



PCCP

## Supplementary Information

### A DFT study of 2-aminopurine-containing dinucleotides: prediction of stacked conformations with B-DNA structure

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#### Supplementary Information

**Table S1** Base-step parameters obtained by analysis of structural data reported for d(GpN) and d(ApN) dinucleotides in the Supplementary Information of Barone *et al.*<sup>1</sup> Values for idealised B-DNA and mean values from B-DNA crystal structures are presented for comparison.

	Shift / Å	Slide / Å	Rise / Å	Tilt / °	Roll / °	Twist / °
B-DNA Ideal <sup>a</sup>	0.00	0.00	3.34	0.00	0.00	36.00
B-DNA Mean <sup>b</sup>	−0.02	0.23	3.32	−0.10	0.60	36.00
(Std. Dev.)	(0.45)	(0.81)	(0.19)	(2.50)	(5.20)	(6.80)
d(GpA)	1.13	−0.15	3.17	0.75	1.02	53.77
d(ApA)	3.55	1.35	3.02	7.49	10.70	53.98
d(GpG)	1.61	0.57	3.12	10.91	−6.72	58.84
d(ApG)	3.32	2.59	3.10	18.64	8.06	62.64
d(GpC)	0.52	−1.36	3.72	−9.01	0.99	46.12
d(ApC)	0.47	−0.29	3.46	−3.35	0.48	37.66
d(GpT)	−1.13	−0.35	3.70	−4.19	−16.01	22.42
d(ApT)	0.53	−0.04	3.22	2.15	−5.57	35.18

<sup>a</sup> From Lu and Olson.<sup>2</sup> <sup>b</sup> From Olson *et al.*<sup>3</sup>

**Table S2** Base-step parameters for computed structures of twisted d(2pN) dinucleotides and the corresponding 2|N dimers.

	Shift / Å	Slide / Å	Rise / Å	Tilt / °	Roll / °	Twist / °
d(2pA)	1.53	−0.13	3.14	0.46	−0.32	60.60
2 A	1.55	−0.21	3.11	−0.12	1.66	58.45
d(2pG)	1.46	−0.18	3.07	4.74	−4.05	59.12
2 G	1.57	−0.23	3.05	3.86	−3.76	59.56
d(2pC)	0.49	−1.54	3.68	−8.75	−1.19	45.61
2 C	−0.89	−2.30	3.12	1.87	−2.04	17.47
d(2pT)	−0.14	−1.55	3.43	−2.13	−5.92	38.81
2 T	−0.85	−2.46	3.16	1.19	−3.30	15.54

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**Table S3** Base-step parameters for computed structures of twisted d(ApN) dinucleotides and the corresponding A|N dimers.

	Shift /Å	Slide /Å	Rise /Å	Tilt /°	Roll /°	Twist /°
d(2pA)	1.21	−0.05	3.24	−2.49	0.43	51.53
A A	1.43	−0.22	3.12	−0.44	3.80	55.91
d(ApG)	1.45	−0.11	3.19	0.53	−3.59	50.13
A G	1.44	−0.33	3.08	2.40	1.53	42.89
d(ApC)	−0.13	−1.17	3.67	−9.10	6.62	40.42
A C	2.44	−1.86	3.06	0.85	3.06	75.02
d(ApT)	−0.70	−1.20	3.22	0.79	−3.17	33.81
A T	2.16	−2.03	2.92	5.56	−2.27	69.20

**Table S4** Sugar pucker parameters for computed twisted structures of d(2pN) and d(ApN) dinucleotides in comparison with those of ideal B-DNA. P is the phase angle of pseudorotation.<sup>a</sup>

	5'-Base		3'-Base	
	P /°	Pucker	P /°	Pucker
B-DNA Ideal <sup>b</sup>	144-180	C2'-endo	144-180	C2'-endo
d(2pA)	170.9	C2'-endo	2.6	C3'-endo
d(ApA)	181.6	C3'-exo	12.8	C3'-endo
d(2pG)	169.9	C2'-endo	2.2	C3'-endo
d(ApG)	183.3	C3'-exo	15.7	C3'-endo
d(2pC)	137.5	C1'-exo	22.0	C3'-endo
d(ApC)	136.3	C1'-exo	21.3	C3'-endo
d(2pT)	146.0	C2'-endo	26.7	C3'-endo
d(ApT)	149.1	C2'-endo	25.9	C3'-endo

<sup>a</sup> The range of P values corresponding to each conformational form is as follows: 04'-endo, 72-108°; C1'-exo, 108-144°; C2'-endo, 144-180°; C3'-exo, 180-216°.<sup>b</sup> From Altona and Sundaralingam.<sup>4</sup>**Table S5** Base-step parameters for computed unstacked structures of d(2pN) and d(ApN) dinucleotides.

	Shift /Å	Slide /Å	Rise /Å	Tilt /°	Roll /°	Twist /°
d(2pG)	−17.69	−5.67	1.55	44.54	−38.16	−148.06
d(ApG)	−17.42	−5.86	2.16	42.17	−41.74	−152.49
d(2pT)	−17.98	−5.59	0.99	43.32	−32.05	−146.75
d(ApT)	−17.96	−5.72	1.20	42.85	−30.97	−149.47

**Table S6** Backbone torsional angles (degrees) for computed unstacked structures of d(2pN) and d(ApN) dinucleotides in comparison with mean values from B-DNA crystal structures. Standard deviations in the latter are small (<1.2) and are not shown. Torsional angles are defined in Figure 1 (main text).

	$\gamma_1$	$\delta_1$	$\epsilon_1$	$\zeta_1$	$\alpha_2$	$\beta_2$	$\gamma_2$	$\delta_2$	$\chi_1$	$\chi_2$
B-DNA Mean <sup>a</sup>	48.4	132.8	−178.3	−96.8	−61.0	179.3	48.4	132.8	−109.7	−109.7
d(2pG)	−68.8	142.9	−147.5	57.9	59.6	−174.7	−68.8	150.4	−117.7	−123.4
d(ApG)	−68.6	142.6	−147.7	57.9	60.2	−171.4	−68.9	150.6	−119.3	−119.0
d(2pT)	−68.4	142.0	−147.9	57.9	60.1	−171.8	−69.2	149.6	−118.4	−133.0
d(ApT)	−68.8	142.5	−149.7	57.2	60.2	−170.2	−69.3	149.3	−118.2	−133.0

<sup>a</sup> From Svozil *et al.*<sup>5</sup>

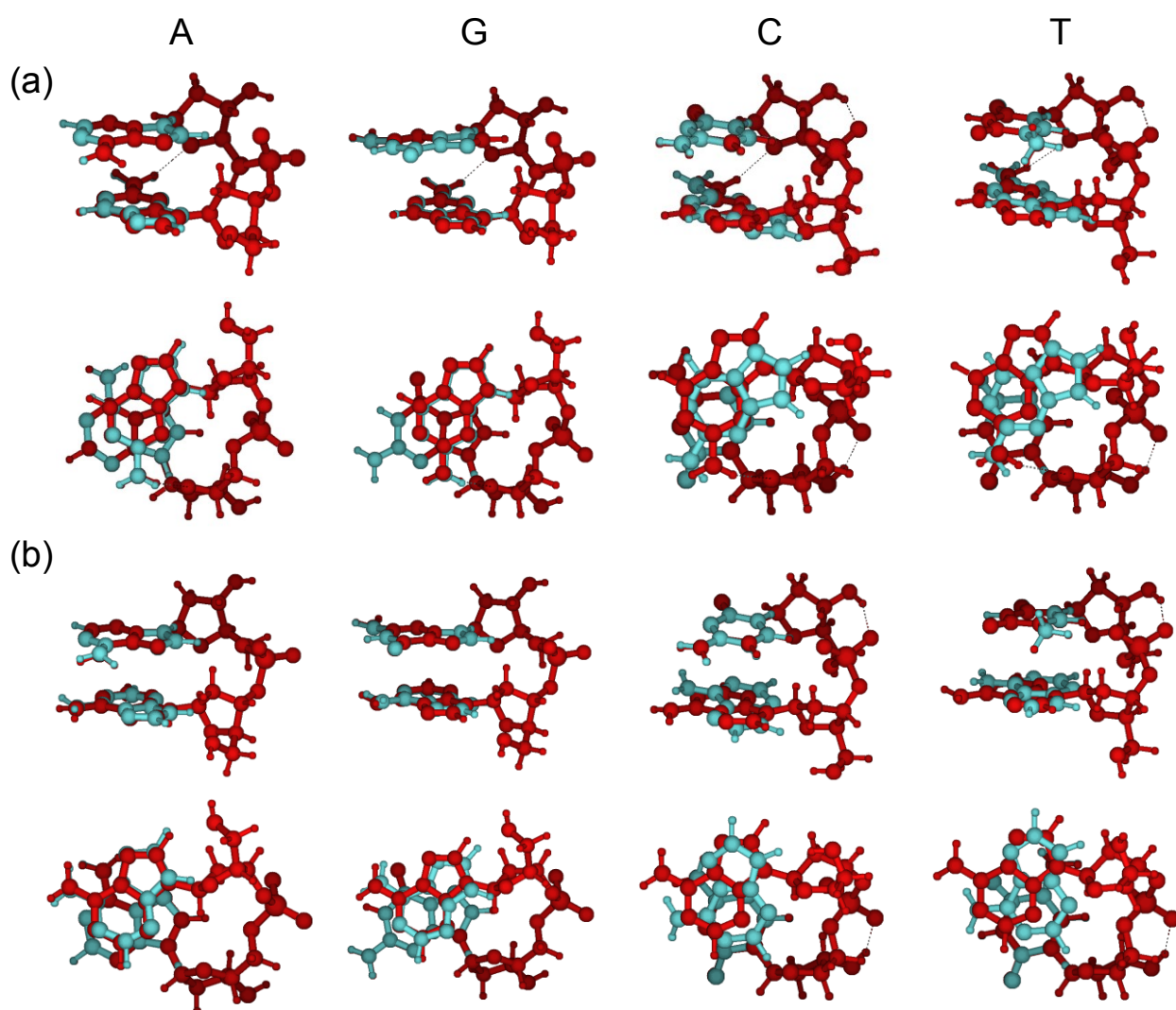
**Table S7** Sugar pucker parameters for computed unstacked structures of d(2pN) and d(ApN) dinucleotides in comparison with those of ideal B-DNA. P is the phase angle of pseudorotation.<sup>a</sup>

	5'-Base		3'-Base	
	P /°	Pucker	P /°	Pucker
B-DNA Ideal <sup>b</sup>	144-180	C2'-endo	144-180	C2'-endo
d(2pG)	155.1	C2'-endo	168.6	C2'-endo
d(ApG)	154.8	C2'-endo	169.2	C2'-endo
d(2pT)	153.8	C2'-endo	167.2	C2'-endo
d(ApT)	154.9	C2'-endo	166.3	C2'-endo

<sup>a</sup> The range of P values corresponding to each conformational form is as follows: O4'-endo, 72-108°; C1'-exo, 108-144°; C2'-endo, 144-180°; C3'-exo, 180-216°.

<sup>b</sup> From Altona and Sundaralingam.<sup>4</sup>

**Figure S1** Comparison of the optimised structures of the twisted conformers of the dinucleotides and the optimised structures of the unbound dimers. The structure of each dinucleotide (red) is overlaid with the structure of the corresponding dimer (blue). (a) d(2pN) dinucleotides (red) and 2|N dimers (blue). (b) d(ApN) dinucleotides (red) and A|N dimers (blue). In each case two alternative views are shown: perpendicular to the backbone (top row) and looking along the backbone from the 5' end (bottom row).



## Cartesian coordinates of all optimised minima

The Cartesian coordinates are given in xyz format (first line: number of atoms; second line: title; following lines: atom symbol and Cartesian coordinates in Hartree). The title line gives information on the system (d(XpY): dinucleoside monophosphate containing bases X and Y; W|Z: dimer containing bases W and Z; d: deoxy; p: phosphate; 2: 2-aminopurine; A: adenine; C: cytosine; G: guanine; T: thymine; B-form: stacked structure in B-DNA conformation; Twisted: stacked structure in twisted conformation; Unstacked: open conformation; Dimer: dimer structure; pcm: polarizable continuum model, water).

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d(2pA)-B-form-pcm
C  -3.02107200  -4.22093000   0.10435000
O  -2.18111000  -4.21393700  -1.04275200
C  -2.99040700  -2.84629800   0.74338900
O  -1.70531500  -2.58707900   1.32480700
C  -3.24636200  -1.70051600  -0.24108100
O  -3.95730900  -0.68586400   0.46815200
C  -1.83825600  -1.25503200  -0.62481600
C  -1.02477100  -1.54680900   0.63717200
N   3.96051600  -0.97796800   1.80865200
C   2.87120200  -0.27385300   2.19383100
N   1.60324500  -0.48297900   1.81895300
C   1.47807600  -1.49239400   0.96676800
C   2.52201500  -2.29873600   0.47929600
C   3.78983000  -1.98726000   0.95661400
N   2.02601800  -3.25887000  -0.39032400
C   0.74021200  -3.03119500  -0.41895400
N   0.33854500  -1.97242800   0.37384500
P  -4.47624200   0.65465300  -0.33677800
C  -2.77588500   2.10152500   1.03185200
O  -3.14859400   1.62189300  -0.25352400
C  -1.46270400   2.84083800   0.92318900
O  -0.41631800   1.90479500   0.63891700
C  -1.41421200   3.91646900  -0.19589000
O  -0.88498800   5.14712300   0.28176100
C  -0.40485900   3.33977100  -1.17949200
C   0.49424200   2.54102700  -0.24000400
N   5.25448000   0.68297700  -0.77910300
C   4.77643500   1.71883500  -0.07144400
N   3.52076700   2.14476400   0.03209200
C   2.68422200   1.39764700  -0.70163800
C   3.03001200   0.29980800  -1.48413400
C   4.39187500  -0.06137100  -1.48618500
N   4.85043100  -1.11505900  -2.19951500
N   1.92271800  -0.22936800  -2.11714800
C   0.93933700   0.54102400  -1.72766400
N   1.32599900   1.54433000  -0.86927700
O  -5.56410900   1.24233400   0.51231000
O  -4.65932200   0.33060800  -1.78920000
H   0.00390700  -3.60338100  -0.97122000
H  -0.93687000  -0.66662700   1.28179300
H  -1.47763500  -1.85578800  -1.46389900
H  -1.80766600  -0.19581200  -0.88294500
H  -3.83150800  -2.01973900  -1.10751600
H  -3.73471600  -2.81957300   1.54567300
H  -2.67621600  -4.96222100   0.83533200
H  -4.05670900  -4.45497600  -0.17466700
H  -2.20343400  -5.08996500  -1.45447300
H  -2.66745800   1.26369900   1.73322800

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H	-3.54550400	2.78154900	1.41610200
H	-1.25376200	3.32522000	1.88720100
H	-2.39941700	4.07147100	-0.64625100
H	-0.90476200	2.66105100	-1.87717600
H	0.12586800	4.11608500	-1.73378400
H	1.17714600	3.19636300	0.31436600
H	-1.52076300	5.55122700	0.89194500
H	5.51881300	2.27947500	0.49156300
H	4.18225100	-1.79891100	-2.53171700
H	5.78625200	-1.44685600	-2.00413800
H	-0.09062500	0.43470000	-2.03883500
N	3.09181400	0.72732900	3.11252800
H	4.03781100	1.08921600	3.11472400
H	2.38250800	1.45079100	3.12252900
H	4.67732900	-2.54017800	0.65416100

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d(2pC)-B-form-pcm

C	-2.45510900	-4.32049000	0.23795100
O	-1.64392000	-4.27162400	-0.92881600
C	-2.50695100	-2.93804000	0.85823200
O	-1.22936000	-2.58168500	1.40325900
C	-2.86882600	-1.82778700	-0.13442300
O	-3.64132900	-0.86046100	0.57719000
C	-1.50656100	-1.28133900	-0.55192200
C	-0.64935300	-1.49333300	0.69740700
N	4.32933100	-0.57680100	1.73660300
C	3.20793400	0.06165900	2.14710000
N	1.94620200	-0.22348900	1.80213700
C	1.85924200	-1.24765000	0.96000900
C	2.94011200	-1.98428300	0.44520300
C	4.19907800	-1.59065500	0.88588800
N	2.48642200	-2.98250100	-0.40456300
C	1.18746400	-2.84777600	-0.39073700
N	0.73755600	-1.81280100	0.40736800
P	-4.32820800	0.39543800	-0.23734400
C	-2.63370500	2.00815800	0.93820000
O	-3.08421800	1.46961600	-0.29688300
C	-1.30823300	2.70049400	0.73152800
O	-0.32639700	1.74491700	0.34317500
C	-1.26933200	3.80978800	-0.35084700
O	-1.27255700	5.10912400	0.22211100
C	0.07071100	3.56553400	-1.05510200
C	0.74835100	2.50869600	-0.17384400
N	1.65877900	1.61783900	-0.87309900
C	3.04708200	1.71099600	-0.62658300
O	3.46623100	2.58580000	0.13544600
N	3.86423400	0.82539500	-1.25583700
C	3.36478700	-0.09486700	-2.06846300
C	1.96593000	-0.18638800	-2.37444500
C	1.15952000	0.70109700	-1.74654100
O	-5.39573100	0.93000100	0.67088500
O	-4.59213400	-0.00676000	-1.65756600
H	0.47642300	-3.47622300	-0.91442400
H	-0.62074600	-0.60404600	1.33363600
H	-1.11699500	-1.86745500	-1.38854300
H	-1.55716500	-0.22756700	-0.82702400
H	-3.44594900	-2.20264000	-0.98391900

H	-3.23220700	-2.95261300	1.67819800
H	-2.04231100	-5.02537400	0.96975000
H	-3.47778900	-4.63031100	-0.01348800
H	-1.61696500	-5.15235300	-1.33009400
H	-2.51243300	1.20846600	1.68028500
H	-3.36395200	2.72949000	1.32525900
H	-1.00697300	3.16240500	1.68537500
H	-2.10912000	3.70245700	-1.04453700
H	-0.08377400	3.16195900	-2.06018400
H	0.65614200	4.48438000	-1.13240300
H	1.32241600	2.96187300	0.63843800
H	-2.16563600	5.31486200	0.53760300
H	0.08448500	0.72422600	-1.88750400
N	4.22805200	-0.95281600	-2.64502700
H	5.18784800	-0.95913300	-2.32504000
H	3.88883800	-1.77683700	-3.12125200
H	1.57203000	-0.92586500	-3.06000800
N	3.38932500	1.07377500	3.06222800
H	4.30582500	1.50316300	3.02426800
H	2.63466900	1.74953700	3.08705700
H	5.10964500	-2.08849500	0.55795100

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d(2pG)-B-form-pcm

C	-3.39890400	-4.06535300	0.16079400
O	-2.60642500	-4.09532900	-1.01936800
C	-3.25680100	-2.70342300	0.81199500
O	-1.94159100	-2.53623200	1.35858700
C	-3.46641600	-1.53321800	-0.15495000
O	-4.11123400	-0.49074100	0.57618100
C	-2.04306800	-1.16092000	-0.56344300
C	-1.21258800	-1.53275500	0.66656000
N	3.85914300	-1.34881600	1.61192300
C	2.84716600	-0.56589900	2.05364600
N	1.54981900	-0.67427100	1.73972600
C	1.30459900	-1.66751400	0.89370800
C	2.25794700	-2.55634900	0.36368200
C	3.56779700	-2.34330300	0.77379800
N	1.64957100	-3.47481800	-0.47848900
C	0.38724600	-3.14217200	-0.45486600
N	0.10662800	-2.05226000	0.34842600
P	-4.61529500	0.86201800	-0.21685900
C	-2.79301100	2.23790700	1.06396900
O	-3.24877200	1.77604500	-0.20093300
C	-1.43929600	2.88549400	0.89117400
O	-0.47108200	1.87691900	0.57885900
C	-1.36878000	3.93818400	-0.24842800
O	-0.73351100	5.13561100	0.18199100
C	-0.44928600	3.27605900	-1.26621300
C	0.43891400	2.44152900	-0.34868700
N	4.99136200	0.33475600	-0.81197400
C	4.58290300	1.36108600	0.00055600
N	3.35559100	1.82521800	0.01787100
C	2.52654800	1.14459300	-0.80677100
C	2.81924200	0.06630800	-1.62902900
C	4.16390000	-0.42508900	-1.66112500
N	1.69029300	-0.36307600	-2.29646700
C	0.74761100	0.44696800	-1.89497500

N	1.19111800	1.39092500	-0.99012900
O	-5.64170900	1.49680200	0.67403800
O	-4.87649700	0.53522300	-1.65682100
H	-0.41648900	-3.65236900	-0.97286800
H	-1.04067600	-0.67380200	1.32247300
H	-1.74023800	-1.76049600	-1.42614500
H	-1.95257400	-0.09915300	-0.79818600
H	-4.08314200	-1.81097500	-1.01362000
H	-3.97419800	-2.63640600	1.63607900
H	-3.07299400	-4.83664800	0.86904800
H	-4.45741700	-4.22981000	-0.07904000
H	-2.70106300	-4.96178200	-1.44087200
H	-2.71085700	1.39981100	1.76838000
H	-3.49887000	2.97083100	1.47259400
H	-1.15716100	3.36887300	1.83678300
H	-2.36086500	4.15504500	-0.65607000
H	-1.02825400	2.61811500	-1.92110400
H	0.10322700	4.00343300	-1.86384800
H	1.17639600	3.06723100	0.16787800
H	-1.30887100	5.58934100	0.81682900
H	-0.28155600	0.41928100	-2.22449600
N	5.50271200	1.86256600	0.87198400
H	6.48652000	1.76637400	0.65131600
H	5.25311000	2.75717300	1.27704700
H	5.94784300	-0.00081800	-0.74035800
O	4.63265800	-1.36551800	-2.29592900
N	3.19491900	0.41417800	2.95653900
H	4.16261200	0.71069200	2.88500500
H	2.54401000	1.19016700	2.99340900
H	4.39380500	-2.96023600	0.42559200

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d(2pT)-B-form-pcm

C	2.39913300	-4.31505900	-0.50774000
O	1.58177400	-4.30875300	0.65581300
C	2.48093600	-2.90405400	-1.05619200
O	1.21772300	-2.50004200	-1.60257100
C	2.84451400	-1.85335300	-0.00088500
O	3.66015300	-0.87261500	-0.64129100
C	1.48533300	-1.29664300	0.41520300
C	0.63924800	-1.44334800	-0.85146400
N	-4.34042600	-0.42921700	-1.82182300
C	-3.21283700	0.19631600	-2.23860500
N	-1.95174600	-0.11685100	-1.91397400
C	-1.87008300	-1.16988500	-1.10769000
C	-2.95683000	-1.91288200	-0.61178300
C	-4.21519400	-1.48014700	-1.01437800
N	-2.50893000	-2.94992800	0.19234700
C	-1.20927300	-2.82937400	0.17452200
N	-0.75219600	-1.76702300	-0.58333300
P	4.32781200	0.33774700	0.25531500
C	2.72427500	2.00282100	-0.96791500
O	3.10420300	1.43690800	0.27885600
C	1.42977100	2.75947000	-0.79619400
O	0.38683600	1.84160200	-0.46627100
C	1.42558000	3.84970200	0.31280000
O	1.21914900	5.14688500	-0.22966400
C	0.20902100	3.48419600	1.16253900

C	-0.59746400	2.60187900	0.20890000
N	-1.53867100	1.69192500	0.83883300
C	-2.87968200	1.78643100	0.50764400
O	-3.33841100	2.61814400	-0.26158900
N	-3.67846500	0.85733900	1.13725500
C	-3.29783000	-0.13986800	2.03243400
O	-4.14113800	-0.88268800	2.51848500
C	-1.86748900	-0.18793300	2.31512200
C	-1.07816600	0.72514400	1.71104500
C	-1.36308000	-1.21897100	3.27863500
O	5.45686300	0.87885300	-0.57057300
O	4.49977400	-0.11842800	1.67314900
H	-0.50171100	-3.48710100	0.66658900
H	0.61992700	-0.52482000	-1.44525700
H	1.07438300	-1.90735300	1.22377600
H	1.55049100	-0.25549600	0.73277300
H	3.38943800	-2.28546900	0.84248500
H	3.21833600	-2.88763500	-1.86510300
H	1.97799000	-4.97427500	-1.27632200
H	3.41407600	-4.65627900	-0.26614000
H	1.53841600	-5.20670800	1.01539100
H	2.58795300	1.21276500	-1.71769100
H	3.50205300	2.68910900	-1.32470500
H	1.18398500	3.25178800	-1.74923000
H	2.35220500	3.82593500	0.89452900
H	0.51482600	2.90614700	2.03945100
H	-0.33812400	4.36986400	1.49159600
H	-1.17635900	3.20161000	-0.49920800
H	2.01233600	5.41631000	-0.71781700
H	-4.66728900	0.91353200	0.90810700
H	-1.63174700	-2.22557000	2.94314900
H	-0.27620800	-1.15799600	3.37679000
H	-1.80841300	-1.07411300	4.26850300
H	-0.00647000	0.74976400	1.87826200
N	-3.38813300	1.22847300	-3.12965600
H	-4.29895300	1.66852100	-3.07958500
H	-2.62356100	1.89311000	-3.15218000
H	-5.12950100	-1.97046400	-0.68616100

63

d (ApA) -B-form-pcm

C	2.70537500	-4.35252200	0.07258900
O	1.80875100	-4.21663000	1.16765500
C	2.83134600	-3.01347100	-0.62729500
O	1.60232900	-2.67079500	-1.28236000
C	3.14683400	-1.84836500	0.31713800
O	3.98261100	-0.93758900	-0.39749600
C	1.76996100	-1.25862300	0.60654100
C	0.99578500	-1.53501600	-0.68296000
N	-3.85265900	-0.46298400	-2.06522600
C	-2.67933300	0.06176700	-2.45477900
N	-1.45506500	-0.25647300	-2.04957500
C	-1.47392500	-1.23118400	-1.13014500
C	-2.60579100	-1.88252700	-0.64221700
C	-3.84371700	-1.44499300	-1.15309700
N	-2.26271300	-2.84762500	0.28341300
C	-0.95590300	-2.77154400	0.35120900
N	-0.41518900	-1.81010600	-0.47096700



P	4.60652200	0.37420500	0.37955000
C	3.04295200	1.90195700	-1.06167100
O	3.37276500	1.45370200	0.24609300
C	1.75547300	2.68959100	-1.00573200
O	0.67938700	1.80816800	-0.67254600
C	1.72916100	3.84057200	0.03893100
O	1.36935100	5.08079900	-0.55632700
C	0.59883700	3.43035900	0.97569900
C	-0.26509900	2.57104000	0.05440500
N	-5.16864100	1.12459400	0.62685500
C	-4.60147500	2.06473000	-0.14681300
N	-3.31684500	2.39061600	-0.25178900
C	-2.54924400	1.63368900	0.54503200
C	-2.98945600	0.62956000	1.40288000
C	-4.37737500	0.38459300	1.41832100
N	-4.92850600	-0.54750800	2.22499000
N	-1.93492500	0.06177000	2.08938700
C	-0.88836300	0.71781600	1.65725400
N	-1.18495700	1.68130500	0.72113600
O	5.75573800	0.83716700	-0.46599800
O	4.73722600	0.07878000	1.84378900
H	-0.31147700	-3.39664300	0.95787000
H	1.02630100	-0.68546400	-1.37159200
H	1.31504700	-1.78711800	1.44856100
H	1.82124100	-0.18973500	0.81734100
H	3.65817300	-2.17752900	1.22572900
H	3.61107300	-3.09298600	-1.39164500
H	2.33498200	-5.09577300	-0.64375600
H	3.69957800	-4.66173900	0.42061900
H	1.72477800	-5.07208100	1.61335000
H	2.91805800	1.04530600	-1.73686300
H	3.84339100	2.54084500	-1.45382700
H	1.56696200	3.12200900	-1.99902500
H	2.68820100	3.93098900	0.55817800
H	0.98717100	2.81139700	1.79030800
H	0.07109800	4.29159000	1.38970800
H	-0.87351500	3.18674700	-0.62004400
H	2.09484700	5.38254000	-1.12426300
H	-5.29036300	2.63128600	-0.76836800
H	-4.33124300	-1.22536700	2.67955800
H	-5.90083800	-0.79148300	2.09071800
H	0.12792100	0.55081800	1.98657900
H	-2.74802100	0.85170600	-3.19886200
N	-5.02142000	-2.01213700	-0.78543500
H	-5.85768600	-1.46922100	-0.96515800
H	-5.02858700	-2.55670200	0.06788600
61			
d (ApC) -B-form-pcm			
C	1.91513400	-4.54234400	-0.09617300
O	1.07849400	-4.34143100	1.03588200
C	2.17171900	-3.20288800	-0.75860100
O	0.97247400	-2.70302500	-1.36568800
C	2.64238600	-2.11442800	0.21265000
O	3.56896000	-1.28788100	-0.49196600
C	1.35213800	-1.37414500	0.55396700
C	0.51122900	-1.52842000	-0.71526400
N	-4.26811300	0.02970200	-1.89603000

C	-3.06689600	0.45025900	-2.32285600
N	-1.86102500	0.02295800	-1.96009300
C	-1.93509100	-0.96255900	-1.05480700
C	-3.10525300	-1.50072700	-0.51948700
C	-4.31418900	-0.93975600	-0.97228800
N	-2.82117300	-2.50884200	0.38133500
C	-1.51221400	-2.57305600	0.38192200
N	-0.91318800	-1.66137100	-0.45677000
P	4.37054400	-0.09479000	0.31366800
C	2.96861800	1.65466400	-1.03417200
O	3.27955400	1.13438200	0.25115500
C	1.77382500	2.57077600	-0.92593600
O	0.62986200	1.81134100	-0.54079800
C	1.89874800	3.73080000	0.10174700
O	1.89207400	5.00038300	-0.53746700
C	0.62430800	3.60034800	0.93619100
C	-0.26961900	2.73949500	0.04158600
N	-1.31821300	2.00200400	0.72422100
C	-2.67309800	2.27426500	0.42437700
O	-2.94832600	3.20391100	-0.33734900
N	-3.62078900	1.48856100	1.00332900
C	-3.27644200	0.51131600	1.82806800
C	-1.91693600	0.25677100	2.20865400
C	-0.97814600	1.02844100	1.61321400
O	5.54945200	0.25270800	-0.54626000
O	4.49628900	-0.45933900	1.76261400
H	-0.90912300	-3.27341300	0.94746400
H	0.60787800	-0.66660000	-1.38212400
H	0.86277900	-1.86128700	1.40146500
H	1.53586800	-0.32439200	0.78392400
H	3.12773500	-2.53273300	1.09842800
H	2.91663600	-3.34260900	-1.54853100
H	1.43675100	-5.21307100	-0.81997200
H	2.87793200	-4.97540500	0.20484600
H	0.90376800	-5.19697600	1.45408800
H	2.73830600	0.83655500	-1.72894200
H	3.82345600	2.21565500	-1.43107200
H	1.58965300	3.02066200	-1.91361100
H	2.79991900	3.62112900	0.71315000
H	0.83045000	3.07109600	1.87158500
H	0.18818400	4.57454600	1.16683500
H	-0.76391800	3.33608800	-0.72934100
H	2.72546600	5.11689700	-1.01907100
H	0.08386500	0.90735900	1.79542000
N	-4.26719700	-0.25019300	2.34391000
H	-5.15981500	-0.21222200	1.86302100
H	-4.02301200	-1.14985400	2.73816000
H	-1.65036400	-0.52501200	2.90865500
H	-3.08883800	1.24478200	-3.06456700
N	-5.51818600	-1.31592300	-0.46640100
H	-6.33951000	-1.05013800	-0.99596400
H	-5.56903200	-2.20875300	0.00888700
64			
d (ApG) -B-form-pcm			
C	3.18812200	-4.18935700	-0.00368000
O	2.31515300	-4.12936800	1.11681700
C	3.18854600	-2.84170800	-0.69843100

O	1.92070700	-2.59614200	-1.32233800
C	3.43225400	-1.65820700	0.24436700
O	4.17462500	-0.68153600	-0.48627600
C	2.01984100	-1.18174500	0.56996500
C	1.23877200	-1.51595400	-0.70159500
N	-3.71954600	-0.82870100	-1.93184000
C	-2.60464800	-0.20693600	-2.35069400
N	-1.34779500	-0.42609700	-1.98207800
C	-1.25993800	-1.40891400	-1.07492200
C	-2.31992700	-2.15788800	-0.56470000
C	-3.60371400	-1.81624500	-1.03222200
N	-1.87155900	-3.10381700	0.33474800
C	-0.57412000	-2.92105100	0.36641500
N	-0.13869400	-1.90776900	-0.45594700
P	4.72808600	0.66396600	0.28601700
C	3.00498900	2.09337300	-1.07045700
O	3.41288800	1.64895400	0.21656000
C	1.66243500	2.77582400	-0.95610700
O	0.66796400	1.80347000	-0.61954700
C	1.57987600	3.89024600	0.12472600
O	1.07762600	5.10700500	-0.41343100
C	0.53642700	3.35035400	1.09521400
C	-0.29981600	2.46494400	0.17401400
N	-4.98695800	0.65909700	0.71260300
C	-4.53370600	1.67444900	-0.09358000
N	-3.27749900	2.05293900	-0.14092000
C	-2.47816300	1.32532300	0.67289300
C	-2.82924800	0.28777600	1.52580200
C	-4.19804700	-0.12671700	1.57481200
N	-1.72532400	-0.19426300	2.19759200
C	-0.73739100	0.54380000	1.76771300
N	-1.12702500	1.48683100	0.83825200
O	5.80526500	1.22170700	-0.59637300
O	4.93907700	0.36178100	1.73938200
H	0.13766500	-3.49862700	0.94430100
H	1.18185800	-0.66417000	-1.38574300
H	1.62923400	-1.74801500	1.41972300
H	1.98807300	-0.11292900	0.78543800
H	3.99062300	-1.94779500	1.13864200
H	3.95331700	-2.85524800	-1.48164700
H	2.85758900	-4.95667500	-0.71415300
H	4.21304400	-4.42058100	0.31454300
H	2.31366000	-4.99000400	1.56046700
H	2.92442100	1.24210600	-1.75914200
H	3.73974800	2.80003400	-1.47471600
H	1.41169900	3.21910100	-1.93057200
H	2.54982800	4.05593100	0.60357200
H	1.01587700	2.73075400	1.85913500
H	-0.03669700	4.14702000	1.57327800
H	-0.97563300	3.06028100	-0.45207700
H	1.74120400	5.48998200	-1.00742700
H	0.29144800	0.46138200	2.08876800
N	-5.44833600	2.26624800	-0.90773000
H	-6.42555800	2.24689500	-0.64531600
H	-5.14216000	3.13358400	-1.33092800
H	-5.97041600	0.40409900	0.68257400
O	-4.71262400	-1.02833800	2.23135000

H	-2.76038400	0.58194500	-3.08280300
N	-4.72113500	-2.47631900	-0.63125100
H	-5.60473900	-2.02455300	-0.83450100
H	-4.67860300	-2.95952000	0.25797600

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d (ApT) -B-form-pcm

C	2.26628500	-4.40851800	-0.18463200
O	1.36160700	-4.26159300	0.90240200
C	2.48160700	-3.05401100	-0.83129400
O	1.28044000	-2.61310800	-1.48017900
C	2.85904600	-1.94497700	0.15760400
O	3.74129300	-1.05250600	-0.52356700
C	1.51484100	-1.29425800	0.46623900
C	0.74813600	-1.45972000	-0.84661200
N	-4.02632100	-0.00193300	-2.17698500
C	-2.82136800	0.40729400	-2.60963800
N	-1.61813800	-0.00342000	-2.22315600
C	-1.69752200	-0.97115700	-1.29675600
C	-2.87071600	-1.52040900	-0.78049100
C	-4.07853700	-0.96165400	-1.24232800
N	-2.59382500	-2.51673000	0.13460800
C	-1.28558000	-2.55652400	0.17186000
N	-0.68083100	-1.63804400	-0.65623300
P	4.45369600	0.17822100	0.30778900
C	2.89856600	1.85564100	-0.96520100
O	3.26494200	1.31563800	0.29621500
C	1.61488000	2.63744500	-0.82781500
O	0.54317600	1.75865500	-0.48774700
C	1.60189900	3.75824500	0.24612400
O	1.67656300	5.04989200	-0.33896000
C	0.23319800	3.58628300	0.91438500
C	-0.48492900	2.61239700	-0.02487500
N	-1.52494000	1.80636900	0.59451000
C	-2.84091600	2.04058500	0.23848600
O	-3.18924200	2.89530400	-0.56302100
N	-3.74880600	1.22687800	0.88227800
C	-3.48932100	0.21597400	1.80410400
O	-4.41127200	-0.45690000	2.25063800
C	-2.08310700	0.06280400	2.16228100
C	-1.18715200	0.85870000	1.54149500
C	-1.71788500	-0.96119800	3.19300200
O	5.58745800	0.64453300	-0.55623300
O	4.62880000	-0.21574800	1.74374000
H	-0.68555300	-3.24009800	0.76125100
H	0.85089200	-0.58948700	-1.50108400
H	1.02200100	-1.84963300	1.26823500
H	1.61276600	-0.24470000	0.74465400
H	3.35195100	-2.33573300	1.05192700
H	3.26181800	-3.15258100	-1.59293900
H	1.86410400	-5.10043000	-0.93437700
H	3.23479800	-4.78955900	0.16457700
H	1.20743600	-5.12951800	1.30278800
H	2.75757300	1.05096600	-1.69839600
H	3.68848000	2.52143000	-1.33425000
H	1.39424700	3.11021900	-1.79786400
H	2.41785400	3.62060100	0.96217200
H	0.33742900	3.13355600	1.90489700

H	-0.28972500	4.53980000	1.01445300
H	-0.95688900	3.13240500	-0.86353900
H	2.58221700	5.20777300	-0.64617900
H	-4.72089000	1.37101000	0.62133700
H	-2.08790700	-1.94787600	2.89871000
H	-0.63334700	-1.01406300	3.31906600
H	-2.16802500	-0.71544300	4.16067600
H	-0.12292700	0.79283400	1.74498600
H	-2.84075100	1.18558400	-3.36837200
N	-5.28369000	-1.37719400	-0.78147400
H	-6.08194100	-0.79204400	-0.99568600
H	-5.30385000	-1.84079600	0.11933900

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d(2pA)-Twisted-pcm

C	3.588088	-1.002591	-1.656884
C	2.508030	-0.129794	-1.420635
C	2.814503	1.071836	-0.784704
N	4.031613	1.476562	-0.394564
C	4.964768	0.576502	-0.689504
N	4.818574	-0.615206	-1.290512
N	1.613138	1.726994	-0.654397
C	0.663484	0.894803	-1.200742
N	1.153937	-0.224731	-1.674153
C	1.392451	2.979540	0.062247
O	0.563142	2.731693	1.182363
C	-0.702948	3.399597	1.063166
C	-0.781026	3.892873	-0.390728
C	0.688905	4.060150	-0.759518
C	-1.821678	2.461971	1.480533
O	-1.992483	1.424252	0.523910
P	-3.354805	1.294613	-0.398867
O	-2.909589	1.267666	-1.834684
O	-1.461373	5.127409	-0.517328
N	3.425996	-2.204271	-2.266396
O	-3.868603	-0.194504	0.057147
C	-3.438357	-1.412823	-0.562345
C	-3.634832	-2.522074	0.484701
O	-2.402118	-2.580981	1.221223
C	-1.435714	-1.728127	0.623038
C	-1.936767	-1.467358	-0.789381
C	-3.959860	-3.891114	-0.082001
O	-2.955263	-4.263766	-1.015347
N	-0.133928	-2.355824	0.673530
C	0.253949	-3.557390	0.117890
N	1.537232	-3.793224	0.211830
C	2.044481	-2.670552	0.855809
C	1.009105	-1.765641	1.139615
N	1.138071	-0.573501	1.705070
C	2.408574	-0.272491	1.999093
N	3.494558	-1.060038	1.803885
C	3.316512	-2.250827	1.234539
N	2.628461	0.947604	2.591123
O	-4.373557	2.278793	0.094199
H	-3.156723	-5.148028	-1.353966
H	4.203238	-2.859846	1.067557
H	-4.946403	-3.849543	-0.562208
H	-4.003218	-4.609152	0.746112

H	-4.435551	-2.236329	1.174818
H	-4.021435	-1.584306	-1.472067
H	-1.702820	-2.321230	-1.430371
H	-1.528774	-0.562766	-1.230472
H	-1.342229	-0.798848	1.192224
H	-0.484807	-4.212436	-0.330674
H	1.888504	1.625406	2.423042
H	3.565166	1.311830	2.462026
H	5.982758	0.832882	-0.406652
H	-2.750312	3.031922	1.590306
H	-1.572717	2.002439	2.442986
H	-0.701889	4.271501	1.731332
H	-1.260830	3.136240	-1.023122
H	-2.415769	4.959801	-0.547784
H	0.892211	3.972793	-1.828107
H	1.021982	5.044594	-0.413871
H	2.383922	3.286730	0.403887
H	-0.386422	1.167862	-1.201794
H	4.190795	-2.862206	-2.175657
H	2.498570	-2.612493	-2.249462

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d(2pC)-Twisted-pcm

C	2.506108	-3.526766	0.576378
C	1.205116	-3.485607	0.077283
C	0.437082	-2.402698	0.520259
N	0.815235	-1.448813	1.358763
C	2.091871	-1.575166	1.739242
N	2.943237	-2.575313	1.397907
N	-0.759780	-2.492382	-0.145664
C	-0.659486	-3.614470	-0.947058
N	0.483391	-4.238229	-0.842433
C	-1.721437	-1.418316	-0.109754
O	-2.548999	-1.558789	1.039630
C	-3.704637	-0.728513	0.856513
C	-3.775782	-0.394220	-0.657080
C	-2.699577	-1.304015	-1.268657
O	-3.640075	1.015040	-0.886880
P	-2.238153	1.850341	-0.953725
O	-2.588451	3.315140	-0.958692
C	-4.898826	-1.519920	1.359466
O	-5.055285	-2.725062	0.628481
N	2.576305	-0.613072	2.588178
O	-1.560631	1.470134	0.495895
C	-1.270005	2.443233	1.487511
C	0.110368	3.034440	1.293892
O	1.114958	2.030807	1.479421
C	2.263868	2.346075	0.704958
C	1.926453	3.628222	-0.078382
C	0.403681	3.593323	-0.100674
N	2.578356	1.185539	-0.146956
C	3.914005	0.727122	-0.200219
N	4.187293	-0.372153	-0.951052
C	3.224891	-0.976706	-1.636360
C	1.871964	-0.510045	-1.642937
C	1.598942	0.560626	-0.857346
O	4.783389	1.332743	0.436131
N	3.561667	-2.063264	-2.358679

O	-0.211026	4.835084	-0.343220
O	-1.345688	1.265856	-2.011135
H	-4.234564	-3.232466	0.739197
H	3.209140	-4.312141	0.306714
H	-5.814301	-0.939057	1.219113
H	-4.777462	-1.727135	2.430287
H	-3.592453	0.199860	1.427730
H	-4.761044	-0.636074	-1.059223
H	-3.161869	-2.276112	-1.471125
H	-2.249913	-0.896136	-2.173345
H	-1.125713	-0.510393	-0.009112
H	-1.471723	-3.914495	-1.596161
H	2.067082	0.266358	2.566493
H	3.584603	-0.526438	2.622314
H	-2.006943	3.253354	1.464111
H	-1.328283	1.936996	2.455420
H	0.248715	3.839316	2.032292
H	0.082039	2.876769	-0.862798
H	-1.128501	4.616481	-0.612813
H	2.388658	3.638744	-1.067541
H	2.267105	4.504126	0.484463
H	3.130259	2.468262	1.352549
H	0.586945	0.939269	-0.751399
H	1.089120	-1.007139	-2.204824
H	4.487950	-2.454328	-2.248752
H	2.850372	-2.646153	-2.777422

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d(2pG)-Twisted-pcm

C	3.316754	-1.289517	-1.747046
C	2.323308	-0.297378	-1.466332
C	2.700715	0.841830	-0.767168
N	3.922492	1.164702	-0.279078
C	4.825978	0.242571	-0.516367
N	4.565112	-0.906416	-1.218911
N	1.564760	1.600937	-0.667747
C	0.564773	0.882686	-1.293219
N	0.982028	-0.254709	-1.786110
C	1.440101	2.853401	0.072414
O	0.618310	2.647142	1.207159
C	-0.604597	3.393753	1.119133
C	-0.677728	3.906262	-0.327580
C	0.793128	3.991318	-0.719559
C	-1.770753	2.519573	1.543419
O	-2.023712	1.513088	0.572808
P	-3.352912	1.549980	-0.402492
O	-2.861044	1.490491	-1.822540
O	-1.298881	5.173626	-0.430468
N	6.083897	0.383354	-0.015209
O	3.208863	-2.353015	-2.351767
O	-4.045365	0.122903	0.012264
C	-3.704639	-1.130137	-0.595564
C	-4.037926	-2.222582	0.435893
O	-2.835578	-2.421006	1.198904
C	-1.775609	-1.658475	0.642512
C	-2.208198	-1.325383	-0.776717
C	-4.489882	-3.544104	-0.155384
O	-3.505929	-4.006816	-1.069896

N	-0.541466	-2.411904	0.704864
C	-0.271637	-3.654289	0.167570
N	0.987618	-3.998750	0.238951
C	1.606986	-2.908535	0.838850
C	0.659246	-1.913604	1.130725
N	0.900243	-0.733548	1.683366
C	2.196932	-0.538072	1.949949
N	3.210896	-1.407923	1.720112
C	2.919702	-2.586612	1.169511
N	2.526795	0.653574	2.550417
O	-4.268979	2.643010	0.063384
H	-3.791316	-4.858330	-1.431354
H	3.749781	-3.265351	0.981417
H	-5.454788	-3.394908	-0.657645
H	-4.627279	-4.263196	0.661491
H	-4.819842	-1.861223	1.111961
H	-4.270457	-1.245595	-1.524836
H	-2.038784	-2.188536	-1.426114
H	-1.695349	-0.459588	-1.185452
H	-1.602913	-0.752965	1.231275
H	-1.074983	-4.249729	-0.252136
H	1.839161	1.388261	2.397988
H	3.482901	0.947587	2.385195
H	-2.659934	3.142596	1.685525
H	-1.529037	2.023180	2.489149
H	-0.537894	4.255984	1.796627
H	-1.205164	3.184563	-0.961277
H	-2.260485	5.045741	-0.439899
H	0.972205	3.910588	-1.793103
H	1.194626	4.946006	-0.363243
H	2.454705	3.089464	0.400841
H	-0.455065	1.249850	-1.342052
H	5.307515	-1.588276	-1.346081
H	6.309273	1.317049	0.305450
H	6.848754	-0.099725	-0.469962

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d(2pT)-Twisted-pcm

C	-1.674802	0.713257	0.900724
N	-2.564603	1.366606	0.066602
C	-3.860832	0.913393	-0.093696
N	-4.171715	-0.195409	0.661502
C	-3.347691	-0.892818	1.542151
C	-1.996337	-0.363779	1.650190
C	-2.136252	2.538828	-0.713263
O	-1.004792	2.164600	-1.485317
C	0.048475	3.114673	-1.292744
C	-0.194452	3.654330	0.118919
C	-1.714059	3.751136	0.138337
C	1.397058	2.462885	-1.519883
O	1.664439	1.460952	-0.551001
P	2.362985	1.796453	0.898333
O	1.457043	1.235822	1.958568
O	0.471456	4.866892	0.373248
O	-4.681860	1.432260	-0.840634
O	-3.780449	-1.870676	2.142250
C	-1.019112	-1.055111	2.553144
O	3.731548	0.912473	0.810163



C	3.817080	-0.492786	0.538458
C	3.682778	-0.795486	-0.974154
O	2.434045	-1.472050	-1.153902
C	1.690526	-1.409008	0.053859
C	2.735508	-1.385424	1.159499
N	0.733031	-2.492183	0.078386
C	-0.487940	-2.386099	-0.536259
C	-1.218609	-3.512786	-0.137810
N	-0.446502	-4.309486	0.698909
C	0.688789	-3.669322	0.799021
N	-0.907507	-1.405759	-1.324383
C	-2.177747	-1.563126	-1.711204
N	-3.004354	-2.588878	-1.384912
C	-2.530807	-3.559258	-0.606170
N	-2.684449	-0.607030	-2.553042
C	4.796946	-1.678348	-1.498210
O	4.894463	-2.817214	-0.655005
O	2.771517	3.246572	0.923268
H	5.624410	-3.374238	-0.960405
H	-3.211932	-4.368361	-0.351698
H	5.732901	-1.104235	-1.491692
H	4.570790	-1.972407	-2.530563
H	3.671290	0.146383	-1.533968
H	4.806770	-0.773394	0.901099
H	3.172984	-2.380521	1.284868
H	2.351720	-1.007660	2.106920
H	1.084468	-0.500641	0.061562
H	1.531938	-3.996458	1.393002
H	-2.183448	0.275795	-2.556681
H	-3.693087	-0.539046	-2.604514
H	2.169530	3.239359	-1.498234
H	1.414605	1.971223	-2.496844
H	-0.061046	3.942363	-2.010676
H	0.117482	2.910635	0.857263
H	1.383314	4.605862	0.624458
H	-2.149639	3.722887	1.139298
H	-2.030061	4.674064	-0.359338
H	-2.976342	2.766981	-1.367826
H	-0.659254	1.102456	0.910409
H	-0.957230	-2.123396	2.315783
H	-0.029882	-0.598735	2.451592
H	-1.336089	-0.978893	3.599390
H	-5.116668	-0.549787	0.541818

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d (ApA) -Twisted-pcm

C	-3.666913	0.550091	1.627871
C	-2.356090	0.928870	1.279289
C	-2.242403	2.003782	0.397218
N	-3.250081	2.732743	-0.103880
C	-4.429397	2.305745	0.338845
N	-4.692176	1.277579	1.160747
N	-0.898937	2.128292	0.157396
C	-0.283047	1.146436	0.890655
N	-1.115887	0.402831	1.580640
C	-0.261498	3.022244	-0.809834
O	0.809804	2.318923	-1.402821
C	2.058071	2.965142	-1.126370

C	1.780714	3.851083	0.095098
C	0.340270	4.273734	-0.168153
C	3.148641	1.928469	-0.974205
O	2.966843	1.198031	0.235313
P	4.132754	0.105917	0.650657
O	3.913449	-0.214731	2.098659
O	2.622970	4.982681	0.167788
N	-3.921100	-0.510114	2.438678
O	3.701442	-1.189104	-0.270513
C	2.935467	-2.256159	0.290803
C	2.599715	-3.212138	-0.859264
O	1.363410	-2.733790	-1.408025
C	0.767171	-1.768985	-0.552387
C	1.557215	-1.804900	0.754607
C	2.468731	-4.666669	-0.449594
O	1.546382	-4.766036	0.627273
N	-0.644166	-2.062386	-0.389014
C	-1.223069	-3.015642	0.415689
N	-2.533611	-2.979823	0.415277
C	-2.839158	-1.941777	-0.444322
C	-1.681250	-1.362917	-0.957430
N	-1.619652	-0.327553	-1.805290
C	-2.831509	0.119896	-2.121878
N	-4.025655	-0.331330	-1.707469
C	-4.059088	-1.368389	-0.854833
H	-2.865816	0.964460	-2.806522
O	5.448414	0.586887	0.114435
H	1.441986	-5.698551	0.865394
N	-5.250377	-1.799009	-0.384586
H	3.457584	-5.040040	-0.152597
H	2.119139	-5.244429	-1.313675
H	3.365677	-3.140623	-1.638111
H	3.506856	-2.743313	1.086055
H	1.148837	-2.555133	1.433630
H	1.580045	-0.845308	1.267518
H	0.809999	-0.784342	-1.032632
H	-0.613580	-3.727257	0.957831
H	-5.299643	2.853776	-0.013776
H	4.121663	2.431788	-0.959907
H	3.125654	1.247569	-1.834914
H	2.323485	3.616200	-1.972098
H	1.855035	3.255173	1.013029
H	3.456999	4.733844	0.593252
H	-0.205502	4.587659	0.723373
H	0.343596	5.093913	-0.894269
H	-1.027474	3.248569	-1.556051
H	0.794731	1.032738	0.851608
H	-4.862758	-0.881840	2.388334
H	-3.191439	-1.210761	2.512168
H	-6.092490	-1.460181	-0.830590
H	-5.299572	-2.691666	0.087916
61			
d (ApC) -Twisted-pcm			
C	-0.675478	-1.604180	-0.747472
N	-1.039429	-2.673287	0.013888
C	-2.388196	-3.087471	0.073941
N	-3.317614	-2.347234	-0.591240

C	-2.953103	-1.301811	-1.319698
C	-1.586034	-0.902373	-1.464252
C	-0.030745	-3.397203	0.808352
O	0.690708	-2.448030	1.578427
C	2.092762	-2.574934	1.336418
C	2.179841	-3.184040	-0.065561
C	1.011970	-4.162578	-0.029360
C	2.760722	-1.226931	1.507040
O	2.301877	-0.310088	0.523349
P	3.051433	-0.149872	-0.930929
O	1.982992	-0.280101	-1.979344
O	3.431403	-3.766690	-0.341075
O	-2.683652	-4.095997	0.722571
N	-3.923296	-0.615937	-1.963849
O	3.567183	1.397641	-0.848499
C	2.731049	2.532891	-0.591738
C	2.413795	2.692703	0.917778
O	0.992402	2.544709	1.059280
C	0.474056	1.959923	-0.127111
C	1.341432	2.528294	-1.242357
N	-0.941552	2.246915	-0.220503
C	-1.901421	1.577731	0.505115
C	-3.118354	2.010189	-0.008575
N	-2.928952	2.915761	-1.034718
C	-1.626532	3.024289	-1.126607
N	-1.720594	0.666367	1.472079
C	-2.878860	0.181248	1.906428
N	-4.122600	0.497019	1.506691
C	-4.273692	1.411282	0.537210
H	-2.819862	-0.571507	2.689244
C	2.766370	4.064492	1.465942
O	2.106660	5.088622	0.739766
O	4.270250	-1.033304	-0.957262
H	1.152456	4.929508	0.826516
N	-5.512100	1.687844	0.076151
H	3.840509	4.240126	1.362604
H	2.505696	4.112334	2.530815
H	2.928075	1.910112	1.485590
H	3.318107	3.380099	-0.950386
H	1.069499	3.572942	-1.425965
H	1.294090	1.951409	-2.165221
H	0.557649	0.872595	-0.062363
H	-1.109974	3.646408	-1.844502
H	3.846814	-1.351960	1.445572
H	2.503981	-0.803612	2.482479
H	2.535907	-3.281813	2.055018
H	1.971001	-2.421124	-0.819878
H	4.002995	-3.020711	-0.618909
H	0.629306	-4.437185	-1.014531
H	1.310758	-5.072470	0.502507
H	-0.602305	-4.052767	1.461740
H	0.372000	-1.321004	-0.746472
H	-1.288424	-0.054944	-2.071969
H	-4.883937	-0.788096	-1.694383
H	-3.719372	0.296460	-2.351070
H	-6.307987	1.351634	0.602293
H	-5.651591	2.496273	-0.514949

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d (ApG) -Twisted-pcm

C	-3.614434	-1.961752	-0.804883
C	-2.318183	-2.355768	-0.421347
C	-1.266245	-1.608612	-0.947170
N	-1.371080	-0.593095	-1.815190
C	-2.638103	-0.342912	-2.128584
N	-3.747446	-0.950148	-1.675826
N	-0.129651	-2.137028	-0.383681
C	-0.550877	-3.171981	0.419957
N	-1.850396	-3.338061	0.428774
C	1.218323	-1.623085	-0.551258
O	1.944327	-2.447611	-1.452285
C	3.236944	-2.775543	-0.923356
C	3.445893	-1.832676	0.267291
C	2.021477	-1.590786	0.748314
O	4.067789	-0.653430	-0.244374
P	4.273677	0.669664	0.713753
O	5.495110	1.372352	0.200298
C	3.310283	-4.250206	-0.576464
O	2.418805	-4.519449	0.497065
H	-2.807352	0.466864	-2.834609
O	2.944998	1.560692	0.309141
C	2.991829	2.249846	-0.936368
C	1.726272	3.049539	-1.138446
O	0.623255	2.161188	-1.344167
C	-0.565226	2.715349	-0.819982
C	-0.199470	4.096577	-0.270140
C	1.289183	3.951195	0.021754
N	-1.065360	1.804488	0.209488
C	-2.371748	1.486778	0.440117
C	-2.341177	0.490303	1.409643
N	-1.042236	0.197527	1.770275
C	-0.313877	0.999645	1.033410
N	-3.445672	2.044112	-0.169899
C	-4.581132	1.511339	0.216069
N	-4.664491	0.511771	1.153135
C	-3.581316	-0.096824	1.819423
O	-3.788887	-1.006466	2.618063
N	-5.748882	1.912568	-0.357688
O	1.921193	5.214252	0.018797
O	4.102160	0.285483	2.152478
H	2.438479	-5.467581	0.691655
N	-4.725373	-2.589812	-0.346541
H	4.343399	-4.496308	-0.297632
H	3.036625	-4.833899	-1.463657
H	3.981466	-2.565739	-1.698020
H	4.077885	-2.273673	1.043668
H	1.730899	-2.411585	1.405335
H	1.915177	-0.654427	1.292470
H	1.100251	-0.624761	-0.989806
H	0.162905	-3.786301	0.952955
H	3.852391	2.928376	-0.953362
H	3.102803	1.532950	-1.760481
H	1.861228	3.678284	-2.031144
H	1.455569	3.437253	0.976841
H	2.790840	5.137053	0.439035

H	-0.803177	4.371831	0.596499
H	-0.329942	4.851897	-1.052820
H	-1.340910	2.751305	-1.589185
H	0.768125	1.060321	1.018827
H	-5.575296	0.124543	1.383904
H	-5.685900	2.776965	-0.881340
H	-6.611594	1.798933	0.159646
H	-5.612244	-2.124372	-0.493490
H	-4.643182	-3.137786	0.500483

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d (ApT) -Twisted-pcm

C	4.241606	1.516436	-0.562104
C	3.061001	2.111878	-0.067729
C	1.863413	1.566149	-0.516558
N	1.723531	0.558201	-1.392310
C	2.901656	0.095331	-1.794364
N	4.130601	0.502090	-1.432852
N	2.831358	3.137097	0.828093
C	1.524825	3.198058	0.912979
N	0.875499	2.274641	0.127656
C	-0.530808	1.920391	0.069554
O	-1.064632	2.348031	-1.171577
C	-2.462208	2.629181	-1.032058
C	-2.795271	2.535205	0.476650
C	-1.409817	2.573614	1.129501
O	-3.623545	1.408227	0.788434
P	-3.103525	-0.135233	0.897167
O	-4.322421	-1.019844	0.934478
C	-2.740798	4.002487	-1.608850
O	-2.100970	4.967445	-0.785927
H	2.876109	-0.726388	-2.507459
O	-2.350513	-0.311970	-0.550654
C	-2.810283	-1.235253	-1.526337
C	-2.151616	-2.586050	-1.336978
O	-0.750322	-2.470578	-1.585298
C	-0.035421	-3.428652	-0.821864
C	-1.067316	-4.137457	0.077468
C	-2.237434	-3.161704	0.078767
N	1.036069	-2.730790	-0.095478
C	0.733563	-1.739729	0.822182
C	1.660013	-1.047943	1.519570
C	3.064074	-1.332511	1.259261
N	3.284587	-2.322567	0.306235
C	2.347440	-3.035182	-0.411086
O	2.679263	-3.868163	-1.245273
O	4.014652	-0.776426	1.798926
C	1.316592	0.012821	2.521596
O	-3.486620	-3.741839	0.368901
O	-2.042552	-0.249667	1.955912
H	-2.297967	5.852106	-1.125110
N	5.469529	1.956838	-0.212916
H	-3.826878	4.162554	-1.629476
H	-2.358003	4.047388	-2.635848
H	-3.039320	1.879739	-1.584139
H	-3.390635	3.393920	0.790048
H	-1.143892	3.629632	1.230813
H	-1.367767	2.069388	2.094683

H	-0.563817	0.828815	0.129725
H	0.982839	3.885969	1.546851
H	-3.897514	-1.353386	-1.469801
H	-2.545412	-0.824607	-2.505167
H	-2.601702	-3.303515	-2.040583
H	-2.033228	-2.376245	0.809557
H	-4.058158	-2.990279	0.632827
H	-0.670501	-4.355760	1.071352
H	-1.372591	-5.077339	-0.394463
H	0.478676	-4.122877	-1.484245
H	-0.322266	-1.514725	0.950867
H	1.879385	0.930839	2.318849
H	0.243492	0.224559	2.493333
H	1.586166	-0.307923	3.534410
H	4.252803	-2.524781	0.072878
H	6.266418	1.377440	-0.442516
H	5.560442	2.571247	0.585149

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d(2pG)-Unstacked-pcm

H	-0.24656400	-0.47459200	-3.13057700
O	0.13537700	-0.35179100	-2.24941700
C	1.47355200	-0.82370500	-2.25215300
H	2.09332300	-0.25734100	-2.96211000
H	1.52435400	-1.88688100	-2.51553000
C	1.99824100	-0.63079900	-0.83981700
H	1.31900600	-1.11130900	-0.12613200
O	3.29148100	-1.23926600	-0.74664600
C	4.23407600	-0.29359100	-0.26056100
H	4.34583800	-0.38466700	0.82513800
N	5.52682300	-0.61362000	-0.82359800
C	5.86271900	-0.68708200	-2.16314300
H	5.13364700	-0.46624500	-2.93243800
N	7.09507500	-1.05279300	-2.38176200
C	7.62468200	-1.24176800	-1.11270900
C	8.86870500	-1.63471000	-0.62996000
H	9.70046400	-1.86984600	-1.29040900
N	9.08148600	-1.73886800	0.67910400
C	8.05791400	-1.45449100	1.52094400
N	8.34346000	-1.52463800	2.85867500
H	9.14861800	-2.08259000	3.11089000
H	7.55010500	-1.60389300	3.48154300
N	6.81996400	-1.07003900	1.18151900
C	6.65382900	-0.97894600	-0.13226900
C	3.67470100	1.06811100	-0.66035600
H	3.89879000	1.27174200	-1.71307700
H	4.05295500	1.88786600	-0.04779700
C	2.17826700	0.84842400	-0.46690700
H	1.56225800	1.49127400	-1.10369700
O	1.81468000	1.01249900	0.90130400
P	1.13362000	2.44176100	1.35329500
O	0.70219800	2.24875700	2.77607000
O	1.99559000	3.59023400	0.92143300
O	-0.17223400	2.47571300	0.35472900
C	-1.11926100	1.42140500	0.44452500
H	-1.60550400	1.43033800	1.42971300
H	-0.63258700	0.44904500	0.29909400
C	-2.13721300	1.62836800	-0.66481800

H	-1.61993900	1.69195000	-1.62741500
O	-3.01554400	0.49304900	-0.68610700
C	-4.34542600	0.89240700	-0.39493700
H	-4.93742700	0.94711500	-1.31332100
N	-4.96543000	-0.13486200	0.41892400
C	-4.49964700	-0.64799500	1.61188000
N	-5.26602800	-1.58659000	2.10029200
C	-6.29263300	-1.70192800	1.18537500
C	-6.11912700	-0.81302400	0.13250900
C	-4.22411200	2.25387000	0.28576900
H	-3.99772000	2.12765800	1.35018900
H	-5.13281700	2.85265600	0.19206800
C	-3.02819200	2.85299800	-0.45077700
H	-2.51199300	3.62870000	0.12422300
O	-3.39605000	3.33364900	-1.73707500
H	-3.96765000	4.10935000	-1.63054300
H	-3.57816000	-0.29365200	2.05485400
C	-7.43562200	-2.56417000	1.17107100
N	-8.21692800	-2.33396000	0.01999100
C	-7.95261800	-1.41658600	-0.96661000
N	-6.90739700	-0.62187200	-0.95075600
O	-7.77987300	-3.41556100	1.98490900
H	-9.03342500	-2.93304400	-0.06545400
N	-8.80414400	-1.39135300	-2.02574700
H	-9.75362300	-1.72054000	-1.90655600
H	-8.70642000	-0.58836900	-2.63452600

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d(2pT)-Unstacked-pcm

H	0.61080600	-1.15758400	-3.16449300
O	0.26945100	-0.81951500	-2.32388500
C	-1.09254500	-0.45544800	-2.48573600
H	-1.70615100	-1.32385700	-2.76523700
H	-1.21349800	0.31906100	-3.25243700
C	-1.54839400	0.08943700	-1.14334800
H	-0.87161900	0.89012300	-0.82316200
O	-2.87188700	0.61647500	-1.28920300
C	-3.72751700	0.04076800	-0.31172100
H	-3.78668400	0.68136900	0.57478800
N	-5.06491000	-0.01124600	-0.85832800
C	-5.47058100	-0.64751200	-2.01710800
H	-4.76604500	-1.20828100	-2.61828000
N	-6.73388500	-0.48571600	-2.29669800
C	-7.21155300	0.31134400	-1.26554100
C	-8.45370300	0.85625700	-0.95708500
H	-9.33093400	0.69163900	-1.57892100
N	-8.60811400	1.61138500	0.12721700
C	-7.52736300	1.83342500	0.91460800
N	-7.75039500	2.57258800	2.04593000
H	-8.57752900	3.15484000	2.03841800
H	-6.93418500	2.98611500	2.47772700
N	-6.28475400	1.36898400	0.72528900
C	-6.17810000	0.62090400	-0.36603600
C	-3.10811500	-1.31595800	0.00895400
H	-3.37524600	-2.04240000	-0.76622100
H	-3.40201900	-1.70713900	0.98410800
C	-1.61963800	-0.99110200	-0.05357000
H	-1.00049400	-1.85469900	-0.31623900

O	-1.17354300	-0.41825500	1.17288600
P	-0.39466300	-1.39552700	2.24452100
O	0.10431100	-0.48707400	3.32777300
O	-1.21693600	-2.61638700	2.53027900
O	0.85513700	-1.91838100	1.31195000
C	1.75347900	-0.95361700	0.78515600
H	2.32611300	-0.48883200	1.60007500
H	1.21006800	-0.17010000	0.24209100
C	2.67168400	-1.67341300	-0.18898400
H	2.06698900	-2.19721600	-0.93554900
O	3.48068900	-0.69275500	-0.85784200
C	4.85184300	-0.91310500	-0.57812000
H	5.33834300	-1.41675900	-1.41439400
N	5.50792100	0.38952600	-0.45156400
C	4.93596300	1.36817400	0.33717300
H	3.99050300	1.08350500	0.78721300
C	5.47053600	2.59194900	0.52586000
C	4.84441300	3.65563600	1.37566200
H	4.63041900	4.55003300	0.78207400
H	3.91119400	3.29787800	1.81647800
H	5.52047500	3.95439600	2.18297100
C	6.72875200	2.89350400	-0.14716800
O	7.33067800	3.95787300	-0.07215500
N	7.23725300	1.85511500	-0.92242300
H	8.11621200	2.02971300	-1.40186400
C	6.70168400	0.59886200	-1.11382900
O	7.25465000	-0.24318700	-1.80759500
C	4.87859900	-1.76009100	0.69174100
H	4.75890500	-1.12414300	1.57653100
H	5.80412500	-2.33092500	0.79663600
C	3.64529500	-2.63833900	0.49058300
H	3.23424700	-3.02761500	1.42778200
O	3.90001100	-3.69238800	-0.42851400
H	4.51521600	-4.32194800	-0.02236500

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d (ApG) -Unstacked-pcm

H	-0.24110600	-1.03365800	-2.80115000
O	0.11872100	-0.73947400	-1.95179200
C	1.45476800	-1.20065200	-1.82669400
H	2.09377300	-0.78854800	-2.62070400
H	1.50806500	-2.29505500	-1.86887400
C	1.94505700	-0.72650500	-0.46948600
H	1.24776400	-1.05688700	0.30906400
O	3.23450500	-1.29990700	-0.22523200
C	4.16574100	-0.27455400	0.08929200
H	4.25254800	-0.15147100	1.17406200
N	5.47189100	-0.69514800	-0.37035300
C	5.83398800	-1.04133600	-1.65206300
H	5.12178700	-1.00469200	-2.46646600
N	7.08150100	-1.42235400	-1.76026000
C	7.57415200	-1.32519100	-0.47342000
C	8.84228400	-1.58310900	0.08768100
N	9.87557500	-2.03866300	-0.64730200
N	9.00971700	-1.39084100	1.40680000
C	7.96479200	-0.96321600	2.13232300
H	8.16051400	-0.82779800	3.19308600
N	6.73041400	-0.68300500	1.72488300



C	6.59051000	-0.88279800	0.40665800
C	3.61959100	0.98186000	-0.58235000
H	3.87627100	0.98035600	-1.64728700
H	3.97974800	1.90615600	-0.12803500
C	2.11748900	0.79799600	-0.39362500
H	1.52171000	1.29908600	-1.16316400
O	1.71367800	1.22919800	0.90333800
P	1.02719900	2.71905200	1.04365600
O	0.55415000	2.81061500	2.46338100
O	1.90663400	3.75964700	0.41709500
O	-0.25008000	2.55379500	0.02179000
C	-1.21039600	1.54466800	0.29676600
H	-1.76270400	1.78741700	1.21510200
H	-0.72470600	0.56938900	0.42536400
C	-2.14506500	1.46968000	-0.89942200
H	-1.55767400	1.30317100	-1.80770700
O	-3.02941500	0.35515200	-0.71058600
C	-4.37327500	0.80141600	-0.61378000
H	-4.90046400	0.62689000	-1.55636900
N	-5.05553600	-0.00398300	0.37943500
C	-4.70568500	-0.16858800	1.70399300
N	-5.48773000	-0.99784100	2.34194000
C	-6.40213600	-1.40628500	1.39240300
C	-6.14482600	-0.80554900	0.16718200
C	-4.28836400	2.28842500	-0.27709700
H	-4.13781800	2.42866600	0.79880600
H	-5.18360500	2.83786600	-0.57654600
C	-3.03893500	2.70119100	-1.05193000
H	-2.55809100	3.59841600	-0.64861400
O	-3.31201300	2.85014400	-2.43911400
H	-3.88374300	3.62261200	-2.56607200
H	-3.85215200	0.34343400	2.12877500
C	-7.50253300	-2.31705300	1.49011400
N	-8.15827700	-2.43857100	0.24784100
C	-7.82026200	-1.78670300	-0.91214600
N	-6.81363900	-0.94798000	-1.00052100
O	-7.90172900	-2.95533400	2.45908600
H	-8.93387100	-3.09509600	0.24004900
N	-8.54940500	-2.08621400	-2.01934400
H	-9.49322300	-2.43560800	-1.91266900
H	-8.41411200	-1.46054900	-2.80368900
H	10.79438000	-2.08535400	-0.22815600
H	9.81015600	-2.05518600	-1.65559200

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d (ApT) -Unstacked-pcm

H	0.52958300	-0.24042900	-3.23722100
O	0.22856500	-0.10590500	-2.32691600
C	-1.14016600	0.26758300	-2.33782100
H	-1.76370000	-0.51800500	-2.78819400
H	-1.29845500	1.19997400	-2.89276100
C	-1.53621200	0.47325700	-0.88600100
H	-0.84412900	1.17956700	-0.41300900
O	-2.86326100	1.01036600	-0.84598700
C	-3.68408000	0.20254000	-0.01417000
H	-3.71841400	0.60714300	1.00290900
N	-5.03976100	0.26845400	-0.51544100
C	-5.48394500	-0.07801100	-1.77110600

H	-4.80654100	-0.47135200	-2.51827700
N	-6.76282600	0.13340500	-1.95228100
C	-7.19063000	0.65330600	-0.74613800
C	-8.45016000	1.08993400	-0.28525200
N	-9.55964500	1.01926900	-1.04684700
N	-8.54329800	1.56721600	0.96708500
C	-7.43661000	1.60443100	1.72536000
H	-7.57402700	2.00143500	2.72803600
N	-6.20237300	1.22163100	1.41180900
C	-6.13648400	0.75323000	0.15742300
C	-3.04936700	-1.18406700	-0.05249300
H	-3.34020900	-1.70439400	-0.97148700
H	-3.30694100	-1.80301500	0.80821600
C	-1.56503900	-0.83634000	-0.08418300
H	-0.95196800	-1.60513000	-0.56561300
O	-1.07757300	-0.56584800	1.22737400
P	-0.29732300	-1.77304200	2.02987000
O	0.25926800	-1.13703900	3.26832000
O	-1.14645900	-3.00820400	2.06908000
O	0.90880600	-2.10498700	0.96221000
C	1.81973100	-1.06814900	0.62975300
H	2.44853500	-0.82840100	1.49842400
H	1.28398000	-0.16207200	0.31944400
C	2.66057300	-1.56052800	-0.53660800
H	2.00005000	-1.87463900	-1.35073000
O	3.47511200	-0.47137500	-0.99830300
C	4.84811300	-0.79441200	-0.86768400
H	5.26447800	-1.09981600	-1.82854400
N	5.56790500	0.42028000	-0.48103100
C	5.08381600	1.20286600	0.54862300
H	4.15311700	0.84914000	0.97986800
C	5.68065500	2.33216200	0.98178000
C	5.14791700	3.18376400	2.09381500
H	4.94091700	4.19872800	1.74007700
H	4.22522300	2.75990100	2.49659100
H	5.87859800	3.26381900	2.90480600
C	6.91180600	2.74627400	0.31854700
O	7.56300800	3.74509800	0.60010100
N	7.33122100	1.90374100	-0.70718000
H	8.18984400	2.15924900	-1.18717000
C	6.73137800	0.74411300	-1.15109100
O	7.20810300	0.07262500	-2.05555400
C	4.90600600	-1.91936900	0.16255100
H	4.86307600	-1.50848000	1.17783600
H	5.80927500	-2.52704700	0.07123700
C	3.62597300	-2.68712000	-0.16152100
H	3.24876800	-3.27370600	0.68265300
O	3.78486400	-3.50226700	-1.31521300
H	4.39640500	-4.22523600	-1.10766000
H	-10.40629300	1.46722600	-0.72332100
H	-9.48301300	0.80069900	-2.03055300
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2 A-Dimer-Twisted-pcm			
N	0.003965	-0.005533	0.000929
C	-0.018669	0.023453	1.355435
N	1.036198	0.020270	2.180052
C	2.193561	-0.050707	1.532093

C	2.359384	-0.120084	0.137777
C	1.184436	-0.078857	-0.607033
N	3.459001	-0.108535	2.042828
C	4.311076	-0.237683	0.971298
N	3.703356	-0.245425	-0.185805
N	-1.262811	0.106533	1.932968
H	-2.014102	-0.272081	1.368629
H	-1.300617	-0.170258	2.906454
H	3.717513	-0.116749	3.021840
H	5.380071	-0.317973	1.115976
H	1.184652	-0.121377	-1.694752
N	0.060459	-3.174680	-1.257641
C	-1.092894	-3.120645	-0.570945
N	-1.274265	-3.081212	0.745223
C	-0.106751	-3.111688	1.404996
C	1.164108	-3.172657	0.833244
C	1.213862	-3.188637	-0.574976
N	0.121428	-3.085264	2.755178
C	1.480561	-3.126239	2.928664
N	2.147540	-3.182032	1.802210
H	-1.994279	-3.103569	-1.178482
H	-0.576948	-3.039244	3.487326
H	1.921090	-3.110555	3.916355
N	2.386908	-3.241212	-1.253778
H	3.221208	-2.931978	-0.768028
H	2.348838	-3.014522	-2.240233

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2|C-Dimer-Twisted-pcm

N	-0.329094	0.226102	-0.183107
C	-0.077440	0.104711	1.142646
N	1.247256	0.127564	1.505565
C	-1.593885	0.188579	-0.591554
C	-2.625646	0.022177	0.327160
C	-2.223911	-0.105426	1.669076
N	-0.975171	-0.074263	2.120510
N	-4.008229	-0.033174	0.225368
C	-4.412899	-0.187017	1.457327
N	-3.387093	-0.238650	2.374208
C	-1.261081	3.116735	2.310836
N	0.036032	3.087227	2.708698
C	1.107299	3.199815	1.816839
N	0.816772	3.351842	0.497495
C	-0.451207	3.384206	0.098028
C	-1.565053	3.269723	0.999622
O	2.257347	3.145089	2.265265
N	-0.684507	3.538055	-1.215484
H	-1.777131	0.298354	-1.658507
H	-5.444342	-0.271556	1.772088
H	1.426696	0.357090	2.475781
H	1.857356	0.606697	0.853677
H	-2.008122	3.005993	3.088689
H	-2.589696	3.291956	0.651213
H	0.094791	3.557240	-1.859524
H	-1.620690	3.515727	-1.593396
H	-3.481341	-0.353838	3.375992
H	0.271825	2.965423	3.687085

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## 2|G-Dimer-Twisted-pcm

N	-0.017649	-0.009426	0.048662
C	-0.009276	-0.003024	1.403907
N	1.063984	-0.019586	2.203829
C	2.207107	-0.053701	1.528698
C	2.342839	-0.068611	0.128650
C	1.150681	-0.042254	-0.587540
N	3.485326	-0.091044	2.008296
C	4.316581	-0.134230	0.912144
N	3.682431	-0.118741	-0.229251
N	-1.241023	0.069341	2.010880
C	-0.213707	-3.059898	1.379645
C	1.048540	-3.208765	0.815397
C	1.160753	-3.226176	-0.612480
N	-0.102991	-3.059974	-1.211719
C	-1.295818	-2.895690	-0.552524
N	-1.406527	-2.908420	0.755596
N	2.016823	-3.318945	1.792115
C	1.353330	-3.237665	2.916303
N	0.000338	-3.087029	2.725744
O	2.159164	-3.357949	-1.314538
N	-2.393536	-2.664532	-1.321502
H	3.769219	-0.110921	2.980071
H	-0.705289	-3.001070	3.447255
H	1.126603	-0.058000	-1.675692
H	5.391201	-0.172680	1.030069
H	-1.248472	-0.209146	2.984872
H	-1.995485	-0.334870	1.467586
H	1.781574	-3.279902	3.908024
H	-0.090290	-3.024689	-2.227099
H	-3.279470	-2.756522	-0.840121
H	-2.399071	-2.981318	-2.282807

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## 2|T-Dimer-Twisted-pcm

C	-0.006123	0.019434	-0.051574
C	0.031052	-0.043585	1.296758
N	1.209417	-0.066807	2.007500
C	2.449205	-0.040129	1.420438
N	2.403131	0.012270	0.044016
C	1.267102	0.045245	-0.766216
O	3.496168	-0.068050	2.053174
O	1.386359	0.092787	-1.984336
N	2.510903	-3.148301	1.546254
C	1.304583	-3.159803	0.896007
N	1.362325	-3.148998	-0.458391
C	0.220633	-3.212287	-1.138442
C	-0.995595	-3.284461	-0.467178
C	-0.912736	-3.271570	0.936854
N	0.202905	-3.216840	1.656211
N	-2.209459	-3.310310	1.366420
C	-2.998536	-3.347796	0.238093
N	-2.319925	-3.333529	-0.877098
H	0.285539	-3.194263	-2.224537
H	-4.076838	-3.385409	0.315396
H	2.499384	-2.858574	2.515893
H	3.305170	-2.825036	1.008984
H	-0.868514	-0.078988	1.902245

C	-1.272579	0.074296	-0.851143
H	-2.532047	-3.320921	2.326457
H	1.193756	-0.122574	3.019287
H	3.302260	0.024495	-0.429631
H	-2.141417	-0.089188	-0.207764
H	-1.380938	1.046597	-1.343818
H	-1.272575	-0.691851	-1.632405

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A|A-Dimer-Twisted-pcm

N	-0.007236	0.063143	-0.055762
C	-0.051299	0.101980	1.285468
N	0.958441	0.073196	2.150589
C	1.188869	-0.029627	-0.655700
C	2.344053	-0.092663	0.148762
C	2.140621	-0.025708	1.526798
N	3.684138	-0.251421	-0.148928
C	4.267981	-0.265411	1.025391
N	3.393769	-0.120029	2.068891
N	1.249489	-0.032799	-2.008677
C	-0.089879	-3.105393	1.430981
C	1.168107	-3.140810	0.829875
C	1.186174	-3.133781	-0.579389
N	0.017934	-3.111934	-1.236913
C	-1.119629	-3.079705	-0.522825
N	-1.271528	-3.072216	0.797432
N	2.172818	-3.167198	1.775969
C	1.530421	-3.146140	2.918164
N	0.167986	-3.116333	2.775742
N	2.343889	-3.177406	-1.282500
H	3.626160	-0.142146	3.054247
H	-0.513844	-3.077465	3.523373
H	-1.048220	0.164068	1.715655
H	5.330762	-0.374475	1.193381
H	-2.034625	-3.055741	-1.109502
H	1.992480	-3.152315	3.896097
H	2.287344	-2.979114	-2.273633
H	3.194424	-2.883028	-0.816593
H	0.402716	-0.270723	-2.509915
H	2.121429	-0.300800	-2.446202

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A|C-Dimer-Twisted-pcm

N	0.050077	0.045670	0.658950
C	-0.273751	-0.198967	1.938577
H	0.568719	-0.315821	2.616331
C	-0.937620	0.203981	-0.234934
C	-2.271629	0.122471	0.213535
C	-2.450222	-0.133305	1.572810
N	-1.482132	-0.310176	2.482564
N	-3.484007	0.298265	-0.424419
C	-4.368853	0.144693	0.530774
N	-3.808024	-0.118469	1.753118
C	-0.551810	2.954061	2.433235
N	0.751242	3.024186	2.061811
C	1.156754	3.211909	0.737230
N	0.185984	3.346075	-0.207170
C	-1.091898	3.271164	0.146015
C	-1.527832	3.078614	1.501424

O	2.365669	3.251123	0.488183
N	-2.013701	3.393463	-0.828378
N	-0.623577	0.410444	-1.535501
H	-5.441150	0.210982	0.407020
H	-0.746958	2.795779	3.487691
H	-2.577393	3.026216	1.763208
H	-1.701876	3.440014	-1.789623
H	-2.983936	3.166304	-0.657817
H	-4.305082	-0.267252	2.622946
H	1.489083	2.920253	2.748868
H	0.310493	0.750849	-1.729758
H	-1.354740	0.752769	-2.146059

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A|G-Dimer-Twisted-pcm

N	-0.047098	0.158635	-0.197559
C	-0.221176	0.270916	1.130069
N	0.691940	0.204459	2.093048
C	1.921073	-0.001924	1.596761
C	2.258131	-0.129870	0.248935
C	1.191375	-0.045685	-0.668594
N	3.108694	-0.134274	2.265500
C	4.075819	-0.342182	1.318405
N	3.612362	-0.342769	0.092310
N	1.382502	-0.132634	-2.008793
C	0.033020	-3.012993	1.327219
C	1.196066	-3.207594	0.589809
C	1.109179	-3.194478	-0.838970
N	-0.221967	-2.998600	-1.254179
C	-1.307996	-2.820615	-0.432255
N	-1.231692	-2.830893	0.877498
N	2.290090	-3.346460	1.418167
C	1.796359	-3.241015	2.625133
N	0.436377	-3.046733	2.628966
O	2.002026	-3.313842	-1.674300
N	-2.500380	-2.574350	-1.040476
H	3.244767	-0.108681	3.268654
H	-1.247303	0.430918	1.451613
H	-0.151159	-2.908420	3.442202
H	5.111636	-0.483861	1.595119
H	2.360099	-3.297263	3.546092
H	-0.351842	-2.959132	-2.261130
H	-3.309347	-2.654040	-0.436829
H	-2.646735	-2.903980	-1.986261
H	0.555915	-0.278003	-2.575570
H	2.222416	-0.597446	-2.331751

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A|T-Dimer-Twisted-pcm

N	0.033991	-0.116340	0.817740
C	0.409475	0.078935	2.092366
N	1.637215	0.200485	2.586638
C	2.567396	0.111928	1.624349
C	2.334711	-0.083430	0.263090
C	0.983643	-0.200974	-0.126887
N	3.930182	0.188375	1.735839
C	4.441672	0.040315	0.473200
N	3.519485	-0.126390	-0.443995
H	-0.404298	0.135569	2.811764

C	-1.209808	-3.084238	0.925922
N	-0.644397	-3.006751	2.173997
C	0.712040	-3.051195	2.396916
C	1.609353	-3.199683	1.398390
C	1.099364	-3.316906	0.036090
N	-0.288758	-3.267106	-0.083962
O	-2.414310	-3.015733	0.724716
C	3.092107	-3.250295	1.608016
O	1.794570	-3.447922	-0.965397
H	4.461072	0.324438	2.587640
H	-1.284592	-2.868020	2.947178
N	0.618255	-0.365976	-1.416954
H	5.507664	0.063994	0.292508
H	1.009117	-2.953920	3.435608
H	3.597562	-2.533303	0.952518
H	3.343801	-3.015793	2.645535
H	3.489425	-4.242330	1.367816
H	-0.669527	-3.347062	-1.022643
H	-0.343922	-0.616560	-1.606168
H	1.312624	-0.684204	-2.080598

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