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Ethyl 7-methyl-2-phenylpyrazolo[1,5-*a*]-pyrimidine-5-carboxylate

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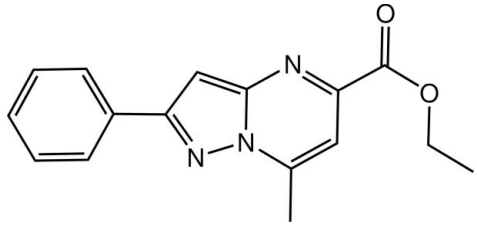
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.170; data-to-parameter ratio = 14.6.

The fused pyrazole and pyrimidine rings in the title compound, $C_{16}H_{15}N_3O_2$, are almost coplanar, being inclined to one another by 1.31 (12)°. The mean plane of this fused ring system is nearly coplanar with the phenyl ring, as indicated by the dihedral angle between their planes of 1.31 (12)°. The fused-ring system and the phenyl ring are nearly coplanar, as indicated by the dihedral angle of 1.27 (10)°. In the crystal, molecules form inversion dimers *via* pairs of C—H···O hydrogen bonds. C—H···N interactions connect the dimers into a three-dimensional network. In addition, π–π contacts are observed, with centroid–centroid distances of 3.426 (2) Å.

Related literature

For pharmacological and biochemical properties of pyrazolo-[1,5-*a*]pyrimidine derivatives, see: Selleri *et al.* (2005); Almansa *et al.* (2001); Suzuki *et al.* (2001); Chen *et al.* (2004). For related structures, see: Chimichi *et al.* (1992).



Experimental

Crystal data

$C_{16}H_{15}N_3O_2$
M_r = 281.31
Orthorhombic, *Pbca*
a = 8.0542 (8) Å
b = 16.4104 (19) Å
c = 21.635 (2) Å
V = 2859.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.41 × 0.32 × 0.21 mm

Data collection

Bruker X8 APEXII area-detector diffractometer
12894 measured reflections
2783 independent reflections
1919 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.170
S = 1.04
2783 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.93	2.36	3.258 (3)	161
C6—H6···N3^{ii}	0.93	2.62	3.507 (3)	161

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

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 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5057).

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supplementary materials

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Ethyl 7-methyl-2-phenylpyrazolo[1,5-*a*]pyrimidine-5-carboxylate

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Comment

Pyrazolo[1,5-*a*]pyrimidines have attracted considerable interest because of their biological activity. For instance, they are known for their potent utility as selective peripheral benzodiazepine receptor ligands (Selleri *et al.*, 2005), COX-2 selective inhibitors (Almansa *et al.*, 2001), HMG-CoA reductase inhibitors (Suzuki *et al.*, 2001) and CRF1 antagonists (Chen *et al.*, 2004).

The condensation of 5-amino-3-arylpyrazoles with ethyl 2,4-dioxopentanoate leads to the title compound ethyl-7-methyl-2-phenylpyrazolo[1,5-*a*]pyrimidine- 5-carboxylate and its isomeric ethyl 5-methyl-2-phenylpyrazolo[1,5-*a*]pyrimidine-7-carboxylate (Chimichi *et al.*, 1992).

The crystal structure of the title compound is built up from two fused five and six-membered rings (N1/N2/C2–C4 and N2/N3/C1/C2/C11/C12) linked to a methyl, a phenyl (C5–C10) and to an ethylcarboxylate group (C14/O1/O2/C15/C16) as shown in Fig. 1. The pyrazole and pyrimidine rings are almost planar with a maximum deviation for atom C6 of 0.002 (2) Å and 0.004 (2) Å, respectively. The mean plane through the two fused rings is slightly folded around the common edge as indicated by the dihedral angle between them of 1.31 (12)°. The dihedral angle between the phenyl ring and the fused-ring system is 1.27 (10)°.

In the crystal structure C12–H12···O1 hydrogen bonds form inversion dimers. Intermolecular C6—H6···N3 interactions connect the dimers into a three dimensional network. In addition, the molecules are connected by π–π contacts, with centroid–centroid distances of 3.426 (2) Å.

Experimental

A solution of ethyl 2,4-dioxopentanoate (1.64 g, 10.4 mmol) and 5-amino-3-phenylpyrazole (1.5 g, 9.4 mmol) in 10 ml of EtOH was heated to reflux for 30 min. After evaporation of solvent under reduced pressure, the residue was purified on silica gel by column chromatography using a 8:2 (*v*/*v*) mixture of petroleum ether and ethyl acetate as eluent. Ethyl-7-methyl-2-phenylpyrazolo[1,5-*a*]pyrimidine-5-carboxylate was recrystallized from cyclohexane to give colourless crystals.

Refinement

All H atoms could be located in a difference Fourier map and treated as riding with C—H = 0.93 Å (aromatic), C—H = 0.97 Å (methylene) and C—H = 0.96 Å (methyl), and with U_{iso}(H) = 1.2 U_{eq}(aromatic, methylene) or U_{iso}(H) = 1.5 U_{eq} (methyl).

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

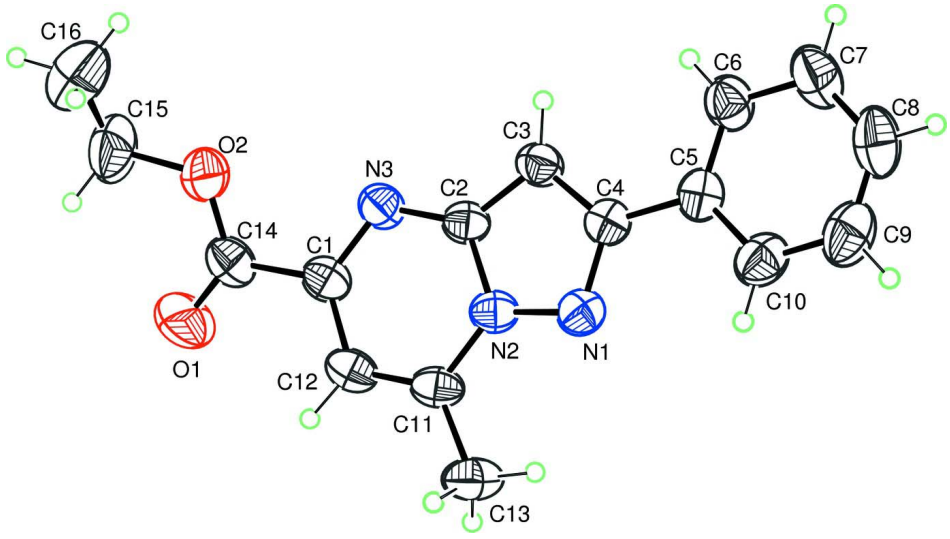

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as small circles.

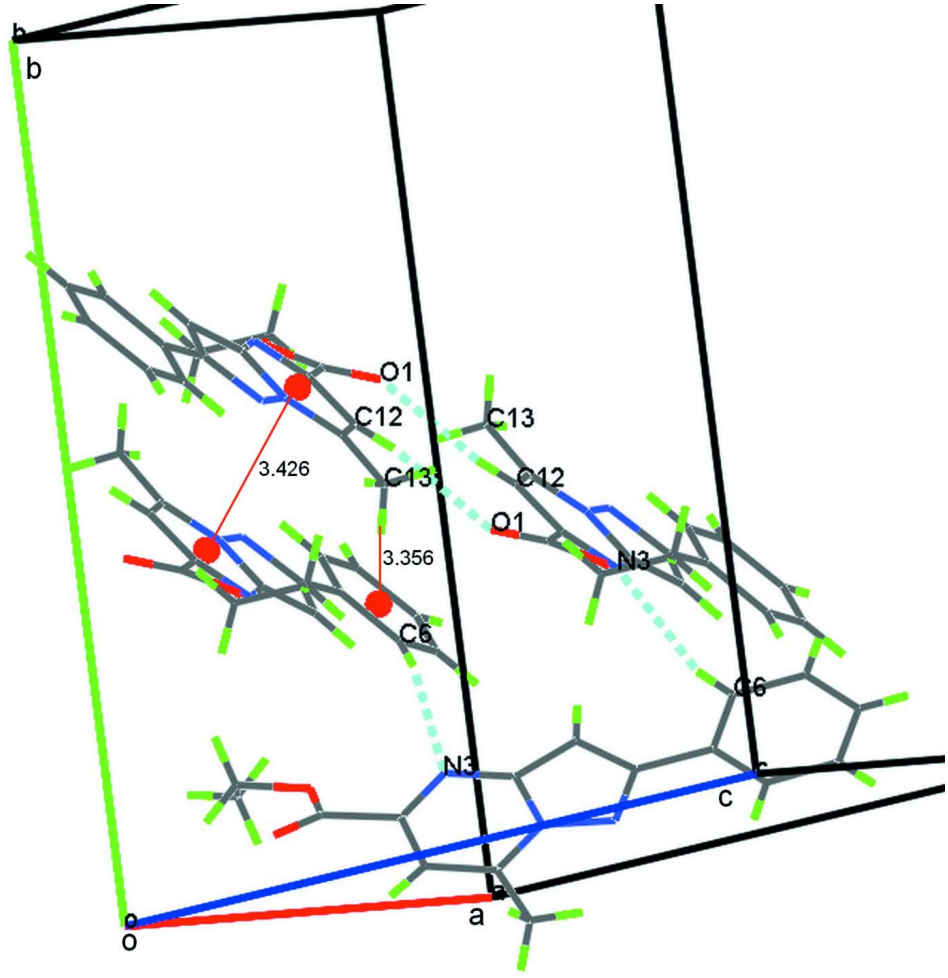

Figure 2

Crystal packing of the title compound showing C12–H12···O1 and C6–H6···N3 hydrogen bonds as blue dashed lines, with C—H···π interactions and a π—π contact (red lines). The red spheres represent the centroids of the C5–C10 and N2/N3/C1/C2/C11/C12 rings and their symmetry partners.

Ethyl 7-methyl-2-phenylpyrazolo[1,5-*a*]pyrimidine-5-carboxylate

Crystal data

$C_{16}H_{15}N_3O_2$
M_r = 281.31
Orthorhombic, *Pbca*
Hall symbol: -p 2ac 2ab
a = 8.0542 (8) Å
b = 16.4104 (19) Å
c = 21.635 (2) Å
V = 2859.5 (5) Å^3
Z = 8
$F(000)$ = 1184
D_x = 1.307 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2783 reflections
θ = 2.5–26.0°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.41 × 0.32 × 0.21 mm

Data collection

Bruker X8 APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
12894 measured reflections
2783 independent reflections
1919 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.5°$
$h = -9 \rightarrow 9$
$k = -20 \rightarrow 19$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.170$
$S = 1.04$
2783 reflections
190 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 1.249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.7015 (3)	0.59846 (13)	−0.00919 (11)	0.0423 (5)
C2	0.4533 (2)	0.62909 (13)	0.03355 (10)	0.0392 (5)
C3	0.2988 (3)	0.66217 (13)	0.04562 (11)	0.0431 (5)
H3	0.2464	0.7041	0.0243	0.052*
C4	0.2383 (3)	0.61938 (13)	0.09644 (10)	0.0404 (5)
C5	0.0780 (3)	0.63145 (14)	0.12822 (10)	0.0426 (5)
C6	−0.0290 (3)	0.69261 (15)	0.10875 (12)	0.0531 (6)
H6	0.0002	0.7255	0.0755	0.064*
C7	−0.1796 (3)	0.70489 (17)	0.13873 (14)	0.0660 (8)
H7	−0.2511	0.7456	0.1252	0.079*
C8	−0.2234 (4)	0.65694 (18)	0.18851 (14)	0.0689 (8)
H8	−0.3243	0.6650	0.2085	0.083*
C9	−0.1158 (3)	0.5968 (2)	0.20843 (13)	0.0681 (8)
H9	−0.1438	0.5649	0.2424	0.082*
C10	0.0323 (3)	0.58363 (17)	0.17833 (12)	0.0557 (7)
H10	0.1025	0.5422	0.1917	0.067*
C11	0.6159 (3)	0.52087 (13)	0.07911 (10)	0.0423 (5)
C12	0.7310 (3)	0.53683 (14)	0.03464 (11)	0.0455 (6)

H12	0.8291	0.5070	0.0332	0.055*
C13	0.6281 (3)	0.45638 (16)	0.12736 (12)	0.0584 (7)
H13A	0.5308	0.4578	0.1530	0.088*
H13B	0.7247	0.4658	0.1523	0.088*
H13C	0.6365	0.4040	0.1079	0.088*
C14	0.8285 (3)	0.61382 (15)	−0.05871 (12)	0.0493 (6)
C15	0.8726 (4)	0.6665 (2)	−0.15930 (14)	0.0784 (9)
H15A	0.9632	0.6276	−0.1601	0.094*
H15B	0.9191	0.7208	−0.1558	0.094*
C16	0.7733 (6)	0.6597 (3)	−0.21607 (16)	0.1145 (15)
H16A	0.8427	0.6700	−0.2513	0.172*
H16B	0.6848	0.6989	−0.2150	0.172*
H16C	0.7276	0.6058	−0.2190	0.172*
N1	0.3450 (2)	0.56159 (11)	0.11673 (9)	0.0435 (5)
N2	0.4760 (2)	0.56790 (11)	0.07779 (8)	0.0395 (5)
N3	0.5670 (2)	0.64421 (11)	−0.01033 (9)	0.0424 (5)
O1	0.9709 (2)	0.59496 (15)	−0.05385 (11)	0.0868 (7)
O2	0.76394 (19)	0.65002 (11)	−0.10746 (8)	0.0575 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0374 (11)	0.0394 (12)	0.0500 (14)	−0.0004 (9)	−0.0033 (9)	−0.0011 (11)
C2	0.0402 (11)	0.0342 (11)	0.0432 (13)	−0.0002 (9)	−0.0029 (9)	0.0031 (10)
C3	0.0424 (11)	0.0386 (12)	0.0484 (14)	0.0045 (9)	0.0018 (10)	0.0049 (10)
C4	0.0398 (11)	0.0401 (11)	0.0411 (13)	−0.0031 (9)	−0.0021 (9)	−0.0020 (10)
C5	0.0410 (11)	0.0439 (12)	0.0429 (13)	−0.0096 (9)	0.0017 (9)	−0.0050 (11)
C6	0.0491 (13)	0.0494 (14)	0.0607 (16)	−0.0019 (11)	0.0115 (11)	0.0015 (12)
C7	0.0535 (14)	0.0578 (16)	0.087 (2)	0.0039 (12)	0.0200 (14)	−0.0032 (16)
C8	0.0566 (16)	0.074 (2)	0.076 (2)	−0.0108 (14)	0.0254 (14)	−0.0131 (17)
C9	0.0625 (16)	0.083 (2)	0.0586 (18)	−0.0192 (15)	0.0127 (13)	0.0060 (15)
C10	0.0517 (13)	0.0662 (16)	0.0492 (15)	−0.0084 (12)	−0.0017 (11)	0.0072 (13)
C11	0.0392 (11)	0.0382 (12)	0.0496 (14)	−0.0004 (9)	−0.0137 (9)	0.0017 (11)
C12	0.0359 (10)	0.0436 (13)	0.0570 (15)	0.0039 (9)	−0.0077 (10)	−0.0002 (12)
C13	0.0522 (14)	0.0578 (15)	0.0650 (17)	0.0032 (12)	−0.0134 (12)	0.0171 (13)
C14	0.0387 (12)	0.0475 (13)	0.0618 (16)	0.0016 (10)	0.0021 (10)	−0.0024 (12)
C15	0.0669 (17)	0.101 (2)	0.068 (2)	−0.0081 (17)	0.0267 (15)	0.0040 (18)
C16	0.124 (3)	0.146 (4)	0.073 (3)	0.013 (3)	0.020 (2)	0.028 (3)
N1	0.0415 (9)	0.0463 (11)	0.0428 (11)	−0.0036 (8)	−0.0023 (8)	0.0023 (9)
N2	0.0384 (9)	0.0375 (10)	0.0425 (11)	−0.0020 (7)	−0.0056 (8)	0.0024 (8)
N3	0.0388 (9)	0.0402 (10)	0.0482 (11)	0.0021 (8)	0.0031 (8)	0.0030 (9)
O1	0.0407 (10)	0.1158 (18)	0.1039 (17)	0.0204 (10)	0.0123 (10)	0.0295 (14)
O2	0.0442 (9)	0.0723 (12)	0.0561 (11)	0.0020 (8)	0.0098 (8)	0.0099 (10)

Geometric parameters (Å, º)

C1—N3	1.318 (3)	C9—H9	0.9300
C1—C12	1.407 (3)	C10—H10	0.9300
C1—C14	1.503 (3)	C11—C12	1.361 (3)
C2—N3	1.342 (3)	C11—N2	1.366 (3)

C2—C3	1.383 (3)	C11—C13	1.490 (3)
C2—N2	1.399 (3)	C12—H12	0.9300
C3—C4	1.393 (3)	C13—H13A	0.9600
C3—H3	0.9300	C13—H13B	0.9600
C4—N1	1.353 (3)	C13—H13C	0.9600
C4—C5	1.476 (3)	C14—O1	1.192 (3)
C5—C10	1.388 (3)	C14—O2	1.318 (3)
C5—C6	1.389 (3)	C15—O2	1.448 (3)
C6—C7	1.390 (3)	C15—C16	1.470 (5)
C6—H6	0.9300	C15—H15A	0.9700
C7—C8	1.380 (4)	C15—H15B	0.9700
C7—H7	0.9300	C16—H16A	0.9600
C8—C9	1.382 (4)	C16—H16B	0.9600
C8—H8	0.9300	C16—H16C	0.9600
C9—C10	1.376 (4)	N1—N2	1.354 (2)

N3—C1—C12	124.1 (2)	N2—C11—C13	118.0 (2)
N3—C1—C14	116.8 (2)	C11—C12—C1	120.0 (2)
C12—C1—C14	119.09 (19)	C11—C12—H12	120.0
N3—C2—C3	132.5 (2)	C1—C12—H12	120.0
N3—C2—N2	121.83 (18)	C11—C13—H13A	109.5
C3—C2—N2	105.69 (18)	C11—C13—H13B	109.5
C2—C3—C4	105.43 (19)	H13A—C13—H13B	109.5
C2—C3—H3	127.3	C11—C13—H13C	109.5
C4—C3—H3	127.3	H13A—C13—H13C	109.5
N1—C4—C3	112.77 (19)	H13B—C13—H13C	109.5
N1—C4—C5	119.9 (2)	O1—C14—O2	124.6 (2)
C3—C4—C5	127.3 (2)	O1—C14—C1	123.3 (2)
C10—C5—C6	118.7 (2)	O2—C14—C1	112.16 (18)
C10—C5—C4	121.3 (2)	O2—C15—C16	107.7 (3)
C6—C5—C4	119.9 (2)	O2—C15—H15A	110.2
C5—C6—C7	120.3 (2)	C16—C15—H15A	110.2
C5—C6—H6	119.8	O2—C15—H15B	110.2
C7—C6—H6	119.8	C16—C15—H15B	110.2
C8—C7—C6	120.3 (3)	H15A—C15—H15B	108.5
C8—C7—H7	119.8	C15—C16—H16A	109.5
C6—C7—H7	119.8	C15—C16—H16B	109.5
C7—C8—C9	119.4 (2)	H16A—C16—H16B	109.5
C7—C8—H8	120.3	C15—C16—H16C	109.5
C9—C8—H8	120.3	H16A—C16—H16C	109.5
C10—C9—C8	120.5 (3)	H16B—C16—H16C	109.5
C10—C9—H9	119.7	C4—N1—N2	103.87 (17)
C8—C9—H9	119.7	N1—N2—C11	125.91 (18)
C9—C10—C5	120.7 (3)	N1—N2—C2	112.24 (16)
C9—C10—H10	119.6	C11—N2—C2	121.85 (18)
C5—C10—H10	119.6	C1—N3—C2	116.24 (19)
C12—C11—N2	115.98 (19)	C14—O2—C15	117.8 (2)
C12—C11—C13	126.0 (2)		

N3—C2—C3—C4	178.2 (2)	N3—C1—C14—O2	−22.0 (3)
N2—C2—C3—C4	0.3 (2)	C12—C1—C14—O2	157.4 (2)
C2—C3—C4—N1	−0.2 (3)	C3—C4—N1—N2	−0.1 (2)
C2—C3—C4—C5	179.4 (2)	C5—C4—N1—N2	−179.70 (18)
N1—C4—C5—C10	−1.1 (3)	C4—N1—N2—C11	−178.94 (19)
C3—C4—C5—C10	179.3 (2)	C4—N1—N2—C2	0.3 (2)
N1—C4—C5—C6	177.8 (2)	C12—C11—N2—N1	178.77 (19)
C3—C4—C5—C6	−1.8 (3)	C13—C11—N2—N1	0.0 (3)
C10—C5—C6—C7	−0.6 (4)	C12—C11—N2—C2	−0.4 (3)
C4—C5—C6—C7	−179.4 (2)	C13—C11—N2—C2	−179.1 (2)
C5—C6—C7—C8	0.6 (4)	N3—C2—N2—N1	−178.54 (18)
C6—C7—C8—C9	0.3 (4)	C3—C2—N2—N1	−0.4 (2)
C7—C8—C9—C10	−1.2 (4)	N3—C2—N2—C11	0.7 (3)
C8—C9—C10—C5	1.3 (4)	C3—C2—N2—C11	178.88 (19)
C6—C5—C10—C9	−0.4 (4)	C12—C1—N3—C2	−0.4 (3)
C4—C5—C10—C9	178.5 (2)	C14—C1—N3—C2	179.02 (19)
N2—C11—C12—C1	−0.3 (3)	C3—C2—N3—C1	−177.9 (2)
C13—C11—C12—C1	178.3 (2)	N2—C2—N3—C1	−0.3 (3)
N3—C1—C12—C11	0.7 (3)	O1—C14—O2—C15	1.4 (4)
C14—C1—C12—C11	−178.7 (2)	C1—C14—O2—C15	−178.5 (2)
N3—C1—C14—O1	158.1 (3)	C16—C15—O2—C14	147.1 (3)
C12—C1—C14—O1	−22.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{i}	0.93	2.36	3.258 (3)	161
C6—H6···N3^{ii}	0.93	2.62	3.507 (3)	161

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) *x*−1/2, −*y*+3/2, −*z*.