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(*Z*)-*N*-(2,6-Diisopropylphenyl)-1-[(2-methoxyphenyl)amino]methanimine oxide

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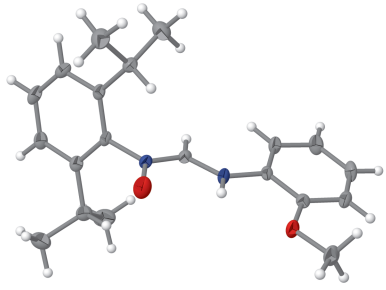
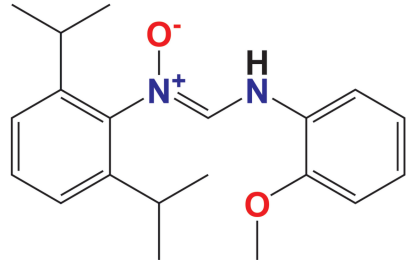
Structural data: full structural data are available from iucrdata.iucr.org

The molecular structure of the title compound, $C_{20}H_{26}N_2O_2$ reveals non-coplanarity between the central formamidine backbone and each of the outer methoxy- and *i*-propyl- substituted benzene rings with dihedral angles of 7.88 (15) and 81.17 (15)°, respectively, indicating significant twists in the molecule. In the crystal, intermolecular C—H···O interactions, forming an $R_4^3(30)$ graph set, occur within a two-dimensional layer that extends along the *ac* plane.

3D view



Chemical scheme



Structure description

The tittle compound is a member of the formamidine class of compounds, which follow the general structure $RN{-}C(R'){=}NR''$, where R, R' and R'' can represent either hydrogen, alkyl or aryl groups (Zamisa *et al.*, 2021; Barker & Kilner, 1994). Their varied structures have led to investigations into their potential medicinal uses, uncovering properties such as antimicrobial and anticancer activities (Clement, 2002; Stojak *et al.*, 2014). Recently, we focused on the application of formamidine metal complexes as catalysts in ring-opening polymerization reactions (Munzeiwa *et al.*, 2018). As part of our work to develop new derivatives with superior catalytic abilities, we synthesized the title compound and analysed its crystal structure.

The title crystal has one molecule in the asymmetric unit, as shown in Fig. 1. The molecular conformation of the title compound is described by a dihedral angle between the 2-methoxybenzene plane and the formamidine backbone of 7.88 (15)°, while that between the 2,6-diisopropylbenzene plane and the backbone measures 81.17 (15)°, suggesting a notable twist of this plane relative to the backbone. Furthermore, the dihedral angle between the two benzene planes is 78.17 (6)°. All other intramolecular bond parameters are comparable with those of (*Z*)-1-[(4-methoxyphenyl)amino]-*N*-phenylmethanimine oxide (CSD refcode: GIKFUB; Giumanini *et al.*, 1999).

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2^{i}	0.95	2.39	3.337 (2)	174
C14—H14*C*···O2^{ii}	0.98	2.47	3.445 (2)	172

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

Intermolecular C—H···O hydrogen bonds were found in the molecular packing of the title compound, Table 1. The oxygen atom is involved in bifurcated C14—H14*C*···O2 and C9—H9···O2 interactions with the hydrogen (H14*C*) atom of the isopropyl substituent and the hydrogen (H9) atom of the 2-methoxyphenyl ring, respectively. The former links neighbouring molecules along [100] whilst the latter joins neighbouring molecules along [001]. Collectively, the two types of C—H···O interactions can be described by an $R_4^3(30)$ graph set within a two-dimensional supramolecular arrangement that propagates along the *ac* plane (Fig. 2).

Synthesis and crystallization

The title compound was synthesized using a modified protocol (Munzeiwa *et al.*, 2017). Thus, *N*-(2,6-diisopropylphenyl)-*N*′-(2-methoxyphenyl)formamidine (1 mmol) was dissolved in dichloromethane (6 ml) followed by the addition of solid sodium hydrogen carbonate (1 mmol). The mixture was cooled to 0°C. A slight excess of *meta*-chloroperoxybenzoic acid (1.2 mmol) in dichloromethane (6 ml) was then added dropwise, and the reaction mixture was allowed to gradually warm to room temperature while stirring for 1 h. The mixture was washed with 2 × 25 ml of 5% potassium carbonate solution. The combined organic layers were dried over anhydrous sodium sulfate, filtered and the solvent evaporated to yield a solid residue. The crude solid was subsequently recrystallized from its methanol solution to produce crystals suitable for X-ray diffraction.

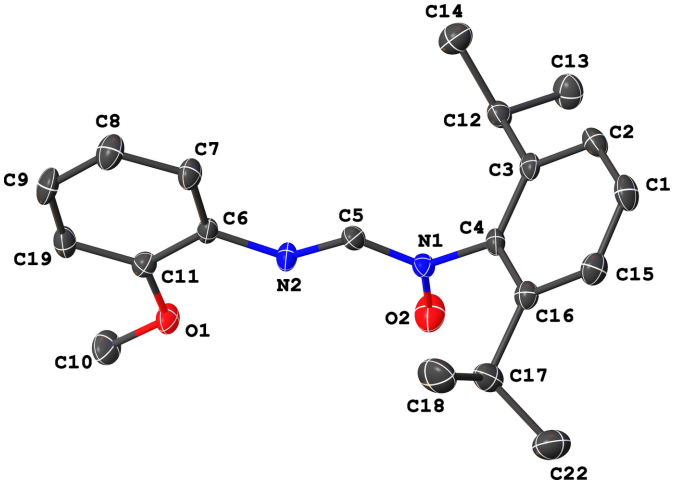


Figure 1
Molecular structure of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. All hydrogen atoms have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{26}N_2O_2$
M_r	326.43
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	10.1243 (4), 23.941 (1), 7.5053 (3)
β (°)	91.315 (3)
V (Å^3)	1818.70 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.22 × 0.18 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.984, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19835, 3268, 2304
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.108, 1.03
No. of reflections	3268
No. of parameters	222
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.34

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystallographic data and structure refinement details are summarized in Table 2.

Acknowledgements

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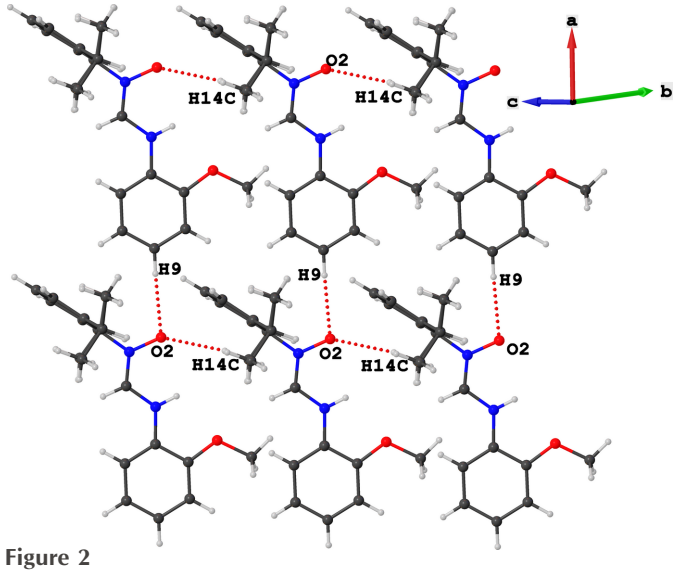

Figure 2
Representation of intermolecular C—H···O interactions (red dotted bonds).

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full crystallographic data

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Crystal data

$C_{20}H_{26}N_2O_2$
M_r = 326.43
Monoclinic, $P2_1/c$
a = 10.1243 (4) Å
b = 23.941 (1) Å
c = 7.5053 (3) Å
β = 91.315 (3)°
V = 1818.70 (13) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.192 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3357 reflections
θ = 2.6–26.1°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.22 × 0.18 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.984, T_{max} = 0.992
19835 measured reflections
3268 independent reflections
2304 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.2°, θ_{min} = 1.7°
h = −12→12
k = −26→28
l = −6→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.03
3268 reflections
222 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.5644P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.24618 (12)	0.68362 (5)	−0.12209 (16)	0.0240 (3)
O2	0.63374 (13)	0.64315 (6)	0.11780 (18)	0.0331 (4)
N1	0.58378 (14)	0.61829 (6)	0.25631 (19)	0.0170 (3)
N2	0.37631 (14)	0.64203 (6)	0.1547 (2)	0.0190 (4)
H2	0.413234	0.658969	0.064484	0.023*
C1	0.82344 (18)	0.54648 (8)	0.6549 (3)	0.0260 (5)
H1	0.874167	0.529441	0.748058	0.031*
C2	0.77386 (18)	0.59966 (8)	0.6781 (2)	0.0225 (4)
H2A	0.791133	0.618873	0.786910	0.027*
C3	0.69884 (16)	0.62541 (7)	0.5438 (2)	0.0180 (4)
C4	0.67049 (16)	0.59410 (7)	0.3911 (2)	0.0164 (4)
C5	0.45720 (17)	0.61710 (7)	0.2758 (2)	0.0182 (4)
H5	0.421147	0.598614	0.375576	0.022*
C6	0.23759 (17)	0.64312 (7)	0.1612 (2)	0.0170 (4)
C7	0.16819 (18)	0.62453 (8)	0.3053 (3)	0.0229 (4)
H7	0.214562	0.610891	0.407812	0.028*
C8	0.03063 (18)	0.62555 (8)	0.3021 (3)	0.0283 (5)
H8	−0.016409	0.612074	0.401349	0.034*
C9	−0.03726 (18)	0.64608 (8)	0.1551 (3)	0.0277 (5)
H9	−0.131108	0.646543	0.152560	0.033*
C10	0.1809 (2)	0.71154 (9)	−0.2667 (3)	0.0317 (5)
H10A	0.120039	0.685618	−0.327481	0.048*
H10B	0.246584	0.724767	−0.350876	0.048*
H10C	0.131282	0.743447	−0.221269	0.048*
C11	0.16860 (17)	0.66476 (7)	0.0128 (2)	0.0188 (4)
C12	0.65352 (17)	0.68551 (8)	0.5626 (2)	0.0210 (4)
H12	0.615423	0.697475	0.444555	0.025*
C13	0.76943 (19)	0.72415 (8)	0.6074 (3)	0.0305 (5)
H13A	0.805030	0.715203	0.726483	0.046*
H13B	0.739196	0.763030	0.604830	0.046*
H13C	0.838529	0.719026	0.519491	0.046*
C14	0.5452 (2)	0.69169 (9)	0.6997 (3)	0.0320 (5)
H14A	0.469131	0.668580	0.664185	0.048*
H14B	0.517834	0.730900	0.706103	0.048*
H14C	0.579024	0.679568	0.816829	0.048*
C15	0.80004 (18)	0.51781 (8)	0.4976 (3)	0.0239 (5)
H15	0.838574	0.482028	0.481773	0.029*
C16	0.72077 (17)	0.54058 (7)	0.3619 (2)	0.0195 (4)
C17	0.68975 (19)	0.50857 (8)	0.1912 (2)	0.0253 (5)
H17	0.652702	0.535657	0.101812	0.030*
C18	0.5848 (2)	0.46398 (9)	0.2228 (3)	0.0419 (6)
H18A	0.620523	0.435607	0.304729	0.063*
H18B	0.559595	0.446378	0.109107	0.063*
H18C	0.506945	0.481362	0.274722	0.063*
C19	0.03187 (17)	0.66612 (7)	0.0105 (3)	0.0233 (4)

H19	−0.014889	0.680792	−0.090184	0.028*
C22	0.8135 (2)	0.48265 (9)	0.1134 (3)	0.0371 (5)
H22A	0.881168	0.511530	0.100393	0.056*
H22B	0.791668	0.466460	−0.003513	0.056*
H22C	0.847068	0.453307	0.193454	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0185 (7)	0.0334 (8)	0.0201 (7)	0.0049 (6)	−0.0014 (6)	0.0075 (6)
O2	0.0261 (8)	0.0423 (9)	0.0311 (8)	−0.0019 (6)	0.0022 (6)	0.0131 (7)
N1	0.0163 (8)	0.0197 (8)	0.0150 (8)	0.0004 (6)	−0.0011 (6)	0.0019 (6)
N2	0.0129 (8)	0.0246 (8)	0.0194 (8)	0.0007 (6)	−0.0006 (6)	0.0055 (7)
C1	0.0223 (10)	0.0292 (11)	0.0260 (11)	−0.0024 (9)	−0.0074 (9)	0.0109 (9)
C2	0.0215 (10)	0.0279 (11)	0.0179 (10)	−0.0056 (8)	−0.0036 (8)	0.0027 (8)
C3	0.0113 (9)	0.0228 (10)	0.0199 (10)	−0.0026 (7)	0.0003 (8)	0.0036 (8)
C4	0.0120 (9)	0.0208 (10)	0.0164 (10)	−0.0012 (7)	−0.0017 (8)	0.0046 (8)
C5	0.0182 (10)	0.0208 (10)	0.0155 (10)	0.0015 (8)	−0.0013 (8)	0.0006 (8)
C6	0.0133 (9)	0.0162 (9)	0.0215 (10)	0.0008 (7)	−0.0010 (8)	−0.0018 (8)
C7	0.0182 (10)	0.0260 (11)	0.0245 (11)	0.0037 (8)	−0.0011 (8)	0.0067 (9)
C8	0.0197 (10)	0.0308 (11)	0.0346 (12)	−0.0001 (9)	0.0042 (9)	0.0088 (10)
C9	0.0125 (10)	0.0282 (11)	0.0423 (13)	0.0000 (8)	0.0008 (9)	0.0037 (10)
C10	0.0286 (11)	0.0422 (13)	0.0240 (11)	0.0090 (10)	−0.0028 (9)	0.0111 (10)
C11	0.0177 (10)	0.0186 (10)	0.0201 (10)	−0.0001 (8)	0.0013 (8)	−0.0005 (8)
C12	0.0204 (10)	0.0236 (10)	0.0189 (10)	0.0001 (8)	−0.0027 (8)	0.0004 (8)
C13	0.0273 (11)	0.0256 (11)	0.0385 (13)	−0.0039 (9)	−0.0030 (10)	−0.0012 (9)
C14	0.0298 (12)	0.0307 (12)	0.0357 (12)	0.0017 (9)	0.0059 (10)	−0.0029 (10)
C15	0.0220 (10)	0.0213 (10)	0.0283 (11)	0.0034 (8)	−0.0003 (9)	0.0062 (9)
C16	0.0163 (9)	0.0205 (10)	0.0218 (10)	−0.0019 (8)	0.0007 (8)	0.0035 (8)
C17	0.0310 (11)	0.0215 (10)	0.0232 (11)	0.0036 (8)	−0.0031 (9)	−0.0002 (8)
C18	0.0421 (14)	0.0421 (14)	0.0414 (14)	−0.0123 (11)	0.0004 (11)	−0.0132 (11)
C19	0.0189 (10)	0.0223 (10)	0.0284 (11)	0.0018 (8)	−0.0066 (9)	−0.0004 (9)
C22	0.0416 (13)	0.0368 (13)	0.0331 (12)	0.0053 (10)	0.0054 (10)	−0.0065 (10)

Geometric parameters (Å, º)

O1—C10	1.424 (2)	C10—H10B	0.9800
O1—C11	1.372 (2)	C10—H10C	0.9800
O2—N1	1.3095 (19)	C11—C19	1.384 (2)
N1—C4	1.445 (2)	C12—H12	1.0000
N1—C5	1.294 (2)	C12—C13	1.526 (3)
N2—H2	0.8800	C12—C14	1.529 (3)
N2—C5	1.349 (2)	C13—H13A	0.9800
N2—C6	1.407 (2)	C13—H13B	0.9800
C1—H1	0.9500	C13—H13C	0.9800
C1—C2	1.381 (3)	C14—H14A	0.9800
C1—C15	1.381 (3)	C14—H14B	0.9800
C2—H2A	0.9500	C14—H14C	0.9800

C2—C3	1.392 (2)	C15—H15	0.9500
C3—C4	1.394 (2)	C15—C16	1.394 (2)
C3—C12	1.518 (3)	C16—C17	1.519 (3)
C4—C16	1.398 (2)	C17—H17	1.0000
C5—H5	0.9500	C17—C18	1.529 (3)
C6—C7	1.377 (3)	C17—C22	1.526 (3)
C6—C11	1.401 (2)	C18—H18A	0.9800
C7—H7	0.9500	C18—H18B	0.9800
C7—C8	1.393 (3)	C18—H18C	0.9800
C8—H8	0.9500	C19—H19	0.9500
C8—C9	1.377 (3)	C22—H22A	0.9800
C9—H9	0.9500	C22—H22B	0.9800
C9—C19	1.390 (3)	C22—H22C	0.9800
C10—H10A	0.9800		

C11—O1—C10	116.96 (14)	C3—C12—C13	111.26 (15)
O2—N1—C4	119.89 (14)	C3—C12—C14	112.18 (15)
C5—N1—O2	120.10 (15)	C13—C12—H12	107.5
C5—N1—C4	119.96 (15)	C13—C12—C14	110.69 (16)
C5—N2—H2	117.4	C14—C12—H12	107.5
C5—N2—C6	125.18 (15)	C12—C13—H13A	109.5
C6—N2—H2	117.4	C12—C13—H13B	109.5
C2—C1—H1	119.7	C12—C13—H13C	109.5
C2—C1—C15	120.67 (17)	H13A—C13—H13B	109.5
C15—C1—H1	119.7	H13A—C13—H13C	109.5
C1—C2—H2A	119.6	H13B—C13—H13C	109.5
C1—C2—C3	120.72 (18)	C12—C14—H14A	109.5
C3—C2—H2A	119.6	C12—C14—H14B	109.5
C2—C3—C4	117.11 (16)	C12—C14—H14C	109.5
C2—C3—C12	120.91 (16)	H14A—C14—H14B	109.5
C4—C3—C12	121.96 (15)	H14A—C14—H14C	109.5
C3—C4—N1	118.05 (15)	H14B—C14—H14C	109.5
C3—C4—C16	123.60 (16)	C1—C15—H15	119.5
C16—C4—N1	118.35 (15)	C1—C15—C16	121.01 (17)
N1—C5—N2	120.13 (16)	C16—C15—H15	119.5
N1—C5—H5	119.9	C4—C16—C17	121.73 (16)
N2—C5—H5	119.9	C15—C16—C4	116.70 (17)
C7—C6—N2	123.31 (16)	C15—C16—C17	121.57 (16)
C7—C6—C11	119.35 (16)	C16—C17—H17	107.8
C11—C6—N2	117.34 (16)	C16—C17—C18	110.65 (16)
C6—C7—H7	119.7	C16—C17—C22	111.84 (16)
C6—C7—C8	120.58 (17)	C18—C17—H17	107.8
C8—C7—H7	119.7	C22—C17—H17	107.8
C7—C8—H8	120.0	C22—C17—C18	110.80 (17)
C9—C8—C7	120.06 (18)	C17—C18—H18A	109.5
C9—C8—H8	120.0	C17—C18—H18B	109.5
C8—C9—H9	120.1	C17—C18—H18C	109.5
C8—C9—C19	119.84 (17)	H18A—C18—H18B	109.5

C19—C9—H9	120.1	H18A—C18—H18C	109.5
O1—C10—H10A	109.5	H18B—C18—H18C	109.5
O1—C10—H10B	109.5	C9—C19—H19	119.9
O1—C10—H10C	109.5	C11—C19—C9	120.24 (17)
H10A—C10—H10B	109.5	C11—C19—H19	119.9
H10A—C10—H10C	109.5	C17—C22—H22A	109.5
H10B—C10—H10C	109.5	C17—C22—H22B	109.5
O1—C11—C6	115.16 (15)	C17—C22—H22C	109.5
O1—C11—C19	124.93 (16)	H22A—C22—H22B	109.5
C19—C11—C6	119.91 (17)	H22A—C22—H22C	109.5
C3—C12—H12	107.5	H22B—C22—H22C	109.5
O1—C11—C19—C9	−179.71 (17)	C4—C3—C12—C14	109.98 (19)
O2—N1—C4—C3	97.35 (19)	C4—C16—C17—C18	−102.6 (2)
O2—N1—C4—C16	−83.0 (2)	C4—C16—C17—C22	133.38 (18)
O2—N1—C5—N2	−0.8 (3)	C5—N1—C4—C3	−80.2 (2)
N1—C4—C16—C15	−177.70 (15)	C5—N1—C4—C16	99.5 (2)
N1—C4—C16—C17	1.8 (2)	C5—N2—C6—C7	8.4 (3)
N2—C6—C7—C8	−178.56 (17)	C5—N2—C6—C11	−172.09 (16)
N2—C6—C11—O1	−1.2 (2)	C6—N2—C5—N1	179.54 (16)
N2—C6—C11—C19	179.04 (16)	C6—C7—C8—C9	−1.0 (3)
C1—C2—C3—C4	3.5 (3)	C6—C11—C19—C9	0.0 (3)
C1—C2—C3—C12	−175.00 (17)	C7—C6—C11—O1	178.31 (16)
C1—C15—C16—C4	2.0 (3)	C7—C6—C11—C19	−1.4 (3)
C1—C15—C16—C17	−177.53 (17)	C7—C8—C9—C19	−0.4 (3)
C2—C1—C15—C16	−3.1 (3)	C8—C9—C19—C11	0.9 (3)
C2—C3—C4—N1	175.00 (15)	C10—O1—C11—C6	−173.25 (16)
C2—C3—C4—C16	−4.7 (3)	C10—O1—C11—C19	6.5 (3)
C2—C3—C12—C13	53.0 (2)	C11—C6—C7—C8	1.9 (3)
C2—C3—C12—C14	−71.6 (2)	C12—C3—C4—N1	−6.5 (2)
C3—C4—C16—C15	2.0 (3)	C12—C3—C4—C16	173.79 (16)
C3—C4—C16—C17	−178.50 (16)	C15—C1—C2—C3	0.2 (3)
C4—N1—C5—N2	176.73 (15)	C15—C16—C17—C18	76.9 (2)
C4—C3—C12—C13	−125.41 (18)	C15—C16—C17—C22	−47.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{i}	0.95	2.39	3.337 (2)	174
C14—H14*C*···O2^{ii}	0.98	2.47	3.445 (2)	172

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