Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*,*N*′,*N*′-Tetrakis(2-hydroxy-5-methylbenzyl)ethane-1,2-diamine dimethylformamide disolvate

Nuan-Sheng Wang,[a] Yong-Tao Wang,[a] Xiu-Kai Guo[b] and Tian-Duo Li[a]*

[a]Shandong Provincial Key Laboratory of Fine Chemicals, Shandong Polytechnic University, Jinan 250353, People's Republic of China, and [b]School of Petrochemical Engineering, Changzhou University, Changzhou 213164, People's Republic of China
Correspondence e-mail: litianduo@163.com

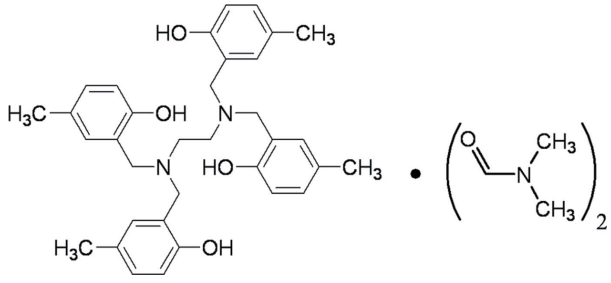
Received 8 May 2011; accepted 12 May 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.154; data-to-parameter ratio = 15.4.

The title compound, $C_{34}H_{40}N_2O_4\cdot 2C_3H_7NO$, was synthesized by the Mannich condensation of ethanediamine, formaldehyde and *p*-cresol. In the crystal, the tetraphenol molecule is arranged around an inversion center. The molecule and the dimethylformamide solvate are linked through an O—H···O hydrogen bond. An intramolecular O—H···N hydrogen bond occurs in the tetraphenol molecule, which may influence the molecular confomation. Futhermore, C—H···O and π–π stacking interactions [centroid–centroid distance = 3.7081 (14) Å] stabilize the crystal packing, building a three-dimensional network.

Related literature

For applications of the title compound, see: Liu *et al.* (2007); Tshuva *et al.* (2000); For related structures, see: Hou *et al.* (2010); Higham *et al.* (2006); Farrell *et al.* (2007).



Experimental

Crystal data

$C_{34}H_{40}N_2O_4\cdot 2C_3H_7NO$ M_r = 686.87
Monoclinic, $P2_1/c$
a = 11.574 (2) Å
b = 6.3557 (12) Å
c = 26.343 (5) Å
β = 94.939 (3)°
V = 1930.7 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.50 × 0.32 × 0.27 mm

Data collection

Bruker SMART APEX diffractometer
9607 measured reflections
3569 independent reflections
2667 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.154
S = 1.07
3569 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.98	2.705 (2)	147
O2—H2···O3	0.82	1.87	2.690 (2)	177
C18—H18···O3^{i}	0.93	2.56	3.368 (3)	145

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

We thank the Shandong Province Higher Educational Science and Technology Program for financial support (J09LB03).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2686).

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supporting information

Acta Cryst. (2011). E**67**, o1438 [doi:10.1107/S1600536811017934]

N,*N*,*N*′,*N*′-Tetrakis(2-hydroxy-5-methylbenzyl)ethane-1,2-diamine dimethylformamide disolvate

Nuan-Sheng Wang, Yong-Tao Wang, Xiu-Kai Guo and Tian-Duo Li

S1. Comment

Multidentate aminophenol are of interest as metallochelators and as ligands for bioinorganic modeling, catalysis, and medical imaging.(Higham *et al.*, 2006; Farrell *et al.*, 2007). Some of them in combination with metals are used as active catalysts for alkenes polymerization (Tshuva *et al.*, 2000) and initiators in the ring-openingpolymerization of lactones (Liu *et al.*, 2007). Herein, we report the crystal structure of the title compound, $'C_{34}H_{40}N_2O_4.(C_3H_7NO)_2'$.

The *N*, *N*′-Tetrakis(2-hydroxy-5-methylbenzyl)-1, 2-ethanediamine molecule is arranged around inversion center located in the middle of the CH_2-CH_2 bond. The DMF solvate is linked to this molecule through O-H···O hydrogen bonds (Fig. 1). There is also a weak intramolecular O-H···N interactions which might influence the conformation of the molecule (Table 1) (Hou *et al.*, 2010).

The occurence of weak C-H···O interactions (Table 1) and π-π stacking between the symmetry related C1—C6 phenyl rings (Centroid to centroid distance of 3.7081 (14)Å, interplanar distance of 3.6891 (8)° and slippage of 0.375Å) result in the formation of a three dimensional network (Fig. 2)

S2. Experimental

The title compound was prepared by mixing ethylenediamine (1.0 mmol), paraformaldehyde (4.0 mmol) and *p*-cresol (10 mmol) were heated to 90°C and stirred for 18 h. This reaction requires no solvent nor inert atmosphere. At the end of the reaction, 10ml of ethanol was added to the mixtures to remove the unreacted *p*-cresol, then sonicated 10 minutes. Finally a white precipitate product was collected by filtration in 56% yield.

S3. Refinement

All H atoms were placed in idealized positions and treated as riding, with C—H = 0.93 Å (CH), 0.97 Å (CH_2), 0.96 Å (CH_3), O—H = 0.82 Å and and U_{iso}(H) = 1.2 U_{eq}(CH and CH_2), U_{iso}(H) = 1.5 *U*eq(CH_3 and OH).

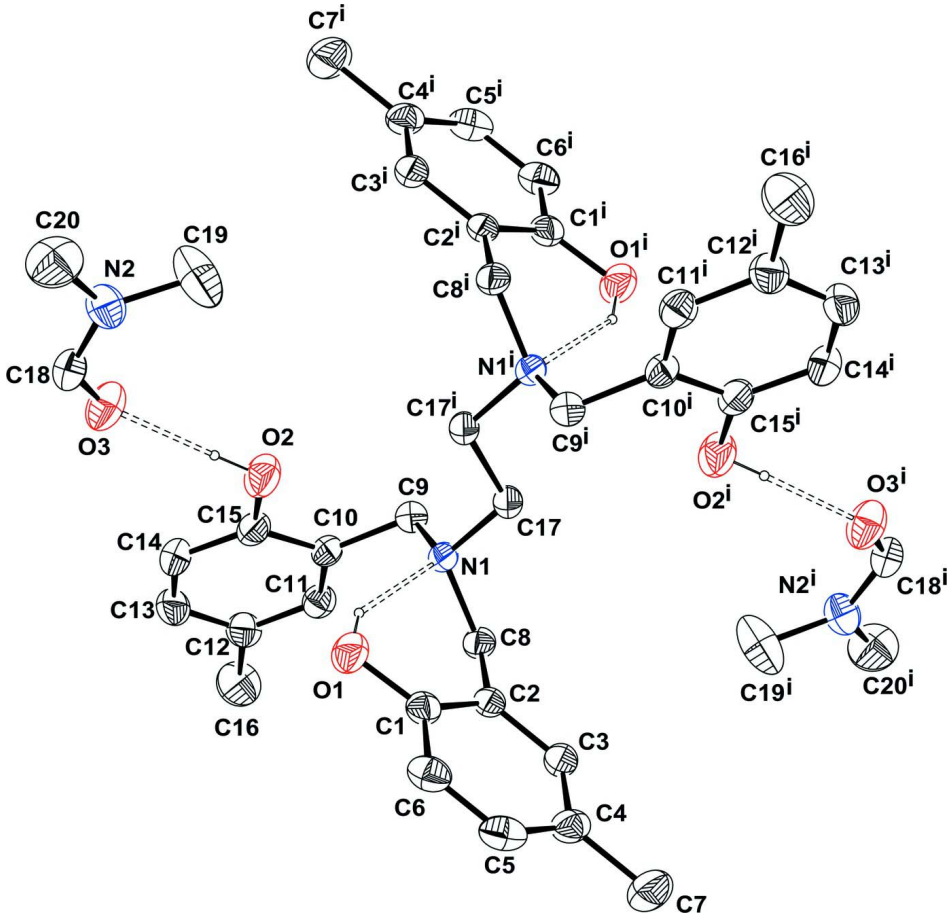

Figure 1

Molecular structure of the title compound with the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small sphere of arbitrary radii. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) -*x*+1, -*y*+1, -*z*+1]

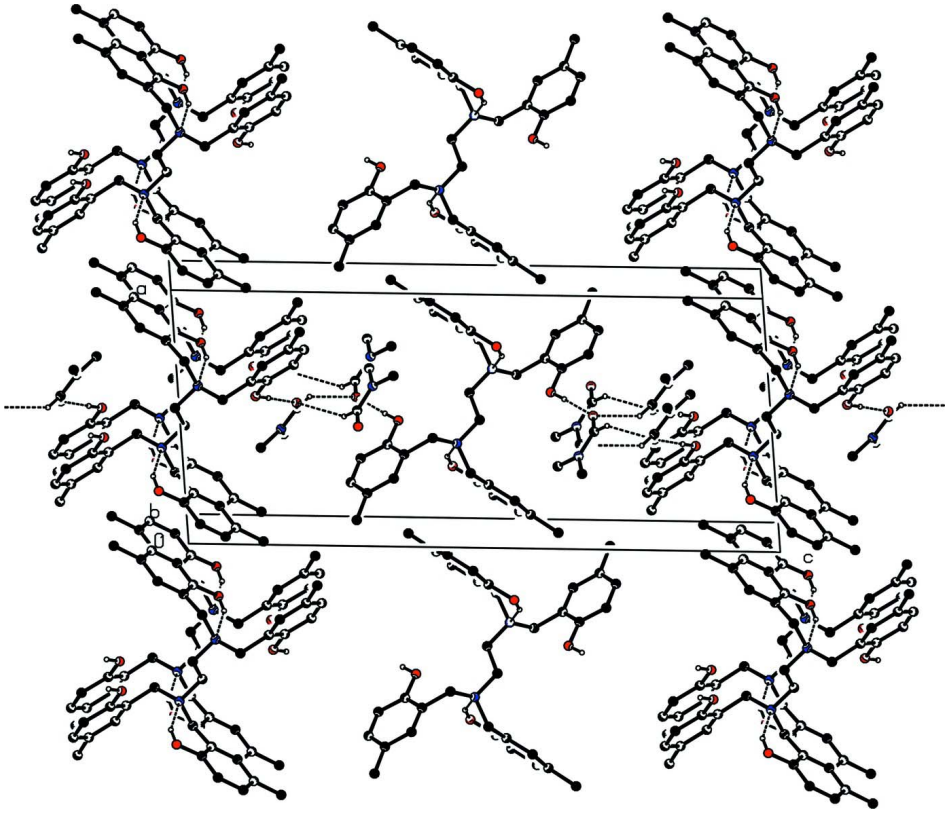

Figure 2

Molecular packing of the title compound viewing along the crystallographic *b*-axis. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

2-{[(2-{bis[(2-hydroxy-5-methylphenyl)methyl]amino}ethyl)[(2-hydroxy-5-methylphenyl)methyl]amino]methyl}-4-methylphenol dimethylformamide disolvate

Crystal data

$C_{34}H_{40}N_2O_4 \cdot 2C_3H_7NO$
$M_r = 686.87$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.574$ (2) Å
$b = 6.3557$ (12) Å
$c = 26.343$ (5) Å
$\beta = 94.939$ (3)°
$V = 1930.7$ (6) Å^3
$Z = 2$
$F(000) = 740$
$D_x = 1.182$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2283 reflections
$\theta = 2.3$–$22.4°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colourless
0.50 × 0.32 × 0.27 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
9607 measured reflections
3569 independent reflections
2667 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.6°$
$h = -13 \rightarrow 13$
$k = 0 \rightarrow 7$
$l = 0 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.154$
$S = 1.07$
3569 reflections
232 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.2941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.81761 (16)	0.6724 (3)	0.50272 (8)	0.0459 (5)
C2	0.80450 (15)	0.4662 (3)	0.48545 (7)	0.0399 (5)
C3	0.86027 (16)	0.4078 (3)	0.44304 (7)	0.0472 (5)
H3	0.8508	0.2709	0.4309	0.057*
C4	0.92929 (17)	0.5440 (4)	0.41797 (8)	0.0546 (6)
C5	0.94148 (18)	0.7469 (4)	0.43666 (9)	0.0602 (6)
H5	0.9880	0.8417	0.4209	0.072*
C6	0.88609 (17)	0.8110 (4)	0.47813 (9)	0.0567 (6)
H6	0.8948	0.9487	0.4897	0.068*
C7	0.9908 (2)	0.4688 (5)	0.37314 (10)	0.0846 (9)
H7A	1.0649	0.4111	0.3851	0.127*
H7B	1.0018	0.5849	0.3508	0.127*
H7C	0.9450	0.3624	0.3551	0.127*
C8	0.74176 (15)	0.3055 (3)	0.51447 (7)	0.0434 (5)
H8A	0.7213	0.1869	0.4923	0.052*
H8B	0.7933	0.2546	0.5428	0.052*
C9	0.59865 (17)	0.2520 (3)	0.57452 (7)	0.0465 (5)
H9A	0.6064	0.1064	0.5642	0.056*
H9B	0.5174	0.2778	0.5787	0.056*
C10	0.66842 (16)	0.2860 (3)	0.62476 (7)	0.0444 (5)
C11	0.74762 (17)	0.1400 (4)	0.64530 (8)	0.0503 (5)
H11	0.7593	0.0176	0.6271	0.060*
C12	0.81018 (19)	0.1691 (4)	0.69194 (8)	0.0571 (6)
C13	0.7899 (2)	0.3509 (5)	0.71814 (8)	0.0648 (7)
H13	0.8299	0.3731	0.7498	0.078*

C14	0.71194 (19)	0.5012 (4)	0.69888 (8)	0.0615 (6)
H14	0.7001	0.6229	0.7174	0.074*
C15	0.65167 (18)	0.4696 (4)	0.65193 (8)	0.0521 (6)
C16	0.8989 (2)	0.0118 (5)	0.71276 (11)	0.0892 (9)
H16A	0.9725	0.0439	0.7004	0.134*
H16B	0.8751	−0.1269	0.7019	0.134*
H16C	0.9057	0.0181	0.7493	0.134*
C17	0.54400 (16)	0.4187 (3)	0.49300 (7)	0.0463 (5)
H17A	0.5051	0.2856	0.4858	0.056*
H17B	0.5782	0.4636	0.4624	0.056*
N1	0.63564 (12)	0.3898 (3)	0.53418 (5)	0.0406 (4)
O1	0.76581 (13)	0.7432 (3)	0.54411 (6)	0.0640 (5)
H1	0.7179	0.6567	0.5520	0.096*
O2	0.57293 (15)	0.6113 (3)	0.63071 (6)	0.0721 (5)
H2	0.5563	0.6957	0.6525	0.108*
C18	0.4736 (2)	1.0737 (4)	0.69918 (8)	0.0546 (6)
H18	0.5089	1.1710	0.7219	0.066*
C19	0.3253 (3)	0.9941 (6)	0.63369 (15)	0.1233 (13)
H19A	0.3785	0.8864	0.6252	0.185*
H19B	0.2982	1.0695	0.6034	0.185*
H19C	0.2606	0.9307	0.6484	0.185*
C20	0.3383 (3)	1.3486 (5)	0.67385 (12)	0.0963 (10)
H20A	0.3860	1.4260	0.6990	0.144*
H20B	0.2604	1.3422	0.6837	0.144*
H20C	0.3385	1.4176	0.6414	0.144*
N2	0.38342 (17)	1.1383 (3)	0.67004 (7)	0.0636 (5)
O3	0.51586 (16)	0.8979 (3)	0.69941 (6)	0.0731 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0384 (10)	0.0481 (13)	0.0502 (12)	0.0064 (9)	−0.0022 (9)	−0.0022 (10)
C2	0.0319 (9)	0.0477 (12)	0.0389 (10)	0.0071 (8)	−0.0024 (8)	0.0010 (9)
C3	0.0417 (11)	0.0552 (13)	0.0442 (11)	0.0071 (9)	0.0001 (9)	−0.0009 (10)
C4	0.0419 (11)	0.0752 (17)	0.0469 (12)	0.0068 (11)	0.0041 (9)	0.0115 (11)
C5	0.0422 (12)	0.0656 (17)	0.0723 (15)	−0.0005 (11)	0.0026 (11)	0.0213 (13)
C6	0.0442 (12)	0.0465 (13)	0.0783 (16)	0.0004 (10)	−0.0007 (11)	0.0036 (11)
C7	0.0739 (17)	0.120 (3)	0.0630 (15)	−0.0014 (17)	0.0253 (14)	0.0050 (16)
C8	0.0400 (10)	0.0458 (12)	0.0440 (11)	0.0088 (9)	0.0025 (8)	−0.0009 (9)
C9	0.0428 (11)	0.0514 (13)	0.0455 (11)	−0.0021 (9)	0.0049 (9)	−0.0026 (9)
C10	0.0452 (11)	0.0516 (13)	0.0377 (10)	−0.0029 (9)	0.0106 (8)	0.0003 (9)
C11	0.0540 (12)	0.0500 (13)	0.0477 (11)	−0.0015 (10)	0.0098 (10)	0.0024 (10)
C12	0.0546 (13)	0.0705 (16)	0.0458 (12)	−0.0007 (11)	0.0019 (10)	0.0075 (11)
C13	0.0586 (14)	0.093 (2)	0.0422 (12)	−0.0093 (13)	−0.0011 (11)	−0.0027 (13)
C14	0.0633 (14)	0.0755 (17)	0.0469 (12)	−0.0021 (12)	0.0109 (11)	−0.0160 (11)
C15	0.0515 (12)	0.0600 (15)	0.0458 (12)	0.0057 (10)	0.0107 (10)	−0.0030 (10)
C16	0.0865 (19)	0.100 (2)	0.0772 (18)	0.0155 (17)	−0.0128 (16)	0.0156 (16)
C17	0.0416 (10)	0.0563 (13)	0.0402 (10)	0.0066 (9)	−0.0011 (8)	−0.0110 (9)

N1	0.0364 (8)	0.0495 (10)	0.0361 (8)	0.0050 (7)	0.0033 (7)	−0.0033 (7)
O1	0.0680 (11)	0.0568 (11)	0.0690 (10)	−0.0011 (8)	0.0163 (8)	−0.0191 (8)
O2	0.0804 (12)	0.0741 (13)	0.0611 (10)	0.0264 (9)	0.0021 (9)	−0.0153 (9)
C18	0.0682 (14)	0.0544 (15)	0.0419 (11)	0.0012 (12)	0.0088 (11)	−0.0042 (10)
C19	0.123 (3)	0.123 (3)	0.114 (3)	−0.020 (2)	−0.048 (2)	−0.016 (2)
C20	0.096 (2)	0.089 (2)	0.103 (2)	0.0314 (18)	0.0033 (18)	0.0172 (18)
N2	0.0689 (12)	0.0650 (14)	0.0549 (11)	−0.0008 (10)	−0.0066 (10)	0.0031 (10)
O3	0.0999 (13)	0.0595 (11)	0.0612 (10)	0.0219 (10)	0.0149 (9)	−0.0026 (8)

Geometric parameters (Å, º)

C1—O1	1.365 (2)	C12—C16	1.502 (4)
C1—C6	1.383 (3)	C13—C14	1.380 (3)
C1—C2	1.391 (3)	C13—H13	0.9300
C2—C3	1.388 (3)	C14—C15	1.381 (3)
C2—C8	1.500 (3)	C14—H14	0.9300
C3—C4	1.384 (3)	C15—O2	1.366 (3)
C3—H3	0.9300	C16—H16A	0.9600
C4—C5	1.383 (3)	C16—H16B	0.9600
C4—C7	1.508 (3)	C16—H16C	0.9600
C5—C6	1.375 (3)	C17—N1	1.462 (2)
C5—H5	0.9300	C17—C17^{i}	1.518 (4)
C6—H6	0.9300	C17—H17A	0.9700
C7—H7A	0.9600	C17—H17B	0.9700
C7—H7B	0.9600	O1—H1	0.8200
C7—H7C	0.9600	O2—H2	0.8200
C8—N1	1.475 (2)	C18—O3	1.219 (3)
C8—H8A	0.9700	C18—N2	1.307 (3)
C8—H8B	0.9700	C18—H18	0.9300
C9—N1	1.469 (2)	C19—N2	1.449 (4)
C9—C10	1.506 (3)	C19—H19A	0.9600
C9—H9A	0.9700	C19—H19B	0.9600
C9—H9B	0.9700	C19—H19C	0.9600
C10—C11	1.381 (3)	C20—N2	1.442 (3)
C10—C15	1.391 (3)	C20—H20A	0.9600
C11—C12	1.384 (3)	C20—H20B	0.9600
C11—H11	0.9300	C20—H20C	0.9600
C12—C13	1.376 (4)		

O1—C1—C6	118.2 (2)	C12—C13—C14	122.1 (2)
O1—C1—C2	121.92 (18)	C12—C13—H13	119.0
C6—C1—C2	119.9 (2)	C14—C13—H13	119.0
C3—C2—C1	118.04 (19)	C13—C14—C15	119.5 (2)
C3—C2—C8	120.45 (18)	C13—C14—H14	120.3
C1—C2—C8	121.25 (17)	C15—C14—H14	120.3
C4—C3—C2	123.0 (2)	O2—C15—C14	122.6 (2)
C4—C3—H3	118.5	O2—C15—C10	117.40 (18)
C2—C3—H3	118.5	C14—C15—C10	120.0 (2)

C5—C4—C3	117.3 (2)	C12—C16—H16A	109.5
C5—C4—C7	122.3 (2)	C12—C16—H16B	109.5
C3—C4—C7	120.4 (2)	H16A—C16—H16B	109.5
C6—C5—C4	121.3 (2)	C12—C16—H16C	109.5
C6—C5—H5	119.4	H16A—C16—H16C	109.5
C4—C5—H5	119.4	H16B—C16—H16C	109.5
C5—C6—C1	120.6 (2)	N1—C17—C17^{i}	111.36 (19)
C5—C6—H6	119.7	N1—C17—H17A	109.4
C1—C6—H6	119.7	C17^{i}—C17—H17A	109.4
C4—C7—H7A	109.5	N1—C17—H17B	109.4
C4—C7—H7B	109.5	C17^{i}—C17—H17B	109.4
H7A—C7—H7B	109.5	H17A—C17—H17B	108.0
C4—C7—H7C	109.5	C17—N1—C9	111.94 (15)
H7A—C7—H7C	109.5	C17—N1—C8	110.94 (14)
H7B—C7—H7C	109.5	C9—N1—C8	109.95 (15)
N1—C8—C2	112.72 (16)	C1—O1—H1	109.5
N1—C8—H8A	109.0	C15—O2—H2	109.5
C2—C8—H8A	109.0	O3—C18—N2	126.2 (2)
N1—C8—H8B	109.0	O3—C18—H18	116.9
C2—C8—H8B	109.0	N2—C18—H18	116.9
H8A—C8—H8B	107.8	N2—C19—H19A	109.5
N1—C9—C10	112.49 (16)	N2—C19—H19B	109.5
N1—C9—H9A	109.1	H19A—C19—H19B	109.5
C10—C9—H9A	109.1	N2—C19—H19C	109.5
N1—C9—H9B	109.1	H19A—C19—H19C	109.5
C10—C9—H9B	109.1	H19B—C19—H19C	109.5
H9A—C9—H9B	107.8	N2—C20—H20A	109.5
C11—C10—C15	118.63 (19)	N2—C20—H20B	109.5
C11—C10—C9	122.36 (19)	H20A—C20—H20B	109.5
C15—C10—C9	119.00 (18)	N2—C20—H20C	109.5
C10—C11—C12	122.5 (2)	H20A—C20—H20C	109.5
C10—C11—H11	118.8	H20B—C20—H20C	109.5
C12—C11—H11	118.8	C18—N2—C20	121.7 (2)
C13—C12—C11	117.3 (2)	C18—N2—C19	119.4 (3)
C13—C12—C16	121.1 (2)	C20—N2—C19	118.8 (3)
C11—C12—C16	121.6 (2)		

O1—C1—C2—C3	179.97 (17)	C10—C11—C12—C13	0.7 (3)
C6—C1—C2—C3	−0.9 (3)	C10—C11—C12—C16	−177.9 (2)
O1—C1—C2—C8	−5.9 (3)	C11—C12—C13—C14	−1.0 (3)
C6—C1—C2—C8	173.23 (18)	C16—C12—C13—C14	177.5 (2)
C1—C2—C3—C4	1.1 (3)	C12—C13—C14—C15	0.2 (4)
C8—C2—C3—C4	−173.15 (18)	C13—C14—C15—O2	179.7 (2)
C2—C3—C4—C5	−0.2 (3)	C13—C14—C15—C10	0.9 (3)
C2—C3—C4—C7	177.9 (2)	C11—C10—C15—O2	179.93 (18)
C3—C4—C5—C6	−0.7 (3)	C9—C10—C15—O2	−0.9 (3)
C7—C4—C5—C6	−178.9 (2)	C11—C10—C15—C14	−1.2 (3)
C4—C5—C6—C1	0.9 (3)	C9—C10—C15—C14	177.91 (19)

O1—C1—C6—C5	179.13 (19)	C17^{i}—C17—N1—C9	80.0 (3)
C2—C1—C6—C5	0.0 (3)	C17^{i}—C17—N1—C8	−156.7 (2)
C3—C2—C8—N1	−144.07 (17)	C10—C9—N1—C17	−157.41 (16)
C1—C2—C8—N1	41.9 (2)	C10—C9—N1—C8	78.8 (2)
N1—C9—C10—C11	−109.0 (2)	C2—C8—N1—C17	73.2 (2)
N1—C9—C10—C15	71.9 (2)	C2—C8—N1—C9	−162.47 (15)
C15—C10—C11—C12	0.4 (3)	O3—C18—N2—C20	178.2 (2)
C9—C10—C11—C12	−178.70 (19)	O3—C18—N2—C19	−0.4 (4)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.98	2.705 (2)	147
O2—H2···O3	0.82	1.87	2.690 (2)	177
C18—H18···O3^{ii}	0.93	2.56	3.368 (3)	145

Symmetry code: (ii) −*x*+1, *y*+1/2, −*z*+3/2.