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Methyl 11,14,16-triphenyl-8,12-dioxa-14,15-diazatetracyclo[8.7.0.0^{2,7}.0^{13,17}]-heptadeca-2(7),3,5,13(17),15-pentaene-10-carboxylate

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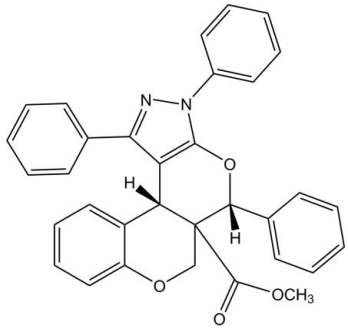
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.129; data-to-parameter ratio = 13.0.

In the title compound, $C_{33}H_{26}N_2O_4$, the pyrazole ring makes dihedral angles of 15.13 (7) and 60.80 (7)° with the adjacent phenyl rings. Both dihydropyran rings exhibit half-chair conformations. A weak intramolecular C—H···O interaction occurs. In the crystal, molecules are linked into inversion dimers through pairs of C—H···N interactions. Weak C—H···π interactions are also observed.

Related literature

For the biological activity of 4*H*-chromenes, see: Cai *et al.* (2006); Gabor (1988); Brooks (1998); Valenti *et al.* (1993); Tang *et al.* (2007). For a related structure, see: Ponnusamy *et al.* (2013).



Experimental

Crystal data

$C_{33}H_{26}N_2O_4$
M_r = 514.56
Monoclinic, $P2_1/n$
a = 11.916 (5) Å
b = 10.876 (5) Å
c = 21.153 (5) Å
β = 105.797 (5)°
V = 2637.9 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.983
40448 measured reflections
4605 independent reflections
3289 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.129
S = 1.01
4605 reflections
354 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

*Cg*1, *Cg*4 and *Cg*6 are the centroids of the N1/N2/C7/C24/C25, C1–C6 and C17–C22 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···N2^{i}	0.93	2.62	3.517 (3)	163
C6—H6···O1	0.93	2.26	2.877 (2)	123
C13—H13···*Cg*6^{ii}	0.93	2.98	3.904 (8)	174
C18—H18···*Cg*1^{i}	0.93	2.88	3.720 (5)	150
C23—H23···*Cg*4^{iii}	0.98	2.86	3.787 (6)	159

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

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5278).

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supplementary materials

Acta Cryst. (2013). E**69**, o1035 [doi:10.1107/S1600536813015213]

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Comment

4*H*-Chromenes and their derivatives exhibit various biological activities such as anti-viral, anti-fungal, anti-inflammatory, antidiabetic, anti-anaphylactic and anti-cancer (Cai *et al.*, 2006; Gabor, 1988; Brooks, 1998; Valenti *et al.*, 1993; Tang *et al.*, 2007).

The geometric parameters of the title molecule (Fig. 1) agree well with a reported similar structure (Ponnusamy *et al.*, 2013). The pyrazole ring makes dihedral angles of 15.13 (7) and 60.80 (7)°, respectively, with two phenyl (C1–C6) and (C26–C31) rings. The molecular structure is stabilized by a weak intramolecular C—H···O interaction and the crystal packing is controlled by weak intermolecular C—H···N and C—H···π interactions (Table 1).

Experimental

A mixture of (*E*)-methyl-2-[(2-formylphenoxy)methyl]-3-phenylacrylate (0.296 g, 1 mmol) and 1,3-diphenyl-4,5-dihydro-1*H*-pyrazol-5-one (0.236 g, 1 mmol) was placed in a round bottom flask and melted at 180 °C for 1 h. After completion of the reaction as indicated by TLC, the crude product was washed with 5 ml of ethylacetate and hexane mixture (1:49 ratio) which successfully provided the title compound as colorless solid in 93% yield.

Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for methine, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl.

Computing details

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

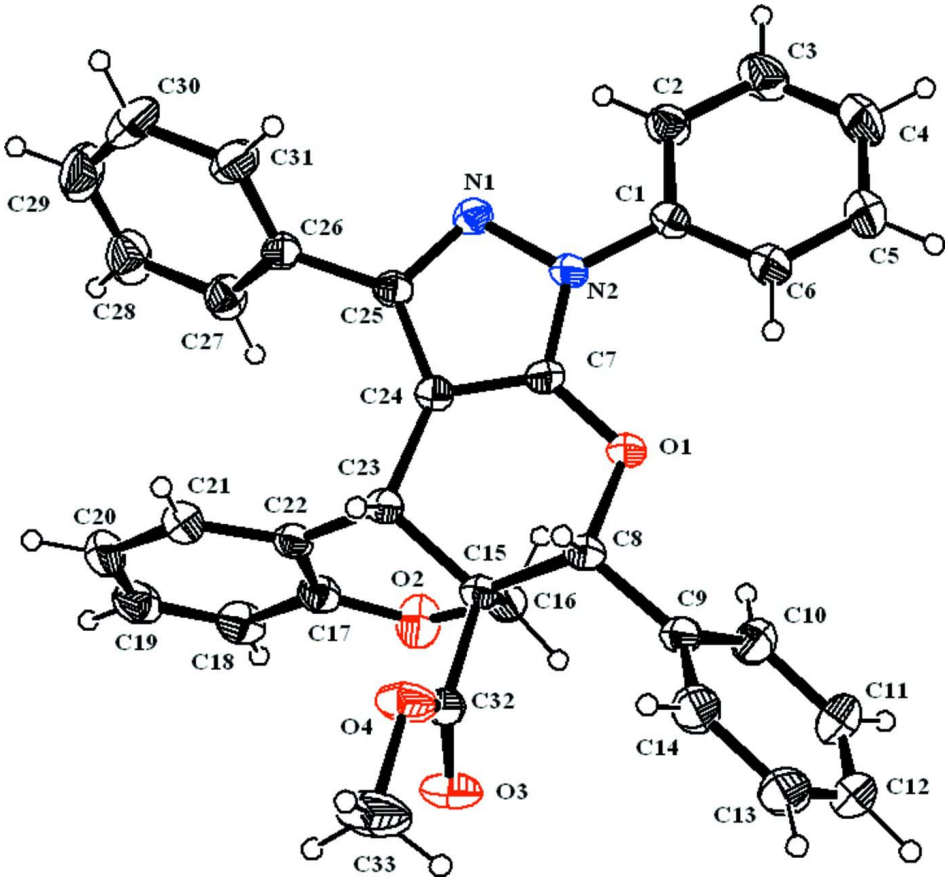

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

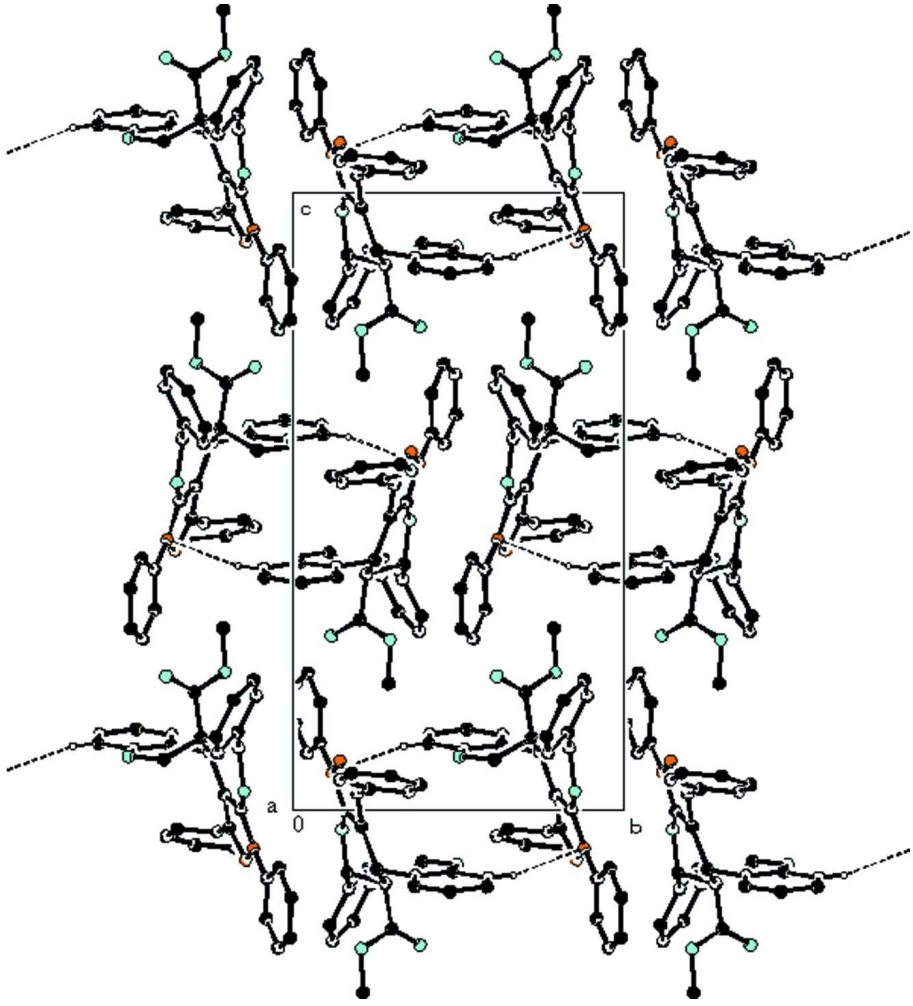

Figure 2

A packing diagram of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

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b = 10.876 (5) Å
c = 21.153 (5) Å
β = 105.797 (5)°
V = 2637.9 (18) Å^3
Z = 4

$F(000)$ = 1080
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9160 reflections
θ = 2.3–25.1°
μ = 0.09 mm^{-1}
T = 295 K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.983

40448 measured reflections
4605 independent reflections
3289 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.1°, θ_{min} = 2.3°
h = −14→14
k = −12→12
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.129
S = 1.01
4605 reflections
354 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
$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2 + 0.2117P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0055 (11)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.05478 (14)	0.91979 (14)	−0.10983 (8)	0.0365 (4)
C2	−0.00894 (17)	0.91873 (17)	−0.17503 (8)	0.0485 (5)
H2	−0.0865	0.8936	−0.1868	0.058*
C3	0.0436 (2)	0.9554 (2)	−0.22240 (9)	0.0640 (6)
H3	0.0008	0.9555	−0.2663	0.077*
C4	0.1577 (2)	0.9914 (2)	−0.20573 (11)	0.0709 (6)
H4	0.1929	1.0147	−0.2381	0.085*
C5	0.21952 (19)	0.9930 (2)	−0.14101 (11)	0.0678 (6)
H5	0.2970	1.0184	−0.1295	0.081*
C6	0.16912 (16)	0.95781 (18)	−0.09264 (9)	0.0525 (5)
H6	0.2119	0.9597	−0.0487	0.063*
C7	0.04554 (14)	0.84233 (14)	0.00130 (8)	0.0340 (4)
C8	0.18737 (14)	0.83563 (15)	0.10115 (8)	0.0365 (4)
H8	0.1595	0.9084	0.1196	0.044*
C9	0.31735 (15)	0.83154 (16)	0.12662 (8)	0.0414 (4)
C10	0.38724 (16)	0.77182 (19)	0.09357 (10)	0.0559 (5)
H10	0.3532	0.7349	0.0532	0.067*
C11	0.50601 (18)	0.7664 (2)	0.11951 (13)	0.0738 (7)
H11	0.5519	0.7268	0.0966	0.089*
C12	0.5564 (2)	0.8188 (3)	0.17848 (14)	0.0864 (9)
H12	0.6365	0.8122	0.1968	0.104*
C13	0.4900 (2)	0.8812 (3)	0.21107 (12)	0.0845 (8)
H13	0.5255	0.9191	0.2509	0.101*
C14	0.37027 (18)	0.8886 (2)	0.18530 (10)	0.0611 (6)

H14	0.3256	0.9320	0.2076	0.073*
C15	0.12185 (14)	0.72167 (14)	0.11748 (7)	0.0342 (4)
O2	0.08181 (11)	0.50306 (10)	0.08741 (7)	0.0573 (4)
C17	−0.02322 (16)	0.51735 (15)	0.09970 (8)	0.0433 (4)
C18	−0.07915 (18)	0.40980 (18)	0.10863 (9)	0.0550 (5)
H18	−0.0453	0.3342	0.1045	0.066*
C19	−0.18357 (19)	0.4139 (2)	0.12349 (10)	0.0625 (6)
H19	−0.2216	0.3412	0.1283	0.075*
C20	−0.23285 (18)	0.5254 (2)	0.13141 (10)	0.0618 (6)
H20	−0.3031	0.5285	0.1426	0.074*
C21	−0.17688 (16)	0.63237 (18)	0.12258 (9)	0.0518 (5)
H21	−0.2099	0.7076	0.1283	0.062*
C22	−0.07280 (14)	0.63042 (15)	0.10545 (8)	0.0381 (4)
C23	−0.01121 (14)	0.74599 (14)	0.09516 (8)	0.0340 (4)
H23	−0.0295	0.8107	0.1230	0.041*
C24	−0.03910 (14)	0.79328 (14)	0.02535 (8)	0.0332 (4)
C25	−0.14127 (14)	0.80602 (14)	−0.02772 (8)	0.0354 (4)
C26	−0.26381 (14)	0.77063 (16)	−0.03464 (8)	0.0393 (4)
C27	−0.29485 (17)	0.64951 (17)	−0.03038 (9)	0.0502 (5)
H27	−0.2372	0.5894	−0.0199	0.060*
C28	−0.4097 (2)	0.6165 (2)	−0.04147 (11)	0.0685 (6)
H28	−0.4294	0.5342	−0.0392	0.082*
C29	−0.4949 (2)	0.7035 (3)	−0.05576 (13)	0.0823 (8)
H29	−0.5726	0.6809	−0.0625	0.099*
C30	−0.46592 (19)	0.8242 (3)	−0.06011 (13)	0.0828 (8)
H30	−0.5241	0.8838	−0.0700	0.099*
C31	−0.35080 (16)	0.85816 (19)	−0.04987 (10)	0.0589 (6)
H31	−0.3318	0.9404	−0.0533	0.071*
C32	0.16275 (15)	0.70167 (16)	0.19162 (8)	0.0397 (4)
C33	0.1692 (2)	0.7890 (3)	0.29487 (10)	0.0889 (9)
H33A	0.1394	0.7163	0.3103	0.133*
H33B	0.1411	0.8604	0.3125	0.133*
H33C	0.2529	0.7878	0.3089	0.133*
N1	−0.11824 (12)	0.85767 (12)	−0.07964 (7)	0.0383 (4)
N2	−0.00009 (11)	0.88050 (12)	−0.06145 (6)	0.0348 (3)
O1	0.16074 (9)	0.85152 (10)	0.03056 (5)	0.0396 (3)
C16	0.14938 (15)	0.60844 (15)	0.08254 (9)	0.0414 (4)
H16A	0.1373	0.6280	0.0364	0.050*
H16B	0.2312	0.5884	0.1005	0.050*
O3	0.21895 (13)	0.61598 (12)	0.21744 (6)	0.0634 (4)
O4	0.13024 (12)	0.79288 (12)	0.22348 (6)	0.0590 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0438 (10)	0.0316 (9)	0.0343 (9)	0.0017 (7)	0.0112 (7)	0.0032 (7)
C2	0.0536 (12)	0.0533 (11)	0.0370 (10)	−0.0019 (9)	0.0097 (9)	0.0021 (8)
C3	0.0802 (16)	0.0792 (15)	0.0332 (10)	−0.0054 (12)	0.0164 (10)	0.0021 (10)
C4	0.0790 (16)	0.0881 (17)	0.0552 (14)	−0.0065 (13)	0.0346 (12)	0.0133 (12)
C5	0.0556 (13)	0.0908 (17)	0.0597 (14)	−0.0093 (12)	0.0203 (11)	0.0206 (12)

C6	0.0492 (12)	0.0646 (12)	0.0421 (11)	−0.0050 (10)	0.0097 (9)	0.0119 (9)
C7	0.0345 (9)	0.0336 (9)	0.0306 (9)	0.0014 (7)	0.0034 (7)	0.0014 (7)
C8	0.0398 (10)	0.0387 (9)	0.0286 (9)	0.0014 (7)	0.0052 (7)	0.0016 (7)
C9	0.0392 (10)	0.0453 (10)	0.0355 (10)	−0.0040 (8)	0.0030 (8)	0.0087 (8)
C10	0.0423 (11)	0.0698 (13)	0.0540 (12)	−0.0001 (10)	0.0104 (9)	0.0010 (10)
C11	0.0376 (12)	0.0990 (18)	0.0830 (17)	0.0050 (11)	0.0135 (12)	0.0177 (14)
C12	0.0410 (13)	0.133 (2)	0.0752 (18)	−0.0137 (14)	−0.0012 (13)	0.0407 (17)
C13	0.0637 (16)	0.128 (2)	0.0460 (13)	−0.0416 (15)	−0.0112 (12)	0.0112 (14)
C14	0.0566 (13)	0.0784 (14)	0.0430 (11)	−0.0212 (11)	0.0047 (10)	−0.0017 (10)
C15	0.0365 (9)	0.0359 (9)	0.0287 (9)	0.0023 (7)	0.0064 (7)	0.0017 (7)
O2	0.0600 (9)	0.0364 (7)	0.0816 (10)	−0.0005 (6)	0.0295 (8)	−0.0085 (6)
C17	0.0499 (11)	0.0406 (10)	0.0369 (10)	−0.0043 (8)	0.0077 (8)	0.0007 (8)
C18	0.0671 (14)	0.0420 (11)	0.0510 (12)	−0.0099 (10)	0.0078 (10)	−0.0007 (9)
C19	0.0683 (15)	0.0590 (14)	0.0527 (13)	−0.0229 (11)	0.0038 (11)	0.0119 (10)
C20	0.0508 (12)	0.0781 (16)	0.0574 (13)	−0.0135 (11)	0.0160 (10)	0.0157 (11)
C21	0.0474 (12)	0.0582 (12)	0.0511 (12)	−0.0007 (9)	0.0155 (9)	0.0119 (9)
C22	0.0400 (10)	0.0412 (10)	0.0304 (9)	−0.0014 (7)	0.0052 (7)	0.0049 (7)
C23	0.0361 (9)	0.0344 (9)	0.0306 (9)	0.0032 (7)	0.0077 (7)	0.0017 (7)
C24	0.0354 (9)	0.0315 (8)	0.0317 (9)	0.0019 (7)	0.0075 (7)	0.0007 (7)
C25	0.0386 (10)	0.0336 (9)	0.0323 (9)	−0.0001 (7)	0.0067 (7)	−0.0004 (7)
C26	0.0361 (10)	0.0492 (11)	0.0298 (9)	−0.0017 (8)	0.0045 (7)	−0.0003 (7)
C27	0.0477 (12)	0.0523 (11)	0.0494 (12)	−0.0088 (9)	0.0113 (9)	−0.0032 (9)
C28	0.0628 (15)	0.0766 (15)	0.0662 (15)	−0.0275 (12)	0.0177 (12)	−0.0068 (12)
C29	0.0417 (13)	0.124 (2)	0.0783 (17)	−0.0230 (15)	0.0107 (12)	−0.0044 (16)
C30	0.0375 (13)	0.104 (2)	0.099 (2)	0.0145 (13)	0.0047 (12)	0.0103 (16)
C31	0.0408 (12)	0.0642 (13)	0.0651 (14)	0.0062 (9)	0.0032 (10)	0.0074 (10)
C32	0.0392 (10)	0.0408 (10)	0.0370 (10)	0.0023 (8)	0.0066 (8)	0.0043 (8)
C33	0.118 (2)	0.113 (2)	0.0290 (11)	0.0323 (17)	0.0092 (12)	−0.0018 (12)
N1	0.0350 (8)	0.0413 (8)	0.0354 (8)	−0.0010 (6)	0.0044 (6)	0.0021 (6)
N2	0.0343 (8)	0.0374 (8)	0.0305 (7)	−0.0002 (6)	0.0051 (6)	0.0046 (6)
O1	0.0354 (7)	0.0497 (7)	0.0307 (6)	−0.0011 (5)	0.0039 (5)	0.0076 (5)
C16	0.0434 (10)	0.0387 (10)	0.0429 (10)	0.0022 (8)	0.0132 (8)	0.0009 (8)
O3	0.0791 (10)	0.0559 (8)	0.0451 (8)	0.0196 (7)	−0.0004 (7)	0.0125 (6)
O4	0.0785 (10)	0.0661 (9)	0.0288 (7)	0.0220 (7)	0.0082 (6)	−0.0019 (6)

Geometric parameters (Å, º)

C1—C6	1.375 (2)	C17—C18	1.384 (3)
C1—C2	1.382 (2)	C18—C19	1.364 (3)
C1—N2	1.422 (2)	C18—H18	0.9300
C2—C3	1.377 (3)	C19—C20	1.378 (3)
C2—H2	0.9300	C19—H19	0.9300
C3—C4	1.366 (3)	C20—C21	1.379 (3)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.367 (3)	C21—C22	1.384 (3)
C4—H4	0.9300	C21—H21	0.9300
C5—C6	1.374 (3)	C22—C23	1.501 (2)
C5—H5	0.9300	C23—C24	1.513 (2)
C6—H6	0.9300	C23—H23	0.9800
C7—O1	1.3472 (19)	C24—C25	1.420 (2)

C7—N2	1.355 (2)	C25—N1	1.327 (2)
C7—C24	1.356 (2)	C25—C26	1.478 (2)
C8—O1	1.4500 (19)	C26—C27	1.378 (2)
C8—C9	1.496 (2)	C26—C31	1.379 (3)
C8—C15	1.553 (2)	C27—C28	1.372 (3)
C8—H8	0.9800	C27—H27	0.9300
C9—C14	1.377 (3)	C28—C29	1.360 (3)
C9—C10	1.386 (3)	C28—H28	0.9300
C10—C11	1.373 (3)	C29—C30	1.368 (4)
C10—H10	0.9300	C29—H29	0.9300
C11—C12	1.354 (4)	C30—C31	1.380 (3)
C11—H11	0.9300	C30—H30	0.9300
C12—C13	1.363 (4)	C31—H31	0.9300
C12—H12	0.9300	C32—O3	1.190 (2)
C13—C14	1.384 (3)	C32—O4	1.315 (2)
C13—H13	0.9300	C33—O4	1.455 (2)
C14—H14	0.9300	C33—H33A	0.9600
C15—C16	1.517 (2)	C33—H33B	0.9600
C15—C32	1.526 (2)	C33—H33C	0.9600
C15—C23	1.549 (2)	N1—N2	1.3772 (19)
O2—C17	1.355 (2)	C16—H16A	0.9700
O2—C16	1.420 (2)	C16—H16B	0.9700
C17—C22	1.384 (2)		

C6—C1—C2	120.15 (16)	C19—C20—C21	119.2 (2)
C6—C1—N2	121.12 (15)	C19—C20—H20	120.4
C2—C1—N2	118.73 (15)	C21—C20—H20	120.4
C3—C2—C1	119.27 (18)	C20—C21—C22	121.58 (19)
C3—C2—H2	120.4	C20—C21—H21	119.2
C1—C2—H2	120.4	C22—C21—H21	119.2
C4—C3—C2	120.86 (19)	C21—C22—C17	118.11 (16)
C4—C3—H3	119.6	C21—C22—C23	122.26 (16)
C2—C3—H3	119.6	C17—C22—C23	119.60 (16)
C3—C4—C5	119.3 (2)	C22—C23—C24	116.12 (13)
C3—C4—H4	120.3	C22—C23—C15	108.25 (13)
C5—C4—H4	120.3	C24—C23—C15	106.87 (13)
C4—C5—C6	121.1 (2)	C22—C23—H23	108.5
C4—C5—H5	119.5	C24—C23—H23	108.5
C6—C5—H5	119.5	C15—C23—H23	108.5
C5—C6—C1	119.30 (18)	C7—C24—C25	103.30 (14)
C5—C6—H6	120.4	C7—C24—C23	120.77 (14)
C1—C6—H6	120.4	C25—C24—C23	135.88 (15)
O1—C7—N2	120.94 (14)	N1—C25—C24	111.68 (14)
O1—C7—C24	128.72 (14)	N1—C25—C26	116.71 (14)
N2—C7—C24	110.29 (14)	C24—C25—C26	131.59 (15)
O1—C8—C9	106.82 (13)	C27—C26—C31	118.50 (17)
O1—C8—C15	109.99 (12)	C27—C26—C25	121.20 (16)
C9—C8—C15	115.48 (13)	C31—C26—C25	120.17 (16)
O1—C8—H8	108.1	C28—C27—C26	120.8 (2)

C9—C8—H8	108.1	C28—C27—H27	119.6
C15—C8—H8	108.1	C26—C27—H27	119.6
C14—C9—C10	118.36 (18)	C29—C28—C27	120.4 (2)
C14—C9—C8	119.10 (17)	C29—C28—H28	119.8
C10—C9—C8	122.54 (16)	C27—C28—H28	119.8
C11—C10—C9	120.9 (2)	C28—C29—C30	119.7 (2)
C11—C10—H10	119.5	C28—C29—H29	120.1
C9—C10—H10	119.5	C30—C29—H29	120.1
C12—C11—C10	120.0 (2)	C29—C30—C31	120.3 (2)
C12—C11—H11	120.0	C29—C30—H30	119.8
C10—C11—H11	120.0	C31—C30—H30	119.8
C11—C12—C13	120.2 (2)	C26—C31—C30	120.3 (2)
C11—C12—H12	119.9	C26—C31—H31	119.9
C13—C12—H12	119.9	C30—C31—H31	119.9
C12—C13—C14	120.5 (2)	O3—C32—O4	124.26 (16)
C12—C13—H13	119.8	O3—C32—C15	124.45 (16)
C14—C13—H13	119.8	O4—C32—C15	111.28 (14)
C9—C14—C13	119.9 (2)	O4—C33—H33A	109.5
C9—C14—H14	120.0	O4—C33—H33B	109.5
C13—C14—H14	120.0	H33A—C33—H33B	109.5
C16—C15—C32	109.52 (13)	O4—C33—H33C	109.5
C16—C15—C23	109.22 (13)	H33A—C33—H33C	109.5
C32—C15—C23	110.59 (13)	H33B—C33—H33C	109.5
C16—C15—C8	110.55 (14)	C25—N1—N2	105.72 (12)
C32—C15—C8	107.64 (13)	C7—N2—N1	109.00 (12)
C23—C15—C8	109.31 (12)	C7—N2—C1	131.03 (14)
C17—O2—C16	119.54 (13)	N1—N2—C1	119.23 (12)
O2—C17—C22	123.89 (15)	C7—O1—C8	111.98 (12)
O2—C17—C18	115.69 (16)	O2—C16—C15	114.68 (14)
C22—C17—C18	120.38 (18)	O2—C16—H16A	108.6
C19—C18—C17	120.47 (19)	C15—C16—H16A	108.6
C19—C18—H18	119.8	O2—C16—H16B	108.6
C17—C18—H18	119.8	C15—C16—H16B	108.6
C18—C19—C20	120.14 (19)	H16A—C16—H16B	107.6
C18—C19—H19	119.9	C32—O4—C33	117.05 (15)
C20—C19—H19	119.9		

C6—C1—C2—C3	0.4 (3)	O1—C7—C24—C23	3.7 (3)
N2—C1—C2—C3	−179.34 (17)	N2—C7—C24—C23	−178.75 (13)
C1—C2—C3—C4	0.6 (3)	C22—C23—C24—C7	−141.22 (16)
C2—C3—C4—C5	−1.1 (4)	C15—C23—C24—C7	−20.34 (19)
C3—C4—C5—C6	0.6 (4)	C22—C23—C24—C25	41.6 (3)
C4—C5—C6—C1	0.3 (3)	C15—C23—C24—C25	162.47 (17)
C2—C1—C6—C5	−0.9 (3)	C7—C24—C25—N1	0.66 (18)
N2—C1—C6—C5	178.87 (17)	C23—C24—C25—N1	178.18 (16)
O1—C8—C9—C14	141.20 (16)	C7—C24—C25—C26	179.51 (17)
C15—C8—C9—C14	−96.15 (19)	C23—C24—C25—C26	−3.0 (3)
O1—C8—C9—C10	−39.1 (2)	N1—C25—C26—C27	116.90 (18)
C15—C8—C9—C10	83.5 (2)	C24—C25—C26—C27	−61.9 (2)

C14—C9—C10—C11	1.9 (3)	N1—C25—C26—C31	−58.8 (2)
C8—C9—C10—C11	−177.79 (18)	C24—C25—C26—C31	122.4 (2)
C9—C10—C11—C12	0.7 (3)	C31—C26—C27—C28	0.4 (3)
C10—C11—C12—C13	−2.6 (4)	C25—C26—C27—C28	−175.35 (18)
C11—C12—C13—C14	2.0 (4)	C26—C27—C28—C29	−1.2 (3)
C10—C9—C14—C13	−2.5 (3)	C27—C28—C29—C30	1.0 (4)
C8—C9—C14—C13	177.18 (18)	C28—C29—C30—C31	−0.2 (4)
C12—C13—C14—C9	0.6 (4)	C27—C26—C31—C30	0.4 (3)
O1—C8—C15—C16	54.65 (17)	C25—C26—C31—C30	176.2 (2)
C9—C8—C15—C16	−66.31 (18)	C29—C30—C31—C26	−0.5 (4)
O1—C8—C15—C32	174.23 (12)	C16—C15—C32—O3	7.7 (2)
C9—C8—C15—C32	53.27 (18)	C23—C15—C32—O3	128.08 (18)
O1—C8—C15—C23	−65.61 (16)	C8—C15—C32—O3	−112.56 (19)
C9—C8—C15—C23	173.44 (13)	C16—C15—C32—O4	−173.82 (14)
C16—O2—C17—C22	2.7 (3)	C23—C15—C32—O4	−53.41 (18)
C16—O2—C17—C18	−175.26 (15)	C8—C15—C32—O4	65.95 (18)
O2—C17—C18—C19	177.76 (17)	C24—C25—N1—N2	−0.31 (18)
C22—C17—C18—C19	−0.3 (3)	C26—C25—N1—N2	−179.34 (13)
C17—C18—C19—C20	−1.7 (3)	O1—C7—N2—N1	178.36 (13)
C18—C19—C20—C21	1.6 (3)	C24—C7—N2—N1	0.63 (18)
C19—C20—C21—C22	0.5 (3)	O1—C7—N2—C1	8.5 (3)
C20—C21—C22—C17	−2.4 (3)	C24—C7—N2—C1	−169.21 (15)
C20—C21—C22—C23	179.53 (16)	C25—N1—N2—C7	−0.18 (17)
O2—C17—C22—C21	−175.60 (16)	C25—N1—N2—C1	171.04 (13)
C18—C17—C22—C21	2.3 (3)	C6—C1—N2—C7	−19.0 (3)
O2—C17—C22—C23	2.5 (3)	C2—C1—N2—C7	160.76 (16)
C18—C17—C22—C23	−179.60 (16)	C6—C1—N2—N1	172.05 (15)
C21—C22—C23—C24	−93.1 (2)	C2—C1—N2—N1	−8.2 (2)
C17—C22—C23—C24	88.85 (18)	N2—C7—O1—C8	165.39 (14)
C21—C22—C23—C15	146.77 (16)	C24—C7—O1—C8	−17.3 (2)
C17—C22—C23—C15	−31.3 (2)	C9—C8—O1—C7	172.87 (13)
C16—C15—C23—C22	53.54 (17)	C15—C8—O1—C7	46.85 (17)
C32—C15—C23—C22	−67.05 (16)	C17—O2—C16—C15	23.4 (2)
C8—C15—C23—C22	174.61 (13)	C32—C15—C16—O2	69.47 (18)
C16—C15—C23—C24	−72.22 (16)	C23—C15—C16—O2	−51.78 (18)
C32—C15—C23—C24	167.19 (13)	C8—C15—C16—O2	−172.09 (13)
C8—C15—C23—C24	48.85 (16)	O3—C32—O4—C33	1.9 (3)
O1—C7—C24—C25	−178.27 (15)	C15—C32—O4—C33	−176.62 (18)
N2—C7—C24—C25	−0.76 (17)		

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*4 and *Cg*6 are the centroids of the N1/N2/C7/C24/C25, C1–C6 and C17–C22 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···N2^{i}	0.93	2.62	3.517 (3)	163
C6—H6···O1	0.93	2.26	2.877 (2)	123
C13—H13···*Cg*6^{ii}	0.93	2.98	3.904 (8)	174

C18—H18···*Cg*1^{i}	0.93	2.88	3.720 (5)	150
C23—H23···*Cg*4^{iii}	0.98	2.86	3.787 (6)	159

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