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N-(4-Bromobenzoyl)-*N*,*N*′-dicyclohexylurea

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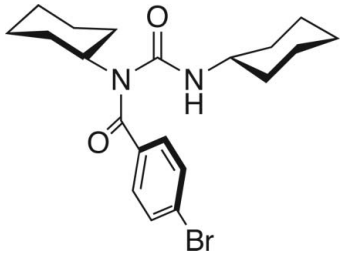
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.078; data-to-parameter ratio = 19.6.

In the title compound, $C_{20}H_{27}BrN_2O_2$, molecules are linked into one-dimensional chains through (amide)N—H···O=C(amide) intermolecular hydrogen bonds.

Related literature

For related literature, see: Bohne *et al.* (2005); Bondy *et al.* (2004); Bruker (2000); Ślebioda (1995). For literature on related crystal structures, see: Ball *et al.* (1990); Chérioux *et al.* (2002); Gallagher *et al.* (1999); Govindasamy & Subramanian (1997); Toniolo *et al.* (1990); Wu *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{27}BrN_2O_2$
M_r = 407.35
Monoclinic, $P2_1/n$
a = 13.501 (2) Å
b = 9.5621 (10) Å
c = 16.306 (2) Å
β = 114.443 (6)°
V = 1916.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.16 mm^{-1}
T = 113 (2) K
0.38 × 0.16 × 0.14 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*REQABS*; Jacobson, 1998)
T_{min} = 0.484, T_{max} = 0.739
17461 measured reflections
4526 independent reflections
3651 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.078
S = 1.06
4526 reflections
231 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.898 (10)	2.072 (11)	2.961 (2)	170 (2)

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

Data collection: *CrystalClear* (Jacobson, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2071).

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N-(4-Bromobenzoyl)-*N*,*N*′-dicyclohexylurea

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S1. Comment

The first conscious total synthesis of a natural product was that of urea in 1828 by Wohler, which marks the beginnings of organic synthesis. Since then, many urea derivatives have been prepared and have demonstrated a wide range of uses, including fluorescence probes (Bohne *et al.*, 2005) and anion receptors (Bondy *et al.*, 2004).

The title compound, an *N*-acylurea derivative, can be conveniently prepared from dicyclohexylcarbodiimide (DCC) and *p*-bromobenzoic acid according to reported methods (Ślebioda, 1995). The molecular structure is shown in Fig.1. Each cyclohexyl group adopts the chair conformation, as is required for energy minimization. The two carbonyl groups are twisted substantially at the central atom, N1, with a dihedral angle of 66.43 (10)° between the O1/C7/N1 and O2/C14/N2 planes, which increases the distance between atoms O1 and N2. As a result, no intramolecular N2–H2A···O1 hydrogen bond is formed. However, molecules are linked into chains through (amide) N–H···O=C (amide) intermolecular hydrogen bonds, reinforced by C–H···O=C interactions. Surprisingly, this supramolecular arrangement is not observed in a closely related X-ray structure (Gallagher *et al.*, 1999).

S2. Experimental

p-bromobenzoic acid (201 mg, 1 mmol) was dissolved in $CHCl_3$ (5 ml) and DCC (206 mg, 1 mmol) and *N*,*N*-dimethyl-pyridin-4-amine (122 mg, 1 mmol) were added to the solution. The resulting mixture was stirred for 1 h at 298 K. After evaporation of the solvent, a colorless solid was isolated. Single crystals suitable for X-ray structure determination were obtained by slow evaporation of a EtOAc solution over a period of several days.

S3. Refinement

The H atom bonded to N2 was found in a difference map and refined freely to obtain an unbiased geometry for the hydrogen bonding scheme. The H atoms bonded to C were placed geometrically (C—H values were set to 1.00, 0.99 and 0.95 A° for atoms CH_2 and CH, respectively) and refined with a riding model, with U_{iso}(H) = 1.2 times U_{eq}(C).

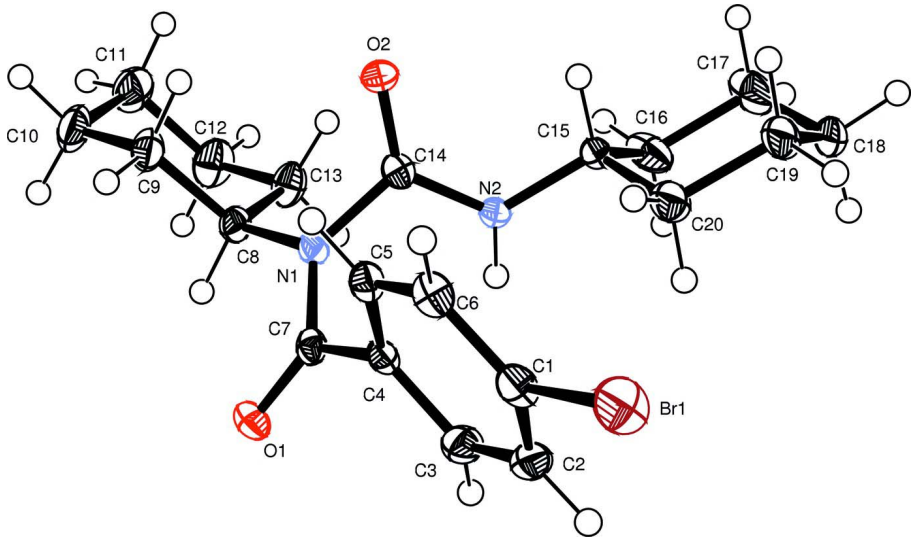

Figure 1

An ellipsoid plot of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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Crystal data

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$a = 13.501\ (2)$ Å
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$\beta = 114.443\ (6)°$
$V = 1916.3\ (4)$ Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 4164 reflections
$\theta = 1.7–27.9°$
$\mu = 2.16$ mm^{-1}
$T = 113$ K
Prism, colorless
0.38 × 0.16 × 0.14 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: Rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (REQABS; Jacobson, 1998)
$T_{min} = 0.484$, $T_{max} = 0.739$
17461 measured reflections
4526 independent reflections
3651 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.7°$
$h = -17\rightarrow17$
$k = -12\rightarrow12$
$l = -21\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.078$
$S = 1.06$
4526 reflections
231 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Special details

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 $F^2 > 2\sigma(F^2)$ 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}
Br1	0.615319 (17)	0.39160 (2)	1.092233 (14)	0.03591 (9)
N1	0.86443 (11)	0.53780 (15)	0.80694 (9)	0.0172 (3)
N2	0.67615 (11)	0.53992 (16)	0.73657 (10)	0.0180 (3)
O1	0.95485 (9)	0.68643 (13)	0.92419 (8)	0.0226 (3)
O2	0.76754 (10)	0.34042 (13)	0.73292 (8)	0.0234 (3)
C1	0.69576 (14)	0.4583 (2)	1.02792 (12)	0.0233 (4)
C2	0.69278 (15)	0.5987 (2)	1.00682 (13)	0.0267 (4)
H2	0.6508	0.6624	1.0240	0.032*
C3	0.75215 (15)	0.6450 (2)	0.96011 (13)	0.0246 (4)
H3	0.7519	0.7414	0.9460	0.029*
C4	0.81235 (13)	0.55047 (19)	0.93373 (11)	0.0176 (4)
C5	0.81418 (14)	0.40955 (19)	0.95585 (12)	0.0205 (4)
H5	0.8551	0.3450	0.9381	0.025*
C6	0.75616 (14)	0.3634 (2)	1.00396 (12)	0.0223 (4)
H6	0.7581	0.2677	1.0202	0.027*
C7	0.88221 (13)	0.60122 (18)	0.88777 (12)	0.0179 (4)
C8	0.94261 (14)	0.55666 (19)	0.76516 (12)	0.0199 (4)
H8	0.9907	0.6372	0.7963	0.024*
C9	1.01578 (15)	0.4287 (2)	0.77921 (14)	0.0259 (4)
H9A	0.9702	0.3452	0.7531	0.031*
H9B	1.0574	0.4122	0.8445	0.031*
C10	1.09504 (16)	0.4493 (2)	0.73482 (14)	0.0331 (5)
H10A	1.1462	0.5260	0.7656	0.040*
H10B	1.1380	0.3628	0.7415	0.040*
C11	1.03445 (17)	0.4842 (2)	0.63510 (14)	0.0361 (5)
H11A	0.9878	0.4043	0.6032	0.043*
H11B	1.0874	0.5007	0.6086	0.043*
C12	0.96424 (17)	0.6143 (2)	0.62288 (14)	0.0341 (5)
H12A	0.9238	0.6338	0.5578	0.041*
H12B	1.0117	0.6956	0.6507	0.041*
C13	0.88348 (15)	0.5955 (2)	0.66570 (13)	0.0268 (4)
H13A	0.8424	0.6834	0.6599	0.032*
H13B	0.8308	0.5210	0.6335	0.032*
C14	0.76568 (14)	0.4618 (2)	0.75616 (11)	0.0180 (4)
C15	0.56540 (13)	0.48403 (19)	0.69141 (12)	0.0180 (4)

H15	0.5702	0.3853	0.6733	0.022*
C16	0.50196 (16)	0.5682 (2)	0.60708 (13)	0.0313 (5)
H16A	0.5392	0.5639	0.5661	0.038*
H16B	0.4987	0.6673	0.6233	0.038*
C17	0.38642 (16)	0.5099 (2)	0.55931 (15)	0.0399 (6)
H17A	0.3452	0.5668	0.5051	0.048*
H17B	0.3899	0.4128	0.5396	0.048*
C18	0.32755 (16)	0.5114 (2)	0.62076 (18)	0.0509 (7)
H18A	0.3189	0.6091	0.6368	0.061*
H18B	0.2542	0.4702	0.5890	0.061*
C19	0.39104 (16)	0.4288 (2)	0.70547 (16)	0.0403 (6)
H19A	0.3934	0.3293	0.6896	0.048*
H19B	0.3535	0.4344	0.7462	0.048*
C20	0.50804 (16)	0.4842 (2)	0.75473 (14)	0.0296 (5)
H20A	0.5063	0.5805	0.7764	0.036*
H20B	0.5487	0.4245	0.8077	0.036*
H2A	0.6851 (15)	0.6326 (10)	0.7456 (12)	0.023 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03720 (13)	0.04748 (17)	0.03229 (13)	−0.01255 (10)	0.02362 (10)	−0.00410 (10)
N1	0.0147 (7)	0.0164 (8)	0.0206 (8)	−0.0024 (6)	0.0075 (6)	−0.0004 (6)
N2	0.0154 (7)	0.0136 (9)	0.0238 (8)	−0.0013 (6)	0.0070 (6)	−0.0024 (7)
O1	0.0190 (6)	0.0223 (7)	0.0233 (7)	−0.0054 (6)	0.0056 (5)	−0.0015 (6)
O2	0.0213 (6)	0.0140 (7)	0.0322 (8)	0.0006 (5)	0.0084 (6)	−0.0032 (6)
C1	0.0217 (9)	0.0320 (12)	0.0174 (9)	−0.0071 (8)	0.0093 (8)	−0.0027 (9)
C2	0.0257 (10)	0.0269 (12)	0.0320 (11)	−0.0048 (8)	0.0165 (9)	−0.0102 (9)
C3	0.0259 (10)	0.0198 (11)	0.0297 (10)	−0.0034 (8)	0.0132 (8)	−0.0030 (9)
C4	0.0141 (8)	0.0212 (10)	0.0151 (8)	−0.0030 (7)	0.0037 (7)	−0.0019 (8)
C5	0.0164 (8)	0.0239 (11)	0.0194 (9)	0.0003 (8)	0.0057 (7)	0.0005 (8)
C6	0.0218 (9)	0.0244 (11)	0.0191 (9)	−0.0012 (8)	0.0067 (8)	0.0040 (8)
C7	0.0145 (8)	0.0166 (10)	0.0198 (9)	0.0026 (7)	0.0045 (7)	0.0037 (8)
C8	0.0171 (9)	0.0203 (10)	0.0252 (10)	−0.0019 (7)	0.0117 (8)	−0.0001 (8)
C9	0.0188 (9)	0.0267 (11)	0.0306 (11)	0.0044 (8)	0.0087 (8)	0.0030 (9)
C10	0.0221 (10)	0.0396 (13)	0.0405 (12)	0.0087 (9)	0.0159 (9)	0.0002 (11)
C11	0.0321 (11)	0.0479 (14)	0.0351 (12)	0.0045 (10)	0.0209 (10)	−0.0050 (11)
C12	0.0348 (11)	0.0463 (14)	0.0290 (11)	0.0046 (10)	0.0210 (10)	0.0048 (10)
C13	0.0245 (10)	0.0332 (12)	0.0264 (10)	0.0058 (9)	0.0144 (8)	0.0065 (9)
C14	0.0176 (9)	0.0184 (10)	0.0179 (9)	−0.0019 (7)	0.0074 (7)	0.0019 (8)
C15	0.0141 (8)	0.0162 (10)	0.0219 (9)	−0.0008 (7)	0.0055 (7)	−0.0019 (8)
C16	0.0314 (11)	0.0229 (11)	0.0270 (11)	−0.0040 (9)	−0.0006 (9)	0.0023 (9)
C17	0.0268 (11)	0.0284 (13)	0.0408 (13)	0.0028 (9)	−0.0096 (10)	0.0015 (10)
C18	0.0150 (10)	0.0391 (14)	0.0841 (19)	0.0034 (10)	0.0060 (12)	−0.0301 (14)
C19	0.0277 (11)	0.0528 (15)	0.0518 (15)	−0.0179 (10)	0.0279 (11)	−0.0276 (12)
C20	0.0262 (10)	0.0367 (13)	0.0304 (11)	−0.0088 (9)	0.0163 (9)	−0.0101 (10)

Geometric parameters (Å, º)

Br1—C1	1.9048 (18)	C10—H10A	0.9900
N1—C7	1.379 (2)	C10—H10B	0.9900
N1—C14	1.441 (2)	C11—C12	1.526 (3)
N1—C8	1.485 (2)	C11—H11A	0.9900
N2—C14	1.342 (2)	C11—H11B	0.9900
N2—C15	1.467 (2)	C12—C13	1.529 (2)
N2—H2A	0.898 (9)	C12—H12A	0.9900
O1—C7	1.223 (2)	C12—H12B	0.9900
O2—C14	1.225 (2)	C13—H13A	0.9900
C1—C6	1.380 (3)	C13—H13B	0.9900
C1—C2	1.382 (3)	C15—C16	1.516 (2)
C2—C3	1.387 (3)	C15—C20	1.526 (2)
C2—H2	0.9500	C15—H15	1.0000
C3—C4	1.397 (3)	C16—C17	1.531 (3)
C3—H3	0.9500	C16—H16A	0.9900
C4—C5	1.393 (3)	C16—H16B	0.9900
C4—C7	1.507 (2)	C17—C18	1.515 (3)
C5—C6	1.390 (2)	C17—H17A	0.9900
C5—H5	0.9500	C17—H17B	0.9900
C6—H6	0.9500	C18—C19	1.512 (3)
C8—C13	1.528 (2)	C18—H18A	0.9900
C8—C9	1.529 (3)	C18—H18B	0.9900
C8—H8	1.0000	C19—C20	1.540 (3)
C9—C10	1.532 (3)	C19—H19A	0.9900
C9—H9A	0.9900	C19—H19B	0.9900
C9—H9B	0.9900	C20—H20A	0.9900
C10—C11	1.524 (3)	C20—H20B	0.9900
C7—N1—C14	121.65 (14)	C11—C12—C13	111.49 (17)
C7—N1—C8	120.63 (14)	C11—C12—H12A	109.3
C14—N1—C8	117.50 (14)	C13—C12—H12A	109.3
C14—N2—C15	123.18 (15)	C11—C12—H12B	109.3
C14—N2—H2A	117.5 (12)	C13—C12—H12B	109.3
C15—N2—H2A	118.8 (12)	H12A—C12—H12B	108.0
C6—C1—C2	121.85 (17)	C8—C13—C12	110.81 (16)
C6—C1—Br1	118.30 (15)	C8—C13—H13A	109.5
C2—C1—Br1	119.85 (14)	C12—C13—H13A	109.5
C1—C2—C3	118.86 (18)	C8—C13—H13B	109.5
C1—C2—H2	120.6	C12—C13—H13B	109.5
C3—C2—H2	120.6	H13A—C13—H13B	108.1
C2—C3—C4	120.33 (18)	O2—C14—N2	125.83 (16)
C2—C3—H3	119.8	O2—C14—N1	121.54 (16)
C4—C3—H3	119.8	N2—C14—N1	112.60 (16)
C5—C4—C3	119.75 (17)	N2—C15—C16	109.75 (14)
C5—C4—C7	119.52 (16)	N2—C15—C20	110.93 (14)
C3—C4—C7	120.56 (17)	C16—C15—C20	111.03 (16)

C6—C5—C4	119.98 (17)	N2—C15—H15	108.3
C6—C5—H5	120.0	C16—C15—H15	108.3
C4—C5—H5	120.0	C20—C15—H15	108.3
C1—C6—C5	119.22 (18)	C15—C16—C17	110.02 (16)
C1—C6—H6	120.4	C15—C16—H16A	109.7
C5—C6—H6	120.4	C17—C16—H16A	109.7
O1—C7—N1	122.99 (16)	C15—C16—H16B	109.7
O1—C7—C4	120.93 (16)	C17—C16—H16B	109.7
N1—C7—C4	115.88 (15)	H16A—C16—H16B	108.2
N1—C8—C13	110.98 (14)	C18—C17—C16	111.28 (18)
N1—C8—C9	111.83 (15)	C18—C17—H17A	109.4
C13—C8—C9	112.02 (16)	C16—C17—H17A	109.4
N1—C8—H8	107.2	C18—C17—H17B	109.4
C13—C8—H8	107.2	C16—C17—H17B	109.4
C9—C8—H8	107.2	H17A—C17—H17B	108.0
C8—C9—C10	111.13 (16)	C19—C18—C17	110.18 (17)
C8—C9—H9A	109.4	C19—C18—H18A	109.6
C10—C9—H9A	109.4	C17—C18—H18A	109.6
C8—C9—H9B	109.4	C19—C18—H18B	109.6
C10—C9—H9B	109.4	C17—C18—H18B	109.6
H9A—C9—H9B	108.0	H18A—C18—H18B	108.1
C11—C10—C9	111.13 (16)	C18—C19—C20	111.59 (18)
C11—C10—H10A	109.4	C18—C19—H19A	109.3
C9—C10—H10A	109.4	C20—C19—H19A	109.3
C11—C10—H10B	109.4	C18—C19—H19B	109.3
C9—C10—H10B	109.4	C20—C19—H19B	109.3
H10A—C10—H10B	108.0	H19A—C19—H19B	108.0
C10—C11—C12	110.37 (17)	C15—C20—C19	110.18 (16)
C10—C11—H11A	109.6	C15—C20—H20A	109.6
C12—C11—H11A	109.6	C19—C20—H20A	109.6
C10—C11—H11B	109.6	C15—C20—H20B	109.6
C12—C11—H11B	109.6	C19—C20—H20B	109.6
H11A—C11—H11B	108.1	H20A—C20—H20B	108.1

C6—C1—C2—C3	0.1 (3)	C13—C8—C9—C10	54.1 (2)
Br1—C1—C2—C3	179.88 (14)	C8—C9—C10—C11	−55.5 (2)
C1—C2—C3—C4	1.0 (3)	C9—C10—C11—C12	57.0 (2)
C2—C3—C4—C5	−1.1 (3)	C10—C11—C12—C13	−57.3 (2)
C2—C3—C4—C7	−176.41 (17)	N1—C8—C13—C12	−179.79 (15)
C3—C4—C5—C6	0.0 (3)	C9—C8—C13—C12	−54.0 (2)
C7—C4—C5—C6	175.39 (15)	C11—C12—C13—C8	55.7 (2)
C2—C1—C6—C5	−1.2 (3)	C15—N2—C14—O2	6.6 (3)
Br1—C1—C6—C5	179.06 (13)	C15—N2—C14—N1	−175.26 (14)
C4—C5—C6—C1	1.1 (3)	C7—N1—C14—O2	−125.42 (18)
C14—N1—C7—O1	−166.44 (16)	C8—N1—C14—O2	60.0 (2)
C8—N1—C7—O1	7.9 (2)	C7—N1—C14—N2	56.4 (2)
C14—N1—C7—C4	18.6 (2)	C8—N1—C14—N2	−118.19 (17)
C8—N1—C7—C4	−167.06 (14)	C14—N2—C15—C16	−124.11 (18)

C5—C4—C7—O1	−117.18 (19)	C14—N2—C15—C20	112.83 (19)
C3—C4—C7—O1	58.1 (2)	N2—C15—C16—C17	179.70 (16)
C5—C4—C7—N1	57.9 (2)	C20—C15—C16—C17	−57.3 (2)
C3—C4—C7—N1	−126.75 (18)	C15—C16—C17—C18	57.9 (2)
C7—N1—C8—C13	−131.60 (17)	C16—C17—C18—C19	−57.3 (2)
C14—N1—C8—C13	43.0 (2)	C17—C18—C19—C20	56.3 (2)
C7—N1—C8—C9	102.52 (19)	N2—C15—C20—C19	178.56 (17)
C14—N1—C8—C9	−82.87 (19)	C16—C15—C20—C19	56.2 (2)
N1—C8—C9—C10	179.38 (15)	C18—C19—C20—C15	−55.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.90 (1)	2.07 (1)	2.961 (2)	170 (2)

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