Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl N-(2-benzoyl-3-oxo-3-phenylpropanoyl)carbamate

Mehmet Akkurt,[a]* Ahmet Oral Sarıoğlu,[b] Mehmet Sönmez[b] and Muhammad Nawaz Tahir[c]*

[a]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Gaziantep University, 27310 Şehitkamil–Gaziantep, Turkey, and [c]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: akkurt@erciyes.edu.tr, dmntahir_uos@yahoo.com

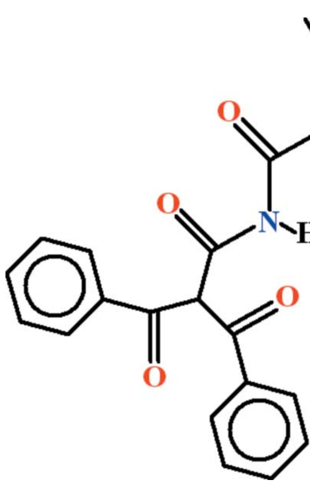
Received 4 January 2013; accepted 5 January 2013

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.049; wR factor = 0.132; data-to-parameter ratio = 15.3.

In the title compound, $C_{19}H_{17}NO_5$, the dihedral angle between the phenyl groups is 79.55 (15)°. The terminal ethoxy group is disordered over two orientations in a 0.873 (6):0.127 (6) ratio. In the crystal, molecules are linked by N—H⋯O and C—H⋯O hydrogen bonds into [001] chains which incorporate $R_1^2(6)$ loops. A very weak C—H⋯π contact also occurs.

Related literature

For background to the carboxamide [–C(O)NH–] group, see: Sönmez (2001). For further synthetic details, see: Fabian *et al.* (1992).



Experimental

Crystal data

$C_{19}H_{17}NO_5$
M_r = 339.34
Monoclinic, $C2/c$
a = 33.088 (8) Å
b = 12.732 (3) Å
c = 8.7110 (18) Å
β = 97.896 (9)°
V = 3635.0 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.35 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009) T_{min} = 0.981, T_{max} = 0.986
14531 measured reflections
3579 independent reflections
1910 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.132
S = 1.01
3579 reflections
234 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

$Cg2$ is the centroid of the C10–C15 phenyl ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O3^{i}	0.86	2.37	3.025 (2)	133
N1—H1⋯O4^{i}	0.86	2.08	2.842 (2)	147
C8—H8⋯O3^{i}	0.98	2.38	3.263 (3)	150
C19B—H19F⋯$Cg2^{ii}$	0.96	2.96	3.786 (5)	145

Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $x, -y+1, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7023).

References

Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fabian, W. F., Kollenz, G., Akcamur, Y., Kök, T. R., Tezcan, M., Akkurt, M. & Hiller, W. (1992). *Monatsch. Chem.* **123**, 265–275.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sönmez, M. (2001). *Turk. J. Chem.* **25**, 181–185.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2013). E**69**, o220 [doi:10.1107/S1600536813000445]

Ethyl *N*-(2-benzoyl-3-oxo-3-phenylpropanoyl)carbamate

Mehmet Akkurt, Ahmet Oral Sarıoğlu, Mehmet Sönmez and Muhammad Nawaz Tahir

S1. Comment

The carboxamide [–C(O)NH–] group, which seems to be everywhere throughout nature in the primary structure of proteins, is an important ligand construction unit for coordination chemists (Sönmez, 2001). The high stability of the amide linkage toward hydrolysis is of crucial importance to biological systems, since it allows the construction of peptides from relatively simple amino acid precursors.

In the title compound (I), (Fig. 1), the C1–C6 and C10–C15 phenyl rings make a dihedral angle of 79.55 (15)° with each other. The C7–C8–C16–O3, C8–C16–N1–C17, O3–C16–N1–C17, C16–N1–C17–O4 and C16–N1–C17–O5 torsion angles are -23.0 (3), -176.6 (2), 3.9 (4), 2.6 (4) and -177.2 (2)°, respectively.

In the crystal structure, N—H···O and C—H···O hydrogen bonds (Table 1, Fig. 2) connect the neighbouring molecules, into chains running along the *c* axis, forming the $R^2_1(6)$ motifs (Fig. 2). Furthermore, C—H···*π* interactions between the H19F hydrogen atom of the methyl group and the C10–C15 phenyl ring (with centroid *Cg*2) is also observed (Table 1).

S2. Experimental

Dibenzoylaceticacid-*N*-carboxyethylamide was prepared from reaction of 4-benzoyl-5-phenyl-2,3-furandione and ethyl urethane as the method reported earlier (Fabian *et al.*, 1992). These compounds were refluxed in benzene for 5 h. The solvent was evaporated under reduced pressure to give an oily residue which was treated with ether and finally crystallized from absolute ethanol as colourless needles. Analysis calculated for ($C_{19}H_{17}NO_5$): C 67.25, H 5.01, N 4.14. Found: C 67.22, H 5.06, N 4.30.

S3. Refinement

All H atoms were positioned geometrically and refined by using a riding model, with N—H = 0.86 Å (amine), C—H = 0.93 (aromatic), C—H = 0.96 (methyl), C—H = 0.97 (methylene) and 0.98 Å (methine), and U_{iso}(H) = 1.2 or 1.5U_{eq}(C,*N*). The C atoms of the terminal ethoxy group are disordered over two positions with occupancy ratio 0.873 (6):0.127 (6). The temperature factors of the disordered C atoms were refined with the EADP restraint.

The unit cell contains a pair of voids of 44 (2)Å^3 volume located about an inversion centre but the residual electron density (highest peak = 0.160 e Å^{-3}and deepest hole = -0.126 e Å^{-3}) in the difference Fourier map suggests that no solvent molecule occupies this void.

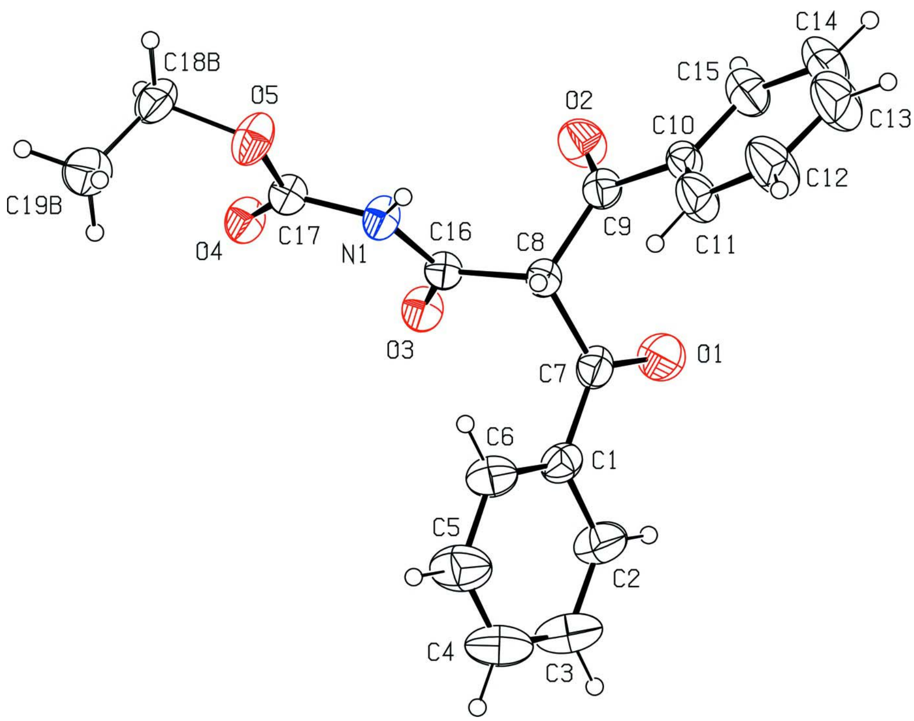


Figure 1

The molecular structure of (I) with displacement ellipsoids for non-H atoms drawn at the 30% probability level. Only the major disorder component is shown.

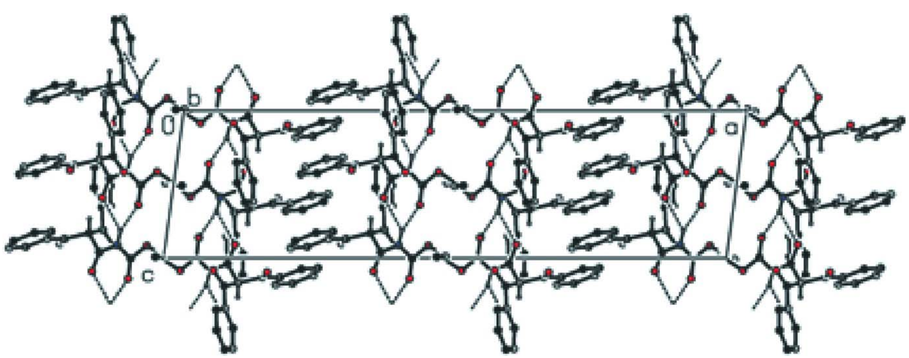


Figure 2

The packing and hydrogen bonding of the title compound, viewing along the *b* axis. H atoms not involved in hydrogen bonding and the minor disordered component are omitted for clarity.

Ethyl *N*-(2-benzoyl-3-oxo-3-phenylpropanoyl)carbamate

Crystal data

$C_{19}H_{17}NO_5$
M_r = 339.34
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 33.088 (8) Å
b = 12.732 (3) Å
c = 8.7110 (18) Å
β = 97.896 (9)°
V = 3635.0 (14) Å^3
Z = 8
F(000) = 1424
D_x = 1.240 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 270 reflections
θ = 3.1–21.4°
μ = 0.09 mm^{-1}

T = 296 K
Needle, white

0.35 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.981, T_{max} = 0.986

14531 measured reflections
3579 independent reflections
1910 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.0°, θ_{min} = 1.2°
$h = -37 \rightarrow 40$
$k = -15 \rightarrow 15$
$l = -8 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.132
S = 1.01
3579 reflections
234 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.910P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $FC^* = KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Extinction coefficient: 0.0030 (4)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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}	Occ. (<1)
O1	0.18768 (6)	0.74420 (16)	0.0969 (2)	0.0913 (9)	
O2	0.09155 (6)	0.76202 (14)	0.08336 (19)	0.0757 (8)	
O3	0.12375 (5)	0.56205 (12)	−0.09053 (15)	0.0564 (6)	
O4	0.05773 (5)	0.42206 (13)	−0.13912 (16)	0.0578 (6)	
O5	0.03265 (5)	0.39586 (14)	0.08394 (17)	0.0693 (7)	
N1	0.08534 (6)	0.50073 (15)	0.08736 (18)	0.0494 (7)	
C1	0.21155 (8)	0.5710 (2)	0.1313 (2)	0.0558 (10)	
C2	0.24785 (9)	0.5949 (3)	0.0759 (3)	0.0819 (12)	
C3	0.27677 (11)	0.5189 (4)	0.0679 (4)	0.1085 (18)	
C4	0.27046 (12)	0.4194 (3)	0.1159 (4)	0.1102 (17)	
C5	0.23524 (12)	0.3949 (3)	0.1725 (4)	0.0984 (17)	
C6	0.20565 (9)	0.4704 (2)	0.1804 (3)	0.0707 (11)	

C7	0.18068 (8)	0.6541 (2)	0.1304 (3)	0.0553 (10)	
C8	0.13836 (7)	0.62652 (16)	0.1695 (2)	0.0435 (8)	
C9	0.11479 (8)	0.72705 (18)	0.1908 (3)	0.0511 (9)	
C10	0.12157 (8)	0.78140 (18)	0.3436 (3)	0.0520 (9)	
C11	0.14062 (9)	0.7351 (2)	0.4765 (3)	0.0754 (11)	
C12	0.14478 (11)	0.7874 (3)	0.6156 (3)	0.1070 (18)	
C13	0.13103 (12)	0.8877 (3)	0.6216 (4)	0.1085 (18)	
C14	0.11213 (11)	0.9365 (2)	0.4910 (4)	0.0946 (14)	
C15	0.10659 (9)	0.8823 (2)	0.3516 (3)	0.0717 (11)	
C16	0.11539 (7)	0.56060 (17)	0.0400 (2)	0.0444 (8)	
C17	0.05827 (7)	0.43737 (18)	−0.0035 (2)	0.0475 (8)	
C18B	−0.00031 (11)	0.3297 (3)	0.0107 (4)	0.0681 (16)	0.874 (6)
C19B	0.01476 (14)	0.2202 (3)	0.0081 (6)	0.122 (2)	0.874 (6)
C19A	−0.0059 (10)	0.230 (2)	0.104 (4)	0.122 (2)	0.127 (6)
C18A	0.0143 (10)	0.302 (2)	−0.003 (3)	0.0681 (16)	0.127 (6)
H2	0.25255	0.66297	0.04389	0.0984*	
H1	0.08306	0.50283	0.18448	0.0593*	
H5	0.23111	0.32685	0.20608	0.1180*	
H6	0.18166	0.45305	0.21893	0.0846*	
H8	0.14126	0.58613	0.26611	0.0522*	
H11	0.15087	0.66726	0.47217	0.0903*	
H12	0.15696	0.75432	0.70541	0.1281*	
H13	0.13449	0.92367	0.71546	0.1301*	
H14	0.10307	1.00540	0.49576	0.1135*	
H15	0.09279	0.91396	0.26339	0.0861*	
H18C	−0.00918	0.35382	−0.09419	0.0818*	0.874 (6)
H18D	−0.02337	0.33326	0.06829	0.0818*	0.874 (6)
H19D	−0.00633	0.17611	−0.04401	0.1830*	0.874 (6)
H19E	0.02221	0.19582	0.11238	0.1830*	0.874 (6)
H19F	0.03817	0.21784	−0.04587	0.1830*	0.874 (6)
H3	0.30085	0.53546	0.02943	0.1298*	
H4	0.29018	0.36801	0.11008	0.1319*	
H18A	0.03551	0.26331	−0.04608	0.0818*	0.127 (6)
H18B	−0.00573	0.32448	−0.08842	0.0818*	0.127 (6)
H19A	−0.02677	0.18932	0.04337	0.1830*	0.127 (6)
H19B	−0.01783	0.27177	0.17740	0.1830*	0.127 (6)
H19C	0.01418	0.18378	0.15742	0.1830*	0.127 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0800 (16)	0.0636 (13)	0.1396 (18)	−0.0162 (11)	0.0482 (13)	−0.0004 (12)
O2	0.0850 (15)	0.0718 (13)	0.0665 (12)	0.0153 (10)	−0.0035 (10)	−0.0004 (9)
O3	0.0666 (12)	0.0714 (11)	0.0345 (8)	−0.0136 (9)	0.0190 (7)	−0.0040 (7)
O4	0.0639 (12)	0.0765 (12)	0.0335 (9)	−0.0142 (9)	0.0081 (7)	−0.0070 (7)
O5	0.0696 (13)	0.0926 (13)	0.0477 (9)	−0.0354 (10)	0.0153 (8)	0.0001 (8)
N1	0.0573 (14)	0.0659 (13)	0.0265 (9)	−0.0173 (10)	0.0107 (8)	−0.0042 (8)
C1	0.0473 (18)	0.0715 (19)	0.0478 (14)	−0.0040 (14)	0.0034 (11)	−0.0022 (12)

C2	0.056 (2)	0.095 (2)	0.097 (2)	0.0000 (18)	0.0189 (16)	0.0082 (17)
C3	0.059 (2)	0.146 (4)	0.125 (3)	0.022 (2)	0.029 (2)	0.017 (3)
C4	0.077 (3)	0.127 (3)	0.127 (3)	0.045 (2)	0.015 (2)	0.017 (2)
C5	0.083 (3)	0.097 (3)	0.115 (3)	0.028 (2)	0.013 (2)	0.026 (2)
C6	0.058 (2)	0.081 (2)	0.0727 (18)	0.0107 (16)	0.0079 (13)	0.0116 (15)
C7	0.0559 (19)	0.0575 (16)	0.0534 (14)	−0.0127 (14)	0.0111 (12)	−0.0060 (12)
C8	0.0475 (16)	0.0496 (14)	0.0339 (11)	−0.0052 (11)	0.0075 (9)	−0.0025 (9)
C9	0.0540 (18)	0.0521 (15)	0.0488 (14)	−0.0059 (12)	0.0131 (12)	0.0011 (11)
C10	0.0574 (17)	0.0474 (15)	0.0547 (14)	−0.0077 (12)	0.0205 (12)	−0.0095 (11)
C11	0.096 (2)	0.0686 (18)	0.0586 (17)	0.0088 (16)	0.0003 (15)	−0.0192 (14)
C12	0.149 (4)	0.102 (3)	0.065 (2)	0.027 (2)	−0.0033 (19)	−0.0311 (18)
C13	0.142 (4)	0.104 (3)	0.079 (2)	0.011 (2)	0.013 (2)	−0.041 (2)
C14	0.129 (3)	0.064 (2)	0.098 (2)	0.0025 (19)	0.041 (2)	−0.0261 (18)
C15	0.091 (2)	0.0568 (18)	0.0722 (18)	−0.0022 (15)	0.0287 (15)	−0.0056 (13)
C16	0.0494 (16)	0.0486 (14)	0.0363 (12)	−0.0022 (11)	0.0102 (10)	0.0017 (10)
C17	0.0522 (17)	0.0552 (14)	0.0357 (12)	−0.0056 (12)	0.0080 (10)	0.0028 (10)
C18B	0.050 (3)	0.079 (3)	0.076 (2)	−0.020 (2)	0.0109 (19)	−0.0027 (16)
C19B	0.079 (3)	0.079 (3)	0.211 (6)	−0.007 (2)	0.032 (3)	−0.025 (3)
C19A	0.079 (3)	0.079 (3)	0.211 (6)	−0.007 (2)	0.032 (3)	−0.025 (3)
C18A	0.050 (3)	0.079 (3)	0.076 (2)	−0.020 (2)	0.0109 (19)	−0.0027 (16)

Geometric parameters (Å, º)

O1—C7	1.214 (3)	C13—C14	1.370 (5)
O2—C9	1.212 (3)	C14—C15	1.387 (4)
O3—C16	1.207 (2)	C18A—C19A	1.53 (4)
O4—C17	1.195 (2)	C18B—C19B	1.482 (5)
O5—C17	1.325 (3)	C2—H2	0.9300
O5—C18B	1.454 (4)	C3—H3	0.9300
O5—C18A	1.50 (3)	C4—H4	0.9300
N1—C16	1.361 (3)	C5—H5	0.9300
N1—C17	1.373 (3)	C6—H6	0.9300
N1—H1	0.8600	C8—H8	0.9800
C1—C2	1.388 (4)	C11—H11	0.9300
C1—C7	1.470 (4)	C12—H12	0.9300
C1—C6	1.373 (4)	C13—H13	0.9300
C2—C3	1.369 (6)	C14—H14	0.9300
C3—C4	1.359 (6)	C15—H15	0.9300
C4—C5	1.363 (6)	C18A—H18B	0.9700
C5—C6	1.381 (5)	C18A—H18A	0.9700
C7—C8	1.527 (4)	C18B—H18D	0.9700
C8—C9	1.523 (3)	C18B—H18C	0.9700
C8—C16	1.523 (3)	C19A—H19A	0.9600
C9—C10	1.490 (4)	C19A—H19C	0.9600
C10—C11	1.373 (4)	C19A—H19B	0.9600
C10—C15	1.382 (4)	C19B—H19E	0.9600
C11—C12	1.373 (4)	C19B—H19F	0.9600
C12—C13	1.359 (5)	C19B—H19D	0.9600

C17—O5—C18B	118.64 (19)	C3—C4—H4	120.00
C17—O5—C18A	105.9 (11)	C5—C4—H4	120.00
C16—N1—C17	126.89 (16)	C4—C5—H5	120.00
C17—N1—H1	117.00	C6—C5—H5	120.00
C16—N1—H1	117.00	C1—C6—H6	120.00
C2—C1—C7	118.3 (3)	C5—C6—H6	120.00
C2—C1—C6	118.7 (3)	C7—C8—H8	109.00
C6—C1—C7	123.0 (2)	C9—C8—H8	109.00
C1—C2—C3	120.5 (3)	C16—C8—H8	109.00
C2—C3—C4	120.3 (3)	C10—C11—H11	119.00
C3—C4—C5	120.0 (4)	C12—C11—H11	120.00
C4—C5—C6	120.4 (3)	C11—C12—H12	120.00
C1—C6—C5	120.1 (3)	C13—C12—H12	120.00
C1—C7—C8	119.4 (2)	C12—C13—H13	120.00
O1—C7—C1	121.8 (2)	C14—C13—H13	120.00
O1—C7—C8	118.8 (2)	C13—C14—H14	120.00
C9—C8—C16	109.97 (19)	C15—C14—H14	120.00
C7—C8—C9	109.54 (19)	C10—C15—H15	120.00
C7—C8—C16	109.95 (17)	C14—C15—H15	120.00
O2—C9—C8	119.7 (2)	H18A—C18A—H18B	108.00
O2—C9—C10	121.4 (2)	O5—C18A—H18A	110.00
C8—C9—C10	118.8 (2)	O5—C18A—H18B	110.00
C9—C10—C11	123.3 (2)	C19A—C18A—H18A	109.00
C11—C10—C15	118.9 (2)	C19A—C18A—H18B	110.00
C9—C10—C15	117.8 (2)	C19B—C18B—H18C	110.00
C10—C11—C12	121.0 (3)	C19B—C18B—H18D	110.00
C11—C12—C13	119.8 (3)	O5—C18B—H18D	110.00
C12—C13—C14	120.8 (3)	O5—C18B—H18C	110.00
C13—C14—C15	119.5 (3)	H18C—C18B—H18D	108.00
C10—C15—C14	120.1 (3)	C18A—C19A—H19A	109.00
O3—C16—N1	124.45 (19)	C18A—C19A—H19B	109.00
N1—C16—C8	113.28 (16)	H19A—C19A—H19C	109.00
O3—C16—C8	122.3 (2)	H19B—C19A—H19C	110.00
O4—C17—N1	125.9 (2)	C18A—C19A—H19C	109.00
O4—C17—O5	125.4 (2)	H19A—C19A—H19B	110.00
O5—C17—N1	108.74 (16)	C18B—C19B—H19F	109.00
O5—C18A—C19A	111 (2)	H19E—C19B—H19F	109.00
O5—C18B—C19B	108.5 (3)	H19D—C19B—H19E	110.00
C1—C2—H2	120.00	H19D—C19B—H19F	109.00
C3—C2—H2	120.00	C18B—C19B—H19D	109.00
C2—C3—H3	120.00	C18B—C19B—H19E	109.00
C4—C3—H3	120.00		

C18B—O5—C17—O4	−3.0 (4)	C1—C7—C8—C16	−69.7 (3)
C18B—O5—C17—N1	176.9 (2)	C7—C8—C9—O2	95.7 (3)
C17—O5—C18B—C19B	88.0 (3)	C7—C8—C9—C10	−83.1 (3)
C16—N1—C17—O4	2.7 (4)	C16—C8—C9—O2	−25.2 (3)

C16—N1—C17—O5	−177.2 (2)	C16—C8—C9—C10	156.0 (2)
C17—N1—C16—O3	−3.9 (4)	C7—C8—C16—O3	−23.0 (3)
C17—N1—C16—C8	176.6 (2)	C9—C8—C16—N1	−82.8 (2)
C6—C1—C2—C3	1.2 (4)	C7—C8—C16—N1	156.55 (19)
C7—C1—C2—C3	−177.1 (3)	C9—C8—C16—O3	97.7 (3)
C2—C1—C6—C5	−0.8 (4)	C8—C9—C10—C15	167.1 (2)
C7—C1—C6—C5	177.4 (3)	O2—C9—C10—C11	166.1 (3)
C2—C1—C7—O1	−7.1 (4)	O2—C9—C10—C15	−11.7 (4)
C6—C1—C7—O1	174.7 (2)	C8—C9—C10—C11	−15.1 (4)
C6—C1—C7—C8	−6.5 (3)	C9—C10—C11—C12	−177.6 (3)
C2—C1—C7—C8	171.7 (2)	C15—C10—C11—C12	0.2 (4)
C1—C2—C3—C4	−0.8 (5)	C9—C10—C15—C14	−179.9 (3)
C2—C3—C4—C5	−0.1 (5)	C11—C10—C15—C14	2.2 (4)
C3—C4—C5—C6	0.5 (5)	C10—C11—C12—C13	−2.1 (5)
C4—C5—C6—C1	−0.1 (5)	C11—C12—C13—C14	1.6 (6)
O1—C7—C8—C16	109.2 (2)	C12—C13—C14—C15	0.8 (6)
O1—C7—C8—C9	−11.8 (3)	C13—C14—C15—C10	−2.7 (5)
C1—C7—C8—C9	169.4 (2)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C10–C15 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.86	2.37	3.025 (2)	133
N1—H1···O4^{i}	0.86	2.08	2.842 (2)	147
C8—H8···O3^{i}	0.98	2.38	3.263 (3)	150
C19*B*—H19*F*···*Cg*2^{ii}	0.96	2.96	3.786 (5)	145

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2; (ii) *x*, −*y*+1, *z*−1/2.