IUCrData

ISSN 2414-3146

# 4-[(4-Hydroxymethyl-2*H*-1,2,3-triazol-2-yl)-methyl]-6,8-dimethyl-2*H*-chromen-2-one. Corrigendum

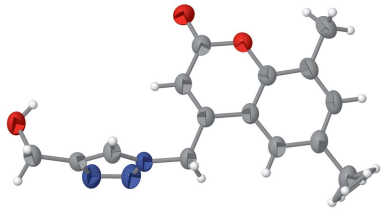
Nasseem El-Khatatneh,[a] Chandra,[a] D. Shamala,[b] K. Shivashankar[b] and M. Mahendra[a]*

[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

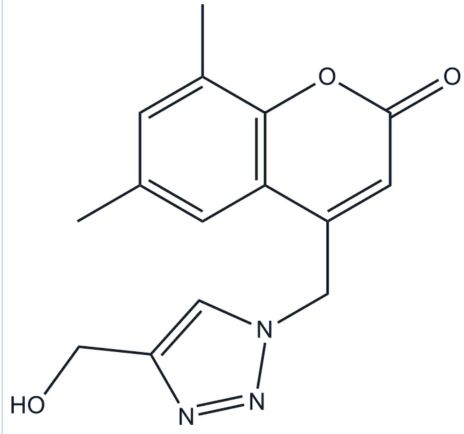
In the paper by El-Khatatneh *et al.* [*IUCrData* (2016), **1**, x161644], the scheme and chemical name in the title are corrected.

In the paper by El-Khatatneh *et al.* (2016), the chemical scheme should be as shown here.

3D view



Chemical scheme




The chemical name in the title is then corrected as '4-[(4-Hydroxymethyl-1*H*-1,2,3-triazol-1-yl)methyl]-6,8-dimethyl-2*H*-chromen-2-one'.

## References

El-Khatatneh, N., Chandra, Shamala, D., Shivashankar, K. & Mahendra, M. (2016). *IUCrData*, **1**, x161644.

IUCrData

ISSN 2414-3146

# 4-[(4-Hydroxymethyl-2*H*-1,2,3-triazol-2-yl)-methyl]-6,8-dimethyl-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 13 October 2016
Accepted 15 October 2016

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

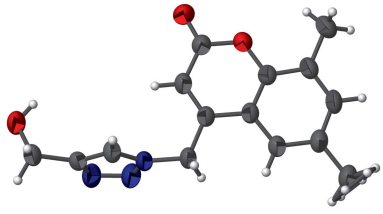
**Keywords:** crystal structure; chromene; triazole; hydrogen bonds.

**CCDC reference**: 1510042

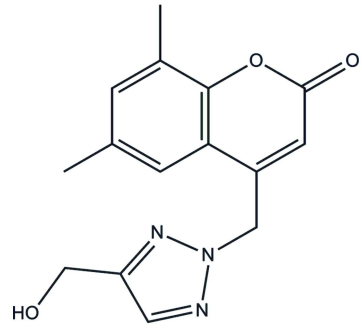
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{15}H_{15}N_3O_3$, the dihedral angle between the triazole ring and coumarin ring system [r.m.s. deviation = 0.040 Å] is 77.40 (6)°. The O atom of the hydroxymethyl group deviates from the triazole ring plane by 1.345 (1) Å. In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(22)$ loops; C—H···O and C—H···N interactions link the dimers into a three-dimensional network.

**3D view**



**Chemical scheme**






## Structure description

Coumarin derivatives represent an important class of natural and synthetic heterocycles that are often linked to a broad array of biological activities (Gaspar *et al.*, 2015). As part of our ongoing studies of coumarin–triazole derivatives (El-Khatatneh *et al.*, 2016), the title compound (Fig. 1) was synthesized and its crystal structure is now reported.

The dihedral angle between the triazole ring and coumarin ring system [r.m.s. deviation = 0.040 Å] is 77.40 (6)°. Key inter-ring torsion angles include 97.34 (15)° for N19—N15—C14—C13) and −173.30 (13)° for C6—C13—C14—N15. The O atom of the hydroxymethyl group is displaced from the triazole ring plane by 1.345 (1) Å.

In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds (Table 1) generate $R_2^2(22)$ loops. The dimers are linked by weak C—H···O and C—H···N hydrogen bonds, generating a three-dimensional network (Fig. 2).

## Synthesis and crystallization

A mixture of propargyl alcohol (1.9 mmol), sodium azide (0.14 g, 2.0 mmol), copper(I) iodide (10 mol%) and triethylamine (0.19 g, 1.9 mmol) in 20 ml of acetone was taken in a

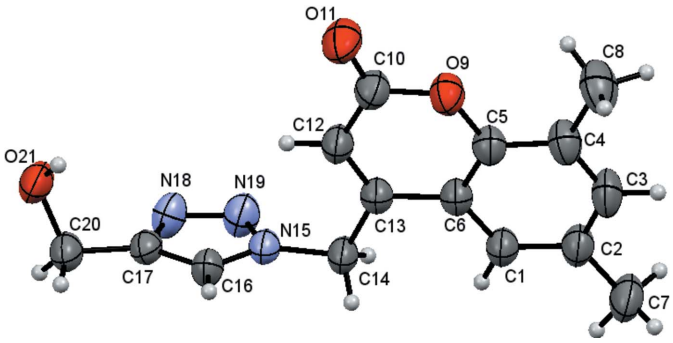



**Figure 1**
The molecular structure of the title compound with 50% probability displacement ellipsoids.

round-bottom flask and stirred for 1 h. To this mixture, 4-bromomethylcoumarin (1.9 mmol) was added and the stirring continued for 8 h (the reaction was monitored by TLC). After the completion of the reaction, the copper catalyst was filtered through celite and the product was extracted with diethyl ether (3.10 ml). The solvent was removed under vacuum. The crude product was dried and recrystallized from ethyl acetate solution to give colourless blocks.

Yield 92%; colourless solid; m.p. 210–212 °C; IR (KBr, $cm^{-1}$): 1742 $cm^{-1}$ (lactone C=O), 3311 $cm^{-1}$ (OH); $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 1.70 (*s*, 1H, OH), 2.37 (*s*, 3H, $C_6-CH_3$) 2.42 (*s*, 3H, $C_8-CH_3$) 4.83 (*s*, 2H, $-CH_2O-$), 5.43 (*s*, 1H, $C_3-H$), 5.70 (*s*, 2H, $-CH_2N-$), 7.21-7.24 (*m*, 1H, $C_7-H$), 7.60 (*s*, 1H, $C_5-H$), 7.75 (*s*, 1H, Tr—H) p.p.m. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 15.0, 20.3, 49.0, 55.0, 113.0, 116.5, 122.0, 123.8, 125.3, 133.1, 134.5, 148.6, 149.5, 150.6, 159.5 p.p.m. Analysis

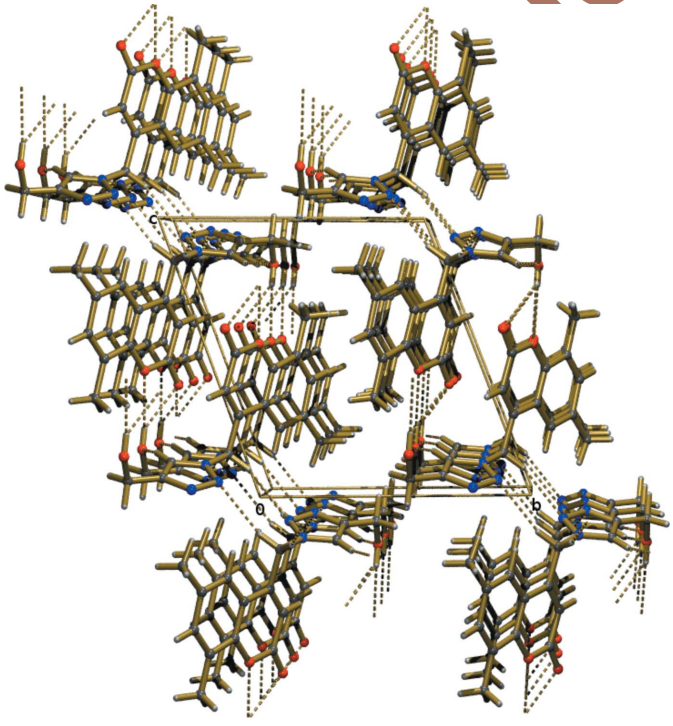



**Figure 2**
The packing viewed along [100] with hydrogen bonds indicated by dashed lines.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O21—H21···O11$^{i}$ | 0.82 | 2.10 | 2.9155 (19) | 176 |
| C14—H14$A$···N19$^{ii}$ | 0.97 | 2.55 | 3.486 (2) | 162 |
| C14—H14$B$···N18$^{iii}$ | 0.97 | 2.41 | 3.344 (2) | 162 |
| C16—H16···O21$^{iii}$ | 0.93 | 2.47 | 3.284 (2) | 146 |

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $-x+1, -y+2, -z+2$; (iii) $x+1, y, z$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{15}H_{15}N_3O_3$ |
| $M_r$ | 285.30 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 293 |
| $a, b, c$ (Å) | 6.0265 (16), 11.062 (3), 11.848 (3) |
| $\alpha, \beta, \gamma$ (°) | 108.812 (7), 103.950 (8), 100.848 (8) |
| $V$ (Å$^3$) | 694.5 (3) |
| $Z$ | 2 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ ($mm^{-1}$) | 0.80 |
| Crystal size (mm) | 0.30 × 0.20 × 0.10 |
| Data collection | |
| Diffractometer | Bruker X8 Proteum |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 8218, 2217, 2142 |
| $R_{int}$ | 0.030 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.587 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.042, 0.114, 1.04 |
| No. of reflections | 2217 |
| No. of parameters | 194 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.14, −0.14 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL2016/4* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

$C_{15}H_{15}N_3O_3$. Calculated for: C, 63.15; H, 5.30; N, 14.73%. Found: C, 63.08; H, 5.26; N, 14.68%.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

MM thanks UGC, New Delhi, Government of India, for awarding a project under the title F. No. 41–920/2012(SR) dated: 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

Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc.,Madison, Wisconsin, USA.
El-Khatatneh, N., Chandra Shamala, D., Shivashankarb, K. & Mahendra, M. (2016). *IUCrData*, **1**, x161618.

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.
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.

# full crystallographic data

*IUCrData* (2016). **1**, x161644 [https://doi.org/10.1107/S2414314616016448]

## 4-[(4-Hydroxymethyl-2*H*-1,2,3-triazol-2-yl)methyl]-6,8-dimethyl-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]-6,8-dimethyl-2*H*-chromen-2-one

*Crystal data*

$C_{15}H_{15}N_3O_3$
$M_r = 285.30$
Triclinic, $P\overline{1}$
$a = 6.0265$ (16) Å
$b = 11.062$ (3) Å
$c = 11.848$ (3) Å
$\alpha = 108.812$ (7)°
$\beta = 103.950$ (8)°
$\gamma = 100.848$ (8)°
$V = 694.5$ (3) Å$^3$
$Z = 2$
$F(000) = 300$
$D_x = 1.364$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2217 reflections
$\theta = 7.2$–64.7°
$\mu = 0.80$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.10 mm

*Data collection*

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
8218 measured reflections
2217 independent reflections
2142 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 64.7°$, $\theta_{min} = 7.2°$
$h = -6\rightarrow7$
$k = -12\rightarrow12$
$l = -13\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.114$
$S = 1.04$
2217 reflections
194 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
$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.126P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.14$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O9 | 0.37402 (19) | 0.76949 (10) | 0.45209 (9) | 0.0574 (3) | |
| O21 | −0.04447 (19) | 1.36437 (12) | 0.82987 (11) | 0.0658 (3) | |
| H21 | −0.055031 | 1.305321 | 0.763928 | 0.099* | |
| O11 | 0.0867 (2) | 0.85556 (13) | 0.39863 (11) | 0.0757 (4) | |
| C6 | 0.6271 (2) | 0.84311 (13) | 0.66749 (13) | 0.0452 (3) | |
| N19 | 0.2818 (2) | 1.08969 (13) | 0.92565 (13) | 0.0596 (4) | |
| N15 | 0.44456 (19) | 1.12365 (11) | 0.87345 (10) | 0.0450 (3) | |
| C13 | 0.5024 (2) | 0.94266 (13) | 0.70280 (13) | 0.0458 (3) | |
| C5 | 0.5580 (3) | 0.75918 (14) | 0.54097 (13) | 0.0485 (3) | |
| N18 | 0.1788 (2) | 1.18550 (14) | 0.94803 (13) | 0.0598 (4) | |
| C1 | 0.8117 (3) | 0.82578 (14) | 0.75347 (14) | 0.0500 (4) | |
| H1 | 0.860125 | 0.880475 | 0.838505 | 0.060* | |
| C12 | 0.3208 (3) | 0.94819 (14) | 0.61462 (14) | 0.0523 (4) | |
| H12 | 0.240245 | 1.011061 | 0.638265 | 0.063* | |
| C4 | 0.6663 (3) | 0.66137 (15) | 0.49641 (14) | 0.0560 (4) | |
| C2 | 0.9229 (3) | 0.72895 (15) | 0.71413 (15) | 0.0542 (4) | |
| C17 | 0.2756 (2) | 1.28047 (13) | 0.91088 (12) | 0.0454 (3) | |
| C20 | 0.1846 (3) | 1.39858 (15) | 0.91808 (14) | 0.0556 (4) | |
| H20A | 0.178228 | 1.440812 | 1.002359 | 0.067* | |
| H20B | 0.295413 | 1.462794 | 0.903203 | 0.067* | |
| C14 | 0.5903 (3) | 1.03629 (14) | 0.83948 (13) | 0.0517 (4) | |
| H14A | 0.597759 | 0.983779 | 0.891184 | 0.062* | |
| H14B | 0.751444 | 1.090828 | 0.859203 | 0.062* | |
| C10 | 0.2480 (3) | 0.85893 (15) | 0.48426 (14) | 0.0552 (4) | |
| C3 | 0.8477 (3) | 0.64959 (16) | 0.58574 (16) | 0.0614 (4) | |
| H3 | 0.923601 | 0.585243 | 0.558673 | 0.074* | |
| C16 | 0.4471 (2) | 1.24121 (13) | 0.86378 (13) | 0.0477 (3) | |
| H16 | 0.545138 | 1.286513 | 0.831682 | 0.057* | |
| C7 | 1.1162 (3) | 0.70920 (19) | 0.80743 (18) | 0.0718 (5) | |
| H7A | 1.168804 | 0.636256 | 0.764247 | 0.108* | 0.31 (2) |
| H7B | 1.055076 | 0.689718 | 0.869294 | 0.108* | 0.31 (2) |
| H7C | 1.248294 | 0.789024 | 0.848366 | 0.108* | 0.31 (2) |
| H7D | 1.145979 | 0.773742 | 0.890357 | 0.108* | 0.69 (2) |
| H7E | 1.259707 | 0.720281 | 0.785311 | 0.108* | 0.69 (2) |
| H7F | 1.066488 | 0.620975 | 0.806239 | 0.108* | 0.69 (2) |
| C8 | 0.5915 (4) | 0.57393 (19) | 0.35871 (16) | 0.0760 (5) | |
| H8A | 0.690144 | 0.613072 | 0.319554 | 0.114* | |
| H8B | 0.427523 | 0.565734 | 0.318815 | 0.114* | |
| H8C | 0.609121 | 0.487213 | 0.349891 | 0.114* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O9 | 0.0673 (7) | 0.0594 (6) | 0.0445 (5) | 0.0320 (5) | 0.0145 (5) | 0.0135 (4) |
| O21 | 0.0540 (6) | 0.0732 (7) | 0.0627 (7) | 0.0362 (5) | 0.0113 (5) | 0.0124 (5) |
| O11 | 0.0765 (8) | 0.0868 (8) | 0.0507 (6) | 0.0440 (7) | 0.0024 (6) | 0.0120 (6) |
| C6 | 0.0468 (7) | 0.0422 (7) | 0.0487 (7) | 0.0192 (6) | 0.0170 (6) | 0.0156 (6) |
| N19 | 0.0560 (7) | 0.0609 (7) | 0.0744 (9) | 0.0269 (6) | 0.0276 (6) | 0.0316 (6) |
| N15 | 0.0420 (6) | 0.0456 (6) | 0.0436 (6) | 0.0198 (5) | 0.0113 (5) | 0.0105 (5) |
| C13 | 0.0457 (7) | 0.0434 (7) | 0.0477 (7) | 0.0186 (6) | 0.0143 (6) | 0.0143 (6) |
| C5 | 0.0549 (8) | 0.0481 (7) | 0.0481 (8) | 0.0228 (6) | 0.0189 (6) | 0.0197 (6) |
| N18 | 0.0546 (7) | 0.0692 (8) | 0.0696 (8) | 0.0322 (6) | 0.0297 (6) | 0.0294 (7) |
| C1 | 0.0504 (8) | 0.0486 (7) | 0.0508 (8) | 0.0237 (6) | 0.0155 (6) | 0.0144 (6) |
| C12 | 0.0518 (8) | 0.0524 (8) | 0.0514 (8) | 0.0272 (6) | 0.0136 (6) | 0.0136 (6) |
| C4 | 0.0723 (10) | 0.0526 (8) | 0.0518 (8) | 0.0309 (7) | 0.0283 (7) | 0.0180 (7) |
| C2 | 0.0564 (8) | 0.0527 (8) | 0.0607 (9) | 0.0290 (7) | 0.0213 (7) | 0.0218 (7) |
| C17 | 0.0420 (7) | 0.0472 (7) | 0.0401 (7) | 0.0183 (6) | 0.0094 (5) | 0.0082 (5) |
| C20 | 0.0553 (8) | 0.0534 (8) | 0.0509 (8) | 0.0274 (6) | 0.0126 (6) | 0.0080 (6) |
| C14 | 0.0488 (8) | 0.0502 (8) | 0.0502 (8) | 0.0271 (6) | 0.0099 (6) | 0.0093 (6) |
| C10 | 0.0560 (8) | 0.0583 (8) | 0.0493 (8) | 0.0268 (7) | 0.0117 (7) | 0.0163 (7) |
| C3 | 0.0766 (11) | 0.0591 (9) | 0.0647 (9) | 0.0434 (8) | 0.0329 (8) | 0.0237 (7) |
| C16 | 0.0467 (7) | 0.0452 (7) | 0.0535 (8) | 0.0203 (6) | 0.0196 (6) | 0.0156 (6) |
| C7 | 0.0739 (11) | 0.0756 (11) | 0.0714 (11) | 0.0479 (9) | 0.0187 (9) | 0.0242 (9) |
| C8 | 0.1070 (15) | 0.0748 (11) | 0.0542 (10) | 0.0497 (11) | 0.0331 (10) | 0.0167 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O9—C10 | 1.3712 (18) | C4—C8 | 1.505 (2) |
| O9—C5 | 1.3833 (18) | C2—C3 | 1.395 (2) |
| O21—C20 | 1.4118 (18) | C2—C7 | 1.503 (2) |
| O21—H21 | 0.8200 | C17—C16 | 1.3635 (19) |
| O11—C10 | 1.2089 (19) | C17—C20 | 1.4952 (19) |
| C6—C5 | 1.392 (2) | C20—H20A | 0.9700 |
| C6—C1 | 1.404 (2) | C20—H20B | 0.9700 |
| C6—C13 | 1.4554 (18) | C14—H14A | 0.9700 |
| N19—N18 | 1.3135 (18) | C14—H14B | 0.9700 |
| N19—N15 | 1.3375 (17) | C3—H3 | 0.9300 |
| N15—C16 | 1.3395 (18) | C16—H16 | 0.9300 |
| N15—C14 | 1.4513 (16) | C7—H7A | 0.9600 |
| C13—C12 | 1.345 (2) | C7—H7B | 0.9600 |
| C13—C14 | 1.5080 (19) | C7—H7C | 0.9600 |
| C5—C4 | 1.392 (2) | C7—H7D | 0.9600 |
| N18—C17 | 1.352 (2) | C7—H7E | 0.9600 |
| C1—C2 | 1.3829 (19) | C7—H7F | 0.9600 |
| C1—H1 | 0.9300 | C8—H8A | 0.9600 |
| C12—C10 | 1.442 (2) | C8—H8B | 0.9600 |
| C12—H12 | 0.9300 | C8—H8C | 0.9600 |
| C4—C3 | 1.384 (2) | | |

| | | | |
|---|---|---|---|
| C10—O9—C5 | 122.09 (11) | N15—C14—H14B | 108.6 |
| C20—O21—H21 | 109.5 | C13—C14—H14B | 108.6 |
| C5—C6—C1 | 117.93 (12) | H14A—C14—H14B | 107.6 |
| C5—C6—C13 | 118.08 (12) | O11—C10—O9 | 115.82 (13) |
| C1—C6—C13 | 123.98 (12) | O11—C10—C12 | 126.45 (14) |
| N18—N19—N15 | 106.63 (11) | O9—C10—C12 | 117.73 (13) |
| N19—N15—C16 | 110.78 (11) | C4—C3—C2 | 123.61 (13) |
| N19—N15—C14 | 119.15 (12) | C4—C3—H3 | 118.2 |
| C16—N15—C14 | 130.04 (12) | C2—C3—H3 | 118.2 |
| C12—C13—C6 | 119.78 (12) | N15—C16—C17 | 105.51 (12) |
| C12—C13—C14 | 123.64 (12) | N15—C16—H16 | 127.2 |
| C6—C13—C14 | 116.58 (11) | C17—C16—H16 | 127.2 |
| O9—C5—C6 | 120.68 (12) | C2—C7—H7A | 109.5 |
| O9—C5—C4 | 116.33 (13) | C2—C7—H7B | 109.5 |
| C6—C5—C4 | 122.99 (13) | H7A—C7—H7B | 109.5 |
| N19—N18—C17 | 109.68 (12) | C2—C7—H7C | 109.5 |
| C2—C1—C6 | 121.27 (14) | H7A—C7—H7C | 109.5 |
| C2—C1—H1 | 119.4 | H7B—C7—H7C | 109.5 |
| C6—C1—H1 | 119.4 | C2—C7—H7D | 109.5 |
| C13—C12—C10 | 121.56 (13) | H7A—C7—H7D | 141.1 |
| C13—C12—H12 | 119.2 | H7B—C7—H7D | 56.3 |
| C10—C12—H12 | 119.2 | H7C—C7—H7D | 56.3 |
| C3—C4—C5 | 116.29 (14) | C2—C7—H7E | 109.5 |
| C3—C4—C8 | 121.84 (14) | H7A—C7—H7E | 56.3 |
| C5—C4—C8 | 121.87 (14) | H7B—C7—H7E | 141.1 |
| C1—C2—C3 | 117.89 (14) | H7C—C7—H7E | 56.3 |
| C1—C2—C7 | 120.78 (14) | H7D—C7—H7E | 109.5 |
| C3—C2—C7 | 121.33 (13) | C2—C7—H7F | 109.5 |
| N18—C17—C16 | 107.39 (12) | H7A—C7—H7F | 56.3 |
| N18—C17—C20 | 121.83 (13) | H7B—C7—H7F | 56.3 |
| C16—C17—C20 | 130.68 (14) | H7C—C7—H7F | 141.1 |
| O21—C20—C17 | 112.70 (12) | H7D—C7—H7F | 109.5 |
| O21—C20—H20A | 109.1 | H7E—C7—H7F | 109.5 |
| C17—C20—H20A | 109.1 | C4—C8—H8A | 109.5 |
| O21—C20—H20B | 109.1 | C4—C8—H8B | 109.5 |
| C17—C20—H20B | 109.1 | H8A—C8—H8B | 109.5 |
| H20A—C20—H20B | 107.8 | C4—C8—H8C | 109.5 |
| N15—C14—C13 | 114.71 (11) | H8A—C8—H8C | 109.5 |
| N15—C14—H14A | 108.6 | H8B—C8—H8C | 109.5 |
| C13—C14—H14A | 108.6 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O21—H21···O11$^{i}$ | 0.82 | 2.10 | 2.9155 (19) | 176 |
| C14—H14*A*···N19$^{ii}$ | 0.97 | 2.55 | 3.486 (2) | 162 |

| | | | | |
|---|---|---|---|---|
| C14—H14*B*···N18$^{iii}$ | 0.97 | 2.41 | 3.344 (2) | 162 |
| C16—H16···O21$^{iii}$ | 0.93 | 2.47 | 3.284 (2) | 146 |

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