

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

4-[(5*R**,10*bR**)-2-Methyl-1,10*b*-dihydro-pyrazolo[1,5-*c*][1,3]benzoxazin-5-yl]-benzoic acid

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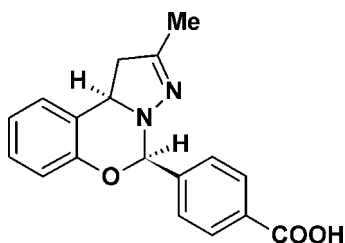
Received 25 January 2008; accepted 1 February 2008

 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.051; wR factor = 0.152; data-to-parameter ratio = 20.5.

In the title compound, $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_3$, a potential inhibitor of the cyclooxygenase-2 isoenzyme, the pyrazoline ring exists in a flattened envelope conformation with one C atom deviating by 0.463 Å from the mean plane of the remaining four atoms. The puckering of the central oxazine ring is more severe, with one N atom and one C atom displaced by 0.235 (6) and 0.370 (2) Å, respectively, on opposite sides of the mean plane defined by the other four atoms; the conformation is that of a half-chair. As a result, the molecule as a whole is not planar. The carboxyl group is involved in an intermolecular O—H···N hydrogen bond, which links the molecules into centrosymmetric dimers.

Related literature

For related literature, see: Palomer *et al.* (2002); Subbaramaiah *et al.* (2002); Světlík *et al.* (2005).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_3$	$\gamma = 79.15$ (2)°
$M_r = 308.33$	$V = 750.1$ (4) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 6.638$ (2) Å	Mo $K\alpha$ radiation
$b = 10.997$ (3) Å	$\mu = 0.09$ mm ⁻¹
$c = 11.141$ (3) Å	$T = 296$ (2) K
$\alpha = 70.78$ (2)°	$0.30 \times 0.20 \times 0.15$ mm
$\beta = 80.85$ (3)°	

Data collection

Siemens P4 diffractometer	$R_{\text{int}} = 0.019$
Absorption correction: none	3 standard reflections
5341 measured reflections	every 97 reflections
4312 independent reflections	intensity decay: none
3216 reflections with $I > 2\sigma(I)$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$	210 parameters
$wR(F^2) = 0.152$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.29$ e Å ⁻³
4312 reflections	$\Delta\rho_{\text{min}} = -0.22$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O8—H8A···N3 ⁱ	0.82	1.93	2.7356 (17)	168

 Symmetry code: (i) $-x - 1, -y + 1, -z + 1$.

Data collection: XSCANS (Siemens, 1991); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

This work was supported by the Grant Agency of the Slovak Republic, project Nos. 1/4298/07 and 1/4299/07.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: B12280).

References

- Palomer, A., Cabré, F., Pascual, J., Campos, J., Trujillo, M. A., Entrena, A., Gallo, M. A., Garcia, L., Mauleón, D. & Espinosa, A. (2002). *J. Med. Chem.* **45**, 1402–1411.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Siemens (1991). XSCANS. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Subbaramaiah, K., Norton, L., Gerald, W. & Dannenberg, A. J. (2002). *J. Biol. Chem.* **277**, 18649–18659.
- Světlík, J., Pronayova, N. & Kubista, J. (2005). *J. Heterocycl. Chem.* **42**, 1143–1147.

supporting information

Acta Cryst. (2008). E64, o563 [doi:10.1107/S1600536808003607]

4-[(5*R**,10*bR**)-2-Methyl-1,10*b*-dihydropyrazolo[1,5-*c*][1,3]benzoxazin-5-yl]benzoic acid

Viktor Kettmann and Jan Světlík

S1. Comment

Recently, based on a pharmacophoric model of the cyclooxygenase-2 (COX-2) inhibitors (Palomer *et al.*, 2002) as novel anticancer drugs (Subbaramaiah *et al.*, 2002), we designed and prepared a series of 2- and 5-substituted derivatives containing the tricyclic system shown in Fig. 1. In order to recognize enzyme binding requirements for this fused heterocycle, we selected the 2-methyl-5-carboxyphenyl derivative, for single-crystal X-ray analysis. The compound was obtained as a 1:1 mixture of the *cis* (1a) and *trans* (1b) diastereomers and we report here the structure of the *cis* isomer.

The molecular structure and atom-numbering scheme is shown in Fig. 2. Bond distances and angles are close to those generally expected. The atom O6 is essentially *sp*²-hybridized and involved in conjugation with the benzo ring as indicated by the valence angle at this atom and a non-equivalency of the O6—C5 and O6—C7 bonds.

The most interesting feature of the structure—the spatial relationship between the pharmacophoric elements (hydrophobic groups and H-bond donors/acceptors)—is given by conformation of the (partially) saturated rings. Thus, the pyrazoline ring adopts a flat-envelope conformation with atom C13 (at the flap) deviating by 0.463 Å from the mean plane of the remaining atoms. The central oxazine ring is also non-planar and is puckered in such a manner that the four atoms O6, C7, C12 and C13 are planar to within 0.006 (2) Å, while atoms N4 and C5 are displaced by 0.235 (6) and 0.370 (2) Å, respectively, on opposite sides of the plane. As a result of the relatively severe puckering of the central ring, the molecule as a whole is non-planar but consists of two approximately planar segments, C5/O6/C7—C13 and C13/C1/C2/N3/N4/C5, folded about the C5...C13 line [dihedral angle 71.7 (1)°]. The carboxyphenyl substituent is rotated by 39.8 (1)° from the mean plane of the oxazine ring.

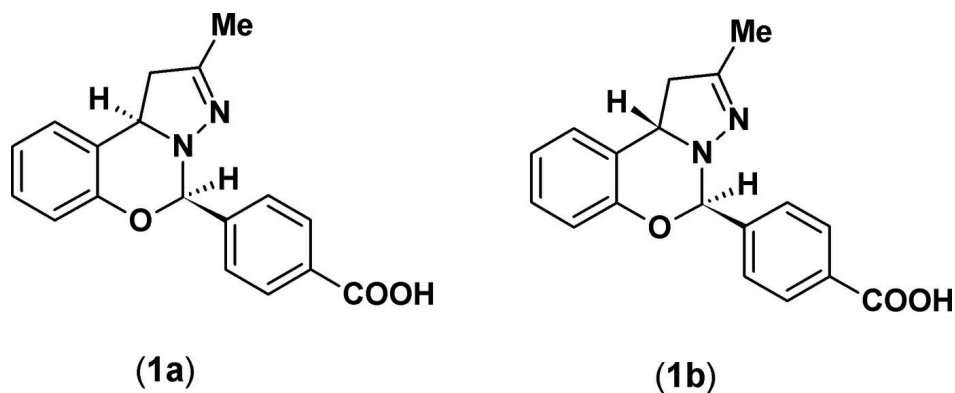
The crystal packing is dominated by a hydrogen bond between centrosymmetrically related molecules (Table 1) which result in formation of hydrogen-bonded dimers.

S2. Experimental

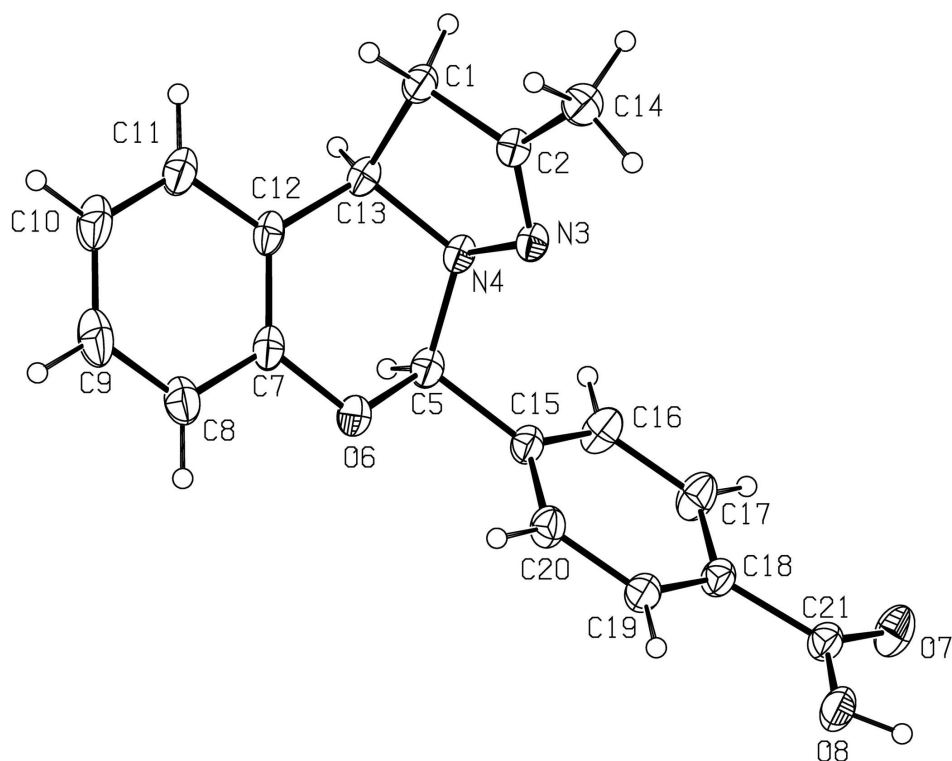
Synthesis of the title compound has been described previously (Světlík *et al.*, 2005). In short, a solution of 4-carboxybenzaldehyde (0.30 g, 2 mmol) and pyrazoline (0.35 g, 2 mmol) in ethyl acetate (14 ml) and methanol (1 ml) was left to react at room temperature for 1 h. The resulting precipitate was filtered off and crystallized from ethanol to obtain (1a) (70% yield; m.p. 474–480 K) as colourless crystals. Crystals suitable for the X-ray analysis were obtained by slow crystallization from acetone.

S3. Refinement

H atoms were visible in difference maps, but were placed geometrically and subsequently treated as riding atoms with distances C—H = 0.93 Å (CH_{arom}), 0.97 Å (CH₂) or 0.98 Å (CH) and 0.96 Å (CH₃) and O—H = 0.82 Å (COOH); *U*_{iso} of the H atoms were set to 1.2 (1.5 for the methyl and carboxy H atoms) times *U*_{eq} of the parent atom.

**Figure 1**

The *cis* title compound (1a) and its *trans* isomer (1 b).

**Figure 2**

Molecular structure with displacement ellipsoids drawn at 35% probability for non-H atoms.

4-[(5*R**,10*bR**)-2-Methyl-1,10*b*-dihydropyrazolo[1,5-*c*][1,3]benzoxazin-5-yl]benzoic acid

Crystal data

$C_{18}H_{16}N_2O_3$

$M_r = 308.33$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 6.638\ (2)\ \text{\AA}$

$b = 10.997\ (3)\ \text{\AA}$

$c = 11.141\ (3)\ \text{\AA}$

$\alpha = 70.78\ (2)^\circ$

$\beta = 80.85\ (3)^\circ$

$\gamma = 79.15\ (2)^\circ$

$V = 750.1\ (4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 324$

$D_x = 1.365\ \text{Mg m}^{-3}$

Melting point: 477 K

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 20 reflections
 $\theta = 7\text{--}18^\circ$
 $\mu = 0.09 \text{ mm}^{-1}$

$T = 296 \text{ K}$
 Prism, colourless
 $0.30 \times 0.20 \times 0.15 \text{ mm}$

Data collection

Siemens P4
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 $\omega/2\theta$ scans
 5341 measured reflections
 4312 independent reflections
 3216 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$
 $\theta_{\text{max}} = 30.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -1 \rightarrow 9$
 $k = -14 \rightarrow 14$
 $l = -15 \rightarrow 15$
 3 standard reflections every 97 reflections
 intensity decay: none

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.152$
 $S = 1.01$
 4312 reflections
 210 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
 $w = 1/[\sigma^2(F_o^2) + (0.0853P)^2 + 0.0987P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{Å}^{-3}$

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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3065 (2)	0.63515 (13)	0.03856 (13)	0.0364 (3)
H1A	0.3369	0.6320	-0.0485	0.044*
H1B	0.4338	0.6149	0.0780	0.044*
C2	0.1553 (2)	0.54630 (12)	0.11427 (12)	0.0324 (3)
N3	0.01255 (17)	0.59887 (10)	0.18002 (10)	0.0314 (2)
N4	0.05040 (17)	0.72620 (10)	0.16410 (10)	0.0304 (2)
C5	-0.1328 (2)	0.81721 (13)	0.17228 (12)	0.0342 (3)
H5	-0.0911	0.8976	0.1736	0.041*
O6	-0.25382 (16)	0.84950 (11)	0.06661 (9)	0.0440 (3)
C7	-0.1451 (2)	0.87381 (13)	-0.05137 (12)	0.0371 (3)
C8	-0.2589 (3)	0.93655 (15)	-0.15442 (14)	0.0479 (4)
H8	-0.3999	0.9630	-0.1409	0.057*
C9	-0.1623 (3)	0.95933 (18)	-0.27641 (16)	0.0586 (5)

H9	-0.2381	1.0010	-0.3458	0.070*
C10	0.0466 (3)	0.92058 (17)	-0.29635 (15)	0.0560 (5)
H10	0.1116	0.9354	-0.3792	0.067*
C11	0.1589 (3)	0.86000 (14)	-0.19372 (13)	0.0449 (4)
H11	0.3003	0.8352	-0.2079	0.054*
C12	0.0646 (2)	0.83525 (12)	-0.06896 (12)	0.0347 (3)
C13	0.1871 (2)	0.76641 (13)	0.04385 (12)	0.0330 (3)
H13	0.2808	0.8222	0.0510	0.040*
C14	0.1724 (2)	0.40903 (14)	0.11858 (15)	0.0418 (3)
H14A	0.2925	0.3598	0.1589	0.063*
H14B	0.1840	0.4044	0.0332	0.063*
H14C	0.0517	0.3737	0.1665	0.063*
C15	-0.2727 (2)	0.76809 (12)	0.29245 (12)	0.0329 (3)
C16	-0.2086 (2)	0.75161 (17)	0.40981 (14)	0.0448 (4)
H16	-0.0830	0.7752	0.4137	0.054*
C17	-0.3307 (3)	0.70033 (17)	0.52093 (14)	0.0462 (4)
H17	-0.2865	0.6890	0.5995	0.055*
C18	-0.5184 (2)	0.66557 (13)	0.51636 (12)	0.0342 (3)
C19	-0.5837 (2)	0.68431 (14)	0.39930 (13)	0.0374 (3)
H19	-0.7103	0.6621	0.3952	0.045*
C20	-0.4614 (2)	0.73595 (14)	0.28820 (13)	0.0381 (3)
H20	-0.5070	0.7492	0.2096	0.046*
C21	-0.6403 (2)	0.60087 (13)	0.63696 (13)	0.0361 (3)
O7	-0.5895 (2)	0.58142 (13)	0.74163 (10)	0.0520 (3)
O8	-0.80628 (16)	0.56450 (11)	0.61698 (10)	0.0454 (3)
H8A	-0.8571	0.5179	0.6845	0.068*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (7)	0.0364 (7)	0.0318 (6)	-0.0088 (5)	0.0038 (5)	-0.0084 (5)
C2	0.0362 (6)	0.0317 (6)	0.0286 (6)	-0.0074 (5)	-0.0017 (5)	-0.0077 (5)
N3	0.0364 (6)	0.0285 (5)	0.0281 (5)	-0.0088 (4)	-0.0002 (4)	-0.0065 (4)
N4	0.0362 (5)	0.0290 (5)	0.0256 (5)	-0.0104 (4)	0.0017 (4)	-0.0072 (4)
C5	0.0423 (7)	0.0310 (6)	0.0282 (6)	-0.0086 (5)	0.0016 (5)	-0.0082 (5)
O6	0.0434 (5)	0.0498 (6)	0.0273 (5)	-0.0018 (5)	-0.0005 (4)	-0.0009 (4)
C7	0.0514 (8)	0.0290 (6)	0.0273 (6)	-0.0098 (6)	-0.0004 (5)	-0.0034 (5)
C8	0.0585 (9)	0.0417 (8)	0.0359 (7)	-0.0042 (7)	-0.0097 (7)	-0.0015 (6)
C9	0.0890 (14)	0.0478 (9)	0.0316 (7)	-0.0059 (9)	-0.0143 (8)	-0.0009 (6)
C10	0.0856 (13)	0.0474 (9)	0.0279 (7)	-0.0115 (9)	0.0037 (8)	-0.0058 (6)
C11	0.0624 (9)	0.0362 (7)	0.0313 (7)	-0.0126 (7)	0.0087 (6)	-0.0072 (5)
C12	0.0507 (8)	0.0253 (6)	0.0270 (6)	-0.0126 (5)	0.0018 (5)	-0.0055 (4)
C13	0.0368 (6)	0.0331 (6)	0.0288 (6)	-0.0134 (5)	0.0036 (5)	-0.0079 (5)
C14	0.0464 (8)	0.0351 (7)	0.0449 (8)	-0.0074 (6)	-0.0004 (6)	-0.0149 (6)
C15	0.0403 (7)	0.0287 (6)	0.0276 (6)	-0.0059 (5)	0.0024 (5)	-0.0081 (5)
C16	0.0447 (8)	0.0600 (9)	0.0340 (7)	-0.0227 (7)	0.0018 (6)	-0.0147 (6)
C17	0.0524 (9)	0.0628 (10)	0.0270 (6)	-0.0203 (7)	-0.0002 (6)	-0.0139 (6)
C18	0.0396 (7)	0.0322 (6)	0.0289 (6)	-0.0055 (5)	0.0031 (5)	-0.0098 (5)

C19	0.0359 (7)	0.0410 (7)	0.0329 (6)	-0.0087 (5)	-0.0014 (5)	-0.0076 (5)
C20	0.0426 (7)	0.0417 (7)	0.0277 (6)	-0.0085 (6)	-0.0042 (5)	-0.0063 (5)
C21	0.0405 (7)	0.0337 (6)	0.0311 (6)	-0.0055 (5)	0.0038 (5)	-0.0097 (5)
O7	0.0637 (7)	0.0646 (7)	0.0285 (5)	-0.0204 (6)	0.0024 (5)	-0.0126 (5)
O8	0.0457 (6)	0.0506 (6)	0.0336 (5)	-0.0165 (5)	0.0032 (4)	-0.0029 (4)

Geometric parameters (Å, °)

C1—C2	1.4934 (19)	C11—C12	1.3915 (19)
C1—C13	1.5249 (19)	C11—H11	0.930
C1—H1A	0.970	C12—C13	1.5101 (19)
C1—H1B	0.970	C13—H13	0.980
C2—N3	1.2730 (17)	C14—H14A	0.960
C2—C14	1.4776 (19)	C14—H14B	0.960
N3—N4	1.4178 (15)	C14—H14C	0.960
N4—C5	1.4335 (18)	C15—C20	1.376 (2)
N4—C13	1.4793 (17)	C15—C16	1.3839 (19)
C5—O6	1.4409 (17)	C16—C17	1.379 (2)
C5—C15	1.5047 (18)	C16—H16	0.930
C5—H5	0.980	C17—C18	1.384 (2)
O6—C7	1.3637 (17)	C17—H17	0.930
C7—C12	1.379 (2)	C18—C19	1.3783 (19)
C7—C8	1.387 (2)	C18—C21	1.4856 (19)
C8—C9	1.371 (2)	C19—C20	1.380 (2)
C8—H8	0.930	C19—H19	0.930
C9—C10	1.377 (3)	C20—H20	0.930
C9—H9	0.930	C21—O7	1.2053 (17)
C10—C11	1.375 (2)	C21—O8	1.3140 (18)
C10—H10	0.930	O8—H8A	0.820
C2—C1—C13	100.79 (11)	C7—C12—C13	120.90 (12)
C2—C1—H1A	111.6	C11—C12—C13	121.16 (14)
C13—C1—H1A	111.6	N4—C13—C12	111.46 (11)
C2—C1—H1B	111.6	N4—C13—C1	100.98 (10)
C13—C1—H1B	111.6	C12—C13—C1	112.93 (11)
H1A—C1—H1B	109.4	N4—C13—H13	110.4
N3—C2—C14	122.55 (13)	C12—C13—H13	110.4
N3—C2—C1	113.23 (12)	C1—C13—H13	110.4
C14—C2—C1	124.16 (12)	C2—C14—H14A	109.5
C2—N3—N4	108.71 (11)	C2—C14—H14B	109.5
N3—N4—C5	114.05 (10)	H14A—C14—H14B	109.5
N3—N4—C13	107.26 (9)	C2—C14—H14C	109.5
C5—N4—C13	114.20 (10)	H14A—C14—H14C	109.5
N4—C5—O6	113.73 (11)	H14B—C14—H14C	109.5
N4—C5—C15	112.11 (11)	C20—C15—C16	119.21 (13)
O6—C5—C15	106.99 (11)	C20—C15—C5	121.22 (12)
N4—C5—H5	107.9	C16—C15—C5	119.55 (13)
O6—C5—H5	107.9	C17—C16—C15	120.12 (14)

C15—C5—H5	107.9	C17—C16—H16	119.9
C7—O6—C5	115.49 (11)	C15—C16—H16	119.9
O6—C7—C12	122.64 (12)	C16—C17—C18	120.50 (13)
O6—C7—C8	116.04 (14)	C16—C17—H17	119.8
C12—C7—C8	121.29 (14)	C18—C17—H17	119.8
C9—C8—C7	119.60 (17)	C19—C18—C17	119.28 (13)
C9—C8—H8	120.2	C19—C18—C21	120.86 (13)
C7—C8—H8	120.2	C17—C18—C21	119.74 (13)
C8—C9—C10	120.15 (16)	C18—C19—C20	120.10 (13)
C8—C9—H9	119.9	C18—C19—H19	119.9
C10—C9—H9	119.9	C20—C19—H19	119.9
C11—C10—C9	119.92 (15)	C15—C20—C19	120.77 (13)
C11—C10—H10	120.0	C15—C20—H20	119.6
C9—C10—H10	120.0	C19—C20—H20	119.6
C10—C11—C12	121.10 (16)	O7—C21—O8	123.78 (13)
C10—C11—H11	119.4	O7—C21—C18	123.50 (14)
C12—C11—H11	119.4	O8—C21—C18	112.71 (12)
C7—C12—C11	117.93 (14)	C21—O8—H8A	109.5
C13—C1—C2—N3	-15.79 (15)	N3—N4—C13—C1	-29.67 (12)
C13—C1—C2—C14	166.98 (12)	C5—N4—C13—C1	-157.08 (11)
C14—C2—N3—N4	174.46 (11)	C7—C12—C13—N4	11.07 (17)
C1—C2—N3—N4	-2.82 (15)	C11—C12—C13—N4	-167.94 (12)
C2—N3—N4—C5	148.89 (11)	C7—C12—C13—C1	123.94 (13)
C2—N3—N4—C13	21.40 (13)	C11—C12—C13—C1	-55.08 (17)
N3—N4—C5—O6	-68.94 (13)	C2—C1—C13—N4	26.12 (12)
C13—N4—C5—O6	54.89 (15)	C2—C1—C13—C12	-93.01 (13)
N3—N4—C5—C15	52.60 (14)	N4—C5—C15—C20	-112.18 (15)
C13—N4—C5—C15	176.43 (10)	O6—C5—C15—C20	13.15 (17)
N4—C5—O6—C7	-44.40 (16)	N4—C5—C15—C16	66.12 (17)
C15—C5—O6—C7	-168.75 (11)	O6—C5—C15—C16	-168.55 (12)
C5—O6—C7—C12	17.97 (19)	C20—C15—C16—C17	1.7 (2)
C5—O6—C7—C8	-164.03 (12)	C5—C15—C16—C17	-176.64 (14)
O6—C7—C8—C9	-177.12 (14)	C15—C16—C17—C18	-0.4 (3)
C12—C7—C8—C9	0.9 (2)	C16—C17—C18—C19	-0.8 (2)
C7—C8—C9—C10	-0.3 (3)	C16—C17—C18—C21	175.18 (15)
C8—C9—C10—C11	-0.6 (3)	C17—C18—C19—C20	0.7 (2)
C9—C10—C11—C12	0.9 (3)	C21—C18—C19—C20	-175.28 (13)
O6—C7—C12—C11	177.24 (13)	C16—C15—C20—C19	-1.9 (2)
C8—C7—C12—C11	-0.7 (2)	C5—C15—C20—C19	176.45 (13)
O6—C7—C12—C13	-1.8 (2)	C18—C19—C20—C15	0.7 (2)
C8—C7—C12—C13	-179.70 (13)	C19—C18—C21—O7	179.54 (14)
C10—C11—C12—C7	-0.2 (2)	C17—C18—C21—O7	3.6 (2)
C10—C11—C12—C13	178.82 (14)	C19—C18—C21—O8	1.05 (19)
N3—N4—C13—C12	90.51 (12)	C17—C18—C21—O8	-174.89 (13)
C5—N4—C13—C12	-36.89 (15)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O8—H8A \cdots N3 ⁱ	0.82	1.93	2.7356 (17)	168

Symmetry code: (i) $-x-1, -y+1, -z+1$.