832456	-0.386633	1.150031
C	-2.985264	-0.247257	-0.337110
O	-1.920574	-1.045216	-0.888851
H	-1.193668	-2.734616	0.045998
H	-1.403697	-1.431700	2.405669
H	-3.481356	0.123235	1.850775
H	-3.942612	-0.672483	-0.683230
C	-2.878480	1.201781	-0.837394
H	-2.789710	1.196023	-1.933035
H	-1.975109	1.652866	-0.421253
O	-3.986650	1.974320	-0.390069
H	-4.761308	1.707683	-0.902305
N	2.651390	1.942466	0.278618
C	0.904282	-0.089946	0.146763
C	2.249130	-0.360712	-0.130216
C	3.136536	0.733238	-0.053397
N	4.458502	0.608470	-0.321995
H	4.853972	-0.309155	-0.445095
H	5.059918	1.394206	-0.134258
N	2.450110	-1.697103	-0.431312
N	0.263291	-1.313644	0.015782
C	1.252245	-2.215620	-0.340655
H	1.009064	-3.256024	-0.515292
C	1.333555	2.052551	0.510640
N	0.390811	1.105935	0.469004
H	0.989755	3.051843	0.769194

d4A 13	X	Y	Z
C	-1.178298	-1.642197	0.171467
C	-1.815224	-1.124196	1.436394
C	-2.851507	-0.352653	1.125507
C	-2.998471	-0.255349	-0.366461
O	-1.942076	-1.089700	-0.885434
H	-1.209593	-2.740388	0.107869
H	-1.442431	-1.375672	2.421657
H	-3.511869	0.156294	1.817285
H	-3.962132	-0.667113	-0.699795
C	-2.854570	1.168537	-0.928397
H	-2.911539	1.121983	-2.020438
H	-1.871317	1.559966	-0.645983
O	-3.924383	1.997229	-0.481649
H	-3.648409	2.407762	0.346671
N	2.644116	1.934330	0.263957
C	0.889857	-0.095574	0.164684
C	2.233184	-0.372265	-0.114668
C	3.125415	0.718158	-0.048167
N	4.455039	0.575458	-0.268584
H	4.797365	-0.290922	-0.651514
H	5.012778	1.410384	-0.351373
N	2.427259	-1.708364	-0.420069
N	0.243654	-1.316945	0.036904
C	1.227741	-2.222049	-0.325219
H	0.979319	-3.260913	-0.501507
C	1.328786	2.049877	0.503915
N	0.382589	1.105574	0.480723
H	0.989434	3.054283	0.748938

d4A 14	X	Y	Z
C	-1.188401	-0.958487	-0.833247
C	-1.510901	-1.894795	0.305374
C	-2.716174	-1.596716	0.782832
C	-3.298660	-0.429671	0.029801
O	-2.347683	-0.184022	-1.027690
H	-0.936232	-1.481272	-1.764699
H	-0.815115	-2.652552	0.640712
H	-3.222270	-2.080245	1.610551
H	-4.259395	-0.660598	-0.449647
C	-3.486805	0.808733	0.904339
H	-2.517939	1.078447	1.349839
H	-4.174981	0.548558	1.726157
O	-4.006042	1.846862	0.090536
H	-4.068843	2.646811	0.627173
N	3.844866	-0.645277	0.329731
C	1.239325	-0.459255	-0.235065
C	1.953003	0.733347	-0.069570
C	3.323651	0.591316	0.230926
N	4.131518	1.660404	0.446072
H	3.795658	2.578248	0.202072
H	5.124535	1.495182	0.491321
N	1.138024	1.835790	-0.251694
N	-0.050578	-0.066028	-0.517388
C	-0.039433	1.317115	-0.520946
H	-0.943965	1.868389	-0.732771
C	3.030179	-1.697511	0.147450
N	1.723327	-1.707093	-0.134762
H	3.503540	-2.672710	0.241449

d4A 15	X	Y	Z
C	-1.102420	0.762156	0.970398
C	-1.541769	1.663074	-0.156378
C	-2.779520	1.338282	-0.518320
C	-3.284374	0.198971	0.319269
O	-2.202234	-0.086841	1.231174
H	-0.837688	1.312798	1.883313
H	-0.886892	2.418823	-0.569339
H	-3.369913	1.780016	-1.311291
H	-4.160121	0.493213	0.920289
C	-3.646291	-1.061091	-0.482799
H	-3.814333	-1.895755	0.212894
H	-2.809616	-1.328037	-1.134703
O	-4.764269	-0.828110	-1.326083
H	-5.556286	-0.800061	-0.773396
N	3.848291	0.786866	-0.518349
C	1.306240	0.422383	0.224510
C	2.103604	-0.715822	0.062164
C	3.436547	-0.481068	-0.335347
N	4.312592	-1.491714	-0.558692
H	4.064565	-2.425432	-0.274158
H	5.282389	-1.254638	-0.693848
N	1.396359	-1.869591	0.345854
N	0.071669	-0.058622	0.607961
C	0.200099	-1.434038	0.670052
H	-0.634684	-2.050043	0.967492
C	2.963929	1.778670	-0.324017
N	1.680939	1.698304	0.043575
H	3.349391	2.782905	-0.487610

d4A 16	X	Y	Z
C	-1.127899	-1.096885	0.266073
C	-1.960229	-1.200381	1.519499
C	-3.195630	-0.773472	1.272928
C	-3.321006	-0.360100	-0.169151
O	-2.007994	-0.565642	-0.717566
H	-0.725592	-2.057783	-0.077322
H	-1.562659	-1.577187	2.454102
H	-4.019535	-0.734002	1.976401
H	-4.025161	-1.009150	-0.712214
C	-3.786188	1.079532	-0.370414
H	-2.993976	1.756603	-0.018388
H	-4.680458	1.250215	0.253657
O	-4.071136	1.258913	-1.746256
H	-4.168040	2.203783	-1.916088
N	3.904855	-0.536819	-0.715479
C	1.322018	-0.527583	-0.030624
C	2.079921	0.603896	0.284271
C	3.439032	0.559015	-0.089645
N	4.299229	1.572872	0.181394
H	3.927933	2.457338	0.488609
H	5.208740	1.543627	-0.251430
N	1.308634	1.566510	0.915911
N	0.049580	-0.249331	0.435474
C	0.118434	1.021780	0.980522
H	-0.754557	1.485528	1.418253
C	3.052737	-1.549390	-0.945903
N	1.754447	-1.637795	-0.639972
H	3.481991	-2.411678	-1.451614

d4A 17	X	Y	Z
C	-1.051906	-1.050954	0.314527
C	-1.961835	-0.903739	1.508954
C	-3.188835	-0.587412	1.102712
C	-3.230023	-0.501221	-0.398525
O	-1.878559	-0.762581	-0.810705
H	-0.621134	-2.054328	0.210473
H	-1.615757	-1.052442	2.524739
H	-4.058659	-0.436749	1.732019
H	-3.889467	-1.277034	-0.815624
C	-3.683450	0.853973	-0.965498
H	-3.577498	0.828873	-2.053626
H	-3.025533	1.648862	-0.586083
O	-5.053006	1.106699	-0.688240
H	-5.122566	1.427841	0.219353
N	4.024265	-0.611678	-0.468778
C	1.403793	-0.506910	0.040754
C	2.132466	0.680422	0.150109
C	3.513067	0.583703	-0.122724
N	4.346996	1.648687	-0.026230
H	3.953634	2.570737	0.070627
H	5.285544	1.544897	-0.377706
N	1.316775	1.740126	0.513799
N	0.102419	-0.160840	0.359751
C	0.128568	1.199067	0.623009
H	-0.772417	1.729084	0.898587
C	3.194985	-1.666512	-0.527764
N	1.880201	-1.712968	-0.289303
H	3.660796	-2.608479	-0.809204

d4A 18	X	Y	Z
C	-1.183762	-0.970595	-0.784468
C	-1.522003	-1.879639	0.371817
C	-2.739708	-1.583291	0.818211
C	-3.314346	-0.439080	0.025625
O	-2.344173	-0.204039	-1.013547
H	-0.917113	-1.517303	-1.697944
H	-0.825321	-2.620661	0.741445
H	-3.256151	-2.048109	1.650136
H	-4.257817	-0.710417	-0.474832
C	-3.543745	0.826588	0.865349
H	-2.626085	1.071907	1.407562
H	-4.325882	0.610306	1.612609
O	-3.852284	1.966000	0.085534
H	-4.635692	1.771696	-0.446571
N	3.861174	-0.644714	0.270614
C	1.244390	-0.461012	-0.233906
C	1.952305	0.731506	-0.049162
C	3.329941	0.590886	0.218238
N	4.134821	1.658641	0.446325
H	3.785705	2.582462	0.248254
H	5.129448	1.500734	0.475911
N	1.125089	1.831971	-0.180093
N	-0.054032	-0.069941	-0.477265
C	-0.055153	1.314016	-0.437086
H	-0.967861	1.866350	-0.609068
C	3.049995	-1.697094	0.075479
N	1.737157	-1.708124	-0.179082
H	3.531477	-2.671193	0.132542

d4A 19	X	Y	Z
C	1.121033	0.733751	-1.036156
C	1.556400	1.677595	0.056889
C	2.785991	1.352497	0.446435
C	3.287809	0.167846	-0.330391
O	2.220777	-0.122783	-1.261139
H	0.862882	1.250391	-1.970521
H	0.908438	2.462066	0.424552
H	3.373686	1.849036	1.209936
H	4.190263	0.411228	-0.907790
C	3.586110	-1.078963	0.519872
H	3.852248	-1.904312	-0.147334
H	2.680175	-1.367792	1.070524
O	4.697004	-0.866481	1.377849
H	4.386201	-0.390871	2.158285
N	-3.799058	0.808577	0.570015
C	-1.276699	0.421862	-0.229712
C	-2.087959	-0.707357	-0.072876
C	-3.409555	-0.461332	0.354856
N	-4.295749	-1.463563	0.575490
H	-4.067197	-2.394429	0.266136
H	-5.259632	-1.215170	0.731428
N	-1.404678	-1.866009	-0.392825
N	-0.057025	-0.070473	-0.646313
C	-0.209051	-1.442530	-0.734374
H	0.610688	-2.064886	-1.059570
C	-2.904342	1.791015	0.376568
N	-1.630151	1.699337	-0.018069
H	-3.271799	2.797466	0.565919

d4A 20	X	Y	Z
C	-1.122423	-1.060171	0.245129
C	-1.934841	-1.194292	1.509062
C	-3.187518	-0.809958	1.280725
C	-3.339642	-0.383842	-0.155825
O	-2.022931	-0.508601	-0.711744
H	-0.725142	-2.015612	-0.120514
H	-1.513045	-1.564669	2.435612
H	-4.003823	-0.804237	1.993965
H	-4.007065	-1.080450	-0.695034
C	-3.889977	1.035068	-0.336462
H	-3.198773	1.749870	0.119748
H	-4.849044	1.103119	0.206085
O	-4.019572	1.422052	-1.689214
H	-4.627807	0.808605	-2.122902
N	3.922690	-0.566689	-0.682595
C	1.330628	-0.516086	-0.038194
C	2.095435	0.613008	0.266670
C	3.459291	0.546694	-0.085987
N	4.326009	1.556793	0.177452
H	3.958383	2.451953	0.457289
H	5.240268	1.510294	-0.243836
N	1.324713	1.595942	0.867004
N	0.054063	-0.214742	0.402122
C	0.127699	1.066528	0.923571
H	-0.747539	1.550674	1.333563
C	3.063566	-1.574407	-0.906211
N	1.759571	-1.642909	-0.618716
H	3.490991	-2.451169	-1.388050

d4A 21	X	Y	Z
C	3.053129	0.001607	-0.024920
O	2.096859	0.800707	-0.747375
C	1.299946	1.554347	0.147460
C	1.813879	1.214022	1.523475
C	2.817042	0.349337	1.419573
C	2.883240	-1.489611	-0.336912
O	3.120606	-1.803423	-1.697590
H	1.407078	2.624985	-0.083875
H	1.391825	1.637826	2.426283
H	3.384972	-0.082717	2.235169
H	4.059122	0.318560	-0.351216
H	1.850869	-1.772181	-0.118541
H	3.546632	-2.059985	0.336175
H	4.041935	-1.591577	-1.898863
N	-0.126479	1.287543	-0.043180
C	-0.852744	0.135184	0.220991
N	-0.442305	-1.019742	0.764412
C	-1.441055	-1.903676	0.856355
N	-2.725434	-1.767348	0.491048
C	-2.152038	0.425884	-0.210548
C	-3.109115	-0.597110	-0.048307
N	-2.241255	1.702288	-0.739530
C	-1.023527	2.166923	-0.627250
H	-1.180483	-2.869655	1.283789
N	-4.409175	-0.430637	-0.397903
H	-4.662942	0.368329	-0.956601
H	-4.998942	-1.247671	-0.410088
H	-0.699795	3.149630	-0.945951

Table SVIII. Cartesian coordinates (in Å) of the 20 d4G conformers located in this work (listed in decreasing order of stability)

d4G 1	X	Y	Z	d4G 2	X	Y	Z
C	-1.490004	-1.674894	-0.013538	C	-1.316803	-1.000610	0.465361
C	-2.140652	-1.274261	1.288929	C	-2.301224	-0.819622	1.592436
C	-3.106546	-0.393335	1.048789	C	-3.529118	-0.692147	1.099980
C	-3.178854	-0.085438	-0.422804	C	-3.506103	-0.813136	-0.398758
O	-2.075916	-0.834201	-0.990603	O	-2.108746	-0.959101	-0.723360
H	-1.685127	-2.732401	-0.252851	H	-0.768479	-1.949248	0.503285
H	-1.843381	-1.694177	2.242129	H	-1.995677	-0.792392	2.631241
H	-3.758531	0.070839	1.778850	H	-4.441542	-0.540399	1.665072
H	-4.110697	-0.468729	-0.869821	H	-4.039926	-1.722045	-0.722364
C	-3.055509	1.404189	-0.770933	C	-4.078313	0.377704	-1.177001
H	-4.031503	1.877704	-0.604526	H	-5.124354	0.530250	-0.889208
H	-2.836961	1.475617	-1.849139	H	-4.061236	0.134160	-2.249701
O	-2.110712	2.083949	0.022438	O	-3.391665	1.583313	-0.907479
H	-1.303607	1.517263	0.071490	H	-2.488007	1.464155	-1.233083
N	2.612141	1.397414	0.082644	N	3.604332	-0.069716	-0.265319
C	1.289530	1.737594	0.153493	C	2.931805	-1.264108	-0.259189
C	0.759343	-0.440593	0.033862	C	1.050152	-0.165543	0.182045
C	2.073247	-0.894400	-0.063000	C	1.624510	1.103992	0.213683
C	3.150093	0.063589	-0.032355	C	3.038591	1.233711	-0.030161
N	2.111474	-2.268259	-0.200554	N	0.672603	2.069415	0.479186
C	0.856190	-2.627386	-0.193678	C	-0.445378	1.403358	0.609531
H	0.491081	-3.641550	-0.288938	H	-1.416938	1.828881	0.818187
N	0.961245	3.059811	0.282526	N	3.660241	-2.391776	-0.563623
H	1.598674	3.749753	-0.085669	H	4.625175	-2.418076	-0.265405
O	4.356973	-0.083295	-0.085714	O	3.763281	2.211705	-0.070440
H	3.326743	2.112608	0.143334	H	4.585234	-0.040807	-0.515778
N	0.326156	0.841058	0.141939	N	1.644461	-1.368803	-0.027885
H	-0.023759	3.258522	0.142290	H	3.149669	-3.246650	-0.391140
N	-0.029119	-1.565376	-0.044942	N	-0.286723	0.029915	0.445006

d4G 3	X	Y	Z
C	-1.297821	0.858090	-0.689990
C	-2.239282	0.597740	-1.839373
C	-3.479042	0.438431	-1.382553
C	-3.503178	0.579589	0.112441
O	-2.130167	0.851039	0.469442
H	-0.779166	1.821656	-0.752379
H	-1.901899	0.553096	-2.867861
H	-4.364699	0.238654	-1.974911
H	-4.107517	1.440113	0.435176
C	-3.976456	-0.654949	0.885619
H	-3.407128	-1.533246	0.541773
H	-5.036925	-0.838413	0.680147
O	-3.852204	-0.458512	2.278896
H	-2.924797	-0.228116	2.436225
N	3.594762	0.143527	0.370496
C	2.879105	1.309171	0.280722
C	1.074918	0.122468	-0.246349
C	1.697496	-1.122972	-0.197186
C	3.096186	-1.188342	0.142185
N	0.802027	-2.133452	-0.493063
C	-0.327256	-1.515252	-0.716467
H	-1.261012	-1.989254	-0.983341
N	3.541071	2.473988	0.594689
H	4.523203	2.530387	0.364940
O	3.853222	-2.134775	0.261551
H	4.557191	0.161604	0.685447
N	1.606907	1.354429	-0.038102
H	3.011351	3.302416	0.361787
N	-0.233827	-0.133458	-0.591223

d4G 4	X	Y	Z
C	-1.267148	-1.066523	0.211023
C	-2.162114	-1.083693	1.425565
C	-3.429425	-0.935414	1.054541
C	-3.515604	-0.818662	-0.443777
O	-2.152294	-0.894313	-0.890926
H	-0.691045	-1.991142	0.084160
H	-1.773631	-1.192088	2.430821
H	-4.297199	-0.893652	1.702114
H	-4.065042	-1.670373	-0.877618
C	-4.190981	0.451742	-0.958193
H	-5.280024	0.341187	-0.828719
H	-3.985814	0.526753	-2.034223
O	-3.706545	1.581688	-0.246710
H	-3.824576	2.364795	-0.797439
N	3.667864	0.003637	-0.169037
C	3.032789	-1.210316	-0.201179
C	1.091430	-0.164883	0.087373
C	1.624326	1.121716	0.148102
C	3.046982	1.291567	0.008834
N	0.624948	2.060474	0.325873
C	-0.479440	1.360734	0.378771
H	-1.483207	1.748031	0.480430
N	3.817609	-2.318572	-0.441292
H	4.750468	-2.314147	-0.052317
O	3.745822	2.290149	0.011178
H	4.663143	0.060515	-0.347142
N	1.736516	-1.352431	-0.063758
H	3.317973	-3.184823	-0.293937
N	-0.265767	-0.006373	0.245239

d4G 5	X	Y	Z
C	-1.193287	-0.911790	0.576782
C	-2.196163	-0.638428	1.669878
C	-3.412132	-0.514276	1.144187
C	-3.349441	-0.712459	-0.344319
O	-1.962191	-0.954365	-0.623443
H	-0.654237	-1.859143	0.691981
H	-1.911536	-0.552680	2.711633
H	-4.337026	-0.303052	1.666003
H	-3.932595	-1.594086	-0.649239
C	-3.840110	0.481456	-1.166617
H	-3.628538	0.285740	-2.227732
H	-3.278227	1.379772	-0.870122
O	-5.232026	0.609688	-0.910361
H	-5.569669	1.346334	-1.434120
N	3.712362	-0.074087	-0.343116
C	3.027777	-1.258602	-0.254529
C	1.174819	-0.117281	0.198766
C	1.763458	1.144983	0.146569
C	3.168770	1.245633	-0.153207
N	0.831317	2.133768	0.398785
C	-0.285978	1.485376	0.598552
H	-1.240263	1.935256	0.832537
N	3.733442	-2.408652	-0.529573
H	4.706766	-2.433031	-0.259604
O	3.901712	2.212118	-0.267165
H	4.683198	-0.069449	-0.631430
N	1.749098	-1.336376	0.027482
H	3.218982	-3.247282	-0.298500
N	-0.149519	0.105979	0.500705

d4G 6	X	Y	Z
C	1.481192	-1.550805	-0.423889
C	1.920921	-0.898968	-1.710705
C	2.887054	-0.021098	-1.461208
C	3.163568	0.043177	0.013460
O	2.246241	-0.915012	0.591778
H	1.699778	-2.629142	-0.418251
H	1.491263	-1.159799	-2.670024
H	3.409283	0.588681	-2.189448
H	4.184350	-0.283295	0.262021
C	2.914513	1.406244	0.663719
H	1.907155	1.743944	0.383216
H	3.647066	2.131419	0.291357
O	3.080451	1.337219	2.068210
H	2.474525	0.646238	2.373023
N	-2.761538	1.324566	-0.066576
C	-1.496781	1.711919	-0.423816
C	-0.801535	-0.389320	-0.161339
C	-2.041861	-0.892504	0.232751
C	-3.173562	-0.002499	0.300744
N	-1.972961	-2.246824	0.493703
C	-0.725641	-2.553233	0.266627
H	-0.289286	-3.538016	0.371880
N	-1.330539	3.029908	-0.787110
H	-1.894460	3.717395	-0.306945
O	-4.337895	-0.206184	0.594046
H	-3.526195	1.987856	-0.102912
N	-0.474358	0.891412	-0.481067
H	-0.358920	3.290723	-0.882825
N	0.050518	-1.476446	-0.147727

d4G 7	X	Y	Z
C	1.397712	0.698928	-1.007941
C	1.649139	1.726670	0.066200
C	2.896938	1.602182	0.506197
C	3.606309	0.492763	-0.217548
O	2.607867	-0.017524	-1.137527
H	1.129093	1.146551	-1.975047
H	0.881733	2.416184	0.389309
H	3.369621	2.189003	1.285055
H	4.449788	0.869173	-0.817190
C	4.124393	-0.641125	0.672656
H	4.970796	-0.265467	1.258626
H	4.505199	-1.442502	0.020447
O	3.171656	-1.113984	1.599980
H	2.414341	-1.454145	1.103027
N	-3.484141	0.176152	0.340128
C	-2.748517	1.317359	0.153856
C	-0.971996	0.058651	-0.313360
C	-1.617494	-1.168586	-0.147642
C	-3.012342	-1.178451	0.214810
N	-0.756763	-2.215009	-0.395712
C	0.379619	-1.638622	-0.702572
H	1.286868	-2.143691	-0.997625
N	-3.419091	2.515045	0.265111
H	-4.170278	2.566088	0.938919
O	-3.788595	-2.097270	0.404000
H	-4.478468	0.237474	0.522814
N	-1.475902	1.315609	-0.166031
H	-2.798767	3.312588	0.278153
N	0.320194	-0.251745	-0.655788

d4G 8	X	Y	Z
C	-1.188897	-0.873586	0.570424
C	-2.176434	-0.594992	1.676412
C	-3.401677	-0.485789	1.169536
C	-3.361432	-0.693255	-0.317944
O	-1.974539	-0.905116	-0.621049
H	-0.657952	-1.826637	0.679345
H	-1.875480	-0.496094	2.712371
H	-4.319087	-0.273787	1.704339
H	-3.922753	-1.600213	-0.601295
C	-3.908127	0.485493	-1.138168
H	-3.669893	0.325705	-2.198739
H	-3.415348	1.409725	-0.823065
O	-5.299568	0.665351	-0.914949
H	-5.771270	-0.029584	-1.392251
N	3.726744	-0.102080	-0.339076
C	3.028562	-1.277527	-0.240208
C	1.186315	-0.109802	0.188554
C	1.788818	1.145040	0.124224
C	3.196976	1.226418	-0.168059
N	0.866056	2.146895	0.359545
C	-0.259406	1.514152	0.561079
H	-1.210000	1.978207	0.782490
N	3.722530	-2.438773	-0.497596
H	4.694254	-2.470591	-0.222697
O	3.942139	2.182550	-0.287492
H	4.699492	-0.111400	-0.620783
N	1.747493	-1.337316	0.035469
H	3.197705	-3.268684	-0.258592
N	-0.137409	0.131868	0.480471

d4G 9	X	Y	Z
C	-1.281792	-1.722055	0.359386
C	-1.846171	-1.000137	1.556892
C	-2.869885	-0.242483	1.178121
C	-3.073804	-0.358393	-0.306079
O	-2.045255	-1.261683	-0.746509
H	-1.392285	-2.813402	0.446294
H	-1.442203	-1.124598	2.553957
H	-3.483942	0.394465	1.802083
H	-4.055507	-0.796159	-0.541554
C	-2.948506	0.962297	-1.067201
H	-2.965647	0.745170	-2.145155
H	-1.981742	1.420766	-0.819116
O	-4.052746	1.768527	-0.667722
H	-4.030122	2.585169	-1.180678
N	2.697293	1.515659	0.030740
C	1.388917	1.798650	0.323413
C	0.895892	-0.365798	0.124778
C	2.192850	-0.768343	-0.197139
C	3.241370	0.218076	-0.262712
N	2.259467	-2.133872	-0.390762
C	1.036609	-2.543887	-0.192748
H	0.696716	-3.568923	-0.263356
N	1.092005	3.108636	0.632300
H	1.603280	3.828357	0.140616
O	4.430959	0.110865	-0.502328
H	3.398264	2.245327	0.076035
N	0.441832	0.892930	0.371292
H	0.098018	3.278935	0.696651
N	0.149208	-1.526828	0.137348

d4G 10	X	Y	Z
C	-1.264105	0.871402	-0.695741
C	-2.193816	0.609922	-1.854190
C	-3.431631	0.429615	-1.401443
C	-3.460376	0.572187	0.096690
O	-2.097894	0.858033	0.456403
H	-0.742915	1.834022	-0.754114
H	-1.852653	0.577704	-2.881849
H	-4.314199	0.222125	-1.995798
H	-4.080289	1.426737	0.407981
C	-3.982970	-0.658768	0.833451
H	-3.255484	-1.473982	0.712107
H	-4.930556	-0.975609	0.364368
O	-4.170967	-0.306635	2.193076
H	-4.242676	-1.118044	2.710023
N	3.620966	0.128920	0.405076
C	2.913527	1.299170	0.306132
C	1.107175	0.124277	-0.239794
C	1.722311	-1.125256	-0.183091
C	3.116284	-1.199282	0.172081
N	0.823868	-2.130494	-0.487202
C	-0.298969	-1.503662	-0.721982
H	-1.232841	-1.971033	-0.999870
N	3.580563	2.459959	0.627464
H	4.563278	2.511245	0.398539
O	3.865944	-2.150962	0.301114
H	4.578810	0.141283	0.733793
N	1.646188	1.352854	-0.027838
H	3.056040	3.290748	0.390888
N	-0.198410	-0.123571	-0.598000

d4G 11	X	Y	Z
C	-1.276407	-1.763336	0.306339
C	-1.853579	-1.091625	1.527119
C	-2.862393	-0.304923	1.168334
C	-3.043839	-0.349040	-0.322237
O	-2.034362	-1.262272	-0.786404
H	-1.380679	-2.857746	0.346308
H	-1.461060	-1.259499	2.522419
H	-3.470644	0.318718	1.811251
H	-4.030846	-0.761894	-0.592417
C	-2.869972	1.011664	-1.013723
H	-2.842984	0.859663	-2.102016
H	-1.913334	1.437521	-0.703938
O	-3.886862	1.926864	-0.622701
H	-4.712950	1.651379	-1.041406
N	2.650511	1.538805	0.047951
C	1.331697	1.799754	0.313611
C	0.883274	-0.375082	0.114706
C	2.192796	-0.755346	-0.181297
C	3.223971	0.250348	-0.229667
N	2.285850	-2.119427	-0.375796
C	1.066173	-2.550239	-0.204916
H	0.745042	-3.580695	-0.284491
N	1.002546	3.104710	0.605363
H	1.515044	3.831386	0.125531
O	4.419603	0.164268	-0.446541
H	3.336584	2.282204	0.098109
N	0.402087	0.874944	0.350170
H	0.004535	3.260394	0.643607
N	0.155281	-1.548370	0.108399

d4G 12	X	Y	Z
C		-0.903231	0.562436
C	-2.185333	-0.633466	1.664143
C	-3.407028	-0.523477	1.148248
C	-3.359618	-0.721703	-0.341661
O	-1.969821	-0.946900	-0.630211
H	-0.650621	-1.850453	0.677075
H	-1.893784	-0.549430	2.704153
H	-4.325243	-0.343209	1.695410
H	-3.933635	-1.613092	-0.635416
C	-3.873845	0.463362	-1.176089
H	-3.703249	0.243402	-2.233749
H	-3.297288	1.365248	-0.927806
O	-5.272262	0.649898	-1.009128
H	-5.413915	1.163096	-0.204137
N	3.720247	-0.078505	-0.331943
C	3.032615	-1.261198	-0.243554
C	1.178814	-0.113865	0.190104
C	1.769979	1.146900	0.136550
C	3.178249	1.243286	-0.151336
N	0.837696	2.138708	0.376259
C	-0.282269	1.493835	0.570156
H	-1.237344	1.947607	0.792917
N	3.737081	-2.413634	-0.508394
H	4.709830	-2.439090	-0.236840
O	3.914029	2.207644	-0.262439
H	4.693374	-0.077038	-0.612558
N	1.751442	-1.334849	0.029624
H	3.219948	-3.251058	-0.279299
N	-0.147835	0.113455	0.480239

d4G 13	X	Y	Z
C	-1.258072	-1.037562	-0.063058
C	-2.009249	-1.258923	1.229268
C	-3.316043	-1.135776	1.015688
C	-3.570786	-0.788573	-0.428807
O	-2.261916	-0.725828	-1.017973
H	-0.696515	-1.928682	-0.371611
H	-1.506537	-1.500754	2.157972
H	-4.108584	-1.260742	1.746011
H	-4.141161	-1.583905	-0.936083
C	-4.331831	0.527203	-0.639039
H	-5.388865	0.360851	-0.374591
H	-4.291047	0.788830	-1.699565
O	-3.787403	1.632250	0.062217
H	-3.829213	1.439816	1.008903
N	3.690091	-0.002484	-0.044740
C	3.049076	-1.211070	-0.119763
C	1.100580	-0.143797	-0.023304
C	1.637398	1.139252	0.067821
C	3.068807	1.294088	0.058883
N	0.635040	2.087842	0.135917
C	-0.477691	1.399929	0.096378
H	-1.481678	1.801811	0.090494
N	3.840468	-2.328919	-0.275119
H	4.739609	-2.326415	0.186170
O	3.775163	2.285269	0.114915
H	4.698167	0.043544	-0.130015
N	1.743815	-1.340231	-0.097186
H	3.323604	-3.190002	-0.162010
N	-0.263370	0.028576	0.002077

d4G 14	X	Y	Z
C	-3.086882	0.214802	-0.090213
O	-2.124802	-0.410750	-0.973269
C	-1.602269	-1.585422	-0.399542
C	-2.320725	-1.733740	0.921587
C	-3.195006	-0.741321	1.064181
C	-2.600111	1.616612	0.350955
O	-2.003482	2.325380	-0.715715
H	-1.793029	-2.439395	-1.066684
H	-2.129569	-2.553413	1.603660
H	-3.859757	-0.582211	1.905779
H	-4.018585	0.311993	-0.662739
H	-1.895303	1.497396	1.184613
H	-3.459755	2.196765	0.704704
H	-1.239795	1.759011	-0.944981
N	-0.128304	-1.522345	-0.294230
C	0.703555	-0.438132	-0.123895
N	0.339162	0.869802	-0.097539
C	1.339731	1.702506	0.083848
N	2.638155	1.289055	0.207095
C	1.991786	-0.967175	-0.034108
C	3.107716	-0.072451	0.150928
N	1.971460	-2.342027	-0.147287
C	0.706663	-2.632519	-0.304652
H	0.304931	-3.628808	-0.436360
H	3.371637	1.959927	0.401623
N	1.067171	3.041006	0.202620
H	1.764091	3.701258	-0.109676
H	0.107276	3.276115	-0.030885
O	4.299235	-0.292885	0.269210

d4G 15	X	Y	Z
C	1.278859	0.930217	-0.799598
C	1.491804	1.883278	0.351929
C	2.736804	1.752639	0.801475
C	3.461435	0.692481	0.014878
O	2.532410	0.332295	-1.028132
H	0.936789	1.429100	-1.715208
H	0.706368	2.531539	0.717036
H	3.186126	2.288515	1.629775
H	4.369162	1.065314	-0.478389
C	3.842054	-0.518604	0.865604
H	2.932353	-0.925373	1.330659
H	4.509018	-0.174394	1.674211
O	4.478560	-1.463971	0.023618
H	4.628387	-2.269645	0.533782
N	-3.596313	-0.037530	0.235227
C	-2.968048	1.161957	0.023730
C	-1.049594	0.068126	-0.246767
C	-1.575101	-1.208327	-0.038424
C	-2.983146	-1.341729	0.233362
N	-0.591764	-2.168469	-0.155286
C	0.498113	-1.491805	-0.425477
H	1.479692	-1.903282	-0.606513
N	-3.763643	2.287799	0.013492
H	-4.552261	2.301497	0.645318
O	-3.677488	-2.321957	0.436739
H	-4.602633	-0.070014	0.344534
N	-1.682233	1.274701	-0.210983
H	-3.226724	3.143972	0.009780
N	0.286352	-0.121866	-0.486316

d4G 16	X	Y	Z
C	-3.490332	0.451278	0.361747
O	-2.390178	0.099222	1.228728
C	-1.207240	0.757592	0.826196
C	-1.596469	1.583649	-0.375322
C	-2.889724	1.407646	-0.630024
C	-4.092813	-0.823726	-0.251643
O	-5.253190	-0.528355	-1.015006
H	-0.815466	1.368971	1.650059
H	-0.881506	2.201918	-0.902290
H	-3.463197	1.873472	-1.423170
H	-4.269156	0.935470	0.967602
H	-4.403244	-1.489821	0.558935
H	-3.325395	-1.343477	-0.841572
H	-4.971336	-0.253399	-1.896191
N	-0.167078	-0.242134	0.517193
C	1.146268	0.040443	0.241272
N	1.687114	1.289266	0.184258
C	2.971463	1.268847	-0.085093
N	3.678534	0.116680	-0.310256
C	1.755075	-1.195468	0.020821
C	3.161479	-1.228750	-0.288152
N	0.844831	-2.221915	0.163583
C	-0.282903	-1.622903	0.457632
H	-1.223090	-2.108874	0.665780
H	4.680970	0.156119	-0.449328
N	3.681910	2.449045	-0.099571
H	4.457190	2.516725	-0.744042
H	3.086091	3.265081	-0.084067
O	3.918634	-2.157170	-0.507818

d4G 17	X	Y	Z
C	-1.279750	-1.750330	0.287103
C	-1.866145	-1.095210	1.512564
C	-2.892109	-0.328999	1.157455
C	-3.071317	-0.359895	-0.335592
O	-2.033515	-1.241959	-0.802561
H	-1.383509	-2.845313	0.322304
H	-1.481028	-1.274222	2.508887
H	-3.528376	0.245047	1.821267
H	-4.048001	-0.784872	-0.610770
C	-2.926607	1.005366	-1.026398
H	-2.981517	0.858155	-2.108738
H	-1.939979	1.418484	-0.783962
O	-3.992827	1.881646	-0.677496
H	-3.809570	2.235111	0.201894
N	2.673752	1.530458	0.048249
C	1.354190	1.803943	0.294006
C	0.888676	-0.368256	0.106714
C	2.199140	-0.760276	-0.170355
C	3.240042	0.235445	-0.211724
N	2.285390	-2.125496	-0.356127
C	1.060948	-2.546797	-0.197931
H	0.733287	-3.575266	-0.276207
N	1.035259	3.116947	0.567097
H	1.564593	3.829354	0.083580
O	4.437503	0.137313	-0.411156
H	3.364840	2.269221	0.098709
N	0.415204	0.888483	0.328838
H	0.038863	3.284082	0.573522
N	0.153065	-1.536926	0.098251

d4G 18	X	Y	Z
C	-1.258316	0.845670	-0.656801
C	-2.159079	0.607071	-1.842901
C	-3.414081	0.454036	-1.429607
C	-3.481555	0.583652	0.069116
O	-2.123070	0.805367	0.474576
H	-0.740553	1.811968	-0.686650
H	-1.787492	0.572914	-2.859920
H	-4.282772	0.270757	-2.051625
H	-4.070530	1.474016	0.353750
C	-4.087691	-0.632557	0.779463
H	-3.453518	-1.505215	0.598904
H	-5.076685	-0.836460	0.333499
O	-4.162382	-0.483181	2.182843
H	-4.738711	0.268134	2.376786
N	3.641695	0.143765	0.387614
C	2.923639	1.307829	0.297949
C	1.117674	0.116582	-0.212506
C	1.743002	-1.127706	-0.163019
C	3.143951	-1.189607	0.166067
N	0.847249	-2.140751	-0.449000
C	-0.284312	-1.524497	-0.666450
H	-1.219831	-2.001104	-0.922085
N	3.586734	2.475059	0.604340
H	4.565241	2.532674	0.359395
O	3.904472	-2.134050	0.281663
H	4.605260	0.164392	0.698720
N	1.650140	1.350380	-0.014267
H	3.052483	3.300911	0.372450
N	-0.192166	-0.142869	-0.547794

d4G 19	X	Y	Z
C	1.272538	0.940392	-0.742273
C	1.510589	1.863407	0.428801
C	2.769205	1.735978	0.840041
C	3.478294	0.701324	0.007385
O	2.524370	0.352095	-1.013818
H	0.909882	1.465106	-1.635252
H	0.728884	2.491781	0.834895
H	3.235378	2.251994	1.671536
H	4.360374	1.113615	-0.508426
C	3.906474	-0.533259	0.815712
H	3.048788	-0.910521	1.379719
H	4.674747	-0.220758	1.543289
O	4.343355	-1.607323	0.006774
H	5.070225	-1.299059	-0.551127
N	-3.606991	-0.034836	0.202004
C	-2.977676	1.163287	-0.012651
C	-1.052667	0.070148	-0.229854
C	-1.577846	-1.204462	-0.013768
C	-2.991042	-1.338015	0.229912
N	-0.588593	-2.162241	-0.094855
C	0.505681	-1.487575	-0.350929
H	1.492152	-1.900969	-0.501019
N	-3.775370	2.287140	-0.053314
H	-4.576128	2.306801	0.562960
O	-3.687962	-2.316627	0.431336
H	-4.615166	-0.068528	0.292176
N	-1.687530	1.276082	-0.223312
H	-3.239955	3.144267	-0.056030
N	0.288686	-0.118465	-0.439282

d4G 20	X	Y	Z
C	-1.423641	-1.623843	0.360125
C	-1.873744	-1.038804	1.675182
C	-2.849317	-0.163033	1.460569
C	-3.120444	-0.044462	-0.015362
O	-2.198531	-0.962621	-0.626849
H	-1.615168	-2.706431	0.308887
H	-1.442112	-1.334698	2.623392
H	-3.380434	0.411218	2.210834
H	-4.143112	-0.384455	-0.258158
C	-2.934202	1.374276	-0.563755
H	-1.888058	1.656357	-0.424319
H	-3.563471	2.059118	0.031805
O	-3.205140	1.484493	-1.948421
H	-4.125378	1.228796	-2.097147
N	2.733610	1.380681	0.080951
C	1.454261	1.724911	0.429619
C	0.825152	-0.392370	0.132410
C	2.084392	-0.852109	-0.255542
C	3.189328	0.071891	-0.299140
N	2.058996	-2.203603	-0.537191
C	0.818622	-2.549896	-0.328585
H	0.412592	-3.545070	-0.455006
N	1.246159	3.034450	0.806958
H	1.786953	3.741009	0.327286
O	4.362888	-0.092586	-0.581183
H	3.476952	2.066633	0.133171
N	0.456926	0.873757	0.467716
H	0.265401	3.262961	0.892615
N	0.007116	-1.503728	0.093730

