

**Ground-State Destabilization in Orotate Phosphoribosyltransferases by
Binding Isotope Effects**

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Supporting Information

Optimized geometries from in vacuo calculations

OMP from *Hs*OPRT crystal structure (PDB code: 2WNS)

-2	1			
P		-3.07508475	-2.76672881	0.21948588
O		-2.47808475	-3.74572881	1.18148588
O		-3.23808475	-3.16572881	-1.23451412
O		-4.30708475	-2.07472881	0.72948588
C		-0.61408475	-1.73972881	0.01548588
O		-2.02208475	-1.56172881	0.21548588
C		-0.29908475	-1.10972881	-1.34051412
O		-0.19408475	0.34227119	-1.30451412
C		1.03091525	-1.56272881	-1.88151412
O		1.05950272	-1.48397722	-3.30905780
C		1.94791525	-0.54172881	-1.26451412
O		3.13925048	-0.41426650	-2.04513806
C		1.16791525	0.78627119	-1.26651412
N		1.49791525	1.53427119	-0.02351412
C		2.79291525	1.78227119	0.25948588
O		3.69691525	1.36527119	-0.52151412
N		3.16591525	2.41727119	1.40748588
C		2.22791525	2.85627119	2.28448588
O		2.61691525	3.49527119	3.40448588
C		0.87991525	2.65227119	2.03948588
C		0.50091525	1.99927119	0.87648588
C		-0.95808475	1.86827119	0.60448588
O		-1.39808475	2.56627119	-0.37051412
O		-1.67608475	1.17527119	1.32448588
H		4.13594376	2.56014762	1.60403362
H		0.14302082	2.99308683	2.73643013
H		1.40467491	1.36420686	-2.13532666
H		2.19217740	-0.82407206	-0.26175877
H		3.90647011	-0.50725549	-1.47564083
H		1.26891992	-2.54909060	-1.54189050
H		1.97081572	-1.46735115	-3.61044160
H		-1.06618544	-1.38369687	-2.03434265
H		-0.06622599	-1.24310456	0.78886491
H		-0.37243820	-2.78200750	0.00275451
H		-1.52046527	-3.69753701	1.13413091

D 8 13 14 21 -12.700 F
D 11 13 14 21 -125.500 F
D 7 13 14 21 -49.7700 F
D 8 13 14 15 167.367 F
D 11 13 14 15 54.5400 F
D 7 13 14 15 130.3200 F
D 8 7 5 6 79.0100 F
D 7 5 6 1 111.70 F
D 5 6 1 2 50.85 F
D 13 14 21 22 -4.685 F
D 14 21 22 24 116.07 F
D 12 11 13 14 -97.51 F

D 8 13 11 9 23.74 F
 D 13 11 9 7 -36.615 F
 D 11 9 7 8 35.38 F
 D 12 11 9 10 -37.98 F
 D 9 7 8 13 -22.44 F
 D 7 8 13 11 -0.65 F

END

Free OMPs in solution with varied O4'-C1'-N1-C2 dihedral angles

OMP1 (O4'-C1'-N1-C2 dihedral angle 81°)

-2	1			
C		-1.00307900	-0.82749000	0.15640800
C		-0.64394400	-1.62615700	-1.10802300
C		0.70137700	-2.24744400	-0.68031000
C		1.30514800	-1.20038300	0.28309000
C		2.45777900	-0.38241500	-0.29577500
H		-2.41558200	-2.42661500	-0.88627300
H		2.05072300	0.40198400	-0.94943900
H		-1.50232400	-1.49451800	0.86191100
H		-0.49516800	-0.93806100	-1.94611700
H		1.36454800	-2.43081100	-1.53846600
H		1.67437800	-1.72487200	1.17162700
H		3.09907100	-1.04488900	-0.89316700
O		-1.59381200	-2.62723900	-1.41999800
O		0.43606400	-3.46381800	0.00668300
O		0.20366500	-0.33962300	0.69121100
P		4.79880500	0.63862600	0.40987800
O		5.42117600	1.00771200	1.71806100
H		-0.42982700	-3.73060200	-0.36126800
N		-1.94902800	0.28903500	-0.06848300
C		-1.79226720	1.05360239	-1.23239418
O		-1.11753600	0.72661697	-2.19644675
N		-2.49197616	2.25394290	-1.22334464
C		-2.92381772	0.60736755	0.87476838
C		-3.41824538	2.71582310	-0.27555284
C		-3.38743857	-0.43055654	1.94907944
H		-2.35293496	2.82544898	-2.04591711
O		-3.97997404	3.79967157	-0.44207226
O		-3.79050670	0.05466793	3.01492710
O		3.22477200	0.18152100	0.75665700
C		-3.61751882	1.77711084	0.80042693
H		-4.35566978	1.98685546	1.56069821
O		5.38846500	-0.34577500	-0.57434400
O		4.52110900	2.03541800	-0.48520000
O		-3.38336018	-1.64359539	1.57935811
H		4.76154300	1.76096800	-1.37995000

D 15 1 19 20 81.00585 F

END

OMP2 (O4'-C1'-N1-C2 dihedral angle 111°)

-2	1			
C		-1.00307900	-0.82749000	0.15640800
C		-0.64394400	-1.62615700	-1.10802300
C		0.70137700	-2.24744400	-0.68031000
C		1.30514800	-1.20038300	0.28309000
C		2.45777900	-0.38241500	-0.29577500
H		-2.41558200	-2.42661500	-0.88627300
H		2.05072300	0.40198400	-0.94943900
H		-1.50232400	-1.49451800	0.86191100
H		-0.49516800	-0.93806100	-1.94611700
H		1.36454800	-2.43081100	-1.53846600
H		1.67437800	-1.72487200	1.17162700
H		3.09907100	-1.04488900	-0.89316700
O		-1.59381200	-2.62723900	-1.41999800
O		0.43606400	-3.46381800	0.00668300
O		0.20366500	-0.33962300	0.69121100
P		4.79880500	0.63862600	0.40987800
O		5.42117600	1.00771200	1.71806100
H		-0.42982700	-3.73060200	-0.36126800
N		-1.94902800	0.28903500	-0.06848300
C		-2.24998602	0.63343969	-1.39310980
O		-2.00852151	-0.06263255	-2.36715155
N		-2.87701026	1.86548437	-1.53238788
C		-2.47497365	1.01278701	0.99961717
C		-3.35487537	2.71905321	-0.52606663
C		-2.49461180	0.42668634	2.44960865
H		-3.06333820	2.13427806	-2.48926246
O		-3.92467012	3.76855791	-0.82916584
O		-2.44444159	1.26464247	3.36024052
O		3.22477200	0.18152100	0.75665700
C		-3.12934311	2.18979810	0.79591949
H		-3.51002361	2.72234210	1.65519320
O		5.38846500	-0.34577500	-0.57434400
O		4.52110900	2.03541800	-0.48520000
O		-2.64889660	-0.82927078	2.53292536
H		4.76154300	1.76096800	-1.37995000

D 15 1 19 20 111.00585 F

END

OMP3 (O4'-C1'-N1-C2 dihedral angle 141°)

-2	1			
C		-1.00307900	-0.82749000	0.15640800
C		-0.64394400	-1.62615700	-1.10802300
C		0.70137700	-2.24744400	-0.68031000
C		1.30514800	-1.20038300	0.28309000
C		2.45777900	-0.38241500	-0.29577500
H		-2.41558200	-2.42661500	-0.88627300

H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800
N	-1.94902800	0.28903500	-0.06848300
C	-2.73889308	0.25298915	-1.22547926
O	-2.90444670	-0.73300682	-1.92689422
N	-3.35649172	1.45958555	-1.53074784
C	-2.00839620	1.36968558	0.80898126
C	-3.39420991	2.63700882	-0.76794442
C	-1.46756291	1.26117011	2.27257228
H	-3.89822875	1.44802992	-2.38454206
O	-4.02509787	3.61375192	-1.17531233
O	-1.05661371	2.32059295	2.76519987
O	3.22477200	0.18152100	0.75665700
C	-2.67692714	2.50867957	0.47610546
H	-2.68618268	3.32525389	1.18320714
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	-1.59142918	0.12479921	2.82165524
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 141.00585 F

END

OMP4 (O4'-C1'-N1-C2 dihedral angle 171°)

-2 1			
C	-1.00307900	-0.82749000	0.15640800
C	-0.64394400	-1.62615700	-1.10802300
C	0.70137700	-2.24744400	-0.68031000
C	1.30514800	-1.20038300	0.28309000
C	2.45777900	-0.38241500	-0.29577500
H	-2.41558200	-2.42661500	-0.88627300
H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800

N	-1.94902800	0.28903500	-0.06848300
C	-3.12798612	0.01419218	-0.77441902
O	-3.56524914	-1.10487958	-0.99364136
N	-3.80194387	1.14500671	-1.21886398
C	-1.64910442	1.58243257	0.35394138
C	-3.52570935	2.49167366	-0.93637524
C	-0.58148881	1.84929552	1.46540709
H	-4.63389836	0.95058420	-1.75981566
O	-4.25434776	3.37673373	-1.38776206
O	0.00110958	2.93957829	1.38924580
O	3.22477200	0.18152100	0.75665700
C	-2.38149541	2.64831122	-0.07332125
H	-2.10489451	3.63404110	0.27120832
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	-0.49430547	0.96297230	2.36818280
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 171.00585 F

END

OMP5 (O4'-C1'-N1-C2 dihedral angle -159°)

-2 1			
C	-1.00307900	-0.82749000	0.15640800
C	-0.64394400	-1.62615700	-1.10802300
C	0.70137700	-2.24744400	-0.68031000
C	1.30514800	-1.20038300	0.28309000
C	2.45777900	-0.38241500	-0.29577500
H	-2.41558200	-2.42661500	-0.88627300
H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800
N	-1.94902800	0.28903500	-0.06848300
C	-3.31300798	-0.01896576	-0.16079032
O	-3.81386735	-1.07860784	0.18254267
N	-4.09400817	1.00603899	-0.68030532
C	-1.49337025	1.59402260	-0.24357489
C	-3.71413851	2.32199017	-0.98622819
C	-0.07381234	2.03347485	0.24439234
H	-5.07322495	0.77523107	-0.78247820
O	-4.55099246	3.12101218	-1.40958929
O	0.44531219	2.95574187	-0.39893589
O	3.22477200	0.18152100	0.75665700
C	-2.32220860	2.57127887	-0.70514219

H	-1.92191478	3.56596445	-0.83643391
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	0.34850113	1.46066069	1.29401562
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 -158.99415 F

END

OMP6 (O4'-C1'-N1-C2 dihedral angle -129°)

-2 1			
C	-1.00307900	-0.82749000	0.15640800
C	-0.64394400	-1.62615700	-1.10802300
C	0.70137700	-2.24744400	-0.68031000
C	1.30514800	-1.20038300	0.28309000
C	2.45777900	-0.38241500	-0.29577500
H	-2.41558200	-2.42661500	-0.88627300
H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800
N	-1.94902800	0.28903500	-0.06848300
C	-3.24438220	0.16239997	0.45098554
O	-3.58368428	-0.66123108	1.28650033
N	-4.15442622	1.07991868	-0.05937822
C	-1.58292253	1.40135013	-0.82346356
C	-3.90900795	2.17342491	-0.90414522
C	-0.08056500	1.76435739	-1.06330207
H	-5.09849132	0.96895627	0.28559355
O	-4.83554627	2.91510764	-1.23494544
O	0.15697038	2.36475267	-2.12020339
O	3.22477200	0.18152100	0.75665700
C	-2.51495258	2.29822326	-1.25006146
H	-2.18627277	3.13926503	-1.84292772
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	0.71116127	1.48450917	-0.11302408
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 -128.99415 F

END

OMP7 (O4'-C1'-N1-C2 dihedral angle -99°)

-2	1			
C		-1.00307900	-0.82749000	0.15640800
C		-0.64394400	-1.62615700	-1.10802300
C		0.70137700	-2.24744400	-0.68031000
C		1.30514800	-1.20038300	0.28309000
C		2.45777900	-0.38241500	-0.29577500
H		-2.41558200	-2.42661500	-0.88627300
H		2.05072300	0.40198400	-0.94943900
H		-1.50232400	-1.49451800	0.86191100
H		-0.49516800	-0.93806100	-1.94611700
H		1.36454800	-2.43081100	-1.53846600
H		1.67437800	-1.72487200	1.17162700
H		3.09907100	-1.04488900	-0.89316700
O		-1.59381200	-2.62723900	-1.41999800
O		0.43606400	-3.46381800	0.00668300
O		0.20366500	-0.33962300	0.69121100
P		4.79880500	0.63862600	0.40987800
O		5.42117600	1.00771200	1.71806100
H		-0.42982700	-3.73060200	-0.36126800
N		-1.94902800	0.28903500	-0.06848300
C		-2.94049700	0.50969257	0.89698370
O		-2.93637730	0.03541493	2.02242704
N		-3.96700906	1.34684978	0.47754040
C		-1.89376581	1.05604159	-1.23034392
C		-4.05810256	2.08578581	-0.71212039
C		-0.59993742	1.11405295	-2.10728047
H		-4.70292737	1.47985128	1.15821061
O		-5.03176322	2.81419208	-0.91062618
O		-0.78665489	1.32496577	-3.31334444
O		3.22477200	0.18152100	0.75665700
C		-2.90808174	1.90230943	-1.56206838
H		-2.82713397	2.46827660	-2.47858390
O		5.38846500	-0.34577500	-0.57434400
O		4.52110900	2.03541800	-0.48520000
O		0.49650045	1.02812757	-1.47592114
H		4.76154300	1.76096800	-1.37995000

D 15 1 19 20 -98.99415 F

END

OMP8 (O4'-C1'-N1-C2 dihedral angle -69°)

-2	1			
C		-1.00307900	-0.82749000	0.15640800
C		-0.64394400	-1.62615700	-1.10802300
C		0.70137700	-2.24744400	-0.68031000
C		1.30514800	-1.20038300	0.28309000
C		2.45777900	-0.38241500	-0.29577500
H		-2.41558200	-2.42661500	-0.88627300

H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800
N	-1.94902800	0.28903500	-0.06848300
C	-2.48277818	0.92985527	1.05769932
O	-2.04539179	0.82466445	2.19313184
N	-3.58197496	1.73530832	0.78658364
C	-2.34260988	0.65062212	-1.35519271
C	-4.12147257	2.08255570	-0.46160660
C	-1.49276419	0.25681007	-2.60780969
H	-3.99252413	2.17102220	1.60155595
O	-5.08706714	2.84530574	-0.52353260
O	-2.13272000	0.11499123	-3.65865787
O	3.22477200	0.18152100	0.75665700
C	-3.39625745	1.48962217	-1.55756094
H	-3.67278014	1.73278996	-2.57307889
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	-0.23796313	0.21380296	-2.42948840
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 -68.99415 F

END

OMP9 (O4'-C1'-N1-C2 dihedral angle -39°)

-2 1			
C	-1.00307900	-0.82749000	0.15640800
C	-0.64394400	-1.62615700	-1.10802300
C	0.70137700	-2.24744400	-0.68031000
C	1.30514800	-1.20038300	0.28309000
C	2.45777900	-0.38241500	-0.29577500
H	-2.41558200	-2.42661500	-0.88627300
H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800

N	-1.94902800	0.28903500	-0.06848300
C	-1.99387112	1.31030581	0.89006878
O	-1.14946660	1.49503872	1.75287451
N	-3.10249349	2.14120714	0.78494360
C	-2.80918734	0.29372355	-1.16455679
C	-4.08213802	2.16460009	-0.21972881
C	-2.51981309	-0.57767370	-2.43077332
H	-3.15763358	2.85727034	1.49683554
O	-4.98663938	3.00011174	-0.17738611
O	-3.52054789	-0.94095926	-3.06361721
O	3.22477200	0.18152100	0.75665700
C	-3.84867342	1.17074070	-1.23774691
H	-4.49662107	1.12987817	-2.10109283
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	-1.29543056	-0.74026704	-2.71821828
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 -38.99415 F

END

OMP10 (O4'-C1'-N1-C2 dihedral angle -9°)

-2 1			
C	-1.00307900	-0.82749000	0.15640800
C	-0.64394400	-1.62615700	-1.10802300
C	0.70137700	-2.24744400	-0.68031000
C	1.30514800	-1.20038300	0.28309000
C	2.45777900	-0.38241500	-0.29577500
H	-2.41558200	-2.42661500	-0.88627300
H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800
N	-1.94902800	0.28903500	-0.06848300
C	-1.60477807	1.54910278	0.43900854
O	-0.48866416	1.86691148	0.81962164
N	-2.65704134	2.45578598	0.47305973
C	-3.16847913	0.08097656	-0.70951690
C	-3.95063858	2.30993525	-0.05129799
C	-3.40588720	-1.16579911	-1.62360811
H	-2.42196398	3.35471606	0.87210913
O	-4.75738949	3.23712993	0.03506361
O	-4.57827119	-1.55994460	-1.68766312
O	3.22477200	0.18152100	0.75665700
C	-4.14410515	1.03110905	-0.68832020

H	-5.07790925	0.82109096	-1.18909400
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	-2.39255428	-1.57844014	-2.26474583
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 -8.99415 F

END

OMP11 (O4'-C1'-N1-C2 dihedral angle 21°)

-2 1			
C	-1.00307900	-0.82749000	0.15640800
C	-0.64394400	-1.62615700	-1.10802300
C	0.70137700	-2.24744400	-0.68031000
C	1.30514800	-1.20038300	0.28309000
C	2.45777900	-0.38241500	-0.29577500
H	-2.41558200	-2.42661500	-0.88627300
H	2.05072300	0.40198400	-0.94943900
H	-1.50232400	-1.49451800	0.86191100
H	-0.49516800	-0.93806100	-1.94611700
H	1.36454800	-2.43081100	-1.53846600
H	1.67437800	-1.72487200	1.17162700
H	3.09907100	-1.04488900	-0.89316700
O	-1.59381200	-2.62723900	-1.41999800
O	0.43606400	-3.46381800	0.00668300
O	0.20366500	-0.33962300	0.69121100
P	4.79880500	0.63862600	0.40987800
O	5.42117600	1.00771200	1.71806100
H	-0.42982700	-3.73060200	-0.36126800
N	-1.94902800	0.28903500	-0.06848300
C	-1.41975621	1.58226072	-0.17462017
O	-0.24004596	1.84063973	-0.35656239
N	-2.36497705	2.59475370	-0.06549893
C	-3.32421330	0.06938654	-0.11200062
C	-3.76220942	2.47961874	-0.00144504
C	-3.91356366	-1.34997843	-0.40259335
H	-1.98263740	3.53006918	-0.10522833
O	-4.46074479	3.49285148	0.05689084
O	-5.02247379	-1.57610817	0.10051858
O	3.22477200	0.18152100	0.75665700
C	-4.20339195	1.10814141	-0.05649926
H	-5.26088897	0.88916761	-0.08145177
O	5.38846500	-0.34577500	-0.57434400
O	4.52110900	2.03541800	-0.48520000
O	-3.23536087	-2.07612852	-1.19057864
H	4.76154300	1.76096800	-1.37995000

D 15 1 19 20 21.00585 F

END

OMP12 (O4'-C1'-N1-C2 dihedral angle 51°)

-2	1			
C		-1.00307900	-0.82749000	0.15640800
C		-0.64394400	-1.62615700	-1.10802300
C		0.70137700	-2.24744400	-0.68031000
C		1.30514800	-1.20038300	0.28309000
C		2.45777900	-0.38241500	-0.29577500
H		-2.41558200	-2.42661500	-0.88627300
H		2.05072300	0.40198400	-0.94943900
H		-1.50232400	-1.49451800	0.86191100
H		-0.49516800	-0.93806100	-1.94611700
H		1.36454800	-2.43081100	-1.53846600
H		1.67437800	-1.72487200	1.17162700
H		3.09907100	-1.04488900	-0.89316700
O		-1.59381200	-2.62723900	-1.41999800
O		0.43606400	-3.46381800	0.00668300
O		0.20366500	-0.33962300	0.69121100
P		4.79880500	0.63862600	0.40987800
O		5.42117600	1.00771200	1.71806100
H		-0.42982700	-3.73060200	-0.36126800
N		-1.94902800	0.28903500	-0.06848300
C		-1.48838199	1.40089499	-0.78639602
O		-0.47022903	1.42326297	-1.46052003
N		-2.30455900	2.52087401	-0.68642603
C		-3.23466101	0.26205902	0.46788804
C		-3.56733998	2.62818400	-0.08352801
C		-3.90681100	-1.08086097	0.90510104
H		-1.95737104	3.33634398	-1.17330006
O		-4.17619099	3.69875601	-0.11775301
O		-4.73413197	-0.98511897	1.82178606
O		3.22477200	0.18152100	0.75665700
C		-4.01064798	1.38119701	0.48842000
H		-4.99653098	1.31586703	0.92504203
O		5.38846500	-0.34577500	-0.57434400
O		4.52110900	2.03541800	-0.48520000
O		-3.59802100	-2.09997700	0.21646105
H		4.76154300	1.76096800	-1.37995000

D 15 1 19 20 51.00585 F

END

OMP13 (O4'-C1'-N1-C2 dihedral angle 180°)

-2	1			
C		0.88514100	1.19944400	0.58157400
C		-0.18081200	1.74194800	-0.41479500
C		-1.46070800	1.73760000	0.43336400
C		-1.24184700	0.52818900	1.33271900
C		-1.75593600	-0.80024200	0.76607000
H		0.97678400	2.99656600	-1.24016900

H	-1.36280200	-1.61033900	1.39249200
H	1.42327100	2.02463600	1.06290600
H	-0.30033100	1.04450200	-1.25364400
H	-2.35598100	1.62585700	-0.18774700
H	-1.69859200	0.69852100	2.31216300
H	-1.37469800	-0.94624400	-0.25113300
O	0.07466300	3.05948600	-0.86793900
O	-1.49901800	2.92581100	1.22991200
O	0.19518000	0.45384200	1.53968600
P	-4.01323600	-0.87140600	-0.64943000
O	-5.46143600	-0.77775300	-0.29100200
H	-1.04292500	3.58570100	0.68283700
N	1.92453300	0.32756100	-0.07770000
C	2.70130524	0.91323741	-1.05664304
O	2.63242729	2.10610963	-1.39973875
N	3.58250671	0.07134422	-1.69407204
C	2.29756545	-0.90755053	0.46512885
C	3.86074682	-1.28337368	-1.39048421
C	2.03234671	-1.26313702	1.97309655
H	4.11250041	0.49041140	-2.44545867
O	4.67180416	-1.89458688	-2.09080828
O	1.59788661	-2.39786560	2.21867170
O	-3.17583800	-0.81539800	0.79856300
C	3.16010218	-1.72142839	-0.22065189
H	3.38929093	-2.69223422	0.19753682
O	-3.31594900	0.02286500	-1.65150900
O	-3.65556000	-2.43688500	-1.14271700
O	2.47866176	-0.34157658	2.69305667
H	-3.08973600	-2.29638400	-1.91343500

D 15 1 19 20 -180.000 F

END