Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-3-(4-Methylphenyl)-1-(3-nitrophenyl)prop-2-en-1-one

Jerry P. Jasinski,[a]* Ray J. Butcher,[b] B. Narayana,[c] K. Lakshmana[c] and H. S. Yathirajan[d]

[a]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [b]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India
Correspondence e-mail: jjasinski@keene.edu

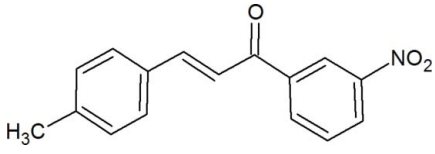
Received 11 November 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.127; data-to-parameter ratio = 23.8.

The title compound, $C_{16}H_{13}NO_3$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The dihedral angle between the mean planes of the 4-methylphenyl and 3-nitrophenyl groups is 4.0 (3)° in molecule *A* and 16.2 (7)° in molecule *B*. Intermolecular C—H···O hydrogen bonding involving the O atoms of the 3-nitrophenyl group of both independent molecules link the molecules into layers approximately parallel to the (110) plane. The layers are held together by π–π stacking interactions between the 4-methylphenyl ring of molecule *A* and the 3-nitrophenyl ring of molecule *B* of the adjacent layer, with the distance between the centroids of interacting rings being 3.6987 (7) Å.

Related literature

For related structures, see: Butcher, Jasinski, Narayana *et al.* (2007); Butcher, Jasinski, Yathirajan, Narayana *et al.* (2007); Butcher, Jasinski, Yathirajan, Veena *et al.* (2007); Rosli *et al.* (2007); Patil *et al.* (2007). For related literature, see: Dimmock *et al.* (1999); Go *et al.* (2005); Goto *et al.* (1991); Uchida *et al.* (1998); Tam *et al.* (1989).



Experimental

Crystal data

$C_{16}H_{13}NO_3$
M_r = 267.27
Triclinic, $P\overline{1}$
a = 8.0951 (3) Å
b = 11.5088 (5) Å
c = 14.6970 (5) Å
α = 80.351 (3)°
β = 74.830 (3)°
γ = 84.416 (3)°
V = 1300.78 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 (2) K
0.41 × 0.35 × 0.28 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.874, T_{max} = 0.974
19776 measured reflections
8636 independent reflections
4667 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.127
S = 0.97
8636 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2*A*—H2*A*···O2*B*	0.93	2.55	3.4644 (16)	170
C11*A*—H11*A*···O2*B*	0.93	2.59	3.5156 (14)	176
C2*B*—H2*B*···O2*A*^{i}	0.93	2.51	3.4311 (16)	171
C14*A*—H14*A*···O3*A*^{ii}	0.93	2.54	3.4455 (16)	164

Symmetry codes: (i) $x+1, y-1, z$; (ii) $x, y, z+1$.

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

KL thanks Mangalore University for use of their research facilities. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2518).

References

Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Butcher, R. J., Jasinski, J. P., Narayana, B., Lakshmana, K. & Yathirajan, H. S. (2007). *Acta Cryst.* E**63**, o3660.
Butcher, R. J., Jasinski, J. P., Yathirajan, H. S., Narayana, B. & Veena, K. (2007). *Acta Cryst.* E**63**, o3833.
Butcher, R. J., Jasinski, J. P., Yathirajan, H. S., Veena, K. & Narayana, B. (2007). *Acta Cryst.* E**63**, o3680.
Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. M. (1999). *Curr. Med. Chem.* **6**, 1125–1149.
Go, M. L., Wu, X. & Liu, X. L. (2005). *Curr. Med. Chem.* **12**, 483–499.
Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
Oxford Diffraction (2007). *CrysAlisPro* (Version 171.31.8) and *CrysAlis RED* (Version 1.171.31.8). Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Patil, P. S., Rosli, M. M., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o785–o786.
Rosli, M. M., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o2692.

 © 2008 International Union of Crystallography

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tam, W., Gurein, B., Calabrese, J. C. & Stevenson, S. H. (1989). *Chem. Phys. Lett.* **154**, 93–96.
Uchida, J., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abdeuyim, A. & Wadanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.

supporting information

Acta Cryst. (2008). E**64**, o1–o2 [https://doi.org/10.1107/S160053680706182X]

(2*E*)-3-(4-Methylphenyl)-1-(3-nitrophenyl)prop-2-en-1-one

Jerry P. Jasinski, Ray J. Butcher, B. Narayana, K. Lakshmana and H. S. Yathirajan

S1. Comment

Chalcones can be easily obtained from the Claisen-Schmidt reaction of aromatic aldehydes and aromatic ketones. Chalcones have been reported to possess many useful properties including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumour and anticancer activities (Dimmock *et al*. 1999; Go *et al.* 2005). They are also important intermediates in organic synthesis. Among several organic compounds reported to have NLO properties, chalcone derivatives are recognized material because of their excellent blue light transmittance and good crystallization ability. They provide necessary configuration to show NLO properties having two planar rings connected through a conjugated double bond (Goto *et al.* 1991; Uchida *et al.* 1998; Tam *et al.* 1989). The crystal structures of 1-(3-hydroxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one (Butcher, Jasinski, Narayana *et al.*, 2007), (2E)-1-(4-methylphenyl)-3-(4-nitrophenyl)prop-2-en-1-one (Butcher, Jasinski, Yathirajan, Veena *et al.*, 2007), (*E*)-3-(4-fluorophenyl)-1-(4-methylphenyl)prop-2-en-1-one (Butcher, Jasinski, Yathirajan, Narayana *et al.* 2007), 3-(dimethylaminophenyl)-1-(3-nitrophenyl)prop-2-en-1-one (Rosli *et al.* 2007) and 3-(5-bromo-2-thienyl)-1-(4-nitrophenyl)prop-2-en-1-one (Patil *et al.* 2007) have been reported. We report here the crystal structure of a new chalcone, the title compound.

The title compound crystallizes with two independent molecules (A and B) in the asymmetric unit (Fig. 1). The dihedral angle between the mean planes of the 4-methylphenyl and 3-nitrophenyl groups is 4.0 (3)° in molecule A and 16.2 (7)° in molecule B. Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding involving the O atoms on the 3-nitrophenyl group of both indpendent molecules. These hydrogen bonds (Table 1) link the molecules into a layer approximately parallel to the (1 1 0) plane (Fig. 2). Intermolecular π-π stacking interactions occur between 4-methylphenyl ring of molecule A at (x, y, z) and 3-nitrophenyl ring of molecule B of the adjacent layer at (1 - x, 1 - y, -z), with the distance between the centroids of interacting rings being 3.6987 (7) Å.

S2. Experimental

A solution of 1-(3-nitrophenyl)ethanone (1.65 g, 0.01 mol) and 4-methylbenzaldehyde (1.20 g, 0.01 mol) in ethanol (25 ml) was stirred well and 10% NaOH solution (5 ml) was added. The reaction mixture was stirred for about 6 h and filtered. The product was crystallized from acetone (m.p. 414–416 K). Single crystals suitable for X-ray structure determination were grown by slow evaporation of an acetone solution of the title compound at room temperature. Analysis found: C 71.82, H 4.85, N 5.20%; $C_{16}H_{13}NO_3$ requires: C 71.90, H 4.90, N 5.24%.

S3. Refinement

All H atoms were placed in calculated positions (C—H = 0.93 or 0.96 Å) and refined using a riding model, with U_{iso}(H) = 1.16–1.21U_{eq}(C).

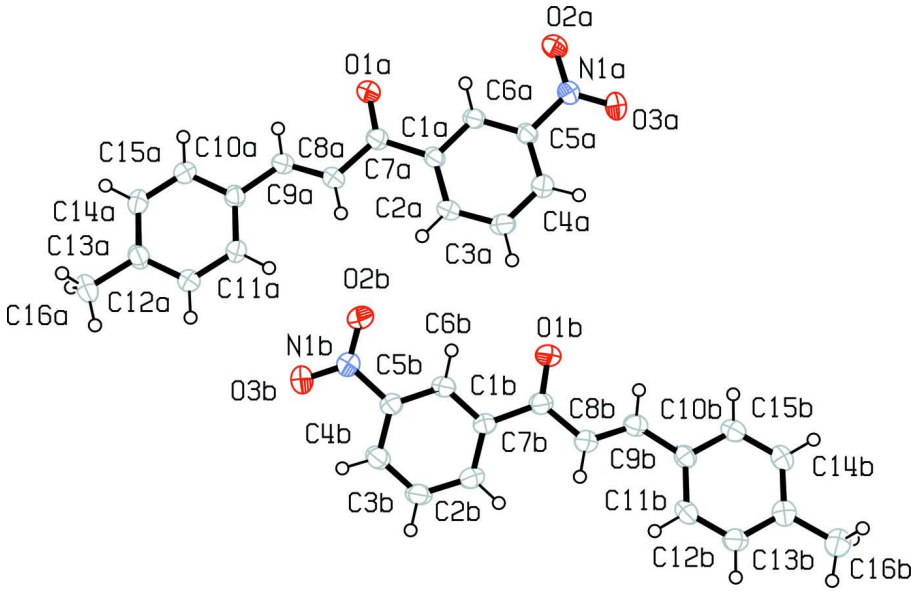


Figure 1

The asymmetric unit of the title compound, showing atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

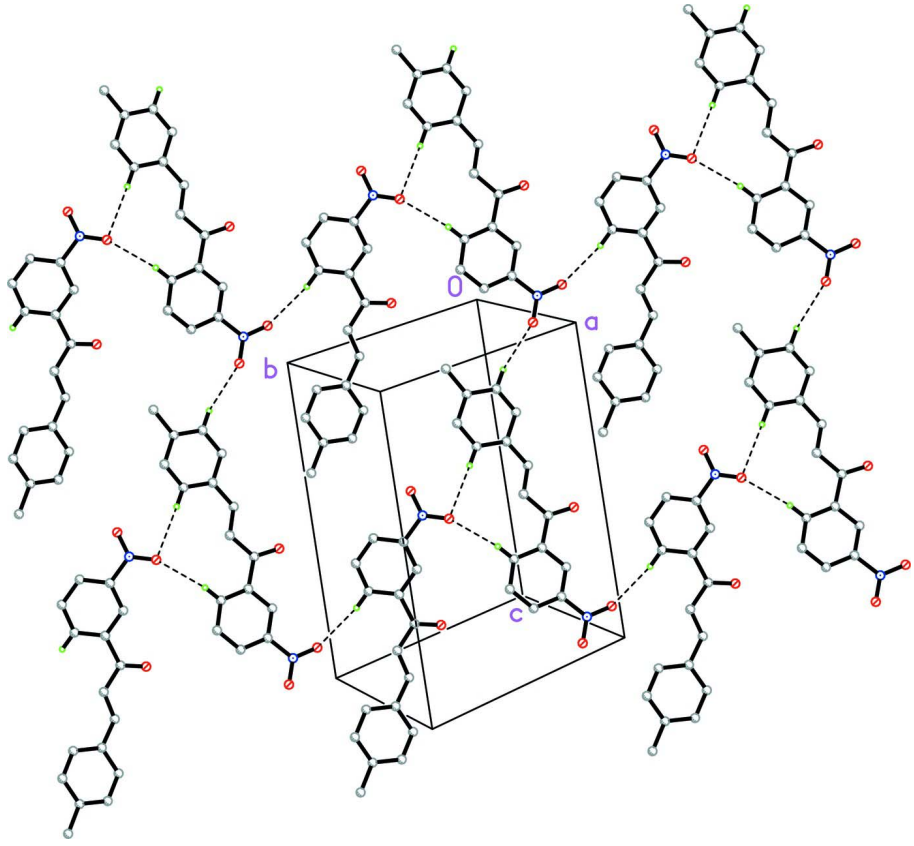


Figure 2

Packing diagram of the title compound, viewed down the *a* axis. Dashed lines indicate intermolecular C—H···O hydrogen bonds.

(2E)-3-(4-Methylphenyl)-1-(3-nitrophenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{13}NO_3$
$M_r = 267.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.0951$ (3) Å
$b = 11.5088$ (5) Å
$c = 14.6970$ (5) Å
$\alpha = 80.351$ (3)°
$\beta = 74.830$ (3)°
$\gamma = 84.416$ (3)°
$V = 1300.78$ (9) Å^3
$Z = 4$
$F(000) = 560$
$D_x = 1.365$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6626 reflections
$\theta = 4.5$–$32.4°$
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Prism, pale yellow
0.41 × 0.35 × 0.28 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.874$, $T_{max} = 0.974$
19776 measured reflections
8636 independent reflections
4667 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 32.5°$, $\theta_{min} = 4.5°$
$h = -12 \rightarrow 12$
$k = -15 \rightarrow 17$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.127$
$S = 0.97$
8636 reflections
363 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
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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}
O1A	−0.10825 (12)	0.78753 (8)	0.47805 (6)	0.0472 (2)
O2A	−0.17664 (12)	0.86596 (9)	0.15922 (6)	0.0496 (2)
O3A	−0.03310 (14)	0.76460 (9)	0.05116 (7)	0.0600 (3)

N1A	−0.07106 (13)	0.78738 (9)	0.13266 (7)	0.0367 (2)
C1A	0.05600 (14)	0.67882 (10)	0.35935 (8)	0.0291 (2)
C2A	0.17987 (15)	0.59163 (10)	0.33036 (8)	0.0342 (3)
H2A	0.2367	0.5488	0.3737	0.041*
C3A	0.22047 (15)	0.56733 (11)	0.23722 (9)	0.0388 (3)
H3A	0.3027	0.5077	0.2191	0.047*
C4A	0.13914 (15)	0.63148 (11)	0.17161 (8)	0.0360 (3)
H4A	0.1660	0.6165	0.1090	0.043*
C5A	0.01681 (14)	0.71848 (10)	0.20163 (8)	0.0294 (2)
C6A	−0.02749 (14)	0.74350 (10)	0.29349 (8)	0.0302 (2)
H6A	−0.1114	0.8023	0.3114	0.036*
C7A	0.00284 (14)	0.70867 (10)	0.45916 (8)	0.0320 (2)
C8A	0.08663 (15)	0.64361 (10)	0.53138 (8)	0.0341 (3)
H8A	0.1754	0.5877	0.5140	0.041*
C9A	0.03681 (15)	0.66381 (10)	0.62182 (8)	0.0341 (3)
H9A	−0.0554	0.7183	0.6359	0.041*
C10A	0.10965 (14)	0.61071 (10)	0.70091 (8)	0.0303 (2)
C11A	0.24015 (15)	0.52191 (10)	0.69233 (8)	0.0329 (3)
H11A	0.2816	0.4930	0.6347	0.039*
C12A	0.30868 (15)	0.47626 (11)	0.76861 (8)	0.0354 (3)
H12A	0.3952	0.4166	0.7616	0.043*
C13A	0.25029 (15)	0.51804 (11)	0.85585 (8)	0.0362 (3)
C14A	0.11819 (16)	0.60523 (12)	0.86462 (8)	0.0400 (3)
H14A	0.0763	0.6336	0.9225	0.048*
C15A	0.04786 (16)	0.65058 (11)	0.78910 (8)	0.0387 (3)
H15A	−0.0415	0.7082	0.7970	0.046*
C16A	0.32905 (19)	0.47144 (14)	0.93769 (9)	0.0519 (4)
H16A	0.3731	0.5354	0.9569	0.078*
H16B	0.4208	0.4144	0.9182	0.078*
H16C	0.2436	0.4348	0.9903	0.078*
O1B	0.39815 (12)	0.28759 (8)	0.17553 (7)	0.0511 (2)
O2B	0.38505 (13)	0.39995 (8)	0.47951 (7)	0.0530 (3)
O3B	0.47675 (14)	0.27633 (10)	0.58517 (7)	0.0658 (3)
N1B	0.45688 (13)	0.30623 (10)	0.50460 (7)	0.0416 (3)
C1B	0.55580 (14)	0.17912 (10)	0.27830 (8)	0.0313 (2)
C2B	0.65291 (15)	0.07736 (11)	0.30205 (9)	0.0371 (3)
H2B	0.6974	0.0269	0.2572	0.045*
C3B	0.68412 (16)	0.05034 (11)	0.39189 (9)	0.0405 (3)
H3B	0.7478	−0.0185	0.4071	0.049*
C4B	0.62101 (15)	0.12525 (11)	0.45862 (9)	0.0391 (3)
H4B	0.6426	0.1084	0.5187	0.047*
C5B	0.52520 (14)	0.22563 (10)	0.43411 (8)	0.0325 (3)
C6B	0.48975 (14)	0.25382 (10)	0.34598 (8)	0.0329 (3)
H6B	0.4229	0.3216	0.3321	0.039*
C7B	0.51234 (15)	0.21124 (11)	0.18375 (8)	0.0359 (3)
C8B	0.60755 (16)	0.15048 (11)	0.10342 (8)	0.0377 (3)
H8B	0.7049	0.1024	0.1084	0.045*
C9B	0.55435 (15)	0.16429 (10)	0.02373 (8)	0.0349 (3)

H9B	0.4563	0.2134	0.0230	0.042*
C10B	0.63097 (14)	0.11180 (10)	−0.06276 (8)	0.0315 (2)
C11B	0.76586 (15)	0.02570 (11)	−0.06979 (9)	0.0371 (3)
H11B	0.8095	−0.0019	−0.0171	0.045*
C12B	0.83539 (15)	−0.01901 (11)	−0.15411 (8)	0.0377 (3)
H12B	0.9257	−0.0760	−0.1574	0.045*
C13B	0.77214 (16)	0.02004 (11)	−0.23457 (9)	0.0368 (3)
C14B	0.63582 (16)	0.10371 (11)	−0.22680 (8)	0.0372 (3)
H14B	0.5906	0.1302	−0.2791	0.045*
C15B	0.56619 (15)	0.14839 (11)	−0.14243 (8)	0.0366 (3)
H15B	0.4742	0.2040	−0.1388	0.044*
C16B	0.84893 (18)	−0.02696 (13)	−0.32704 (9)	0.0475 (3)
H16D	0.8871	0.0373	−0.3767	0.071*
H16E	0.7641	−0.0671	−0.3429	0.071*
H16F	0.9446	−0.0811	−0.3205	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0582 (6)	0.0466 (6)	0.0373 (5)	0.0196 (4)	−0.0185 (4)	−0.0101 (4)
O2A	0.0500 (5)	0.0565 (6)	0.0455 (5)	0.0211 (5)	−0.0237 (4)	−0.0121 (5)
O3A	0.0856 (8)	0.0647 (7)	0.0368 (5)	0.0213 (5)	−0.0313 (5)	−0.0167 (5)
N1A	0.0390 (6)	0.0390 (6)	0.0347 (5)	0.0027 (5)	−0.0154 (4)	−0.0061 (4)
C1A	0.0325 (6)	0.0252 (6)	0.0309 (6)	−0.0012 (4)	−0.0124 (4)	−0.0013 (4)
C2A	0.0374 (6)	0.0291 (6)	0.0359 (6)	0.0043 (5)	−0.0131 (5)	−0.0012 (5)
C3A	0.0396 (7)	0.0336 (7)	0.0410 (7)	0.0071 (5)	−0.0083 (5)	−0.0067 (5)
C4A	0.0418 (7)	0.0341 (7)	0.0326 (6)	0.0000 (5)	−0.0107 (5)	−0.0058 (5)
C5A	0.0300 (5)	0.0293 (6)	0.0299 (5)	−0.0001 (4)	−0.0107 (4)	−0.0028 (5)
C6A	0.0315 (6)	0.0261 (6)	0.0343 (6)	0.0018 (4)	−0.0122 (4)	−0.0041 (5)
C7A	0.0340 (6)	0.0300 (6)	0.0324 (6)	−0.0003 (5)	−0.0103 (5)	−0.0033 (5)
C8A	0.0353 (6)	0.0340 (7)	0.0335 (6)	0.0038 (5)	−0.0130 (5)	−0.0029 (5)
C9A	0.0390 (6)	0.0296 (6)	0.0362 (6)	0.0043 (5)	−0.0150 (5)	−0.0059 (5)
C10A	0.0311 (6)	0.0324 (6)	0.0288 (5)	−0.0020 (5)	−0.0095 (4)	−0.0056 (5)
C11A	0.0385 (6)	0.0328 (6)	0.0293 (6)	−0.0004 (5)	−0.0105 (5)	−0.0077 (5)
C12A	0.0370 (6)	0.0366 (7)	0.0331 (6)	0.0037 (5)	−0.0108 (5)	−0.0063 (5)
C13A	0.0380 (6)	0.0414 (7)	0.0311 (6)	−0.0010 (5)	−0.0136 (5)	−0.0038 (5)
C14A	0.0452 (7)	0.0480 (8)	0.0290 (6)	0.0035 (6)	−0.0105 (5)	−0.0130 (5)
C15A	0.0419 (7)	0.0389 (7)	0.0383 (6)	0.0082 (5)	−0.0147 (5)	−0.0130 (5)
C16A	0.0619 (9)	0.0624 (10)	0.0353 (7)	0.0088 (7)	−0.0240 (6)	−0.0064 (6)
O1B	0.0595 (6)	0.0492 (6)	0.0496 (5)	0.0225 (5)	−0.0259 (4)	−0.0164 (4)
O2B	0.0731 (7)	0.0400 (6)	0.0460 (5)	0.0174 (5)	−0.0179 (5)	−0.0135 (4)
O3B	0.0876 (8)	0.0755 (8)	0.0382 (5)	0.0277 (6)	−0.0280 (5)	−0.0186 (5)
N1B	0.0448 (6)	0.0441 (7)	0.0365 (6)	0.0055 (5)	−0.0113 (5)	−0.0105 (5)
C1B	0.0278 (5)	0.0314 (6)	0.0338 (6)	0.0008 (5)	−0.0060 (4)	−0.0062 (5)
C2B	0.0344 (6)	0.0346 (7)	0.0401 (6)	0.0040 (5)	−0.0053 (5)	−0.0092 (5)
C3B	0.0380 (7)	0.0359 (7)	0.0436 (7)	0.0085 (5)	−0.0098 (5)	−0.0015 (5)
C4B	0.0391 (7)	0.0395 (7)	0.0371 (6)	0.0024 (5)	−0.0122 (5)	0.0006 (5)
C5B	0.0311 (6)	0.0334 (6)	0.0319 (6)	0.0005 (5)	−0.0062 (5)	−0.0059 (5)

C6B	0.0318 (6)	0.0294 (6)	0.0381 (6)	0.0015 (5)	−0.0114 (5)	−0.0043 (5)
C7B	0.0368 (6)	0.0331 (7)	0.0396 (7)	0.0023 (5)	−0.0125 (5)	−0.0086 (5)
C8B	0.0389 (6)	0.0377 (7)	0.0381 (6)	0.0051 (5)	−0.0130 (5)	−0.0082 (5)
C9B	0.0348 (6)	0.0308 (6)	0.0376 (6)	0.0000 (5)	−0.0090 (5)	−0.0018 (5)
C10B	0.0332 (6)	0.0298 (6)	0.0315 (6)	−0.0042 (5)	−0.0096 (4)	−0.0009 (5)
C11B	0.0422 (7)	0.0348 (7)	0.0360 (6)	−0.0011 (5)	−0.0172 (5)	0.0010 (5)
C12B	0.0351 (6)	0.0354 (7)	0.0408 (7)	0.0018 (5)	−0.0087 (5)	−0.0042 (5)
C13B	0.0403 (7)	0.0345 (7)	0.0368 (6)	−0.0098 (5)	−0.0097 (5)	−0.0035 (5)
C14B	0.0399 (7)	0.0398 (7)	0.0344 (6)	−0.0048 (5)	−0.0156 (5)	−0.0010 (5)
C15B	0.0369 (6)	0.0327 (7)	0.0424 (7)	0.0003 (5)	−0.0164 (5)	−0.0029 (5)
C16B	0.0509 (8)	0.0494 (8)	0.0419 (7)	−0.0040 (6)	−0.0095 (6)	−0.0084 (6)

Geometric parameters (Å, º)

O1A—C7A	1.2266 (14)	O2B—N1B	1.2224 (14)
O2A—N1A	1.2222 (13)	O3B—N1B	1.2242 (14)
O3A—N1A	1.2227 (13)	N1B—O2B	1.2224 (14)
N1A—C5A	1.4698 (15)	N1B—C5B	1.4704 (15)
C1A—C2A	1.3849 (16)	C1B—C6B	1.3904 (16)
C1A—C6A	1.3967 (16)	C1B—C2B	1.3924 (17)
C1A—C7A	1.5050 (15)	C1B—C7B	1.5000 (17)
C2A—C3A	1.3910 (16)	C2B—C3B	1.3876 (17)
C2A—H2A	0.93	C2B—H2B	0.93
C3A—C4A	1.3811 (17)	C3B—C4B	1.3790 (18)
C3A—H3A	0.93	C3B—H3B	0.93
C4A—C5A	1.3800 (17)	C4B—C5B	1.3778 (17)
C4A—H4A	0.93	C4B—H4B	0.93
C5A—C6A	1.3751 (15)	C5B—C6B	1.3788 (16)
C6A—H6A	0.93	C6B—H6B	0.93
C7A—C8A	1.4692 (16)	C7B—C8B	1.4739 (16)
C8A—C9A	1.3372 (16)	C8B—C9B	1.3307 (16)
C8A—H8A	0.93	C8B—H8B	0.93
C9A—C10A	1.4571 (16)	C9B—C10B	1.4620 (16)
C9A—H9A	0.93	C9B—H9B	0.93
C10A—C11A	1.3928 (16)	C10B—C15B	1.3916 (16)
C10A—C15A	1.3985 (15)	C10B—C11B	1.3963 (17)
C11A—C12A	1.3827 (16)	C11B—C12B	1.3819 (17)
C11A—H11A	0.93	C11B—H11B	0.93
C12A—C13A	1.3943 (16)	C12B—C13B	1.3988 (17)
C12A—H12A	0.93	C12B—H12B	0.93
C13A—C14A	1.3890 (18)	C13B—C14B	1.3865 (18)
C13A—C16A	1.5031 (17)	C13B—C16B	1.5050 (17)
C14A—C15A	1.3810 (17)	C14B—C15B	1.3825 (17)
C14A—H14A	0.93	C14B—H14B	0.93
C15A—H15A	0.93	C15B—H15B	0.93
C16A—H16A	0.96	C16B—H16D	0.96
C16A—H16B	0.96	C16B—H16E	0.96
C16A—H16C	0.96	C16B—H16F	0.96

O1B—C7B	1.2272 (15)		
O2A—N1A—O3A	123.18 (11)	O2B—N1B—O3B	123.47 (11)
O2A—N1A—C5A	118.36 (9)	O2B—N1B—O3B	123.47 (11)
O3A—N1A—C5A	118.45 (10)	O2B—N1B—C5B	118.42 (10)
C2A—C1A—C6A	119.17 (10)	O2B—N1B—C5B	118.42 (10)
C2A—C1A—C7A	123.95 (10)	O3B—N1B—C5B	118.11 (11)
C6A—C1A—C7A	116.88 (10)	C6B—C1B—C2B	119.13 (11)
C1A—C2A—C3A	120.87 (11)	C6B—C1B—C7B	117.43 (11)
C1A—C2A—H2A	119.6	C2B—C1B—C7B	123.40 (10)
C3A—C2A—H2A	119.6	C3B—C2B—C1B	120.77 (11)
C4A—C3A—C2A	120.24 (12)	C3B—C2B—H2B	119.6
C4A—C3A—H3A	119.9	C1B—C2B—H2B	119.6
C2A—C3A—H3A	119.9	C4B—C3B—C2B	120.20 (12)
C5A—C4A—C3A	118.08 (11)	C4B—C3B—H3B	119.9
C5A—C4A—H4A	121.0	C2B—C3B—H3B	119.9
C3A—C4A—H4A	121.0	C5B—C4B—C3B	118.39 (12)
C6A—C5A—C4A	122.98 (11)	C5B—C4B—H4B	120.8
C6A—C5A—N1A	118.30 (10)	C3B—C4B—H4B	120.8
C4A—C5A—N1A	118.72 (10)	C4B—C5B—C6B	122.72 (11)
C5A—C6A—C1A	118.66 (11)	C4B—C5B—N1B	118.99 (11)
C5A—C6A—H6A	120.7	C6B—C5B—N1B	118.29 (11)
C1A—C6A—H6A	120.7	C5B—C6B—C1B	118.78 (11)
O1A—C7A—C8A	121.56 (10)	C5B—C6B—H6B	120.6
O1A—C7A—C1A	119.20 (10)	C1B—C6B—H6B	120.6
C8A—C7A—C1A	119.24 (10)	O1B—C7B—C8B	121.84 (11)
C9A—C8A—C7A	120.81 (11)	O1B—C7B—C1B	118.90 (11)
C9A—C8A—H8A	119.6	C8B—C7B—C1B	119.26 (11)
C7A—C8A—H8A	119.6	C9B—C8B—C7B	120.09 (12)
C8A—C9A—C10A	127.80 (11)	C9B—C8B—H8B	120.0
C8A—C9A—H9A	116.1	C7B—C8B—H8B	120.0
C10A—C9A—H9A	116.1	C8B—C9B—C10B	128.03 (12)
C11A—C10A—C15A	118.21 (10)	C8B—C9B—H9B	116.0
C11A—C10A—C9A	122.66 (10)	C10B—C9B—H9B	116.0
C15A—C10A—C9A	119.13 (11)	C15B—C10B—C11B	117.82 (11)
C12A—C11A—C10A	120.69 (10)	C15B—C10B—C9B	118.74 (11)
C12A—C11A—H11A	119.7	C11B—C10B—C9B	123.44 (10)
C10A—C11A—H11A	119.7	C12B—C11B—C10B	120.84 (11)
C11A—C12A—C13A	121.17 (12)	C12B—C11B—H11B	119.6
C11A—C12A—H12A	119.4	C10B—C11B—H11B	119.6
C13A—C12A—H12A	119.4	C11B—C12B—C13B	121.04 (12)
C14A—C13A—C12A	117.97 (11)	C11B—C12B—H12B	119.5
C14A—C13A—C16A	120.87 (11)	C13B—C12B—H12B	119.5
C12A—C13A—C16A	121.16 (12)	C14B—C13B—C12B	118.00 (11)
C15A—C14A—C13A	121.26 (11)	C14B—C13B—C16B	120.67 (11)
C15A—C14A—H14A	119.4	C12B—C13B—C16B	121.33 (12)
C13A—C14A—H14A	119.4	C15B—C14B—C13B	120.95 (11)
C14A—C15A—C10A	120.66 (12)	C15B—C14B—H14B	119.5

C14A—C15A—H15A	119.7	C13B—C14B—H14B	119.5
C10A—C15A—H15A	119.7	C14B—C15B—C10B	121.32 (12)
C13A—C16A—H16A	109.5	C14B—C15B—H15B	119.3
C13A—C16A—H16B	109.5	C10B—C15B—H15B	119.3
H16A—C16A—H16B	109.5	C13B—C16B—H16D	109.5
C13A—C16A—H16C	109.5	C13B—C16B—H16E	109.5
H16A—C16A—H16C	109.5	H16D—C16B—H16E	109.5
H16B—C16A—H16C	109.5	C13B—C16B—H16F	109.5
O2B—O2B—N1B	0 (10)	H16D—C16B—H16F	109.5
O2B—N1B—O2B	0.00 (11)	H16E—C16B—H16F	109.5
C6A—C1A—C2A—C3A	−0.59 (16)	C6B—C1B—C2B—C3B	−0.10 (16)
C7A—C1A—C2A—C3A	178.84 (10)	C7B—C1B—C2B—C3B	−177.82 (10)
C1A—C2A—C3A—C4A	1.01 (17)	C1B—C2B—C3B—C4B	−0.93 (17)
C2A—C3A—C4A—C5A	−0.60 (17)	C2B—C3B—C4B—C5B	0.89 (17)
C3A—C4A—C5A—C6A	−0.22 (17)	C3B—C4B—C5B—C6B	0.17 (17)
C3A—C4A—C5A—N1A	−179.90 (10)	C3B—C4B—C5B—N1B	179.91 (10)
O2A—N1A—C5A—C6A	1.82 (15)	O2B—N1B—C5B—C4B	173.67 (11)
O3A—N1A—C5A—C6A	−179.32 (10)	O2B—N1B—C5B—C4B	173.67 (11)
O2A—N1A—C5A—C4A	−178.48 (10)	O3B—N1B—C5B—C4B	−5.53 (16)
O3A—N1A—C5A—C4A	0.38 (15)	O2B—N1B—C5B—C6B	−6.57 (16)
C4A—C5A—C6A—C1A	0.62 (16)	O2B—N1B—C5B—C6B	−6.57 (16)
N1A—C5A—C6A—C1A	−179.69 (9)	O3B—N1B—C5B—C6B	174.22 (11)
C2A—C1A—C6A—C5A	−0.20 (15)	C4B—C5B—C6B—C1B	−1.18 (17)
C7A—C1A—C6A—C5A	−179.68 (9)	N1B—C5B—C6B—C1B	179.07 (9)
C2A—C1A—C7A—O1A	179.98 (11)	C2B—C1B—C6B—C5B	1.12 (15)
C6A—C1A—C7A—O1A	−0.57 (15)	C7B—C1B—C6B—C5B	178.98 (10)
C2A—C1A—C7A—C8A	0.68 (16)	C6B—C1B—C7B—O1B	−13.01 (16)
C6A—C1A—C7A—C8A	−179.87 (9)	C2B—C1B—C7B—O1B	164.75 (11)
O1A—C7A—C8A—C9A	4.01 (17)	C6B—C1B—C7B—C8B	167.00 (10)
C1A—C7A—C8A—C9A	−176.71 (10)	C2B—C1B—C7B—C8B	−15.23 (16)
C7A—C8A—C9A—C10A	−177.55 (10)	O1B—C7B—C8B—C9B	−10.23 (18)
C8A—C9A—C10A—C11A	−4.54 (18)	C1B—C7B—C8B—C9B	169.75 (10)
C8A—C9A—C10A—C15A	174.93 (11)	C7B—C8B—C9B—C10B	−179.97 (10)
C15A—C10A—C11A—C12A	−1.23 (16)	C8B—C9B—C10B—C15B	−172.74 (11)
C9A—C10A—C11A—C12A	178.24 (10)	C8B—C9B—C10B—C11B	7.71 (18)
C10A—C11A—C12A—C13A	−0.41 (17)	C15B—C10B—C11B—C12B	1.75 (16)
C11A—C12A—C13A—C14A	1.45 (17)	C9B—C10B—C11B—C12B	−178.70 (10)
C11A—C12A—C13A—C16A	−177.81 (11)	C10B—C11B—C12B—C13B	−0.39 (17)
C12A—C13A—C14A—C15A	−0.83 (18)	C11B—C12B—C13B—C14B	−0.96 (16)
C16A—C13A—C14A—C15A	178.43 (12)	C11B—C12B—C13B—C16B	179.09 (10)
C13A—C14A—C15A—C10A	−0.82 (19)	C12B—C13B—C14B—C15B	0.92 (17)
C11A—C10A—C15A—C14A	1.84 (17)	C16B—C13B—C14B—C15B	−179.13 (10)
C9A—C10A—C15A—C14A	−177.65 (11)	C13B—C14B—C15B—C10B	0.48 (17)
O2B—O2B—N1B—O3B	0.00 (5)	C11B—C10B—C15B—C14B	−1.80 (16)
O2B—O2B—N1B—C5B	0.00 (8)	C9B—C10B—C15B—C14B	178.63 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2*A*—H2*A*···O2*B*	0.93	2.55	3.4644 (16)	170
C11*A*—H11*A*···O2*B*	0.93	2.59	3.5156 (14)	176
C2*B*—H2*B*···O2*A*^{i}	0.93	2.51	3.4311 (16)	171
C14*A*—H14*A*···O3*A*^{ii}	0.93	2.54	3.4455 (16)	164

Symmetry codes: (i) *x*+1, *y*−1, *z*; (ii) *x*, *y*, *z*+1.