organic compounds

N-Cyclohexyl-3-(4-hydroxy-6-oxo-1,6-dihydropyrimidin-5-yl)-3-p-tolyl-propanamide

Xing-Han Wang, Wen-Juan Hao and Shu-Jiang Tu*

School of Chemistry and Chemical Engineering, Xuzhou Normal University, Xuzhou 221116, People's Republic of China

Correspondence e-mail: laotu2001@263.net

In the molecule of the title compound, $C_{20}H_{25}N_3O_3$, the aromatic rings are oriented at a dihedral angle of 88.36 (3)°. The cyclohexane ring adopts a chair conformation. In the crystal structure, intermolecular N—H⋯O and O—H⋯N hydrogen bonds link the molecules. C—H⋯π interactions are also present.

Related literature

For general background, see: Johar *et al.* (2005); Janeba *et al.* (2005); Soloducho *et al.* (2003); Mathews & Asokan (2007); Lagoja (2005); Michael (2005); Erian (1993). For bond-length data, see: Allen *et al.* (1987). For ring-puckering parameters, see: Cremer & Pople (1975).
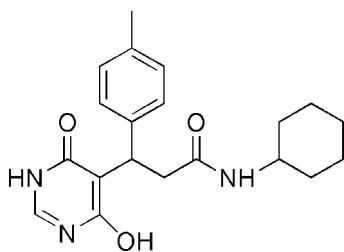
Experimental

Crystal data
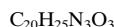
$C_{20}H_{25}N_3O_3$	$V = 1826.5$ (4) Å^3
$M_r = 355.43$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 7.1563$ (12) Å	$\mu = 0.09$ mm^{-1}
$b = 19.637$ (2) Å	$T = 298$ (2) K
$c = 13.2746$ (18) Å	$0.23 \times 0.16 \times 0.14$ mm
$\beta = 101.740$ (2)°	

Data collection

Bruker SMART CCD area-detector diffractometer	9491 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	3216 independent reflections
$T_{min} = 0.980$, $T_{max} = 0.988$	1916 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.073$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	235 parameters
$wR(F^2) = 0.104$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
3216 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O3^i	0.86	1.98	2.813 (3)	162
O1—H1A⋯N2^{ii}	0.82	1.95	2.753 (3)	168
N3—H3⋯O2^{iii}	0.86	2.19	2.992 (4)	155
C17—H17B⋯$Cg2^{iv}$	0.97	2.47	3.440 (3)	177
C20—H20A⋯$Cg2^v$	0.97	2.74	3.629 (3)	152

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+2, -y+2, -z+2$; (iii) $-x+2, -y+2, -z+1$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x, -y, -z+1$. $Cg2$ is centroid of the C8–C13 ring.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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supporting information

N-Cyclohexyl-3-(4-hydroxy-6-oxo-1,6-dihydropyrimidin-5-yl)-3-*p*-tolyl-propanamide

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S1. Comment

The pyrimidines and their derivatives as a class of extremely important heterocyclic compounds are used in a wide array of synthetic and industrial applications. Not only they are an integral part of the genetic materials, *viz*. DNA and RNA as nucleotides and nucleosides but also play critical roles especially in pharmaceutical fields (Johar *et al.*, 2005; Janeba *et al.*, 2005). Some pyrimidine derivatives can give stable and good quality nanomaterials having many important electrical and optical properties (Soloducho *et al.*, 2003; Mathews & Asokan, 2007), and also used as functional materials (Lagoja, 2005; Michael, 2005; Erian, 1993). We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (N1/N2/C1-C4) and B (C8-C13) are, of course, planar, and they are oriented at a dihedral angle of 88.36 (3)°. The cyclohexane ring C (C15-C20), having total puckering amplitude, Q_T, of 0.565 (3) Å, chair conformation [φ = -30.33 (3)° and θ = 4.00 (3)°] (Cremer & Pople, 1975).

In the crystal structure, intermolecular N-H···O and O-H···N hydrogen bonds (Table 1) link the molecules, in which they may be effective in the stabilization of the structure. There also exist C–H···π interactions (Table 1).

S2. Experimental

The title compound was prepared by the reaction of *p*-tolylidene-Meldrum's acid (1 mmol) with 6-hydroxy-pyrimidin-4(3*H*)-one (1 mmol) and cyclohexanamine (1 mmol) at 373 K in glacial acetic acid under microwave irradiation (maximum power 250 W, initial power 100 W) for 18 min (yield; 83%, m.p. 534–536 K). Crystals suitable for X-ray analysis were obtained from an ethanol solution by slow evaporation.

S3. Refinement

H atoms were positioned geometrically, with O-H = 0.82 Å (for OH), N-H = 0.86 Å (for NH) and C-H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,N,O)$, where x = 1.5 for methyl and OH H and x = 1.2 for all other H atoms.
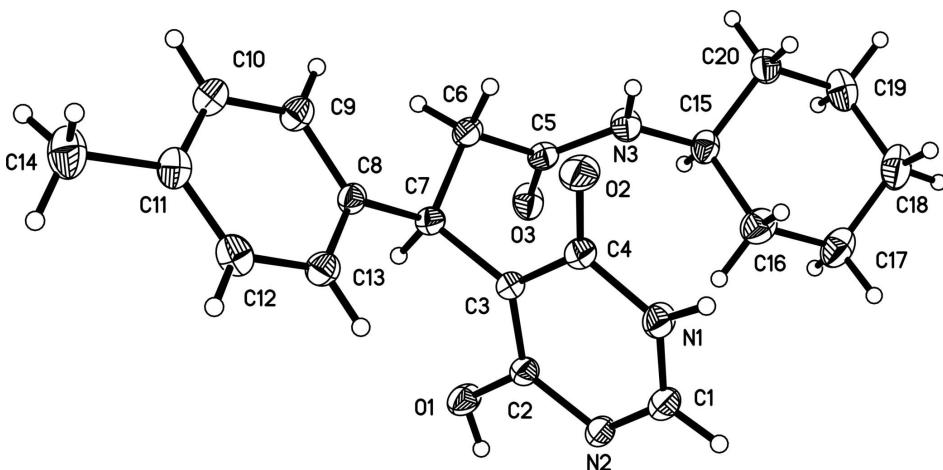
Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

N-Cyclohexyl-3-(4-hydroxy-6-oxo-1,6-dihydropyrimidin-5-yl)- 3-*p*-tolylpropanamide

Crystal data

$C_{20}H_{25}N_3O_3$	$F(000) = 760$
$M_r = 355.43$	$D_x = 1.293$ Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point = 534–536 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.1563$ (12) Å	Cell parameters from 1921 reflections
$b = 19.637$ (2) Å	$\theta = 2.6–27.7°$
$c = 13.2746$ (18) Å	$\mu = 0.09$ mm^{-1}
$\beta = 101.740$ (2)°	$T = 298$ K
$V = 1826.5$ (4) Å^3	Block, colorless
$Z = 4$	$0.23 \times 0.16 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	9491 measured reflections
Radiation source: fine-focus sealed tube	3216 independent reflections
Graphite monochromator	1916 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.073$
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$T_{min} = 0.980$, $T_{max} = 0.988$	$h = -8 \rightarrow 8$
	$k = -23 \rightarrow 21$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.048$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.104$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$
3216 reflections	where $P = (F_o^2 + 2F_c^2)/3$
235 parameters	$(\Delta/\sigma)_{max} = 0.001$
0 restraints	$\Delta\rho_{max} = 0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8327 (2)	1.04303 (8)	0.89288 (11)	0.0456 (5)
H1A	0.8598	1.0297	0.9526	0.068*
O2	1.1335 (2)	1.04358 (9)	0.60752 (11)	0.0511 (5)
O3	0.5892 (2)	0.93937 (8)	0.69802 (11)	0.0447 (4)
N1	1.2782 (3)	1.00038 (10)	0.76292 (14)	0.0387 (5)
H1	1.3786	0.9909	0.7394	0.046*
N2	1.1340 (3)	0.99789 (9)	0.90587 (13)	0.0367 (5)
N3	0.7956 (3)	0.91122 (9)	0.59665 (13)	0.0378 (5)
H3	0.8514	0.9251	0.5488	0.045*
C1	1.2753 (3)	0.98462 (12)	0.86043 (17)	0.0396 (6)
H1B	1.3815	0.9626	0.8987	0.048*
C2	0.9778 (3)	1.02944 (11)	0.84599 (16)	0.0316 (5)
C3	0.9650 (3)	1.04690 (10)	0.74467 (15)	0.0290 (5)
C4	1.1234 (3)	1.03189 (11)	0.69730 (17)	0.0346 (6)
C5	0.6857 (3)	0.95565 (11)	0.63376 (16)	0.0329 (6)
C6	0.6872 (3)	1.02749 (11)	0.59477 (16)	0.0350 (6)
H6A	0.5572	1.0422	0.5679	0.042*
H6B	0.7563	1.0291	0.5391	0.042*
C7	0.7820 (3)	1.07626 (11)	0.68124 (15)	0.0317 (6)
H7	0.6931	1.0795	0.7283	0.038*
C8	0.8005 (3)	1.14835 (11)	0.64204 (16)	0.0302 (5)
C9	0.6815 (3)	1.17248 (12)	0.55327 (17)	0.0366 (6)
H9	0.6022	1.1421	0.5108	0.044*
C10	0.6781 (3)	1.24068 (12)	0.52658 (18)	0.0400 (6)
H10	0.5952	1.2553	0.4672	0.048*
C11	0.7955 (4)	1.28759 (12)	0.58638 (19)	0.0393 (6)
C12	0.9218 (4)	1.26311 (12)	0.67173 (19)	0.0412 (6)
H12	1.0068	1.2931	0.7115	0.049*
C13	0.9251 (3)	1.19530 (12)	0.69940 (17)	0.0367 (6)
H13	1.0118	1.1806	0.7573	0.044*
C14	0.7807 (4)	1.36269 (12)	0.5595 (2)	0.0587 (8)
H14A	0.8643	1.3731	0.5135	0.088*
H14B	0.8168	1.3892	0.6212	0.088*
H14C	0.6517	1.3734	0.5269	0.088*
C15	0.8280 (3)	0.84081 (11)	0.63122 (17)	0.0367 (6)

H15	0.7200	0.8266	0.6614	0.044*
C16	1.0092 (4)	0.83383 (13)	0.71338 (18)	0.0488 (7)
H16A	0.9999	0.8627	0.7714	0.059*
H16B	1.1174	0.8492	0.6857	0.059*
C17	1.0429 (4)	0.76056 (13)	0.75025 (19)	0.0532 (7)
H17A	1.1649	0.7576	0.7979	0.064*
H17B	0.9442	0.7473	0.7868	0.064*
C18	1.0418 (4)	0.71171 (14)	0.6614 (2)	0.0593 (8)
H18A	1.1538	0.7198	0.6324	0.071*
H18B	1.0483	0.6653	0.6869	0.071*
C19	0.8642 (4)	0.72005 (12)	0.5780 (2)	0.0556 (8)
H19A	0.7536	0.7057	0.6043	0.067*
H19B	0.8738	0.6910	0.5202	0.067*
C20	0.8367 (4)	0.79365 (12)	0.54125 (18)	0.0435 (6)
H20A	0.9418	0.8070	0.5095	0.052*
H20B	0.7195	0.7975	0.4900	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0413 (10)	0.0669 (13)	0.0301 (9)	0.0186 (9)	0.0109 (8)	0.0084 (8)
O2	0.0557 (12)	0.0680 (13)	0.0339 (10)	0.0139 (10)	0.0193 (9)	0.0113 (8)
O3	0.0467 (11)	0.0426 (10)	0.0503 (10)	0.0067 (8)	0.0227 (9)	0.0080 (8)
N1	0.0312 (12)	0.0497 (13)	0.0373 (11)	0.0088 (10)	0.0120 (10)	0.0044 (10)
N2	0.0357 (12)	0.0444 (13)	0.0295 (11)	0.0122 (10)	0.0057 (9)	0.0041 (9)
N3	0.0432 (13)	0.0354 (12)	0.0390 (11)	0.0032 (10)	0.0185 (10)	0.0063 (9)
C1	0.0356 (15)	0.0456 (15)	0.0353 (14)	0.0085 (12)	0.0020 (12)	0.0041 (11)
C2	0.0292 (13)	0.0365 (14)	0.0286 (13)	0.0043 (11)	0.0047 (11)	−0.0004 (10)
C3	0.0301 (13)	0.0301 (13)	0.0257 (12)	0.0031 (11)	0.0030 (10)	0.0007 (10)
C4	0.0371 (15)	0.0360 (14)	0.0304 (13)	0.0042 (12)	0.0061 (12)	0.0026 (11)
C5	0.0296 (14)	0.0373 (15)	0.0302 (13)	−0.0008 (11)	0.0024 (11)	0.0011 (11)
C6	0.0363 (15)	0.0344 (14)	0.0319 (13)	0.0028 (11)	0.0016 (11)	0.0038 (10)
C7	0.0340 (14)	0.0347 (14)	0.0263 (12)	0.0042 (11)	0.0059 (11)	0.0018 (10)
C8	0.0277 (13)	0.0324 (14)	0.0305 (13)	0.0052 (11)	0.0063 (11)	0.0021 (11)
C9	0.0315 (14)	0.0359 (15)	0.0403 (14)	−0.0024 (11)	0.0020 (12)	0.0036 (11)
C10	0.0372 (15)	0.0397 (15)	0.0420 (15)	0.0012 (13)	0.0053 (12)	0.0081 (12)
C11	0.0348 (15)	0.0356 (15)	0.0493 (16)	0.0008 (12)	0.0130 (13)	0.0031 (12)
C12	0.0328 (15)	0.0378 (15)	0.0537 (17)	−0.0081 (12)	0.0104 (13)	−0.0084 (12)
C13	0.0292 (14)	0.0418 (15)	0.0376 (14)	0.0014 (12)	0.0034 (12)	−0.0012 (11)
C14	0.066 (2)	0.0381 (17)	0.0760 (19)	0.0006 (14)	0.0241 (16)	0.0061 (14)
C15	0.0355 (15)	0.0356 (15)	0.0413 (14)	0.0049 (11)	0.0132 (12)	0.0074 (11)
C16	0.0460 (17)	0.0539 (17)	0.0462 (16)	0.0012 (14)	0.0090 (14)	0.0077 (13)
C17	0.0423 (17)	0.0642 (19)	0.0551 (17)	0.0101 (14)	0.0148 (14)	0.0224 (15)
C18	0.0567 (19)	0.0523 (19)	0.075 (2)	0.0196 (15)	0.0281 (17)	0.0207 (15)
C19	0.059 (2)	0.0414 (17)	0.071 (2)	0.0062 (14)	0.0233 (17)	−0.0026 (14)
C20	0.0406 (16)	0.0427 (16)	0.0477 (15)	0.0063 (13)	0.0099 (13)	−0.0021 (12)

Geometric parameters (Å, º)

N1—C1	1.335 (3)	C10—H10	0.9300
N1—C4	1.406 (3)	C11—C12	1.384 (3)
N1—H1	0.8600	C11—C14	1.516 (3)
N2—C1	1.305 (3)	C12—C13	1.380 (3)
N2—C2	1.380 (3)	C12—H12	0.9300
N3—C5	1.334 (3)	C13—H13	0.9300
N3—C15	1.460 (3)	C14—H14A	0.9600
N3—H3	0.8600	C14—H14B	0.9600
O1—C2	1.341 (2)	C14—H14C	0.9600
O1—H1A	0.8200	C15—C16	1.522 (3)
O2—C4	1.230 (2)	C15—C20	1.523 (3)
O3—C5	1.244 (2)	C15—H15	0.9800
C1—H1B	0.9300	C16—C17	1.523 (3)
C2—C3	1.373 (3)	C16—H16A	0.9700
C3—C4	1.435 (3)	C16—H16B	0.9700
C3—C7	1.519 (3)	C17—C18	1.519 (4)
C5—C6	1.504 (3)	C17—H17A	0.9700
C6—C7	1.542 (3)	C17—H17B	0.9700
C6—H6A	0.9700	C18—C19	1.515 (4)
C6—H6B	0.9700	C18—H18A	0.9700
C7—C8	1.523 (3)	C18—H18B	0.9700
C7—H7	0.9800	C19—C20	1.525 (3)
C8—C9	1.390 (3)	C19—H19A	0.9700
C8—C13	1.396 (3)	C19—H19B	0.9700
C9—C10	1.384 (3)	C20—H20A	0.9700
C9—H9	0.9300	C20—H20B	0.9700
C10—C11	1.383 (3)		
C1—N1—C4	122.5 (2)	C13—C12—H12	119.1
C1—N1—H1	118.8	C11—C12—H12	119.1
C4—N1—H1	118.8	C12—C13—C8	121.2 (2)
C1—N2—C2	115.89 (18)	C12—C13—H13	119.4
C5—N3—C15	124.82 (18)	C8—C13—H13	119.4
C5—N3—H3	117.6	C11—C14—H14A	109.5
C15—N3—H3	117.6	C11—C14—H14B	109.5
C2—O1—H1A	109.5	H14A—C14—H14B	109.5
N2—C1—N1	124.6 (2)	C11—C14—H14C	109.5
N2—C1—H1B	117.7	H14A—C14—H14C	109.5
N1—C1—H1B	117.7	H14B—C14—H14C	109.5
O1—C2—C3	120.1 (2)	N3—C15—C16	111.59 (19)
O1—C2—N2	115.78 (18)	N3—C15—C20	111.02 (18)
C3—C2—N2	124.1 (2)	C16—C15—C20	110.01 (19)
C2—C3—C4	118.5 (2)	N3—C15—H15	108.0
C2—C3—C7	121.06 (19)	C16—C15—H15	108.0
C4—C3—C7	120.26 (18)	C20—C15—H15	108.0
O2—C4—N1	119.2 (2)	C15—C16—C17	111.8 (2)

O2—C4—C3	126.4 (2)	C15—C16—H16A	109.3
N1—C4—C3	114.34 (18)	C17—C16—H16A	109.3
O3—C5—N3	122.4 (2)	C15—C16—H16B	109.3
O3—C5—C6	121.4 (2)	C17—C16—H16B	109.3
N3—C5—C6	116.14 (19)	H16A—C16—H16B	107.9
C5—C6—C7	111.05 (17)	C18—C17—C16	111.8 (2)
C5—C6—H6A	109.4	C18—C17—H17A	109.3
C7—C6—H6A	109.4	C16—C17—H17A	109.3
C5—C6—H6B	109.4	C18—C17—H17B	109.3
C7—C6—H6B	109.4	C16—C17—H17B	109.3
H6A—C6—H6B	108.0	H17A—C17—H17B	107.9
C3—C7—C8	114.65 (18)	C19—C18—C17	111.7 (2)
C3—C7—C6	112.09 (17)	C19—C18—H18A	109.3
C8—C7—C6	112.24 (17)	C17—C18—H18A	109.3
C3—C7—H7	105.7	C19—C18—H18B	109.3
C8—C7—H7	105.7	C17—C18—H18B	109.3
C6—C7—H7	105.7	H18A—C18—H18B	107.9
C9—C8—C13	116.8 (2)	C18—C19—C20	111.7 (2)
C9—C8—C7	121.7 (2)	C18—C19—H19A	109.3
C13—C8—C7	121.2 (2)	C20—C19—H19A	109.3
C10—C9—C8	121.5 (2)	C18—C19—H19B	109.3
C10—C9—H9	119.2	C20—C19—H19B	109.3
C8—C9—H9	119.2	H19A—C19—H19B	107.9
C11—C10—C9	121.4 (2)	C15—C20—C19	110.4 (2)
C11—C10—H10	119.3	C15—C20—H20A	109.6
C9—C10—H10	119.3	C19—C20—H20A	109.6
C10—C11—C12	117.3 (2)	C15—C20—H20B	109.6
C10—C11—C14	120.5 (2)	C19—C20—H20B	109.6
C12—C11—C14	122.2 (2)	H20A—C20—H20B	108.1
C13—C12—C11	121.7 (2)		
C2—N2—C1—N1	1.1 (3)	C3—C7—C8—C9	153.35 (19)
C4—N1—C1—N2	−1.8 (4)	C6—C7—C8—C9	24.0 (3)
C1—N2—C2—O1	180.0 (2)	C3—C7—C8—C13	−33.2 (3)
C1—N2—C2—C3	−0.1 (3)	C6—C7—C8—C13	−162.62 (19)
O1—C2—C3—C4	179.7 (2)	C13—C8—C9—C10	−4.0 (3)
N2—C2—C3—C4	−0.3 (3)	C7—C8—C9—C10	169.7 (2)
O1—C2—C3—C7	−5.2 (3)	C8—C9—C10—C11	1.0 (3)
N2—C2—C3—C7	174.9 (2)	C9—C10—C11—C12	2.5 (3)
C1—N1—C4—O2	−178.3 (2)	C9—C10—C11—C14	−176.1 (2)
C1—N1—C4—C3	1.3 (3)	C10—C11—C12—C13	−3.1 (3)
C2—C3—C4—O2	179.2 (2)	C14—C11—C12—C13	175.5 (2)
C7—C3—C4—O2	4.0 (4)	C11—C12—C13—C8	0.1 (3)
C2—C3—C4—N1	−0.3 (3)	C9—C8—C13—C12	3.4 (3)
C7—C3—C4—N1	−175.56 (18)	C7—C8—C13—C12	−170.3 (2)
C15—N3—C5—O3	−4.8 (3)	C5—N3—C15—C16	−94.9 (3)
C15—N3—C5—C6	174.2 (2)	C5—N3—C15—C20	142.0 (2)
O3—C5—C6—C7	66.6 (3)	N3—C15—C16—C17	179.60 (18)

N3—C5—C6—C7	−112.4 (2)	C20—C15—C16—C17	−56.7 (3)
C2—C3—C7—C8	117.4 (2)	C15—C16—C17—C18	54.0 (3)
C4—C3—C7—C8	−67.5 (3)	C16—C17—C18—C19	−52.2 (3)
C2—C3—C7—C6	−113.1 (2)	C17—C18—C19—C20	54.0 (3)
C4—C3—C7—C6	62.0 (3)	N3—C15—C20—C19	−178.2 (2)
C5—C6—C7—C3	44.5 (2)	C16—C15—C20—C19	57.8 (3)
C5—C6—C7—C8	175.24 (18)	C18—C19—C20—C15	−57.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3[i]	0.86	1.98	2.813 (3)	162
O1—H1*A*···N2[ii]	0.82	1.95	2.753 (3)	168
N3—H3···O2[iii]	0.86	2.19	2.992 (4)	155
C17—H17*B*···*Cg*2[iv]	0.97	2.47	3.440 (3)	177
C20—H20*A*···*Cg*2[v]	0.97	2.74	3.629 (3)	152

Symmetry codes: (i) $x+1$, y, z; (ii) $-x+2$, $-y+2$, $-z+2$; (iii) $-x+2$, $-y+2$, $-z+1$; (iv) $-x+1/2$, $y+1/2$, $-z+1/2$; (v) $-x$, $-y$, $-z+1$.