IUCrData

ISSN 2414-3146

4-[(4-Hydroxymethyl-2*H*-1,2,3-triazol-2-yl)methyl]-6-isopropyl-2*H*-chromen-2-one

Nasseem El-Khatatneh,[a] Chandra,[a] D. Shamala,[b] K. Shivashankar[b] and M. Mahendra[a]*

[a]Department of Studies in Physics, Manasagangotri University of Mysore, Mysore 570 006, India, and [b]Department of Chemistry, Central College Campus, Bangalore University, Bangalore 560 001, India. *Correspondence e-mail: mahendra@physics.uni-mysore.ac.in

Received 28 November 2016
Accepted 14 December 2016

Edited by E. R. T. Tiekink, Sunway University, Malaysia

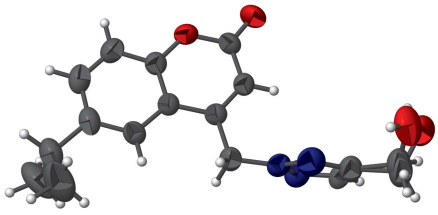
Keywords: crystal structure; chromones; triazole; conformation.

CCDC reference: 1523344

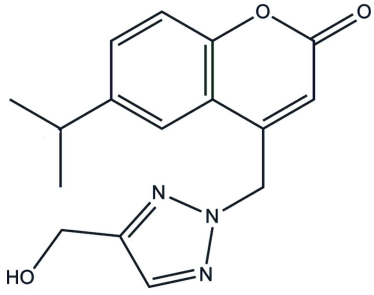
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{17}N_3O_3$, the chromene ring is planar, with a maximum deviation of 0.017 (4) Å for the ring O atom. The triazole and the chromene rings, bridged by a methylene C atom, are inclined to one another by 78.3 (2)°. In the crystal, methylene–triazole C—H···N hydrogen bonds lead to the formation of helical supramolecular chains along the *b* axis. The sample was refined as an inversion twin. The terminal methylhydroxy group is disordered over two sets of sites [site occupancy = 0.610 (13) for the major component].

3D view



Chemical scheme



Structure description

Coumarins and their derivatives form represent an important class of natural and synthetic heterocycles that are often linked to a broad array of biological activities (Gaspar *et al.*, 2015), such as anti-bacterial (Basanagouda *et al.*, 2009), anti-oxidant (Vukovic *et al.*, 2010) and anti-inflammatory (Emmanuel-Giota *et al.*, 2001). These derivatives are also used in the pharmaceutical industry as precursor reagents in the synthesis of a number of synthetic anti-coagulant pharmaceuticals (Bairagi *et al.*, 2012). As part of our ongoing studies of coumarin–triazole derivatives (El-Khatatneh *et al.*, 2016), the title compound was synthesized and its crystal structure is reported herein.

In the molecular structure (Fig. 1), the chromene unit (O19/C9/C10/C18/C20/C22) is planar, with a maximum deviation of 0.017 (4) Å for the ring atom O21. The triazole (N4/N5/N6/C3/C7) and the chromene (O19/C9/C10/C18/C20/C22) rings, bridged *via* a methylene-C8 atom, are inclined to one another by 78.3 (2)°. The intra-ring bond conformation between the chromene and triazole moieties are also characterized by torsion angles of 100.2 (5)° [for N4—N5—C8—C9] and −178.6 (3)° [for C10—C9—C8—N5]. The hydroxymethyl group is not coplanar with the triazole ring, as indicated by

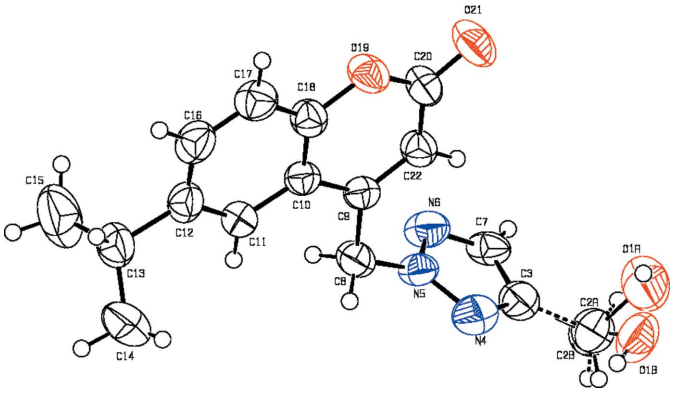


Figure 1
Perspective diagram of the title molecule, showing 50% probability displacement ellipsoids and both components of the disordered hydroxymethyl group.

torsion angle C7—C3—C2*A*—O1*A* = 77 (2)°. One methyl unit of the isopropyl group is not co-planar with the chromene ring, as suggested by the C11—C12—C13—C14 torsion angle of 40.5 (8)°, while the other methyl group is below, with a C11—C12—C13—C15 torsion angle of −88.1 (6)°.

The crystal features C8—H8*A*···N6 hydrogen bonds (Table 1), which lead to helical supramolecular chains along the *b* axis. The molecular packing exhibits layered stacking when viewed along the *b* axis, as shown in Fig. 2.

Synthesis and crystallization

The general procedure for the synthesis of N_2 coumarin 1,2,3-triazoles has been reported (Shamala *et al.*, 2016). To a solution of propargyl alcohol (0.11 g, 1.9 mmol) in acetone, CuI (10 mol%) and triethylamine (0.19 g, 1.9 mmol) were added. The mixture was stirred at room temperature for 15 min. Then, 4-(azidomethyl)-6-isopropyl-2*H*-chromen-2-one (1.9 mmol) was added and the resulting mixture was stirred until the starting material was consumed as judged by TLC. After the completion of the reaction, the catalyst was filtered through celite and the product was extracted with ether (3.10 ml). The solvent was removed under vacuum. The crude product was dried and recrystallized from ethyl acetate to give colourless blocks of the title compound.

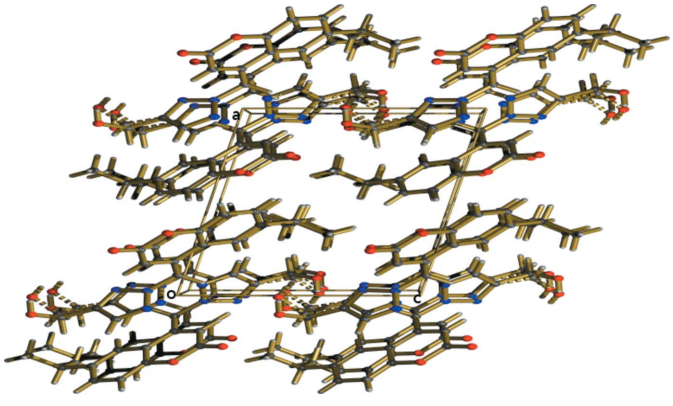


Figure 2
Packing diagram of the molecule viewed parallel to the *b* axis.

Yield 85%; colourless solid; m.p. 466–468 K. IR (KBr, cm^{-1}): 1720 (lactone C═O), 3190 (OH). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.25 (*d*, 6H, 2-CH_3 of *i*-Pr), *J* = 5.2 Hz), 2.06 (*s*, 1H, OH), 2.95 (*m*, 1H, CH of *i*-Pr, *J* = 5.2 Hz), 4.93 (*s*, 2H, –CH_2O–), 5.97 (*s*, 2H, –CH_2N–), 6.21 (*s*, 1H, C_3—H), 7.36 (*d*, 1H, C_7—H, *J* = 8.4 Hz), 7.55 (*d*, 1H, C_8—H, $J_{1,2}$ = 7.6 Hz), 7.70 (*s*, 1H, C_5—H), 8.38 (*s*, 1H, Tr-H) p.p.m. ^{13}C NMR (100 MHz, DMSO-d_6): δ 16.9 (2C), 26.7, 43.3, 49.5, 101.1, 107.9, 109.6, 110.4, 113.7, 124.2, 138.7, 141.0, 142.9, 145.0, 153.0 p.p.m. Analysis calculated for $C_{16}H_{17}N_3O_3$: C, 64.20; H, 5.72; N, 14.04%; found: C, 64.08; H, 5.60; N, 14.00%.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···N6^{i}	0.97	2.55	3.070 (6)	114

Symmetry code: (i) $-x, y-\frac{1}{2}, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{17}N_3O_3$
M_r	299.32
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	273
a, *b*, *c* (Å)	8.715 (5), 7.301 (4), 12.113 (6)
β (°)	101.209 (9)
V (Å^3)	756.0 (7)
Z	2
Radiation type	Mo *Kα*
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.25 × 0.15
Data collection	
Diffractometer	Bruker MicroStar microfocus rotating anode
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7069, 2680, 2307
R_{int}	0.026
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.058, 0.173, 1.06
No. of reflections	2680
No. of parameters	214
No. of restraints	38
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.28
Absolute structure	Flack *x* determined using 884 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.4 (6)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The sample was refined as an inversion twin. The terminal methylhydroxyl group is disor-

dered over two sets of sites (site occupancy = 0.610 (13) for the major component).

Acknowledgements

MM thanks the UGC, New Delhi, India, for awarding a project under the title F. No. 41-920/2012(SR) from 25-07-2012. SD is grateful to the Council of Scientific and Industrial Research, New Delhi, India, for financial assistance [grant No. 02 (0172)/13/EMR-II].

References

Bairagi, S. H., Salaskar, P. P., Loke, S. D., Surve, N. N., Tandel, D. V. & Dusara, M. D. (2012). *Int. J. Pharm. Res.* **4**, 16–19.

Basanagouda, M., Kulkarni, M. V., Sharma, D., Gupta, V. K., Pranesha, Sandhyarani, P. & Rasal, V. P. (2009). *J. Chem. Sci.* **121**, 485–495.

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

El-Khatatneh, N., Chandra, Shamala, D., Shivashankar, K. & Mahendra, M. (2016). *IUCrData*, **1**, x161618.

Emmanuel-Giota, A. A., Fylaktakidou, K. C., Litinas, K. E., Nicolaides, D. N. & Hadjipavlou-Litina, D. J. (2001). *J. Heterocycl. Chem.* **38**, 717–722.

Gaspar, A., Milhazes, N., Santana, L., Uriarte, E., Borges, F. & Matos, M. J. (2015). *Curr. Top. Med. Chem.* **15**, 432–445.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Shamala, D., Shivashankar, K., Chandra & Mahendra, M. (2016). *Synth. Commun.* **46**, 433–441.

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

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

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

Vukovic, N., Sukdolak, S., Solujic, S. & Niciforovic, N. (2010). *Arch. Pharm. Res.* **33**, 5–15.

full crystallographic data

IUCrData (2016). **1**, x161989 [https://doi.org/10.1107/S2414314616019891]

4-[(4-Hydroxymethyl-2*H*-1,2,3-triazol-2-yl)methyl]-6-isopropyl-2*H*-chromen-2-one

Nasseem El-Khatatneh, Chandra, D. Shamala, K. Shivashankar and M. Mahendra

4-[(4-Hydroxymethyl-2*H*-1,2,3-triazol-2-yl)methyl]-6-isopropyl-2*H*-chromen-2-one

Crystal data

$C_{16}H_{17}N_3O_3$
M_r = 299.32
Monoclinic, $P2_1$
a = 8.715 (5) Å
b = 7.301 (4) Å
c = 12.113 (6) Å
β = 101.209 (9)°
V = 756.0 (7) Å^3
Z = 2
$F(000)$ = 316
D_x = 1.315 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2680 reflections
θ = 1.7–25.0°
μ = 0.09 mm^{-1}
T = 273 K
Block, colourless
0.35 × 0.25 × 0.15 mm

Data collection

Bruker MicroStar microfocus rotating anode diffractometer
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
7069 measured reflections
2680 independent reflections
2307 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.0°, θ_{min} = 1.7°
h = −10→10
k = −8→8
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.173
S = 1.06
2680 reflections
214 parameters
38 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
$w = 1/[\sigma^2(F_o^2) + (0.1139P)^2 + 0.0997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack x determined using 884 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.4 (6)

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.

Refinement. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C2A	0.432 (4)	−0.285 (8)	−0.109 (3)	0.080 (3)	0.610 (13)
H2A1	0.474773	−0.398344	−0.075005	0.096*	0.610 (13)
H2A2	0.399222	−0.304324	−0.189741	0.096*	0.610 (13)
O1A	0.5459 (9)	−0.1448 (13)	−0.0887 (7)	0.109 (4)	0.610 (13)
H1A	0.567622	−0.123296	−0.021052	0.164*	0.610 (13)
C2B	0.445 (6)	−0.277 (14)	−0.090 (6)	0.080 (3)	0.390 (13)
H2B1	0.430161	−0.396496	−0.126013	0.096*	0.390 (13)
H2B2	0.467401	−0.191108	−0.145752	0.096*	0.390 (13)
O1B	0.5778 (11)	−0.2871 (17)	−0.0017 (10)	0.089 (4)	0.390 (13)
H1B	0.560748	−0.359343	0.046267	0.133*	0.390 (13)
O19	0.0897 (4)	0.2890 (4)	0.3404 (2)	0.0600 (8)	
C11	−0.1689 (4)	−0.1100 (6)	0.2962 (4)	0.0508 (10)	
H11	−0.191640	−0.210542	0.248665	0.061*	
C9	0.0411 (4)	−0.0058 (5)	0.1920 (3)	0.0446 (9)	
C10	−0.0518 (5)	0.0111 (5)	0.2791 (3)	0.0453 (9)	
C18	−0.0219 (5)	0.1603 (6)	0.3514 (4)	0.0509 (10)	
C20	0.1754 (5)	0.2769 (6)	0.2573 (4)	0.0550 (11)	
C22	0.1485 (5)	0.1217 (6)	0.1844 (3)	0.0488 (10)	
H22	0.208492	0.108718	0.129199	0.059*	
C17	−0.1015 (6)	0.1867 (7)	0.4379 (4)	0.0612 (12)	
H17	−0.078051	0.286037	0.486358	0.073*	
N5	0.1126 (4)	−0.1759 (5)	0.0339 (3)	0.0497 (8)	
C12	−0.2519 (5)	−0.0858 (7)	0.3810 (4)	0.0562 (11)	
C8	0.0117 (5)	−0.1697 (6)	0.1159 (4)	0.0576 (11)	
H8A	0.027464	−0.279960	0.161356	0.069*	
H8B	−0.096445	−0.168051	0.076627	0.069*	
O21	0.2705 (4)	0.3975 (6)	0.2539 (3)	0.0804 (11)	
C7	0.1952 (5)	−0.0965 (6)	−0.1125 (3)	0.0530 (10)	
H7	0.204076	−0.038826	−0.179462	0.064*	
N4	0.2440 (5)	−0.2750 (7)	0.0358 (4)	0.0734 (12)	
C16	−0.2155 (6)	0.0646 (7)	0.4515 (4)	0.0642 (12)	
H16	−0.269929	0.082688	0.509450	0.077*	
N6	0.0842 (5)	−0.0676 (5)	−0.0562 (3)	0.0628 (10)	
C3	0.2948 (6)	−0.2225 (7)	−0.0586 (4)	0.0636 (12)	
C13	−0.3833 (5)	−0.2128 (8)	0.3976 (5)	0.0683 (13)	
H13	−0.392494	−0.200590	0.476651	0.082*	
C14	−0.3496 (9)	−0.4077 (10)	0.3806 (8)	0.121 (3)	
H14A	−0.429774	−0.482233	0.401963	0.182*	
H14B	−0.250109	−0.439262	0.425926	0.182*	
H14C	−0.347001	−0.428504	0.302684	0.182*	
C15	−0.5364 (6)	−0.1510 (13)	0.3291 (7)	0.120 (3)	
H15A	−0.542993	−0.187489	0.252200	0.180*	
H15B	−0.543668	−0.020020	0.333103	0.180*	
H15C	−0.620528	−0.205715	0.358126	0.180*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2A	0.086 (6)	0.071 (6)	0.097 (12)	−0.005 (5)	0.050 (5)	−0.015 (11)
O1A	0.109 (6)	0.109 (7)	0.125 (7)	−0.029 (5)	0.063 (5)	−0.052 (5)
C2B	0.086 (6)	0.071 (6)	0.097 (12)	−0.005 (5)	0.050 (5)	−0.015 (11)
O1B	0.069 (6)	0.093 (8)	0.110 (8)	0.029 (6)	0.033 (6)	0.033 (6)
O19	0.0690 (18)	0.0526 (18)	0.0603 (17)	−0.0160 (15)	0.0173 (15)	−0.0159 (14)
C11	0.048 (2)	0.045 (2)	0.060 (2)	−0.0010 (19)	0.0126 (18)	0.0015 (19)
C9	0.047 (2)	0.0389 (19)	0.047 (2)	0.0028 (17)	0.0077 (16)	0.0007 (16)
C10	0.048 (2)	0.041 (2)	0.048 (2)	0.0023 (16)	0.0110 (16)	0.0018 (17)
C18	0.052 (2)	0.051 (2)	0.051 (2)	−0.0022 (19)	0.0131 (17)	0.0017 (19)
C20	0.053 (2)	0.055 (3)	0.058 (2)	−0.014 (2)	0.0144 (19)	−0.003 (2)
C22	0.052 (2)	0.048 (2)	0.049 (2)	−0.0036 (19)	0.0154 (17)	0.0005 (18)
C17	0.071 (3)	0.060 (3)	0.055 (2)	0.002 (2)	0.019 (2)	−0.006 (2)
N5	0.0589 (19)	0.0377 (17)	0.0539 (19)	0.0035 (16)	0.0139 (15)	−0.0042 (15)
C12	0.049 (2)	0.059 (3)	0.063 (2)	0.007 (2)	0.0184 (18)	0.015 (2)
C8	0.066 (2)	0.046 (2)	0.067 (3)	−0.011 (2)	0.028 (2)	−0.009 (2)
O21	0.083 (2)	0.073 (2)	0.092 (2)	−0.039 (2)	0.0307 (19)	−0.023 (2)
C7	0.080 (3)	0.039 (2)	0.045 (2)	0.001 (2)	0.0247 (19)	0.0076 (18)
N4	0.080 (3)	0.059 (3)	0.084 (3)	0.003 (2)	0.023 (2)	−0.008 (2)
C16	0.065 (3)	0.068 (3)	0.065 (3)	0.011 (2)	0.027 (2)	0.006 (2)
N6	0.077 (2)	0.048 (2)	0.066 (2)	0.0081 (19)	0.0191 (18)	0.0050 (18)
C3	0.070 (3)	0.055 (3)	0.072 (3)	−0.006 (2)	0.030 (2)	−0.009 (2)
C13	0.058 (3)	0.071 (3)	0.080 (3)	−0.002 (2)	0.024 (2)	0.015 (3)
C14	0.119 (6)	0.065 (4)	0.199 (8)	−0.025 (4)	0.079 (6)	0.000 (5)
C15	0.063 (3)	0.134 (7)	0.153 (7)	−0.020 (4)	−0.002 (4)	0.047 (6)

Geometric parameters (Å, º)

C2Aa—O1A	1.41 (4)	C17—C16	1.368 (7)
C2Aa—C3	1.52 (5)	C17—H17	0.9300
C2Aa—H2A1	0.9700	N5—N6	1.331 (5)
C2Aa—H2A2	0.9700	N5—N4	1.351 (5)
O1Aa—H1A	0.8200	N5—C8	1.450 (5)
C2Bb—O1B	1.42 (4)	C12—C16	1.389 (7)
C2Bb—C3	1.49 (8)	C12—C13	1.517 (6)
C2Bb—H2B1	0.9700	C8—H8A	0.9700
C2Bb—H2B2	0.9700	C8—H8B	0.9700
O1Bb—H1B	0.8200	C7—N6	1.305 (6)
O19—C20	1.368 (5)	C7—C3	1.343 (7)
O19—C18	1.377 (5)	C7—H7	0.9300
C11—C12	1.378 (6)	N4—C3	1.359 (7)
C11—C10	1.396 (5)	C16—H16	0.9300
C11—H11	0.9300	C13—C14	1.476 (10)
C9—C22	1.335 (6)	C13—C15	1.497 (8)
C9—C10	1.454 (5)	C13—H13	0.9800
C9—C8	1.502 (6)	C14—H14A	0.9600

C10—C18	1.390 (6)	C14—H14B	0.9600
C18—C17	1.378 (6)	C14—H14C	0.9600
C20—O21	1.215 (5)	C15—H15A	0.9600
C20—C22	1.428 (6)	C15—H15B	0.9600
C22—H22	0.9300	C15—H15C	0.9600
O1Aa—C2Aa—C3	107 (4)	C11—C12—C13	122.7 (5)
O1Aa—C2Aa—H2A1	110.3	C16—C12—C13	119.3 (4)
C3—C2Aa—H2A1	110.3	N5—C8—C9	113.1 (3)
O1Aa—C2Aa—H2A2	110.3	N5—C8—H8A	109.0
C3—C2Aa—H2A2	110.3	C9—C8—H8A	109.0
H2A1a—C2Aa—H2A2	108.5	N5—C8—H8B	109.0
C2Aa—O1Aa—H1A	109.5	C9—C8—H8B	109.0
O1Bb—C2Bb—C3	117 (5)	H8A—C8—H8B	107.8
O1Bb—C2Bb—H2B1	108.1	N6—C7—C3	109.3 (4)
C3—C2Bb—H2B1	108.1	N6—C7—H7	125.3
O1Bb—C2Bb—H2B2	108.1	C3—C7—H7	125.3
C3—C2Bb—H2B2	108.1	N5—N4—C3	104.4 (4)
H2B1b—C2Bb—H2B2	107.3	C17—C16—C12	121.7 (4)
C2Bb—O1Bb—H1B	109.5	C17—C16—H16	119.1
C20—O19—C18	121.6 (3)	C12—C16—H16	119.1
C12—C11—C10	122.3 (4)	C7—N6—N5	107.1 (4)
C12—C11—H11	118.9	C7—C3—N4	108.5 (4)
C10—C11—H11	118.9	C7—C3—C2B	125 (3)
C22—C9—C10	119.2 (4)	N4—C3—C2B	126 (3)
C22—C9—C8	123.5 (4)	C7—C3—C2A	120 (2)
C10—C9—C8	117.4 (3)	N4—C3—C2A	132 (2)
C18—C10—C11	117.1 (4)	C14—C13—C15	113.2 (7)
C18—C10—C9	117.5 (4)	C14—C13—C12	113.3 (5)
C11—C10—C9	125.5 (4)	C15—C13—C12	110.9 (5)
O19—C18—C17	116.6 (4)	C14—C13—H13	106.3
O19—C18—C10	121.5 (4)	C15—C13—H13	106.3
C17—C18—C10	121.9 (4)	C12—C13—H13	106.3
O21—C20—O19	116.8 (4)	C13—C14—H14A	109.5
O21—C20—C22	125.8 (4)	C13—C14—H14B	109.5
O19—C20—C22	117.3 (3)	H14A—C14—H14B	109.5
C9—C22—C20	122.9 (4)	C13—C14—H14C	109.5
C9—C22—H22	118.5	H14A—C14—H14C	109.5
C20—C22—H22	118.5	H14B—C14—H14C	109.5
C16—C17—C18	119.0 (5)	C13—C15—H15A	109.5
C16—C17—H17	120.5	C13—C15—H15B	109.5
C18—C17—H17	120.5	H15A—C15—H15B	109.5
N6—N5—N4	110.7 (4)	C13—C15—H15C	109.5
N6—N5—C8	120.1 (3)	H15A—C15—H15C	109.5
N4—N5—C8	129.1 (4)	H15B—C15—H15C	109.5
C11—C12—C16	118.0 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···N6^{i}	0.97	2.55	3.070 (6)	114

Symmetry code: (i) −*x*, *y*−1/2, −*z*.