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Deoxy-phenyl-β -D-ribofuranose

Crystallization:
- about 5mg solute in about 200µl solvent (5-10% ethyl acetate in toluene)
- solved under heating and stepwise cooling to room temperature, 4°C (over night) and finally to -18°C (over the weekend).

Data collection and reduction:
- on an Enraf-Nonius CAD4 diffractometer (MoK$_\alpha$ λ=0.71069 Å) at room temperature
- crystal dimensions : 0.07 x 0.4 x 0.65 mm
- decay of control reflections during the measurement was observed
- data reduction with the program LAZY included decay correction

Structure determination and refinement:
- direct methods (SHELXS86)
- unrestraint refinement including all hydrogens, anisotropic temperature factors for all non hydrogens (SHELXL93)

Table 1: Crystal data

chemical formula	$C_{11}H_{14}O_4$
chemical formula weight	210.22
temperature	RT
wavelength	0.7107 Å
crystal system	monoclinic
space group (no)	$P2_1$ (4)
a (Å)	6.736(6)Å
b (Å)	6.780(2) Å
c (Å)	11.085(4)Å
α (°)	90
β (°)	99.64(6)
γ (°)	90
volume	501.2(5) Å^3
Z	2

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density	1.393 mg/mm^3
absorption coefficient	0.106mm^-1
F(000)	224
qmax	30°
h,k,l	$-9 \le h \le 9, 0 \le k \le 9\ 0 \le l \le 15$
number of reflections	1582
refinement	Full-matrix least-squares (F^2)
weighting scheme	$w = \frac{1}{\left[\sigma^2(F_{obs}^2) + (0.1001 * P)^2 + 0.0087 * P\right]}$ mit $P = \frac{\left[F_{obs}^2 + 2 * F_{calc}^2\right]}{3}$
extinction coefficient	0.0000(16)
number of parameters	193
max diffrence density	0.338
min diffrence density	-0.281 e.Å^-3
R factor (incl. I>2sigma(I))	**R1 = 0.0545**, wR2 = 0.1342

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Numbering:

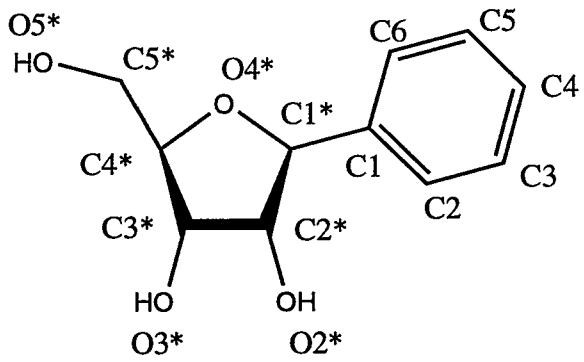

Table 2: Atom coordinates (fractional) and equivalent isotropic temperature factors (Å2)

ATOM	X	Y	Z	U(eq)
O5*	-0.6816(3)	-1.1930(4)	-0.3277(3)	0.0386(6)
H5O	-0.7354(53)	-1.3002(61)	-0.3699(30)	0.014(8)
C5*	-0.4693(5)	-1.2056(6)	-0.3231(4)	0.0335(8)
H51	-0.4329(62)	-1.3460(85)	-0.3364(40)	0.037(11)
H52	-0.4152(66)	-1.2017(82)	-0.2326(43)	0.041(12)
C4*	-0.3977(4)	-1.0581(4)	-0.4068(3)	0.0237(6)
H4*	-0.4782(58)	-1.0806(60)	-0.4863(38)	0.022(8)
O4*	-0.4251(3)	-0.8602(4)	-0.3649(2)	0.0289(5)
C3*	-0.1756(4)	-1.0751(5)	-0.4171(3)	0.0247(6)
H3*	-0.1331(49)	-1.2104(58)	-0.3976(32)	0.014(8)
O3*	-0.1388(4)	-1.0132(4)	-0.5342(2)	0.0339(6)
H3O	-0.1505(60)	-1.1048(73)	-0.5711(39)	0.026(11)
C2*	-0.0802(4)	-0.9302(5)	-0.3190(3)	0.0214(6)
H2*	-0.0843(61)	-0.9885(80)	-0.2324(39)	0.040(12)
O2*	0.1085(3)	-0.8516(4)	-0.3335(2)	0.0298(5)
H2O	0.1628(56)	-0.9566(64)	-0.3184(36)	0.022(9)
C1*	-0.2363(4)	-0.7643(5)	-0.3296(3)	0.0220(6)
H1*	-0.2113(69)	-0.6698(81)	-0.3918(43)	0.039(11)
C1	-0.2337(4)	-0.6441(5)	-0.2142(2)	0.0224(6)
C2	-0.0727(5)	-0.5202(6)	-0.1748(3)	0.0318(7)
H2	0.0342(59)	-0.5157(78)	-0.2167(38)	0.032(10)
C3	-0.0666(6)	-0.4096(6)	-0.0697(4)	0.0397(8)
H3	0.0477(91)	-0.3325(109)	-0.0500(50)	0.077(18)
C4	-0.2203(6)	-0.4199(7)	-0.0028(4)	0.0412(9)
H4	-0.2030(75)	-0.3384(95)	0.0497(44)	0.050(14)
C5	-0.3815(6)	-0.5418(8)	-0.0416(4)	0.0453(10)
H5	-0.4908(67)	-0.5630(65)	0.0047(43)	0.029(9)
C6	-0.3896(5)	-0.6538(6)	-0.1480(3)	0.0345(8)
H6	-0.4945(70)	-0.7431(86)	-0.1750(38)	0.046(13)

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Table 3: Bond distances [Å]

O5*	C5*	1.431(4)	C2*	C1*	1.533(4)
C5*	C4*	1.499(5)	C1*	C1	1.515(4)
C4*	O4*	1.442(4)	C1	C6	1.384(4)
C4*	C3*	1.530(4)	C1	C2	1.387(5)
O4*	C1*	1.427(4)	C2	C3	1.380(5)
C3*	O3*	1.425(4)	C3	C4	1.376(6)
C3*	C2*	1.526(5)	C4	C5	1.378(6)
C2*	O2*	1.416(4)	C5	C6	1.395(5)

Table 4: Bond angles [°]

O4*	C4*	C5*	110.4(3)	O4*	C1*	C2*	105.1(3)
O4*	C4*	C3*	106.0(2)	C1	C1*	C2*	114.8(2)
C5*	C4*	C3*	114.8(3)	C6	C1	C2	119.3(3)
C1*	O4*	C4*	110.8(2)	C6	C1	C1*	121.4(3)
O3*	C3*	C2*	110.0(3)	C2	C1	C1*	119.3(3)
O3*	C3*	C4*	111.7(3)	C3	C2	C1	120.4(3)
C2*	C3*	C4*	101.6(2)	C2	C3	C4	120.6(4)
O2*	C2*	C3*	116.3(2)	C5	C4	C3	119.4(4)
O2*	C2*	C1*	109.7(3)	C4	C5	C6	120.5(3)
C3*	C2*	C1*	102.4(2)	C1	C6	C5	119.8(3)
O4*	C1*	C1	111.1(2)	O5*	C5*	C4*	111.4(3)

Table 5: Torsion angles [°]

sugar pucker:

ν_0: -14.6 ν_1: 32.5 ν_2: -36.9 ν_3: 29.2 ν_4: -9.4

P: 175.7 C_2' endo

backbone:

γ: -174.2 δ: 149.8 χ(O4'-C1'-C1-C2): -171.7

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Picture of the structure:

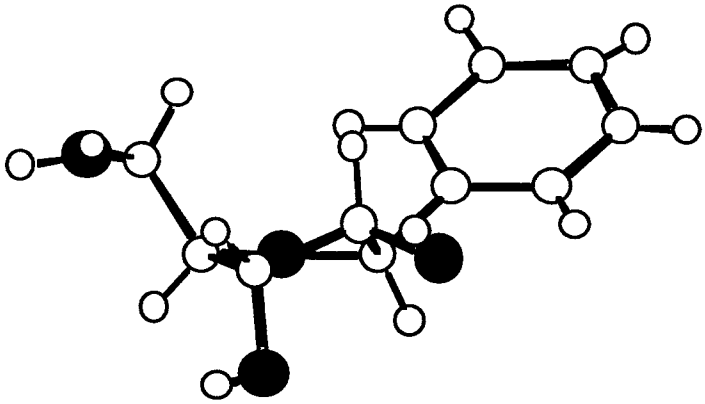

Table 6: Close contacts in the lattice [Å]

O5*	O2*	2.71	O4*	O2*	3.23
O5*	O3*	2.81			
O3*	O2*	2.75			

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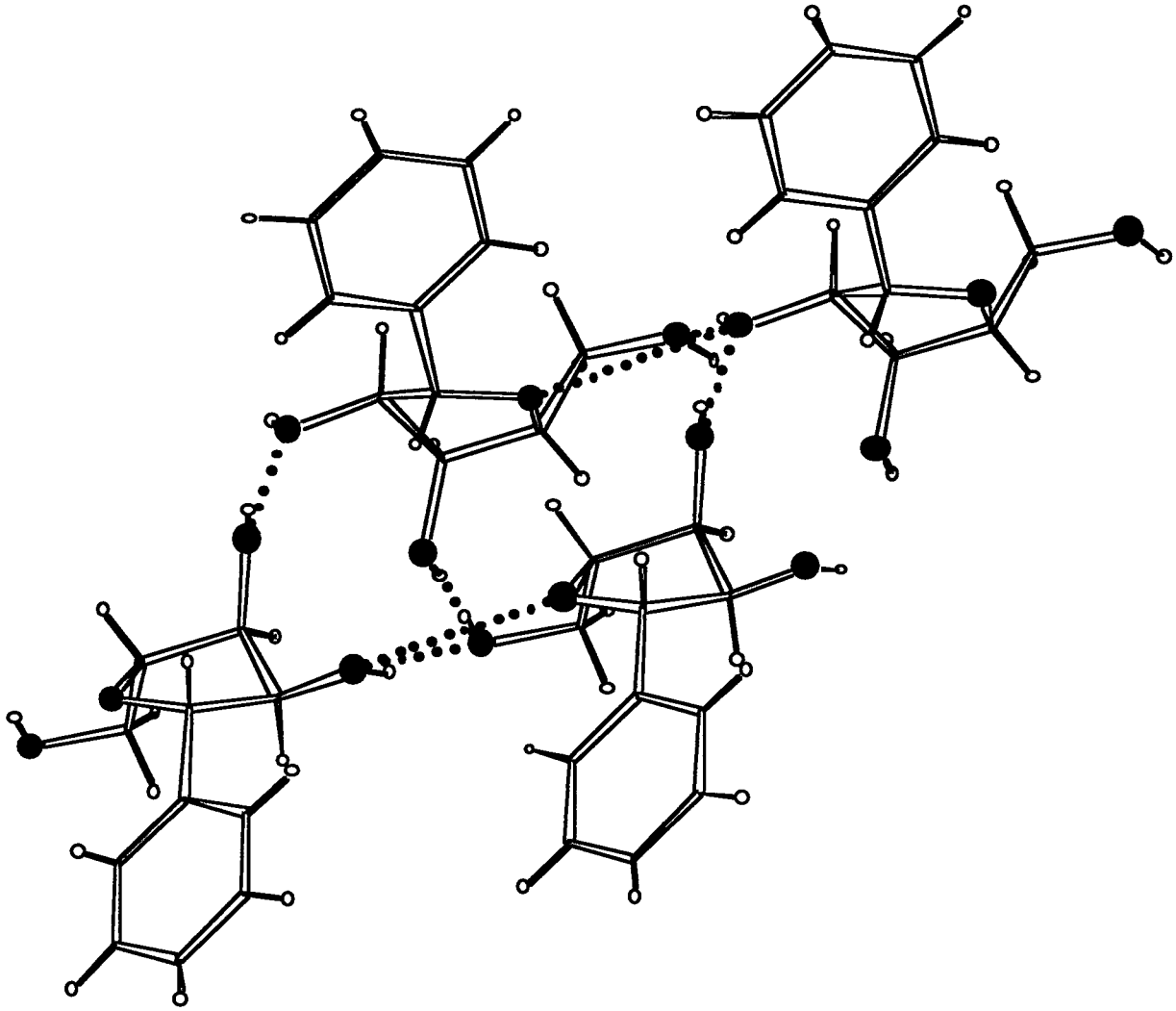
Packing arrangement:



March 95 Stefan Portmann