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N-(3,4-Dimethylphenyl)acetamide

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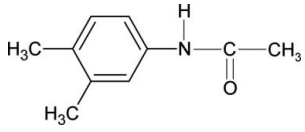
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.064; wR factor = 0.209; data-to-parameter ratio = 14.6.

The conformation of the N—H bond in the title compound (34DMPA), $C_{10}H_{13}NO$, is *syn* to the 3-methyl substituent in the aromatic ring, in contrast to the *anti* conformation observed with respect to the 3-chloro substituent in *N*-(3,4-dichlorophenyl)acetamide (34DCPA). The asymmetric unit of the structure contains three molecules. The bond parameters in 34DMPA are similar to those in 34DCPA, *N*-(2,6-dimethylphenyl)acetamide, *N*-(3,5-dimethylphenyl)acetamide and other acetanilides. The molecules in 34DMPA are linked into infinite chains through N—H···O hydrogen bonding.

Related literature

For related literature, see: Gowda *et al.* (2007*a*,*b*); Gowda, Kozisek, Svoboda & Fuess (2007); Gowda, Kožíšek, Tokarčík & Fuess (2007); Jones *et al.* (1990); Shilpa & Gowda (2007).



Experimental

Crystal data

$C_{10}H_{13}NO$
M_r = 163.21
Triclinic, $P\overline{1}$
a = 6.749 (1) Å
b = 14.281 (2) Å
c = 15.005 (2) Å
α = 85.33 (1)°
β = 79.81 (1)°
γ = 87.58 (1)°
V = 1418.1 (3) Å^3
Z = 6
Cu $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 299 (2) K
0.35 × 0.33 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
5528 measured reflections
5025 independent reflections
3386 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
3 standard reflections
frequency: 120 min
intensity decay: 2.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.210
S = 1.03
5025 reflections
344 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O3	0.88 (3)	2.08 (3)	2.956 (3)	177 (3)
N3—H3*N*···O2	0.86 (3)	2.14 (3)	2.989 (3)	172 (3)
N2—H2*N*···O1^{i}	0.98 (3)	1.92 (3)	2.893 (3)	170 (2)

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

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2051).

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supporting information

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N-(3,4-Dimethylphenyl)acetamide

B. Thimme Gowda, Sabine Foro and Hartmut Fuess

S1. Comment

In the present work, the structure of *N*-(3,4-dimethylphenyl)-acetamide (34DMPA) has been determined to study the effect of substituents on the structures of *N*-aromatic amides (Gowda *et al.*, 2007*a*, *b*; Gowda, Kozisek, Svoboda & Fuess, 2007; Gowda, Kožíšek, Tokarčík & Fuess, 2007). The conformation of the N—H bond in 34DMPA is *syn* to the 3-methyl substituent in the aromatic ring, in contrast to the anti conformation obseved with respect to the 3-chloro substituent in *N*-(3,4-dichlorophenyl)-acetamide (34DCPA) (Jones *et al.*, 1990). The asymmetric unit of the structure contains 3 molecules. The bond parameters in 34DMPA are similar to those in 34DCPA (Jones *et al.*, 1990), *N*-(2,6-dimethylphenyl)-acetamide (Gowda *et al.*, 2007*b*), *N*-(3,5-dimethylphenyl)-acetamide (Gowda, Kožíšek, Tokarčík & Fuess, 2007) and other acetanilides. The molecules in 34DMPA are linked into chains through N—H···O hydrogen bonding (Table 1 & Fig. 2).

S2. Experimental

The title compound was prepared according to the literature method (Shilpa and Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Shilpa and Gowda, 2007). Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

S3. Refinement

The CH atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å. The NH atoms were located in difference map with N—H = 0.86 (3)–0.98 (3) Å. U_{iso}(H) values were set equal to 1.2 U_{eq} of the parent atom.were set equal to 1.2 U_{eq} of the parent atom.

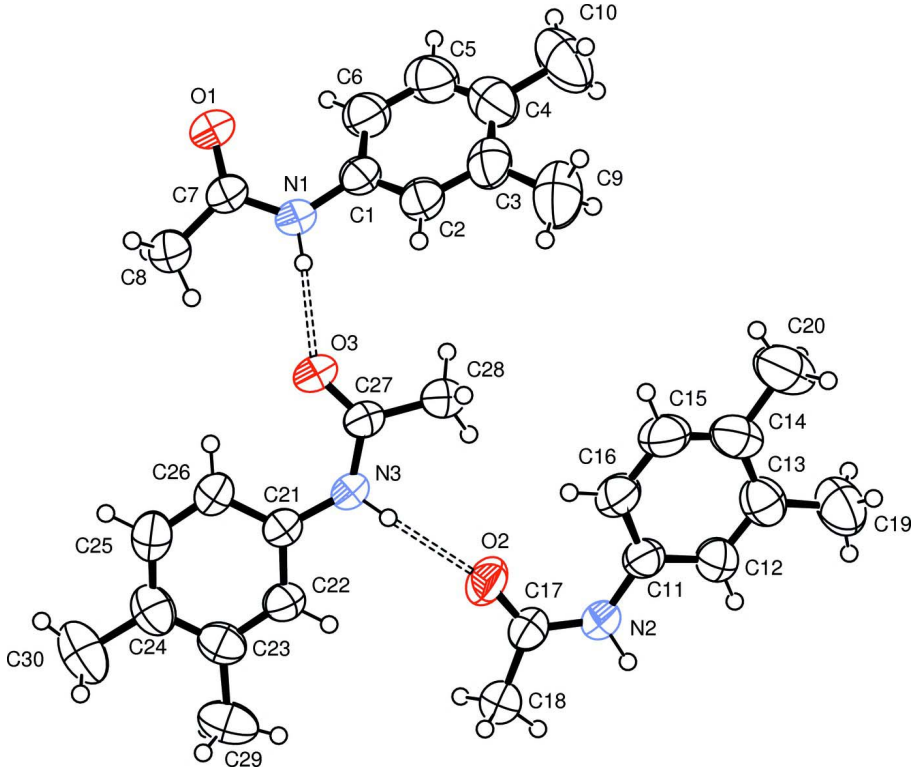

Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

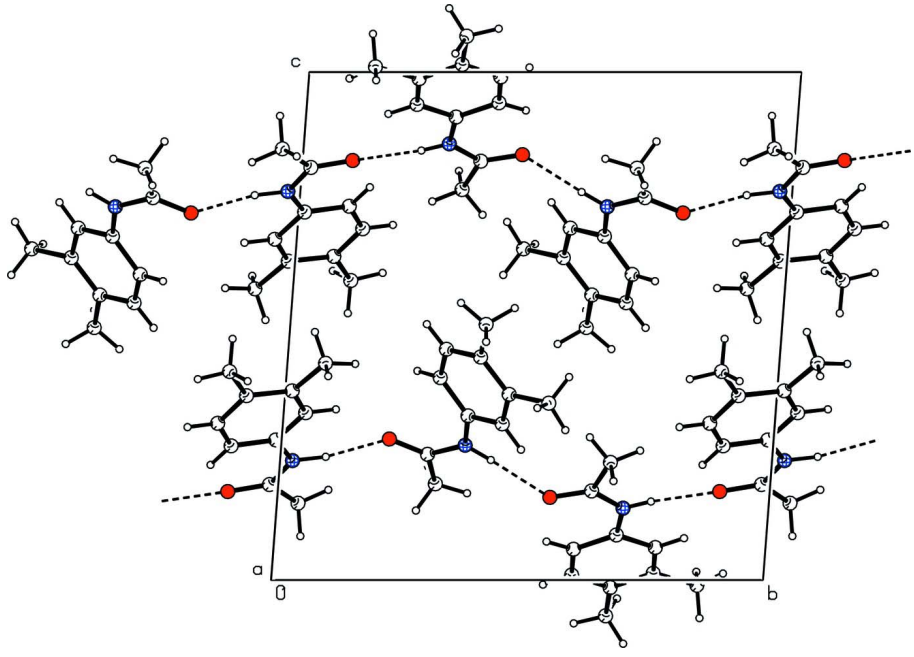

Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

N-(3,4-Dimethylphenyl)acetamide

Crystal data

$C_{10}H_{13}NO$
$M_r = 163.21$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.749$ (1) Å
$b = 14.281$ (2) Å
$c = 15.005$ (2) Å
$\alpha = 85.33$ (1)°
$\beta = 79.81$ (1)°
$\gamma = 87.58$ (1)°
$V = 1418.1$ (3) Å^3
$Z = 6$
$F(000) = 528$
$D_x = 1.147$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 3.1$–22.1°
$\mu = 0.59$ mm^{-1}
$T = 299$ K
Prism, colourless
0.35 × 0.33 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
5528 measured reflections
5025 independent reflections
3386 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 66.9°$, $\theta_{min} = 3.0°$
$h = -8 \rightarrow 1$
$k = -17 \rightarrow 17$
$l = -17 \rightarrow 17$
3 standard reflections every 120 min
intensity decay: 2.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.210$
$S = 1.03$
5025 reflections
344 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1316P)^2 + 0.1229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0022 (7)

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	0.6611 (4)	0.21887 (13)	0.27754 (16)	0.0935 (7)
N1	0.7204 (3)	0.37376 (14)	0.26524 (16)	0.0647 (6)

H1N	0.702 (4)	0.428 (2)	0.2362 (19)	0.078*
C1	0.8633 (4)	0.37519 (17)	0.32314 (17)	0.0633 (6)
C2	1.0021 (4)	0.44579 (19)	0.3073 (2)	0.0713 (7)
H2	1.0045	0.4879	0.2565	0.086*
C3	1.1384 (4)	0.4555 (2)	0.3653 (2)	0.0794 (8)
C4	1.1409 (5)	0.3917 (3)	0.4390 (2)	0.0906 (10)
C5	1.0037 (6)	0.3211 (3)	0.4542 (2)	0.0970 (10)
H5	1.0053	0.2774	0.5036	0.116*
C6	0.8637 (5)	0.3128 (2)	0.3985 (2)	0.0849 (9)
H6	0.7702	0.2654	0.4117	0.102*
C7	0.6247 (4)	0.29887 (17)	0.24731 (19)	0.0658 (6)
C8	0.4682 (4)	0.31912 (19)	0.1893 (2)	0.0778 (8)
H8A	0.4651	0.3850	0.1708	0.093*
H8B	0.3390	0.3016	0.2232	0.093*
H8C	0.4995	0.2838	0.1367	0.093*
C9	1.2754 (5)	0.5374 (3)	0.3480 (3)	0.1155 (13)
H9A	1.2499	0.5751	0.2951	0.139*
H9B	1.4130	0.5149	0.3385	0.139*
H9C	1.2511	0.5747	0.3995	0.139*
C10	1.2889 (7)	0.3980 (4)	0.5030 (3)	0.1352 (18)
H10A	1.4232	0.4007	0.4689	0.162*
H10B	1.2785	0.3437	0.5456	0.162*
H10C	1.2588	0.4537	0.5353	0.162*
O2	0.6415 (3)	0.89842 (12)	0.17410 (15)	0.0810 (6)
N2	0.7398 (3)	1.02533 (14)	0.23505 (15)	0.0625 (5)
H2N	0.709 (4)	1.092 (2)	0.2425 (18)	0.075*
C11	0.9017 (4)	0.98806 (17)	0.27568 (18)	0.0613 (6)
C12	0.9873 (4)	1.04469 (19)	0.32918 (18)	0.0697 (7)
H12	0.9362	1.1057	0.3360	0.084*
C13	1.1444 (5)	1.0139 (2)	0.37231 (19)	0.0775 (8)
C14	1.2212 (4)	0.9219 (2)	0.3629 (2)	0.0810 (8)
C15	1.1404 (5)	0.8675 (2)	0.3084 (3)	0.0908 (10)
H15	1.1927	0.8068	0.3009	0.109*
C16	0.9848 (4)	0.89835 (19)	0.2641 (2)	0.0822 (9)
H16	0.9360	0.8594	0.2267	0.099*
C17	0.6230 (4)	0.98221 (17)	0.18788 (17)	0.0617 (6)
C18	0.4661 (4)	1.04309 (19)	0.1511 (2)	0.0746 (7)
H18A	0.4555	1.1026	0.1774	0.089*
H18B	0.3387	1.0130	0.1660	0.089*
H18C	0.5031	1.0529	0.0863	0.089*
C19	1.2353 (6)	1.0776 (3)	0.4266 (3)	0.1110 (12)
H19A	1.1668	1.1379	0.4254	0.133*
H19B	1.3752	1.0848	0.4013	0.133*
H19C	1.2225	1.0513	0.4882	0.133*
C20	1.3884 (5)	0.8838 (3)	0.4104 (3)	0.1128 (13)
H20A	1.5045	0.9218	0.3914	0.135*
H20B	1.4218	0.8203	0.3953	0.135*
H20C	1.3459	0.8849	0.4748	0.135*

O3	0.6498 (3)	0.55410 (11)	0.16267 (14)	0.0773 (6)
N3	0.5363 (3)	0.70443 (13)	0.14131 (14)	0.0607 (5)
H3N	0.555 (4)	0.760 (2)	0.1545 (18)	0.073*
C21	0.3877 (4)	0.69495 (15)	0.08863 (16)	0.0565 (6)
C22	0.2832 (4)	0.77608 (17)	0.06384 (16)	0.0609 (6)
H22	0.3169	0.8330	0.0823	0.073*
C23	0.1323 (4)	0.7758 (2)	0.01327 (18)	0.0683 (7)
C24	0.0808 (4)	0.6904 (2)	−0.0150 (2)	0.0764 (8)
C25	0.1861 (5)	0.6102 (2)	0.0097 (2)	0.0824 (8)
H25	0.1532	0.5533	−0.0092	0.099*
C26	0.3366 (4)	0.60984 (18)	0.0604 (2)	0.0723 (7)
H26	0.4032	0.5540	0.0756	0.087*
C27	0.6556 (4)	0.63784 (16)	0.17531 (16)	0.0600 (6)
C28	0.7946 (5)	0.67177 (19)	0.2314 (2)	0.0846 (9)
H28A	0.9251	0.6808	0.1947	0.101*
H28B	0.8056	0.6261	0.2810	0.101*
H28C	0.7430	0.7303	0.2546	0.101*
C29	0.0253 (5)	0.8664 (3)	−0.0104 (2)	0.0974 (10)
H29A	−0.1148	0.8630	0.0161	0.117*
H29B	0.0386	0.8766	−0.0752	0.117*
H29C	0.0836	0.9175	0.0127	0.117*
C30	−0.0827 (5)	0.6855 (3)	−0.0706 (2)	0.1065 (12)
H30A	−0.2087	0.7060	−0.0365	0.128*
H30B	−0.0925	0.6218	−0.0854	0.128*
H30C	−0.0511	0.7254	−0.1256	0.128*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1197 (17)	0.0455 (10)	0.1293 (18)	0.0036 (10)	−0.0624 (14)	−0.0039 (10)
N1	0.0750 (14)	0.0435 (10)	0.0809 (14)	0.0084 (9)	−0.0294 (11)	−0.0085 (9)
C1	0.0722 (16)	0.0520 (13)	0.0701 (15)	0.0128 (11)	−0.0214 (13)	−0.0183 (11)
C2	0.0703 (16)	0.0615 (15)	0.0851 (18)	0.0085 (12)	−0.0187 (14)	−0.0180 (13)
C3	0.0669 (17)	0.0801 (19)	0.095 (2)	0.0081 (14)	−0.0113 (15)	−0.0384 (16)
C4	0.094 (2)	0.107 (3)	0.078 (2)	0.0302 (19)	−0.0285 (17)	−0.0381 (19)
C5	0.128 (3)	0.095 (2)	0.0727 (19)	0.019 (2)	−0.033 (2)	−0.0118 (17)
C6	0.112 (2)	0.0733 (18)	0.0740 (17)	0.0072 (16)	−0.0310 (17)	−0.0088 (14)
C7	0.0712 (15)	0.0480 (13)	0.0822 (17)	0.0085 (11)	−0.0229 (13)	−0.0134 (11)
C8	0.0755 (17)	0.0617 (15)	0.104 (2)	0.0046 (13)	−0.0362 (16)	−0.0142 (14)
C9	0.092 (2)	0.126 (3)	0.133 (3)	−0.020 (2)	−0.015 (2)	−0.041 (3)
C10	0.125 (3)	0.190 (5)	0.109 (3)	0.038 (3)	−0.060 (3)	−0.061 (3)
O2	0.0835 (13)	0.0536 (10)	0.1117 (15)	−0.0016 (9)	−0.0232 (11)	−0.0266 (10)
N2	0.0678 (12)	0.0451 (10)	0.0776 (13)	−0.0025 (9)	−0.0202 (11)	−0.0051 (9)
C11	0.0581 (13)	0.0532 (13)	0.0713 (15)	−0.0023 (10)	−0.0100 (12)	0.0011 (11)
C12	0.0714 (16)	0.0664 (16)	0.0741 (16)	0.0001 (12)	−0.0187 (14)	−0.0102 (12)
C13	0.0732 (17)	0.094 (2)	0.0659 (16)	−0.0067 (15)	−0.0133 (14)	−0.0036 (14)
C14	0.0640 (16)	0.089 (2)	0.0840 (19)	0.0010 (15)	−0.0099 (15)	0.0200 (16)
C15	0.0762 (19)	0.0631 (17)	0.132 (3)	0.0055 (14)	−0.0238 (19)	0.0067 (18)

C16	0.0772 (18)	0.0521 (14)	0.122 (2)	0.0023 (12)	−0.0285 (18)	−0.0108 (15)
C17	0.0597 (14)	0.0531 (13)	0.0713 (15)	−0.0071 (10)	−0.0063 (12)	−0.0077 (11)
C18	0.0770 (17)	0.0628 (15)	0.0889 (19)	−0.0060 (13)	−0.0286 (15)	−0.0025 (13)
C19	0.108 (3)	0.130 (3)	0.107 (3)	0.004 (2)	−0.044 (2)	−0.030 (2)
C20	0.088 (2)	0.131 (3)	0.116 (3)	0.004 (2)	−0.029 (2)	0.033 (2)
O3	0.0991 (14)	0.0402 (9)	0.1004 (14)	0.0032 (8)	−0.0406 (11)	−0.0032 (8)
N3	0.0747 (13)	0.0378 (10)	0.0753 (13)	0.0002 (9)	−0.0272 (11)	−0.0072 (9)
C21	0.0622 (14)	0.0466 (12)	0.0624 (13)	0.0019 (10)	−0.0150 (11)	−0.0074 (10)
C22	0.0681 (15)	0.0503 (12)	0.0650 (14)	0.0039 (10)	−0.0144 (12)	−0.0051 (10)
C23	0.0603 (14)	0.0786 (17)	0.0635 (15)	0.0098 (12)	−0.0093 (12)	−0.0006 (12)
C24	0.0604 (15)	0.098 (2)	0.0734 (17)	0.0008 (14)	−0.0160 (13)	−0.0144 (15)
C25	0.085 (2)	0.0730 (18)	0.098 (2)	−0.0096 (15)	−0.0327 (17)	−0.0188 (15)
C26	0.0814 (18)	0.0517 (14)	0.0914 (19)	−0.0013 (12)	−0.0318 (15)	−0.0141 (12)
C27	0.0740 (15)	0.0439 (12)	0.0643 (14)	−0.0023 (10)	−0.0202 (12)	0.0016 (10)
C28	0.111 (2)	0.0558 (15)	0.099 (2)	0.0038 (14)	−0.0545 (19)	−0.0015 (14)
C29	0.085 (2)	0.104 (2)	0.100 (2)	0.0300 (18)	−0.0245 (18)	0.0084 (19)
C30	0.076 (2)	0.159 (4)	0.093 (2)	0.002 (2)	−0.0321 (18)	−0.026 (2)

Geometric parameters (Å, º)

O1—C7	1.226 (3)	C15—H15	0.9300
N1—C7	1.342 (3)	C16—H16	0.9300
N1—C1	1.410 (3)	C17—C18	1.494 (4)
N1—H1N	0.88 (3)	C18—H18A	0.9600
C1—C6	1.382 (4)	C18—H18B	0.9600
C1—C2	1.383 (4)	C18—H18C	0.9600
C2—C3	1.391 (4)	C19—H19A	0.9600
C2—H2	0.9300	C19—H19B	0.9600
C3—C4	1.376 (5)	C19—H19C	0.9600
C3—C9	1.500 (5)	C20—H20A	0.9600
C4—C5	1.376 (5)	C20—H20B	0.9600
C4—C10	1.514 (4)	C20—H20C	0.9600
C5—C6	1.382 (4)	O3—C27	1.229 (3)
C5—H5	0.9300	N3—C27	1.347 (3)
C6—H6	0.9300	N3—C21	1.399 (3)
C7—C8	1.488 (4)	N3—H3N	0.86 (3)
C8—H8A	0.9600	C21—C22	1.390 (3)
C8—H8B	0.9600	C21—C26	1.395 (3)
C8—H8C	0.9600	C22—C23	1.374 (4)
C9—H9A	0.9600	C22—H22	0.9300
C9—H9B	0.9600	C23—C24	1.400 (4)
C9—H9C	0.9600	C23—C29	1.503 (4)
C10—H10A	0.9600	C24—C25	1.382 (4)
C10—H10B	0.9600	C24—C30	1.504 (4)
C10—H10C	0.9600	C25—C26	1.372 (4)
O2—C17	1.228 (3)	C25—H25	0.9300
N2—C17	1.346 (3)	C26—H26	0.9300
N2—C11	1.408 (3)	C27—C28	1.486 (4)

N2—H2N	0.98 (3)	C28—H28A	0.9600
C11—C16	1.388 (4)	C28—H28B	0.9600
C11—C12	1.393 (4)	C28—H28C	0.9600
C12—C13	1.376 (4)	C29—H29A	0.9600
C12—H12	0.9300	C29—H29B	0.9600
C13—C14	1.401 (5)	C29—H29C	0.9600
C13—C19	1.487 (4)	C30—H30A	0.9600
C14—C15	1.366 (5)	C30—H30B	0.9600
C14—C20	1.499 (4)	C30—H30C	0.9600
C15—C16	1.378 (4)		

C7—N1—C1	127.2 (2)	O2—C17—N2	123.6 (2)
C7—N1—H1N	119.3 (19)	O2—C17—C18	120.6 (2)
C1—N1—H1N	113.3 (19)	N2—C17—C18	115.8 (2)
C6—C1—C2	118.2 (3)	C17—C18—H18A	109.5
C6—C1—N1	123.0 (3)	C17—C18—H18B	109.5
C2—C1—N1	118.6 (2)	H18A—C18—H18B	109.5
C1—C2—C3	121.8 (3)	C17—C18—H18C	109.5
C1—C2—H2	119.1	H18A—C18—H18C	109.5
C3—C2—H2	119.1	H18B—C18—H18C	109.5
C4—C3—C2	119.6 (3)	C13—C19—H19A	109.5
C4—C3—C9	121.2 (3)	C13—C19—H19B	109.5
C2—C3—C9	119.2 (3)	H19A—C19—H19B	109.5
C5—C4—C3	118.5 (3)	C13—C19—H19C	109.5
C5—C4—C10	119.9 (4)	H19A—C19—H19C	109.5
C3—C4—C10	121.7 (4)	H19B—C19—H19C	109.5
C4—C5—C6	122.2 (3)	C14—C20—H20A	109.5
C4—C5—H5	118.9	C14—C20—H20B	109.5
C6—C5—H5	118.9	H20A—C20—H20B	109.5
C1—C6—C5	119.7 (3)	C14—C20—H20C	109.5
C1—C6—H6	120.2	H20A—C20—H20C	109.5
C5—C6—H6	120.2	H20B—C20—H20C	109.5
O1—C7—N1	122.5 (2)	C27—N3—C21	129.3 (2)
O1—C7—C8	121.8 (2)	C27—N3—H3N	114.5 (19)
N1—C7—C8	115.7 (2)	C21—N3—H3N	116.2 (18)
C7—C8—H8A	109.5	C22—C21—C26	118.2 (2)
C7—C8—H8B	109.5	C22—C21—N3	117.3 (2)
H8A—C8—H8B	109.5	C26—C21—N3	124.5 (2)
C7—C8—H8C	109.5	C23—C22—C21	122.9 (2)
H8A—C8—H8C	109.5	C23—C22—H22	118.6
H8B—C8—H8C	109.5	C21—C22—H22	118.6
C3—C9—H9A	109.5	C22—C23—C24	119.0 (2)
C3—C9—H9B	109.5	C22—C23—C29	119.8 (3)
H9A—C9—H9B	109.5	C24—C23—C29	121.2 (3)
C3—C9—H9C	109.5	C25—C24—C23	117.7 (3)
H9A—C9—H9C	109.5	C25—C24—C30	120.7 (3)
H9B—C9—H9C	109.5	C23—C24—C30	121.5 (3)
C4—C10—H10A	109.5	C26—C25—C24	123.7 (3)

C4—C10—H10B	109.5	C26—C25—H25	118.2
H10A—C10—H10B	109.5	C24—C25—H25	118.2
C4—C10—H10C	109.5	C25—C26—C21	118.6 (3)
H10A—C10—H10C	109.5	C25—C26—H26	120.7
H10B—C10—H10C	109.5	C21—C26—H26	120.7
C17—N2—C11	129.2 (2)	O3—C27—N3	123.1 (2)
C17—N2—H2N	116.1 (16)	O3—C27—C28	121.4 (2)
C11—N2—H2N	114.7 (16)	N3—C27—C28	115.5 (2)
C16—C11—C12	117.6 (3)	C27—C28—H28A	109.5
C16—C11—N2	123.8 (2)	C27—C28—H28B	109.5
C12—C11—N2	118.5 (2)	H28A—C28—H28B	109.5
C13—C12—C11	122.6 (3)	C27—C28—H28C	109.5
C13—C12—H12	118.7	H28A—C28—H28C	109.5
C11—C12—H12	118.7	H28B—C28—H28C	109.5
C12—C13—C14	119.0 (3)	C23—C29—H29A	109.5
C12—C13—C19	120.8 (3)	C23—C29—H29B	109.5
C14—C13—C19	120.1 (3)	H29A—C29—H29B	109.5
C15—C14—C13	118.1 (3)	C23—C29—H29C	109.5
C15—C14—C20	120.5 (3)	H29A—C29—H29C	109.5
C13—C14—C20	121.3 (3)	H29B—C29—H29C	109.5
C14—C15—C16	123.1 (3)	C24—C30—H30A	109.5
C14—C15—H15	118.5	C24—C30—H30B	109.5
C16—C15—H15	118.5	H30A—C30—H30B	109.5
C15—C16—C11	119.5 (3)	C24—C30—H30C	109.5
C15—C16—H16	120.3	H30A—C30—H30C	109.5
C11—C16—H16	120.3	H30B—C30—H30C	109.5

C7—N1—C1—C6	−29.7 (4)	C19—C13—C14—C20	3.1 (5)
C7—N1—C1—C2	154.5 (3)	C13—C14—C15—C16	−1.3 (5)
C6—C1—C2—C3	−0.6 (4)	C20—C14—C15—C16	179.1 (3)
N1—C1—C2—C3	175.4 (2)	C14—C15—C16—C11	−1.2 (5)
C1—C2—C3—C4	2.2 (4)	C12—C11—C16—C15	2.9 (4)
C1—C2—C3—C9	−175.8 (3)	N2—C11—C16—C15	−178.6 (3)
C2—C3—C4—C5	−1.6 (4)	C11—N2—C17—O2	1.1 (4)
C9—C3—C4—C5	176.3 (3)	C11—N2—C17—C18	−178.3 (2)
C2—C3—C4—C10	178.8 (3)	C27—N3—C21—C22	178.8 (2)
C9—C3—C4—C10	−3.3 (5)	C27—N3—C21—C26	−0.5 (4)
C3—C4—C5—C6	−0.5 (5)	C26—C21—C22—C23	0.2 (4)
C10—C4—C5—C6	179.2 (3)	N3—C21—C22—C23	−179.1 (2)
C2—C1—C6—C5	−1.4 (4)	C21—C22—C23—C24	−0.1 (4)
N1—C1—C6—C5	−177.3 (3)	C21—C22—C23—C29	179.6 (3)
C4—C5—C6—C1	2.0 (5)	C22—C23—C24—C25	−0.1 (4)
C1—N1—C7—O1	−4.0 (5)	C29—C23—C24—C25	−179.9 (3)
C1—N1—C7—C8	175.1 (2)	C22—C23—C24—C30	−179.9 (3)
C17—N2—C11—C16	7.9 (4)	C29—C23—C24—C30	0.4 (4)
C17—N2—C11—C12	−173.6 (3)	C23—C24—C25—C26	0.3 (5)
C16—C11—C12—C13	−2.1 (4)	C30—C24—C25—C26	−179.9 (3)
N2—C11—C12—C13	179.3 (2)	C24—C25—C26—C21	−0.3 (5)

C11—C12—C13—C14	−0.4 (4)	C22—C21—C26—C25	0.0 (4)
C11—C12—C13—C19	178.2 (3)	N3—C21—C26—C25	179.3 (3)
C12—C13—C14—C15	2.1 (4)	C21—N3—C27—O3	0.7 (4)
C19—C13—C14—C15	−176.5 (3)	C21—N3—C27—C28	−178.2 (3)
C12—C13—C14—C20	−178.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3	0.88 (3)	2.08 (3)	2.956 (3)	177 (3)
N3—H3*N*···O2	0.86 (3)	2.14 (3)	2.989 (3)	172 (3)
N2—H2*N*···O1^{i}	0.98 (3)	1.92 (3)	2.893 (3)	170 (2)

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