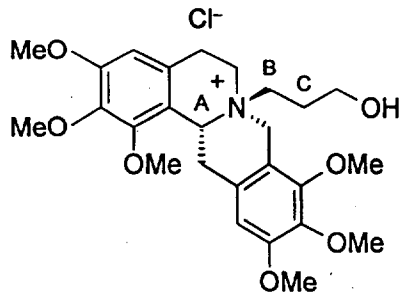
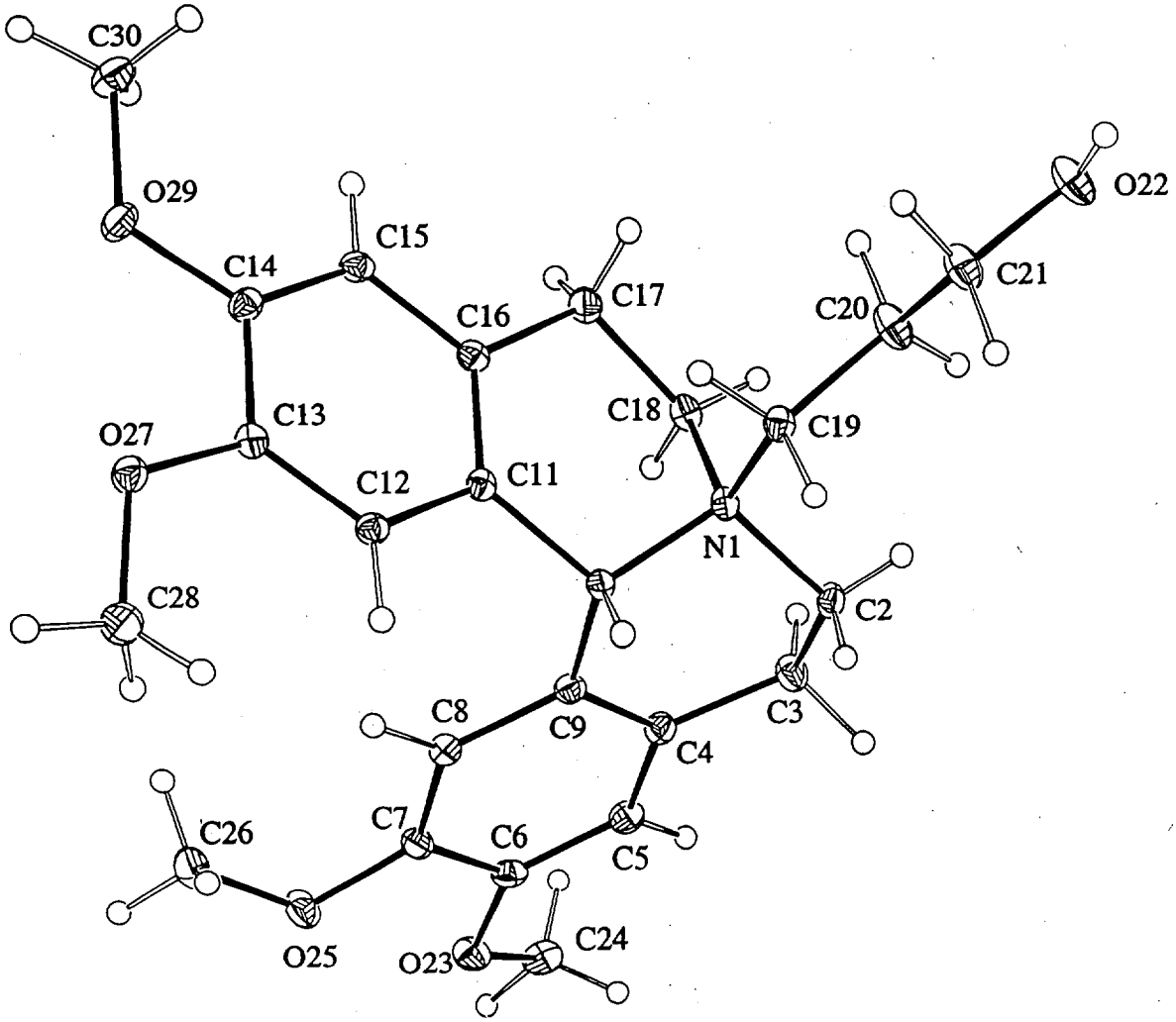


15

500 MHz 2D ROESY Spectrum of **15**
Solvent: DMSO-d_6

Crystal Structure Numbering System
and Conformation of **16**.



C2

Space Group and Cell Dimensions Monoclinic, P $2_1/c$
a 14.1397(6) b 12.0930(5) c 16.9352(7)
beta 108.194(1)
Volume 2751.00(20)A**3

Empirical formula : C24 H44 N O11 Cl

Cell dimensions were obtained from 6573 reflections with 2Theta angle in the range 3.00 - 60.00 degrees.

Crystal dimensions : 0.40 X 0.40 X 0.15 mm

FW = 558.06 Z = 4 F(000) = 1201.40

Dcalc 1.347Mg.m-3, mu 0.20mm-1, lambda 0.71073A, 2Theta(max) 60.0

The intensity data were collected on a Bruker SMART diffractometer, using the omega scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -19 18; Kmin,max 0 16; Lmin,max 0 23
No. of reflections measured 37693
No. of unique reflections 7912
No. of reflections with Inet > 2.5sigma(Inet) 5985
Merging R-value on intensities 0.026
No correction was made for absorption

Details of the last least squares cycle
81 atoms, 462 parameters Full-matrix on Fo Counter wts (k 0.000300)
The residuals are as follows :--
Significant reflections: 5985 Rf 0.057, Rw 0.079
All reflections: 7912 Rf 0.069, Rw 0.081
Included reflections: 7849 Rf 0.069, Rw 0.080 GoF 2.5349
where Rf = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.000.

In the last D-map, the deepest hole was -1.100e/A**3,
and the highest peak 0.830e/A**3.

The following references are relevant to the NRCVAX System.

1. Full System Reference :
Gabe, E.J., Le Page, Y., Charland,.J.-P., Lee, F.L. and White, P.S. (1989) J. Appl. Cryst., 22, 384-387.

2. Scattering Factors from Int. Tab. Vol. 4 :
International Tables for X-ray Crystallography, Vol. IV, (1974) Kynoch Press, Birmingham, England.

The following references may also be relevant.

3. ORTEP Plotting :
Johnson, C.K., (1976) ORTEP - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138, Oak Ridge

4. Pluto Plotting :
S. Motherwell, University Chemical Laboratory, Cambridge, 1978

5. Missing Symmetry Treatment by MISSYM :
Le Page, Y., (1988) J. Appl. Cryst., 21, 983-984.

6. Grouping of Equivalent Reflections in DATRD2 :
Le Page, Y. and Gabe, E.J., (1979) J. Appl. Cryst., 12, 464-466.

17-Nov-1999

Table . Atomic Parameters x,y,z and Biso.
E.S.Ds. refer to the last digit printed.

	x	y	z	Biso
Cl1	0.38550(5)	0.20284(6)	0.23966(4)	2.499(24)
N1	0.74370(13)	0.76904(15)	0.52144(11)	1.29 (6)
C2	0.66939(17)	0.67554(19)	0.49409(15)	1.67 (8)
C3	0.69091(17)	0.58083(20)	0.55554(17)	1.96 (9)
C4	0.79875(16)	0.54728(18)	0.58072(14)	1.53 (8)
C5	0.82619(18)	0.44497(19)	0.62138(15)	1.74 (9)
C6	0.92360(17)	0.40890(18)	0.64484(13)	1.60 (9)
C7	0.99621(16)	0.47450(18)	0.62572(13)	1.51 (8)
C8	0.96980(16)	0.57695(18)	0.58830(13)	1.47 (8)
C9	0.87069(16)	0.61523(17)	0.56596(13)	1.35 (8)
C10	0.84606(15)	0.72756(17)	0.52134(13)	1.23 (8)
C11	0.92389(15)	0.81665(17)	0.55598(12)	1.20 (7)
C12	1.00994(15)	0.81656(17)	0.53060(13)	1.26 (8)
C13	1.08514(15)	0.89305(17)	0.56256(13)	1.32 (7)
C14	1.07313(16)	0.97519(17)	0.61828(13)	1.38 (8)
C15	0.98770(16)	0.97643(18)	0.64084(13)	1.41 (8)
C16	0.91254(15)	0.89720(17)	0.61060(13)	1.32 (7)
C17	0.81855(17)	0.90673(20)	0.63435(15)	1.63 (9)
C18	0.75075(17)	0.80789(20)	0.60823(13)	1.49 (8)
C19	0.71051(16)	0.86151(18)	0.45724(13)	1.43 (8)
C20	0.61512(19)	0.91974(22)	0.45743(16)	2.12 (9)
C21	0.57845(18)	0.99380(22)	0.38195(16)	2.18 (10)
O22	0.48644(13)	1.04149(16)	0.38338(12)	2.61 (8)
O23	0.95729(12)	0.31244(13)	0.68587(11)	2.01 (7)
C24	0.89329(21)	0.25834(21)	0.72489(16)	2.13 (10)
O25	1.08980(12)	0.43041(14)	0.64696(11)	2.08 (7)
C26	1.16840(19)	0.50108(23)	0.63976(18)	2.23 (11)
O27	1.17235(11)	0.89813(13)	0.54396(10)	1.70 (6)
C28	1.19365(21)	0.80776(24)	0.49841(19)	2.45 (11)
O29	1.15101(12)	1.04715(13)	0.64560(10)	1.82 (6)
C30	1.13906(20)	1.13720(21)	0.69702(16)	2.07 (9)
O31	0.54369(20)	0.34678(20)	0.37130(14)	4.57 (12)
O32	0.68701(21)	0.2824 (3)	0.29358(20)	7.26 (18)
O33	0.65580(14)	0.37474(16)	0.13655(13)	3.06 (9)
O34	0.58165(15)	0.30928(16)	0.53969(12)	2.96 (8)
O35	0.52024(20)	0.06435(21)	0.15628(16)	4.73 (12)
O36	0.6974 (3)	0.0896 (4)	0.2494 (3)	9.19 (24)
H2a	0.6104 (19)	0.7050 (20)	0.4860 (15)	1.3 (5)
H2b	0.6742 (17)	0.6569 (20)	0.4401 (16)	1.3 (5)
H3a	0.6717 (23)	0.602 (3)	0.6041 (21)	3.5 (7)
H3b	0.6422 (19)	0.5182 (22)	0.5240 (17)	2.0 (5)
H5	0.7763 (19)	0.4016 (22)	0.6318 (16)	1.8 (5)
H8	1.0233 (20)	0.6237 (22)	0.5758 (17)	2.2 (6)
H10	0.8430 (18)	0.7150 (20)	0.4631 (16)	1.5 (5)
H12	1.0154 (18)	0.7634 (21)	0.4893 (16)	1.4 (5)
H15	0.9807 (18)	1.0262 (21)	0.6783 (17)	1.7 (5)
H17a	0.8316 (22)	0.9105 (25)	0.6862 (21)	2.9 (6)
H17b	0.7831 (20)	0.9713 (23)	0.6129 (17)	2.0 (5)
H18a	0.7754 (17)	0.7474 (20)	0.6431 (15)	0.9 (4)
H18b	0.6901 (20)	0.8214 (20)	0.6097 (16)	1.6 (5)
H19a	0.6994 (19)	0.8236 (21)	0.4059 (17)	1.6 (5)

H19b	0.7657	(18)	0.9114	(21)	0.4711	(15)	1.5 (5)
H20a	0.562	(3)	0.872	(3)	0.4618	(21)	4.3 (8)
H20b	0.6254	(23)	0.969	(3)	0.5083	(22)	3.6 (7)
H21a	0.574	(3)	0.950	(3)	0.3239	(24)	5.3 (9)
H21b	0.6235	(21)	1.0541	(24)	0.3828	(17)	2.4 (6)
H22	0.473	(3)	1.090	(3)	0.3469	(23)	4.4 (8)
H24a	0.8674	(21)	0.3066	(24)	0.7599	(19)	2.6 (6)
H24b	0.8372	(23)	0.2261	(25)	0.6885	(20)	3.0 (6)
H24c	0.9413	(23)	0.200	(3)	0.7612	(21)	3.4 (7)
H26a	1.1604	(20)	0.5213	(23)	0.5842	(19)	2.4 (6)
H26b	1.2271	(21)	0.4607	(22)	0.6678	(17)	2.0 (5)
H26c	1.1796	(21)	0.563	(3)	0.6732	(19)	2.7 (6)
H28a	1.146	(3)	0.779	(3)	0.455	(3)	5.7 (10)
H28b	1.1926	(19)	0.7368	(23)	0.5279	(17)	1.7 (5)
H28c	1.2566	(24)	0.824	(3)	0.4945	(20)	3.6 (7)
H30a	1.1282	(19)	1.1039	(22)	0.7502	(17)	1.9 (5)
H30b	1.1971	(21)	1.1810	(23)	0.7093	(17)	2.3 (6)
H30c	1.0830	(22)	1.1823	(24)	0.6673	(18)	2.4 (6)
H31a	0.481		0.385		0.357		5.4
H31b	0.559		0.318		0.427		5.4
H32a	0.643		0.223		0.267		8.2
H32b	0.652		0.331		0.320		8.2
H33a	0.665		0.340		0.190		3.9
H33b	0.608		0.433		0.129		3.9
H34a	0.557		0.356		0.574		3.8
H34b	0.606		0.242		0.569		3.8
H35a	0.567		0.117		0.189		5.9
H35b	0.459		0.068		0.170		5.9
H36a	0.739		0.041		0.291		10.0
H36b	0.699		0.160		0.270		10.7

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

7

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Cl1	3.15(3)	3.67(3)	2.49(3)	0.91(3)	0.619(23)	0.71(3)
N1	1.34(8)	1.76(8)	1.73(8)	-0.01(7)	0.39 (7)	0.29(7)
C2	1.43(10)	2.07(11)	2.61(12)	-0.27(8)	0.28 (9)	0.16(9)
C3	1.85(11)	2.21(11)	3.37(13)	-0.06(9)	0.82 (10)	0.60(10)
C4	1.85(10)	1.88(10)	2.07(10)	-0.15(8)	0.57 (8)	-0.02(8)
C5	2.52(11)	1.79(10)	2.32(11)	-0.32(9)	0.80 (9)	0.12(9)
C6	2.70(11)	1.50(10)	1.76(10)	0.17(8)	0.54 (9)	0.02(8)
C7	1.90(10)	1.91(10)	1.79(10)	0.34(8)	0.40 (8)	-0.15(8)
C8	1.84(10)	1.83(10)	1.88(10)	-0.05(8)	0.52 (8)	-0.09(8)
C9	1.86(10)	1.59(10)	1.61(10)	0.00(8)	0.43 (8)	-0.11(8)
C10	1.34(9)	1.75(10)	1.57(10)	0.01(7)	0.44 (8)	-0.01(8)
C11	1.49(9)	1.52(10)	1.42(9)	-0.01(7)	0.28 (7)	0.26(7)
C12	1.76(10)	1.50(10)	1.48(9)	0.05(8)	0.44 (8)	-0.01(8)
C13	1.61(10)	1.80(10)	1.61(9)	-0.01(8)	0.54 (8)	0.19(8)
C14	1.87(10)	1.62(10)	1.54(10)	-0.18(8)	0.21 (8)	0.08(8)
C15	2.07(10)	1.66(10)	1.51(10)	0.13(8)	0.40 (8)	-0.15(8)
C16	1.74(10)	1.72(10)	1.50(9)	0.16(8)	0.40 (8)	0.19(8)
C17	1.90(10)	2.54(12)	1.81(11)	0.07(9)	0.67 (8)	-0.37(9)
C18	1.73(10)	2.46(11)	1.59(10)	0.24(9)	0.71 (8)	0.32(8)
C19	1.74(10)	1.96(10)	1.56(10)	0.01(8)	0.30 (8)	0.36(8)
C20	2.30(12)	3.13(13)	2.74(12)	0.88(10)	0.97 (10)	1.16(10)
C21	2.34(12)	3.00(13)	2.86(13)	0.68(10)	0.72 (10)	1.01(10)
O22	2.98(10)	3.34(10)	3.56(10)	1.45(8)	0.97 (8)	1.45(8)
O23	2.89(9)	1.86(8)	2.93(9)	0.29(7)	0.97 (7)	0.61(7)
C24	3.64(14)	2.13(12)	2.37(12)	-0.36(10)	1.00 (11)	0.36(10)
O25	2.08(8)	2.46(9)	3.24(9)	0.56(7)	0.65 (7)	0.60(7)
C26	2.06(12)	2.98(13)	3.33(14)	0.21(10)	0.71 (10)	0.04(11)
O27	1.88(8)	2.20(8)	2.59(8)	-0.43(6)	1.03 (6)	-0.55(6)
C28	2.56(13)	3.42(14)	3.85(15)	-0.46(11)	1.76 (11)	-1.41(12)
O29	2.14(8)	2.21(8)	2.56(8)	-0.76(6)	0.75 (7)	-0.81(7)
C30	3.06(13)	2.24(12)	2.55(12)	-0.81(10)	0.89 (10)	-0.87(10)
O31	8.05(18)	5.46(14)	4.15(13)	-1.96(13)	2.34 (12)	-0.83(11)
O32	5.54(17)	15.3 (3)	7.43(20)	1.74(18)	3.00 (15)	5.17(21)
O33	3.62(11)	3.89(11)	4.45(12)	-0.08(8)	1.75 (9)	0.23(9)
O34	3.83(11)	3.83(11)	3.77(11)	-0.09(9)	1.48 (9)	-0.14(9)
O35	7.56(17)	6.04(15)	5.77(15)	3.26(13)	4.11 (13)	2.26(12)
O36	12.5 (3)	12.3 (3)	10.2 (3)	1.0 (3)	3.63 (24)	1.97(25)
H2a	1.7 (6)					
H2b	1.6 (6)					
H3a	4.4 (9)					
H3b	2.5 (7)					
H5	2.3 (7)					
H8	2.8 (7)					
H10	1.9 (6)					
H12	1.8 (6)					
H15	2.1 (6)					
H17a	3.6 (8)					
H17b	2.5 (7)					
H18a	1.2 (6)					
H18b	2.0 (6)					
H19a	2.0 (6)					
H19b	1.9 (6)					

H20a	5.5	(10)
H20b	4.6	(9)
H21a	6.7	(11)
H21b	3.1	(7)
H22	5.6	(11)
H24a	3.3	(8)
H24b	3.8	(8)
H24c	4.3	(9)
H26a	3.0	(7)
H26b	2.5	(7)
H26c	3.4	(8)
H28a	7.2	(12)
H28b	2.2	(7)
H28c	4.6	(9)
H30a	2.4	(7)
H30b	2.9	(7)
H30c	3.0	(7)
H31a	6.9	
H31b	6.9	
H32a	10.4	
H32b	10.4	
H33a	5.0	
H33b	5.0	
H34a	4.8	
H34b	4.8	
H35a	7.5	
H35b	7.5	
H36a	12.7	
H36b	13.5	

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

DISANG -- The NRCVAX Distance and Angle Program

The Space Group is P 2_1/C Centrosymmetric
The Equivalent Positions are:
1) x y z 2) -x 1/2+y 1/2-z

The Lattice is Primitive. There are no Centering Vectors

N(1)-C(2)	1.514(3)	C(21)-O(22)	1.430(3)
N(1)-C(10)	1.532(3)	C(21)-H(21a)	1.10(4)
N(1)-C(18)	1.516(3)	C(21)-H(21b)	0.97(3)
N(1)-C(19)	1.528(3)	O(22)-H(22)	0.83(4)
C(2)-C(3)	1.513(3)	O(23)-C(24)	1.434(3)
C(2)-H(2a)	0.88(3)	C(24)-H(24a)	0.98(3)
C(2)-H(2b)	0.96(3)	C(24)-H(24b)	0.92(3)
C(3)-C(4)	1.505(3)	C(24)-H(24c)	1.04(3)
C(3)-H(3a)	0.98(3)	O(25)-C(26)	1.437(3)
C(3)-H(3b)	1.05(3)	C(26)-H(26a)	0.94(3)
C(4)-C(5)	1.410(3)	C(26)-H(26b)	0.95(3)
C(4)-C(9)	1.390(3)	C(26)-H(26c)	0.92(3)
C(5)-C(6)	1.380(3)	O(27)-C(28)	1.423(3)
C(5)-H(5)	0.94(3)	C(28)-H(28a)	0.90(4)
C(6)-C(7)	1.413(3)	C(28)-H(28b)	1.00(3)
C(6)-O(23)	1.365(3)	C(28)-H(28c)	0.93(3)
C(7)-C(8)	1.389(3)	O(29)-C(30)	1.437(3)
C(7)-O(25)	1.367(3)	C(30)-H(30a)	1.04(3)
C(8)-C(9)	1.411(3)	C(30)-H(30b)	0.94(3)
C(8)-H(8)	1.02(3)	C(30)-H(30c)	0.96(3)
C(9)-C(10)	1.541(3)	O(31)-H(31a)	0.960(3)
C(10)-C(11)	1.521(3)	O(31)-H(31b)	0.9600(23)
C(10)-H(10)	0.98(3)	O(32)-H(32a)	0.960(4)
C(11)-C(12)	1.411(3)	O(32)-H(32b)	0.960(4)
C(11)-C(16)	1.387(3)	O(32)-H(36b)	1.552(4)
C(12)-C(13)	1.386(3)	O(33)-H(33a)	0.9600(20)
C(12)-H(12)	0.97(3)	O(33)-H(33b)	0.9600(20)
C(13)-C(14)	1.416(3)	O(34)-H(34a)	0.9600(19)
C(13)-O(27)	1.366(3)	O(34)-H(34b)	0.9600(20)
C(14)-C(15)	1.376(3)	O(35)-H(35a)	0.960(3)
C(14)-O(29)	1.366(3)	O(35)-H(35b)	0.9600(23)
C(15)-C(16)	1.404(3)	O(36)-H(36a)	0.960(4)
C(15)-H(15)	0.90(3)	O(36)-H(36b)	0.921(4)
C(16)-C(17)	1.508(3)	H(2a)-H(2b)	1.48(4)
C(17)-C(18)	1.509(3)	H(17a)-H(17b)	1.42(4)
C(17)-H(17a)	0.84(3)	H(18a)-H(18b)	1.47(4)
C(17)-H(17b)	0.94(3)	H(20a)-H(20b)	1.54(5)
C(18)-H(18a)	0.94(3)	H(24a)-H(24b)	1.51(4)
C(18)-H(18b)	0.88(3)	H(26a)-H(26c)	1.53(4)
C(19)-C(20)	1.522(3)	H(26b)-H(26c)	1.42(4)
C(19)-H(19a)	0.95(3)	H(28a)-H(28b)	1.31(5)
C(19)-H(19b)	0.96(3)	H(30b)-H(30c)	1.55(4)
C(20)-C(21)	1.514(3)	H(32a)-H(36b)	1.08334(3)
C(20)-H(20a)	0.96(4)	H(36a)-H(36b)	1.54494(6)
C(20)-H(20b)	1.02(3)		

C(2)-N(1)-C(10)	108.71(16)	H(19a)-C(19)-H(19b)	114.7(21)
C(2)-N(1)-C(18)	110.92(17)	C(19)-C(20)-C(21)	110.00(20)
C(2)-N(1)-C(19)	107.41(16)	C(19)-C(20)-H(20a)	115.3(20)
C(10)-N(1)-C(18)	109.04(16)	C(19)-C(20)-H(20b)	112.4(18)
C(10)-N(1)-C(19)	108.61(15)	C(21)-C(20)-H(20a)	110.6(20)
C(18)-N(1)-C(19)	112.06(17)	C(21)-C(20)-H(20b)	106.5(18)
N(1)-C(2)-C(3)	112.55(18)	H(20a)-C(20)-H(20b)	101(3)
N(1)-C(2)-H(2a)	106.3(16)	C(20)-C(21)-O(22)	107.33(20)
N(1)-C(2)-H(2b)	102.5(14)	C(20)-C(21)-H(21a)	112.0(19)
C(3)-C(2)-H(2a)	113.1(16)	C(20)-C(21)-H(21b)	112.6(17)
C(3)-C(2)-H(2b)	114.6(14)	O(22)-C(21)-H(21a)	114.2(19)
H(2a)-C(2)-H(2b)	106.9(22)	O(22)-C(21)-H(21b)	107.2(16)
C(2)-C(3)-C(4)	111.55(19)	H(21a)-C(21)-H(21b)	103.6(25)
C(2)-C(3)-H(3a)	109.5(18)	C(21)-O(22)-H(22)	106.0(24)
C(2)-C(3)-H(3b)	103.7(14)	C(6)-O(23)-C(24)	117.01(18)
C(4)-C(3)-H(3a)	110.8(18)	O(23)-C(24)-H(24a)	114.6(17)
C(4)-C(3)-H(3b)	113.3(14)	O(23)-C(24)-H(24b)	114.8(19)
H(3a)-C(3)-H(3b)	107.7(23)	O(23)-C(24)-H(24c)	101.2(17)
C(3)-C(4)-C(5)	118.34(20)	H(24a)-C(24)-H(24b)	104.4(25)
C(3)-C(4)-C(9)	121.56(20)	H(24a)-C(24)-H(24c)	110.3(25)
C(5)-C(4)-C(9)	120.09(20)	H(24b)-C(24)-H(24c)	111.8(25)
C(4)-C(5)-C(6)	121.04(21)	C(7)-O(25)-C(26)	117.17(18)
C(4)-C(5)-H(5)	118.2(16)	O(25)-C(26)-H(26a)	112.5(17)
C(6)-C(5)-H(5)	120.7(16)	O(25)-C(26)-H(26b)	103.2(16)
C(5)-C(6)-C(7)	119.22(20)	O(25)-C(26)-H(26c)	114.7(18)
C(5)-C(6)-O(23)	125.10(20)	H(26a)-C(26)-H(26b)	116.5(23)
C(7)-C(6)-O(23)	115.68(19)	H(26a)-C(26)-H(26c)	110.4(25)
C(6)-C(7)-C(8)	119.63(20)	H(26b)-C(26)-H(26c)	98.8(24)
C(6)-C(7)-O(25)	115.71(19)	C(13)-O(27)-C(28)	116.71(18)
C(8)-C(7)-O(25)	124.65(20)	O(27)-C(28)-H(28a)	120(3)
C(7)-C(8)-C(9)	121.21(20)	O(27)-C(28)-H(28b)	110.6(15)
C(7)-C(8)-H(8)	118.6(15)	O(27)-C(28)-H(28c)	104.0(19)
C(9)-C(8)-H(8)	120.2(15)	H(28a)-C(28)-H(28b)	87(3)
C(4)-C(9)-C(8)	118.65(19)	H(28a)-C(28)-H(28c)	120(3)
C(4)-C(9)-C(10)	122.92(19)	H(28b)-C(28)-H(28c)	112.5(24)
C(8)-C(9)-C(10)	118.32(18)	C(14)-O(29)-C(30)	116.95(18)
N(1)-C(10)-C(9)	110.92(16)	O(29)-C(30)-H(30a)	107.9(14)
N(1)-C(10)-C(11)	109.74(16)	O(29)-C(30)-H(30b)	107.4(17)
N(1)-C(10)-H(10)	107.8(14)	O(29)-C(30)-H(30c)	110.2(17)
C(9)-C(10)-C(11)	114.19(17)	H(30a)-C(30)-H(30b)	112.4(22)
C(9)-C(10)-H(10)	106.7(14)	H(30a)-C(30)-H(30c)	110.5(22)
C(11)-C(10)-H(10)	107.2(14)	H(30b)-C(30)-H(30c)	108.3(24)
C(10)-C(11)-C(12)	118.09(18)	H(31a)-O(31)-H(31b)	109.47(23)
C(10)-C(11)-C(16)	122.31(18)	H(32a)-O(32)-H(32b)	109.5(3)
C(12)-C(11)-C(16)	119.60(19)	H(32a)-O(32)-H(36b)	43.62(17)
C(11)-C(12)-C(13)	120.66(19)	H(32b)-O(32)-H(36b)	144.7(3)
C(11)-C(12)-H(12)	119.3(14)	H(33a)-O(33)-H(33b)	109.47(19)
C(13)-C(12)-H(12)	120.0(14)	H(34a)-O(34)-H(34b)	109.47(19)
C(12)-C(13)-C(14)	119.43(19)	H(35a)-O(35)-H(35b)	109.47(24)
C(12)-C(13)-O(27)	125.30(19)	H(36a)-O(36)-H(36b)	110.4(4)
C(14)-C(13)-O(27)	115.26(18)	C(2)-H(2a)-H(2b)	38.5(14)
C(13)-C(14)-C(15)	119.40(19)	C(2)-H(2b)-H(2a)	34.5(13)
C(13)-C(14)-O(29)	114.88(18)	C(17)-H(17a)-H(17b)	39.3(18)
C(15)-C(14)-O(29)	125.72(19)	C(17)-H(17b)-H(17a)	34.7(16)
C(14)-C(15)-C(16)	121.44(20)	C(18)-H(18a)-H(18b)	34.9(13)

C(14)-C(15)-H(15)	120.1(16)	C(18)-H(18b)-H(18a)	37.5(14)
C(16)-C(15)-H(15)	118.4(16)	C(20)-H(20a)-H(20b)	40.6(19)
C(11)-C(16)-C(15)	119.40(19)	C(20)-H(20b)-H(20a)	37.9(17)
C(11)-C(16)-C(17)	121.78(19)	C(24)-H(24a)-H(24b)	36.5(16)
C(15)-C(16)-C(17)	118.71(19)	C(24)-H(24b)-H(24a)	39.1(17)
C(16)-C(17)-C(18)	113.16(19)	C(26)-H(26a)-H(26c)	34.3(15)
C(16)-C(17)-H(17a)	111.0(20)	C(26)-H(26b)-H(26c)	39.8(16)
C(16)-C(17)-H(17b)	111.7(16)	C(26)-H(26c)-H(26a)	35.3(16)
C(18)-C(17)-H(17a)	105.2(20)	C(26)-H(26c)-H(26b)	41.5(17)
C(18)-C(17)-H(17b)	109.4(16)	H(26a)-H(26c)-H(26b)	66.1(20)
H(17a)-C(17)-H(17b)	105(3)	C(28)-H(28a)-H(28b)	49.4(24)
N(1)-C(18)-C(17)	111.89(17)	C(28)-H(28b)-H(28a)	43.1(21)
N(1)-C(18)-H(18a)	105.5(15)	C(30)-H(30b)-H(30c)	36.3(15)
N(1)-C(18)-H(18b)	108.3(17)	C(30)-H(30c)-H(30b)	35.4(15)
C(17)-C(18)-H(18a)	110.9(14)	O(32)-H(32a)-H(36b)	98.69(19)
C(17)-C(18)-H(18b)	112.3(16)	O(36)-H(36a)-H(36b)	33.9(3)
H(18a)-C(18)-H(18b)	107.5(21)	O(32)-H(36b)-O(36)	171.3(3)
N(1)-C(19)-C(20)	114.37(18)	O(32)-H(36b)-H(32a)	37.69(11)
N(1)-C(19)-H(19a)	103.0(15)	O(32)-H(36b)-H(36a)	152.78(11)
N(1)-C(19)-H(19b)	104.0(15)	O(36)-H(36b)-H(32a)	134.8(3)
C(20)-C(19)-H(19a)	109.3(15)	O(36)-H(36b)-H(36a)	35.6(3)
C(20)-C(19)-H(19b)	111.3(15)	H(32a)-H(36b)-H(36a)	151.8

Torsion angles

C10	N1	C2	C3	65.9(3)	C18	N1	C2	C3	-54.0(3)
C19	N1	C2	C3	-176.8(4)	C2	N1	C10	C9	-47.84(23)
C2	N1	C10	C11	-174.9(4)	C18	N1	C10	C9	73.2(3)
C18	N1	C10	C11	-53.90(23)	C19	N1	C10	C9	-164.4(4)
C19	N1	C10	C11	68.5(3)	C2	N1	C18	C17	-175.7(4)
C10	N1	C18	C17	64.6(3)	C19	N1	C18	C17	-55.7(3)
C2	N1	C19	C20	69.2(3)	C10	N1	C19	C20	-173.4(4)
C18	N1	C19	C20	-52.8(3)	N1	C2	C3	C4	-48.33(24)
C2	C3	C4	C5	-165.1(5)	C2	C3	C4	C9	15.92(20)
C3	C4	C5	C6	179.0(5)	C9	C4	C5	C6	-2.04(20)
C3	C4	C9	C8	-177.6(4)	C3	C4	C9	C10	-1.54(19)
C5	C4	C9	C8	3.43(20)	C5	C4	C9	C10	179.5(4)
C4	C5	C6	C7	-1.66(20)	C4	C5	C6	O23	178.6(5)
C5	C6	C7	C8	3.89(21)	C5	C6	C7	O25	-176.6(4)
O23	C6	C7	C8	-176.3(4)	O23	C6	C7	O25	3.19(16)
C5	C6	O23	C24	-15.88(23)	C7	C6	O23	C24	164.4(4)
C6	C7	C8	C9	-2.49(19)	O25	C7	C8	C9	178.0(4)
C6	C7	O25	C26	-171.1(4)	C8	C7	O25	C26	8.38(22)
C7	C8	C9	C4	-1.18(20)	C7	C8	C9	C10	-177.5(4)
C4	C9	C10	N1	18.07(19)	C4	C9	C10	C11	142.7(4)
C8	C9	C10	N1	-165.8(4)	C8	C9	C10	C11	-41.21(22)
N1	C10	C11	C12	-154.0(4)	N1	C10	C11	C16	25.63(19)
C9	C10	C11	C12	80.8(3)	C9	C10	C11	C16	-99.6(3)
C10	C11	C12	C13	-177.5(4)	C16	C11	C12	C13	2.91(19)
C10	C11	C16	C15	179.4(4)	C10	C11	C16	C17	-4.58(19)
C12	C11	C16	C15	-1.01(19)	C12	C11	C16	C17	175.0(4)
C11	C12	C13	C14	-2.96(19)	C11	C12	C13	O27	178.1(4)
C12	C13	C14	C15	1.12(19)	C12	C13	C14	O29	-179.4(4)
O27	C13	C14	C15	-179.8(4)	O27	C13	C14	O29	-0.35(15)
C12	C13	O27	C28	-10.14(23)	C14	C13	O27	C28	170.9(4)
C13	C14	C15	C16	0.76(19)	O29	C14	C15	C16	-178.6(4)
C13	C14	O29	C30	175.2(4)	C15	C14	O29	C30	-5.35(22)
C14	C15	C16	C11	-0.81(19)	C14	C15	C16	C17	-176.9(4)
C11	C16	C17	C18	12.32(19)	C15	C16	C17	C18	-171.6(4)
C16	C17	C18	N1	-42.19(22)	N1	C19	C20	C21	-169.3(4)
C19	C20	C21	O22	177.1(5)					