Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

Crystal structure of 5-(1-benzofuran-2-yl)-3-(4-methylphenyl)-4,5-dihydro-1,2-oxazol-5-ol

A. J. Ravi,[a] A. C. Vinayaka,[b] S. Jeyaseelan,[c] M. P. Sadashiva[b] and H. C. Devarajegowda[a]*

[a]Department of Physics, Yuvaraja's College (Constituent College), University of Mysore, Mysore 570 005, Karnataka, India, [b]Department of Studies in Chemistry, Manasagangotri, University of Mysore, Mysore 570 006, India, and [c]Department of Physics, St. Philomena's College, Mysore, India. *Correspondence e-mail: hcdevarajegowda@ycm.uni-mysore.ac.in

Received 2 June 2015; accepted 9 June 2015

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

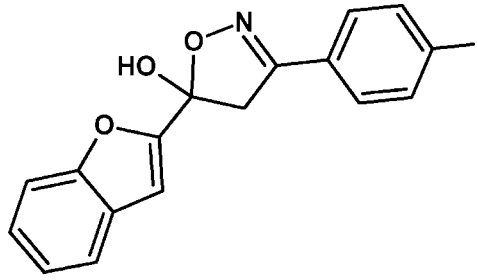
In the title compound, $C_{18}H_{15}NO_3$, the isoxazole moiety adopts a shallow envelope conformation, with the C atom bearing the OH group displaced by 0.148 (1) Å from the mean plane through the other four atoms. The mean plane of this ring (all atoms) subtends dihedral angles of 87.19 (6) and 15.51 (7)° with the benzofuran ring system (r.m.s. deviation = 0.007 Å) and the 4-methylphenyl ring, respectively. In the crystal, molecules are linked by O—H···N hydrogen bonds, generating [001] $C(5)$ chains, with adjacent molecules in the chain related by c-glide symmetry. Weak C—H···O interactions link the chains into a three-dimensional network.

Keywords: crystal structure; benzofuran; 1,2-oxazole; alcohol; biological properties; pharmaceutical properties.

CCDC reference: 1405867

1. Related literature

For the biological and pharmaceutical properties of isoxazoles, see: Eddington *et al.* (2002); Lee *et al.* (2009); Rozman *et al.* (2002); Shin *et al.* (2005).



2. Experimental

2.1. Crystal data

$C_{18}H_{15}NO_3$
M_r = 293.31
Monoclinic, $P2_1/c$
a = 10.2200 (15) Å
b = 14.2289 (19) Å
c = 10.2474 (15) Å
β = 93.058 (7)°
V = 1488.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.20 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
23993 measured reflections
3452 independent reflections
2829 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.123
S = 1.03
3452 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O13—H13···N9^{i}	0.82	2.17	2.9352 (15)	156
C2—H2···O10^{ii}	0.93	2.46	3.2328 (17)	141
C7—H7C···O15^{iii}	0.96	2.58	3.175 (2)	121
C18—H18···O10^{i}	0.93	2.54	3.4183 (17)	158

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{5}{2}$; (iii) $-x, -y, -z+3$.

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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7438).

References

Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Eddington, N. D., Cox, D. S., Roberts, R. R., Butcher, R. J., Edafiogho, I. O., Stables, J. P., Cooke, N., Goodwin, A. M., Smith, C. A. & Scott, K. R. (2002). *Eur. J. Med. Chem.* **37**, 635–648.

Lee, Y., Park, S. M. & Kim, B. H. (2009). *Bioorg. Med. Chem. Lett.* **19**, 1126–1128.

Rozman, B., Praprotnik, S., Logar, D., Tomsic, M., Hojnik, M., Kos-Golja, M., Accetto, R. & Dolenc, P. (2002). *Ann. Rheum. Dis.* **61**, 567–569.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Shin, K. D., Lee, M. Y., Shin, D. S., Lee, S., Son, K. H., Koh, S., Paik, Y. K., Kwon, B. M. & Han, D. C. (2005). *J. Biol. Chem.* **280**, 41439–41448.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2015). E**71**, o492–o493 [doi:10.1107/S2056989015011263]

Crystal structure of 5-(1-benzofuran-2-yl)-3-(4-methylphenyl)-4,5-dihydro-1,2-oxazol-5-ol

A. J. Ravi, A. C. Vinayaka, S. Jeyaseelan, M. P. Sadashiva and H. C. Devarajegowda

S1. Comment

Isoxazole derivatives bearing various substituents are known to have diverse biological and pharmaceutical activities; such as antiviral (Lee *et al.*, 2009), anti-HIV activities (Shin *et al.*, 2005) and anticonvulsant activity (Eddington *et al.*, 2002). In addition, isoxazole derivative is used for the treatment of rheumatoid arthritis (Rozman *et al.*, 2002). As part of our interest in these compounds, the title compound was chosen for the X-ray structure analysis.

In the molecular structure of the title compound (Fig. 1), the isoxazole moiety makes dihedral angles of 87.19 (6)° and 15.51 (7)° with benzofuran and phenyl ring, respectively. The dihedral angle between the benzofuran and phenyl ring is 81.67 (6)° The central isoxazole moiety adopts a slightly flattened envelope conformation with puckering parameter Q = 0.2406 (12) Å and φ = 183.41 (17)° , and the maximum deviation found on the puckered atom at C11 is -0.148 (1) Å. The crystal structure features C—H···O and O—H···N hydrogen bonds. The packing diagram of the molecule when viewed down the *a* axis as shown in Fig. 2.

S2. Experimental

A solution of 2 Eq. of K_2CO_3 in water (1 ml) was added to the stirred solution of 4 Eq. of *N*-hydroxyl-4-toluene-sulfonamide in MeOH/H_2O (5/1 ml). Then 1 Eq. of 1-Benzofuran-2-yl-3-*p*-tolyl-propenone was added and reaction mixture was allowed to stir at room temperature for overnight. After completion of reaction, the reaction mixture was diluted with EtOAc, washed with water and brine. The organic extract was dried and concentrated under reduced pressure to give crude product, which was further purified using column chromatography (60–120 silica gel) to afford pure product.

S3. Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atom, with O–H distance is equal to 0.82 Å and C–H distance in the range of 0.93 to 0.97 Å; U_{iso}(H) = 1.2–1.5U_{eq} (carrier atom) for all H atoms.

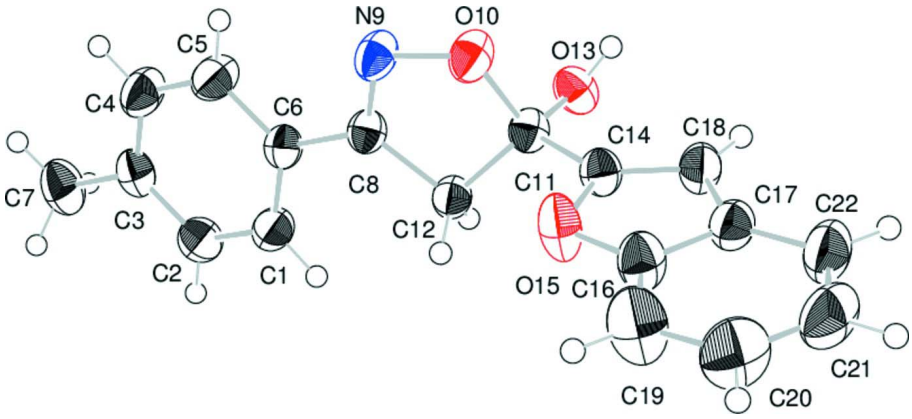


Figure 1

Perspective diagram of the molecule with 50% probability displacement ellipsoids.

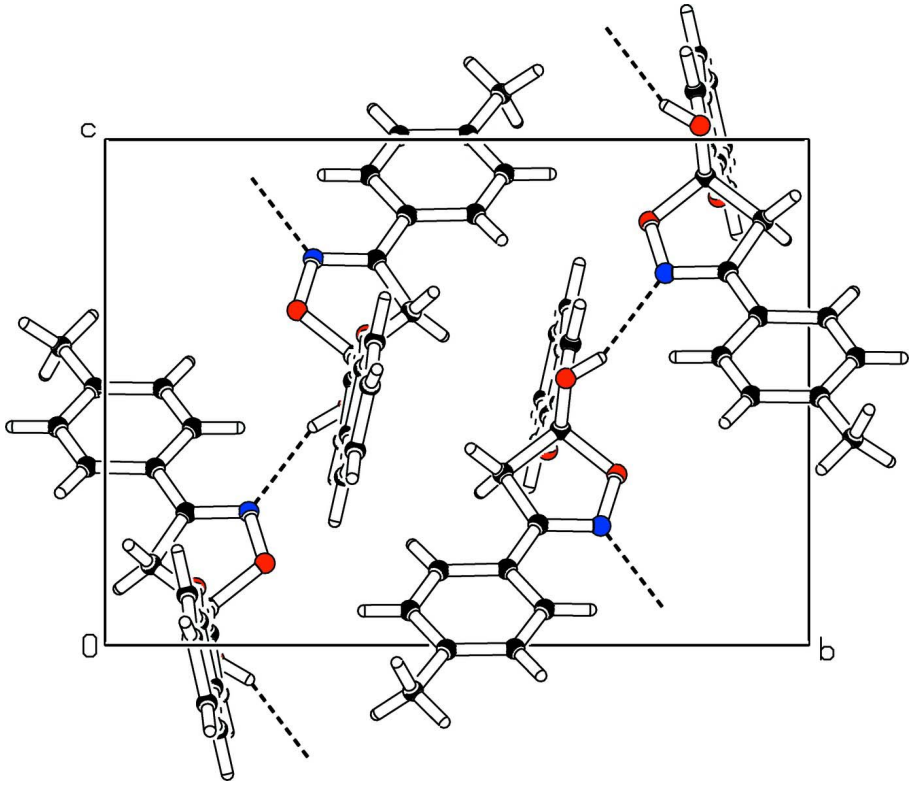


Figure 2

Packing diagram of the molecule viewed down the *a* axis.

5-(1-Benzofuran-2-yl)-3-(4-methylphenyl)-4,5-dihydro-1,2-oxazol-5-ol

Crystal data

$C_{18}H_{15}NO_3$
M_r = 293.31
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.2200 (15) Å
b = 14.2289 (19) Å
c = 10.2474 (15) Å
β = 93.058 (7)°
V = 1488.1 (4) Å^3
Z = 4
$F(000)$ = 616
D_x = 1.309 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3452 reflections
θ = 2.0–27.6°
μ = 0.09 mm^{-1}
T = 293 K
Block, light yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
ω and φ scans
23993 measured reflections
3452 independent reflections
2829 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.6°, θ_{min} = 2.0°
h = −13→13
k = −18→18
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.123
S = 1.03
3452 reflections
200 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
$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.3174P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O10	0.10420 (9)	0.22693 (6)	1.16214 (9)	0.0469 (3)
O13	0.01366 (9)	0.15474 (6)	0.97218 (9)	0.0424 (3)
O15	0.34411 (9)	0.12845 (9)	1.11345 (9)	0.0560 (4)
N9	0.02005 (11)	0.20392 (8)	1.26398 (11)	0.0442 (3)
C1	−0.10566 (14)	−0.02593 (9)	1.35272 (13)	0.0444 (4)
C2	−0.19545 (15)	−0.06737 (10)	1.43143 (14)	0.0490 (5)
C3	−0.27405 (13)	−0.01485 (10)	1.50880 (12)	0.0425 (4)
C4	−0.25865 (15)	0.08194 (11)	1.50733 (15)	0.0514 (5)
C5	−0.16973 (14)	0.12463 (10)	1.42932 (15)	0.0486 (4)
C6	−0.09233 (11)	0.07103 (8)	1.34970 (11)	0.0351 (3)
C7	−0.37282 (16)	−0.06253 (12)	1.59045 (16)	0.0589 (5)
C8	−0.00193 (12)	0.11530 (8)	1.26170 (11)	0.0346 (3)
C11	0.10936 (12)	0.14692 (8)	1.07341 (12)	0.0352 (3)
C12	0.07217 (12)	0.06513 (8)	1.15977 (11)	0.0358 (3)

C14	0.24379 (12)	0.14657 (9)	1.02232 (12)	0.0374 (3)
C16	0.45719 (14)	0.13194 (11)	1.04688 (14)	0.0498 (5)
C17	0.42854 (13)	0.15256 (9)	0.91647 (13)	0.0434 (4)
C18	0.28814 (13)	0.16133 (10)	0.90353 (13)	0.0431 (4)
C19	0.58217 (16)	0.11677 (16)	1.09931 (19)	0.0757 (7)
C20	0.68147 (16)	0.12359 (15)	1.0141 (2)	0.0747 (7)
C21	0.65735 (16)	0.14460 (13)	0.8845 (2)	0.0670 (6)
C22	0.53186 (17)	0.15950 (12)	0.83303 (17)	0.0608 (6)
H1	−0.05400	−0.06330	1.30160	0.0530*
H2	−0.20290	−0.13250	1.43210	0.0590*
H4	−0.30920	0.11890	1.56000	0.0620*
H5	−0.16150	0.18970	1.43000	0.0580*
H7A	−0.44440	−0.08530	1.53470	0.0880*
H7B	−0.40510	−0.01840	1.65190	0.0880*
H7C	−0.33190	−0.11430	1.63680	0.0880*
H12A	0.01720	0.02000	1.11180	0.0430*
H12B	0.14910	0.03350	1.19800	0.0430*
H13	0.02420	0.20390	0.93240	0.0640*
H18	0.23800	0.17470	0.82740	0.0520*
H19	0.59860	0.10270	1.18730	0.0910*
H20	0.76740	0.11370	1.04540	0.0900*
H21	0.72720	0.14890	0.83020	0.0800*
H22	0.51630	0.17380	0.74500	0.0730*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O10	0.0539 (6)	0.0394 (5)	0.0492 (5)	−0.0152 (4)	0.0203 (4)	−0.0082 (4)
O13	0.0359 (5)	0.0471 (5)	0.0441 (5)	−0.0045 (4)	0.0002 (4)	0.0092 (4)
O15	0.0352 (5)	0.0961 (8)	0.0367 (5)	−0.0054 (5)	0.0013 (4)	0.0150 (5)
N9	0.0475 (6)	0.0416 (6)	0.0451 (6)	−0.0103 (5)	0.0175 (5)	−0.0081 (4)
C1	0.0504 (8)	0.0395 (7)	0.0445 (7)	0.0007 (5)	0.0132 (6)	−0.0021 (5)
C2	0.0581 (9)	0.0389 (7)	0.0508 (8)	−0.0041 (6)	0.0115 (7)	0.0050 (6)
C3	0.0395 (7)	0.0531 (8)	0.0351 (6)	−0.0041 (5)	0.0029 (5)	0.0083 (5)
C4	0.0497 (8)	0.0542 (8)	0.0522 (8)	−0.0015 (6)	0.0213 (7)	−0.0052 (6)
C5	0.0519 (8)	0.0382 (6)	0.0576 (8)	−0.0040 (6)	0.0204 (7)	−0.0060 (6)
C6	0.0332 (6)	0.0400 (6)	0.0322 (6)	−0.0031 (5)	0.0033 (5)	−0.0007 (5)
C7	0.0548 (9)	0.0719 (10)	0.0509 (8)	−0.0084 (7)	0.0120 (7)	0.0170 (7)
C8	0.0340 (6)	0.0375 (6)	0.0323 (6)	−0.0035 (5)	0.0029 (5)	−0.0026 (4)
C11	0.0346 (6)	0.0371 (6)	0.0340 (6)	−0.0041 (5)	0.0035 (5)	−0.0021 (4)
C12	0.0385 (6)	0.0357 (6)	0.0337 (6)	−0.0023 (5)	0.0064 (5)	−0.0014 (5)
C14	0.0348 (6)	0.0435 (6)	0.0338 (6)	−0.0034 (5)	0.0012 (5)	0.0015 (5)
C16	0.0354 (7)	0.0679 (9)	0.0464 (8)	−0.0041 (6)	0.0055 (6)	0.0068 (6)
C17	0.0405 (7)	0.0481 (7)	0.0422 (7)	0.0003 (5)	0.0085 (6)	−0.0001 (5)
C18	0.0394 (7)	0.0565 (8)	0.0337 (6)	0.0036 (6)	0.0040 (5)	0.0018 (5)
C19	0.0392 (9)	0.1234 (17)	0.0637 (11)	−0.0029 (9)	−0.0044 (8)	0.0191 (11)
C20	0.0354 (8)	0.0994 (14)	0.0893 (14)	−0.0008 (8)	0.0036 (8)	0.0033 (11)
C21	0.0447 (9)	0.0773 (12)	0.0813 (12)	−0.0022 (7)	0.0260 (8)	−0.0039 (9)

C22	0.0543 (9)	0.0773 (11)	0.0528 (9)	0.0024 (8)	0.0203 (7)	0.0011 (8)

Geometric parameters (Å, º)

O10—N9	1.4254 (15)	C16—C17	1.384 (2)
O10—C11	1.4597 (15)	C17—C18	1.4394 (19)
O13—C11	1.3917 (15)	C17—C22	1.397 (2)
O15—C14	1.3739 (16)	C19—C20	1.377 (3)
O15—C16	1.3739 (17)	C20—C21	1.371 (3)
O13—H13	0.8200	C21—C22	1.377 (2)
N9—C8	1.2808 (16)	C1—H1	0.9300
C1—C2	1.385 (2)	C2—H2	0.9300
C1—C6	1.3869 (17)	C4—H4	0.9300
C2—C3	1.379 (2)	C5—H5	0.9300
C3—C4	1.386 (2)	C7—H7A	0.9600
C3—C7	1.507 (2)	C7—H7B	0.9600
C4—C5	1.383 (2)	C7—H7C	0.9600
C5—C6	1.3935 (19)	C12—H12A	0.9700
C6—C8	1.4671 (16)	C12—H12B	0.9700
C8—C12	1.5028 (17)	C18—H18	0.9300
C11—C14	1.4961 (18)	C19—H19	0.9300
C11—C12	1.5225 (17)	C20—H20	0.9300
C14—C18	1.3380 (18)	C21—H21	0.9300
C16—C19	1.376 (2)	C22—H22	0.9300
N9—O10—C11	108.67 (9)	C16—C19—C20	116.20 (17)
C14—O15—C16	105.83 (10)	C19—C20—C21	121.95 (16)
C11—O13—H13	109.00	C20—C21—C22	121.36 (16)
O10—N9—C8	108.96 (10)	C17—C22—C21	118.27 (16)
C2—C1—C6	120.35 (12)	C2—C1—H1	120.00
C1—C2—C3	121.91 (13)	C6—C1—H1	120.00
C2—C3—C4	117.54 (13)	C1—C2—H2	119.00
C4—C3—C7	122.23 (13)	C3—C2—H2	119.00
C2—C3—C7	120.24 (13)	C3—C4—H4	119.00
C3—C4—C5	121.42 (14)	C5—C4—H4	119.00
C4—C5—C6	120.61 (13)	C4—C5—H5	120.00
C1—C6—C5	118.16 (11)	C6—C5—H5	120.00
C1—C6—C8	120.44 (11)	C3—C7—H7A	109.00
C5—C6—C8	121.38 (11)	C3—C7—H7B	109.00
N9—C8—C6	121.81 (11)	C3—C7—H7C	109.00
N9—C8—C12	112.70 (11)	H7A—C7—H7B	109.00
C6—C8—C12	125.48 (10)	H7A—C7—H7C	109.00
O10—C11—C12	102.46 (9)	H7B—C7—H7C	109.00
O10—C11—C14	106.56 (10)	C8—C12—H12A	112.00
O10—C11—O13	110.77 (9)	C8—C12—H12B	112.00
O13—C11—C14	111.19 (10)	C11—C12—H12A	112.00
C12—C11—C14	117.60 (10)	C11—C12—H12B	112.00
O13—C11—C12	107.88 (10)	H12A—C12—H12B	109.00

C8—C12—C11	101.05 (9)	C14—C18—H18	127.00
O15—C14—C18	111.78 (11)	C17—C18—H18	127.00
C11—C14—C18	132.83 (12)	C16—C19—H19	122.00
O15—C14—C11	115.38 (10)	C20—C19—H19	122.00
O15—C16—C17	110.29 (12)	C19—C20—H20	119.00
C17—C16—C19	123.67 (14)	C21—C20—H20	119.00
O15—C16—C19	126.04 (14)	C20—C21—H21	119.00
C16—C17—C18	105.42 (12)	C22—C21—H21	119.00
C18—C17—C22	136.03 (13)	C17—C22—H22	121.00
C16—C17—C22	118.55 (13)	C21—C22—H22	121.00
C14—C18—C17	106.68 (12)		

C11—O10—N9—C8	13.54 (13)	C6—C8—C12—C11	161.79 (11)
N9—O10—C11—O13	91.49 (11)	O10—C11—C12—C8	23.18 (11)
N9—O10—C11—C12	−23.35 (12)	O13—C11—C12—C8	−93.75 (11)
N9—O10—C11—C14	−147.45 (9)	C14—C11—C12—C8	139.58 (11)
C16—O15—C14—C11	−179.68 (12)	O10—C11—C14—O15	66.25 (13)
C16—O15—C14—C18	−0.19 (16)	O10—C11—C14—C18	−113.10 (16)
C14—O15—C16—C17	0.43 (16)	O13—C11—C14—O15	−172.95 (11)
C14—O15—C16—C19	−179.12 (17)	O13—C11—C14—C18	7.7 (2)
O10—N9—C8—C6	−175.99 (10)	C12—C11—C14—O15	−47.91 (16)
O10—N9—C8—C12	3.06 (14)	C12—C11—C14—C18	132.74 (15)
C6—C1—C2—C3	0.0 (2)	O15—C14—C18—C17	−0.11 (16)
C2—C1—C6—C5	1.11 (19)	C11—C14—C18—C17	179.27 (13)
C2—C1—C6—C8	−177.02 (12)	O15—C16—C17—C18	−0.49 (16)
C1—C2—C3—C4	−1.2 (2)	O15—C16—C17—C22	179.71 (13)
C1—C2—C3—C7	178.48 (13)	C19—C16—C17—C18	179.07 (17)
C2—C3—C4—C5	1.3 (2)	C19—C16—C17—C22	−0.7 (2)
C7—C3—C4—C5	−178.39 (14)	O15—C16—C19—C20	179.82 (17)
C3—C4—C5—C6	−0.2 (2)	C17—C16—C19—C20	0.3 (3)
C4—C5—C6—C1	−1.0 (2)	C16—C17—C18—C14	0.36 (16)
C4—C5—C6—C8	177.08 (13)	C22—C17—C18—C14	−179.89 (16)
C1—C6—C8—N9	−174.48 (12)	C16—C17—C22—C21	0.6 (2)
C1—C6—C8—C12	6.60 (18)	C18—C17—C22—C21	−179.14 (16)
C5—C6—C8—N9	7.46 (19)	C16—C19—C20—C21	0.2 (3)
C5—C6—C8—C12	−171.46 (12)	C19—C20—C21—C22	−0.3 (3)
N9—C8—C12—C11	−17.21 (13)	C20—C21—C22—C17	−0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13—H13···N9^{i}	0.82	2.17	2.9352 (15)	156
C2—H2···O10^{ii}	0.93	2.46	3.2328 (17)	141
C7—H7*C*···O15^{iii}	0.96	2.58	3.175 (2)	121
C18—H18···O10^{i}	0.93	2.54	3.4183 (17)	158

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, *y*−1/2, −*z*+5/2; (iii) −*x*, −*y*, −*z*+3.