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# 4-(3,5-Dimethoxyphenyl)-6-(2-methoxyphenyl)-pyrimidin-2-amine

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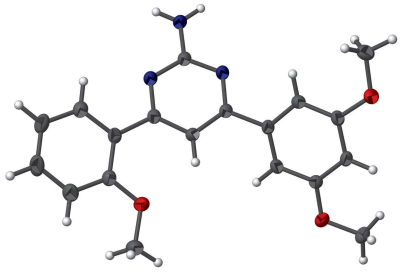
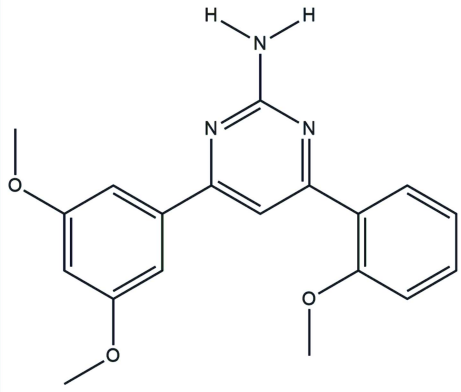
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{19}H_{19}N_3O_3$, the 2-methoxyphenyl and 3,5-dimethoxyphenyl rings are attached at the 4- and 6-positions, respectively, of the central 2-aminopyrimidine ring. The dihedral angles between the planes of the benzene rings and that of the 2-aminopyrimidine ring are 17.31 (9) and 44.39 (6)°, respectively. In the crystal, pairs of N—H···N hydrogen bonds form inversion dimers enclosing $R_2^2(8)$ rings. Pairs of N—H···O hydrogen bonds link the dimers into chains along [010].

**3D view**



**Chemical scheme**




## Structure description

2-Aminopyrimidine pharmacophores have shown a broad spectrum of biological activities including use against Parkinson's disease (Robinson *et al.*, 2016) and displaying antibacterial (Nagarajan *et al.*, 2014), anti-platelet (Giridhar *et al.*, 2012), antidiabetic (Singh *et al.*, 2011) and antitumor properties (Lee *et al.*, 2011). The title 2-aminopyrimidine compound was synthesized in a continuation of our research program to expand the use of novel synthetic chalcones (Lee *et al.* 2016), and its crystal structure was determined and is reported here.

The molecular structure of the title compound is shown in Fig. 1. The central 2-aminopyrimidine ring contains two benzene rings at the C4 and C6 positions respectively. The dihedral angles between central 2-aminopyrimidine ring and the C5–C10 and C12–C17 benzene rings are 17.31 (9) and 44.39 (6)°, respectively. All three methoxy groups on the benzene rings are slightly twisted from the ring plane [C17—C16—O3—C19 = −4.9 (2), C15—C14—O2—C18 = −4.5 (2) and C7—C6—O1—C11 = 3.7 (2)°].

In the crystal, pairs of N3—H3*B*···N2 hydrogen bonds form inversion dimers that enclose $R_2^2(8)$ rings. These dimers are linked into chains along the *b*-axis direction by pairs of N3—H3*A*···O3 hydrogen bonds (Table 1, Fig. 2).

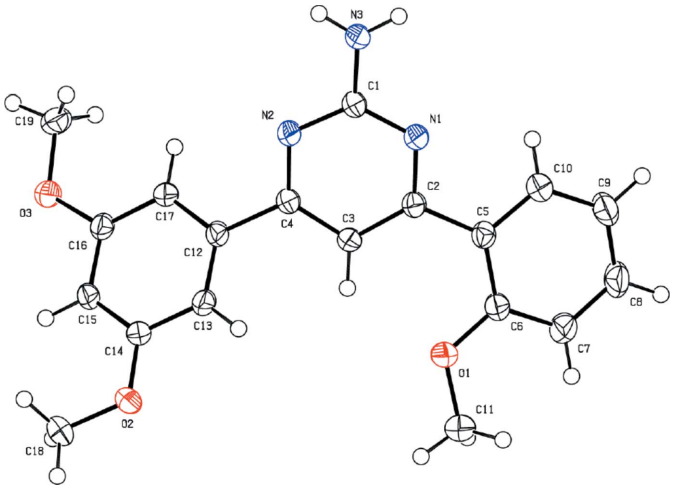



**Figure 1**
The molecular structure of the title compound, showing the atom-labelling scheme with displacement ellipsoids drawn at the 30% probability level.

Some examples of other 2-aminopyrimidine structures have also been published recently (Sangeetha *et al.*, 2016; Thanigaimani *et al.*, 2012).

## Synthesis and crystallization

A synthetic scheme is shown in Fig. 3. The chalcone (*E*)-1-(3,5-dimethoxyphenyl)-3-(2-methoxyphenyl)prop-2-en-1-one was prepared as a starting material by a previously reported method (Koh *et al.* 2016). 2-Amino pyrimidine was obtained by a cyclization reaction of this chalcone with guanidine hydrogen chloride in basic solution. To an ethanol solution of 3,5-dimethoxyacetophenone (I) and 2-methoxybenzaldehyde (II) an excess amount of 50% aqueous KOH was added and the mixture was stirred at room temperature for 20 h. After completion of reaction, the reaction mixture was poured into 6*M* HCl in an ice-bath to give a precipitate of the chalcone (III). The solid was filtered and washed with ethanol and was used for the next reaction without further purification. The chalcone (III, 1 eq.) and the guanidine HCl salt (1.5 eq.) were dissolved in a DMF solution to which was added solid $K_2CO_3$ (3 eq.). The reaction mixture was refluxed for 2 h and cooled to room temperature. The reaction mixture was then poured into 3*M* HCl in an ice bath to give a precipitate of the title 2-aminopyrimidine compound, which was purified by recrystallization from ethanol.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*B*···N2$^{i}$ | 0.87 | 2.28 | 3.1374 (19) | 167 |
| N3—H3*A*···O3$^{ii}$ | 0.87 | 2.39 | 3.2545 (17) | 175 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{19}H_{19}N_3O_3$ |
| $M_r$ | 337.37 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 223 |
| *a*, *b*, *c* (Å) | 7.5867 (7), 10.2680 (7), 11.4684 (8) |
| $\alpha, \beta, \gamma$ (°) | 95.592 (4), 102.147 (4), 109.987 (3) |
| *V* (Å$^3$) | 806.71 (11) |
| *Z* | 2 |
| Radiation type | Mo *Kα* |
| $\mu$ (mm$^{-1}$) | 0.10 |
| Crystal size (mm) | 0.18 × 0.10 × 0.06 |
| | |
| Data collection | |
| Diffractometer | Bruker PHOTON 100 CMOS |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2012) |
| $T_{min}$, $T_{max}$ | 0.690, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 26671, 4065, 2736 |
| $R_{int}$ | 0.063 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.671 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.046, 0.112, 1.02 |
| No. of reflections | 4065 |
| No. of parameters | 229 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.24, −0.21 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

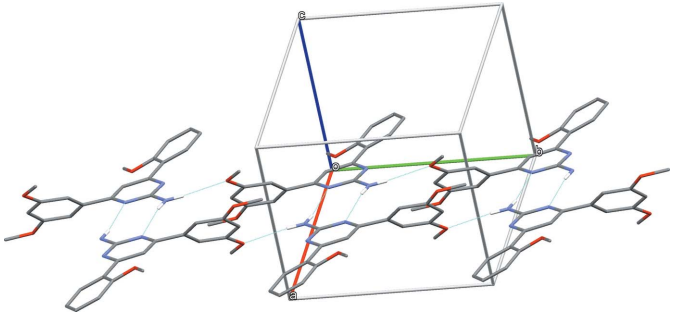


**Figure 2**
Part of the crystal structure with intermolecular hydrogen bonds shown as dashed lines. For clarity only those H atoms involved in hydrogen bonding are shown.

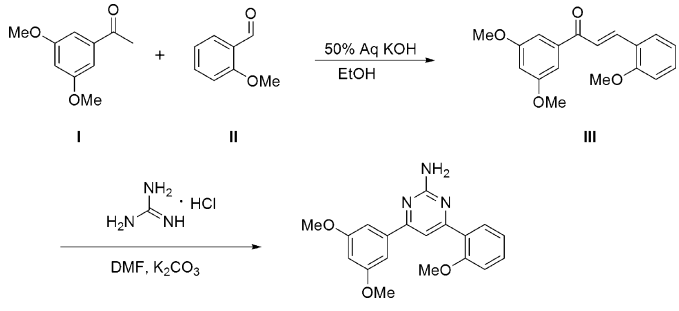



**Figure 3**
Synthetic scheme for the preparation of the title compound.

## Refinement

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

## Funding information

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# full crystallographic data

*IUCrData* (2018). **3**, x180796 [https://doi.org/10.1107/S2414314618007964]

## 4-(3,5-Dimethoxyphenyl)-6-(2-methoxyphenyl)pyrimidin-2-amine

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*Crystal data*

$C_{19}H_{19}N_3O_3$
$M_r$ = 337.37
Triclinic, $P\overline{1}$
$a$ = 7.5867 (7) Å
$b$ = 10.2680 (7) Å
$c$ = 11.4684 (8) Å
$\alpha$ = 95.592 (4)°
$\beta$ = 102.147 (4)°
$\gamma$ = 109.987 (3)°
$V$ = 806.71 (11) Å$^3$
$Z$ = 2
$F(000)$ = 356
$D_x$ = 1.389 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5933 reflections
$\theta$ = 2.6–27.9°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 223 K
Block, yellow
0.18 × 0.10 × 0.06 mm

*Data collection*

Bruker PHOTON 100 CMOS diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
$T_{min}$ = 0.690, $T_{max}$ = 0.746
26671 measured reflections
4065 independent reflections
2736 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.063
$\theta_{max}$ = 28.5°, $\theta_{min}$ = 2.9°
$h$ = −10→10
$k$ = −13→13
$l$ = −15→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.112
$S$ = 1.02
4065 reflections
229 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.2728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 1.2100 (2) | 0.51141 (15) | 0.91277 (13) | 0.0264 (3) |
| N1 | 1.04986 (18) | 0.52945 (13) | 0.85350 (11) | 0.0277 (3) |
| C2 | 0.9093 (2) | 0.41773 (15) | 0.77721 (13) | 0.0240 (3) |
| C3 | 0.9345 (2) | 0.29009 (16) | 0.75753 (14) | 0.0266 (3) |
| H3 | 0.8409 | 0.2128 | 0.7001 | 0.032* |
| C4 | 1.1029 (2) | 0.28096 (15) | 0.82566 (13) | 0.0251 (3) |
| N2 | 1.24219 (18) | 0.38985 (13) | 0.90484 (11) | 0.0277 (3) |
| N3 | 1.3510 (2) | 0.62546 (13) | 0.98728 (12) | 0.0346 (3) |
| H3A | 1.3357 | 0.7058 | 0.9951 | 0.052* |
| H3B | 1.4575 | 0.6189 | 1.0276 | 0.052* |
| C5 | 0.7267 (2) | 0.44012 (15) | 0.72488 (13) | 0.0250 (3) |
| C6 | 0.5714 (2) | 0.34812 (16) | 0.62920 (14) | 0.0282 (3) |
| C7 | 0.4022 (2) | 0.37506 (19) | 0.59430 (17) | 0.0387 (4) |
| H7 | 0.2980 | 0.3120 | 0.5314 | 0.046* |
| C8 | 0.3857 (3) | 0.49308 (19) | 0.65090 (18) | 0.0425 (4) |
| H8 | 0.2704 | 0.5100 | 0.6267 | 0.051* |
| C9 | 0.5371 (3) | 0.58643 (18) | 0.74266 (17) | 0.0382 (4) |
| H9 | 0.5269 | 0.6681 | 0.7803 | 0.046* |
| C10 | 0.7041 (2) | 0.55922 (17) | 0.77906 (15) | 0.0311 (4) |
| H10 | 0.8063 | 0.6230 | 0.8426 | 0.037* |
| O1 | 0.59265 (17) | 0.23350 (12) | 0.57163 (11) | 0.0385 (3) |
| C11 | 0.4395 (3) | 0.14655 (19) | 0.46928 (17) | 0.0456 (5) |
| H11A | 0.3258 | 0.0969 | 0.4961 | 0.068* |
| H11B | 0.4809 | 0.0788 | 0.4292 | 0.068* |
| H11C | 0.4079 | 0.2049 | 0.4130 | 0.068* |
| C12 | 1.1292 (2) | 0.14340 (15) | 0.81773 (14) | 0.0253 (3) |
| C13 | 1.0781 (2) | 0.05546 (16) | 0.70723 (14) | 0.0269 (3) |
| H13 | 1.0340 | 0.0843 | 0.6351 | 0.032* |
| C14 | 1.0924 (2) | −0.07653 (16) | 0.70354 (14) | 0.0259 (3) |
| C15 | 1.1509 (2) | −0.12181 (16) | 0.80938 (14) | 0.0268 (3) |
| H15 | 1.1533 | −0.2130 | 0.8067 | 0.032* |
| C16 | 1.2062 (2) | −0.03059 (15) | 0.91990 (13) | 0.0260 (3) |
| C17 | 1.1975 (2) | 0.10205 (15) | 0.92550 (14) | 0.0259 (3) |
| H17 | 1.2368 | 0.1635 | 1.0004 | 0.031* |
| O2 | 1.04676 (17) | −0.15512 (12) | 0.59013 (10) | 0.0349 (3) |
| C18 | 1.0753 (3) | −0.28546 (17) | 0.58342 (16) | 0.0358 (4) |
| H18A | 1.2073 | −0.2692 | 0.6273 | 0.054* |
| H18B | 1.0534 | −0.3259 | 0.4991 | 0.054* |
| H18C | 0.9848 | −0.3500 | 0.6193 | 0.054* |
| O3 | 1.26833 (17) | −0.08393 (11) | 1.01866 (10) | 0.0348 (3) |
| C19 | 1.3421 (2) | 0.00789 (18) | 1.13319 (14) | 0.0347 (4) |
| H19A | 1.4454 | 0.0932 | 1.1287 | 0.052* |
| H19B | 1.3926 | −0.0386 | 1.1942 | 0.052* |
| H19C | 1.2386 | 0.0318 | 1.1549 | 0.052* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0294 (8) | 0.0204 (8) | 0.0277 (8) | 0.0096 (6) | 0.0031 (6) | 0.0041 (6) |
| N1 | 0.0291 (7) | 0.0207 (7) | 0.0298 (7) | 0.0095 (5) | 0.0008 (5) | 0.0032 (5) |
| C2 | 0.0261 (8) | 0.0215 (7) | 0.0248 (7) | 0.0094 (6) | 0.0052 (6) | 0.0062 (6) |
| C3 | 0.0278 (8) | 0.0191 (7) | 0.0279 (8) | 0.0082 (6) | −0.0010 (6) | 0.0012 (6) |
| C4 | 0.0281 (8) | 0.0193 (7) | 0.0263 (8) | 0.0091 (6) | 0.0031 (6) | 0.0044 (6) |
| N2 | 0.0287 (7) | 0.0199 (6) | 0.0308 (7) | 0.0098 (5) | −0.0007 (5) | 0.0034 (5) |
| N3 | 0.0339 (8) | 0.0200 (7) | 0.0398 (8) | 0.0102 (6) | −0.0078 (6) | −0.0023 (6) |
| C5 | 0.0266 (8) | 0.0226 (8) | 0.0273 (8) | 0.0102 (6) | 0.0069 (6) | 0.0081 (6) |
| C6 | 0.0277 (8) | 0.0245 (8) | 0.0325 (8) | 0.0116 (6) | 0.0051 (7) | 0.0044 (7) |
| C7 | 0.0282 (9) | 0.0333 (9) | 0.0487 (11) | 0.0128 (7) | −0.0018 (8) | 0.0019 (8) |
| C8 | 0.0303 (9) | 0.0382 (10) | 0.0622 (12) | 0.0209 (8) | 0.0055 (8) | 0.0074 (9) |
| C9 | 0.0394 (10) | 0.0306 (9) | 0.0494 (11) | 0.0201 (8) | 0.0113 (8) | 0.0036 (8) |
| C10 | 0.0333 (9) | 0.0261 (8) | 0.0336 (9) | 0.0129 (7) | 0.0058 (7) | 0.0043 (7) |
| O1 | 0.0339 (7) | 0.0347 (7) | 0.0396 (7) | 0.0182 (5) | −0.0071 (5) | −0.0095 (5) |
| C11 | 0.0466 (11) | 0.0345 (10) | 0.0433 (10) | 0.0166 (9) | −0.0108 (9) | −0.0062 (8) |
| C12 | 0.0223 (7) | 0.0183 (7) | 0.0320 (8) | 0.0073 (6) | 0.0007 (6) | 0.0039 (6) |
| C13 | 0.0273 (8) | 0.0232 (8) | 0.0279 (8) | 0.0102 (6) | 0.0001 (6) | 0.0061 (6) |
| C14 | 0.0236 (8) | 0.0228 (8) | 0.0276 (8) | 0.0089 (6) | 0.0006 (6) | 0.0003 (6) |
| C15 | 0.0264 (8) | 0.0189 (7) | 0.0334 (8) | 0.0103 (6) | 0.0022 (6) | 0.0032 (6) |
| C16 | 0.0248 (8) | 0.0226 (8) | 0.0289 (8) | 0.0092 (6) | 0.0021 (6) | 0.0068 (6) |
| C17 | 0.0242 (7) | 0.0215 (8) | 0.0274 (8) | 0.0078 (6) | −0.0002 (6) | 0.0010 (6) |
| O2 | 0.0477 (7) | 0.0272 (6) | 0.0286 (6) | 0.0197 (5) | 0.0010 (5) | −0.0009 (5) |
| C18 | 0.0431 (10) | 0.0292 (9) | 0.0380 (9) | 0.0204 (8) | 0.0075 (8) | −0.0001 (7) |
| O3 | 0.0471 (7) | 0.0255 (6) | 0.0279 (6) | 0.0162 (5) | −0.0027 (5) | 0.0050 (5) |
| C19 | 0.0373 (9) | 0.0333 (9) | 0.0275 (8) | 0.0111 (7) | 0.0001 (7) | 0.0047 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.3428 (19) | O1—C11 | 1.427 (2) |
| C1—N3 | 1.3453 (19) | C11—H11A | 0.9700 |
| C1—N2 | 1.3497 (19) | C11—H11B | 0.9700 |
| N1—C2 | 1.3395 (19) | C11—H11C | 0.9700 |
| C2—C3 | 1.392 (2) | C12—C13 | 1.379 (2) |
| C2—C5 | 1.492 (2) | C12—C17 | 1.400 (2) |
| C3—C4 | 1.388 (2) | C13—C14 | 1.394 (2) |
| C3—H3 | 0.9400 | C13—H13 | 0.9400 |
| C4—N2 | 1.3349 (19) | C14—O2 | 1.3702 (18) |
| C4—C12 | 1.489 (2) | C14—C15 | 1.382 (2) |
| N3—H3A | 0.8700 | C15—C16 | 1.391 (2) |
| N3—H3B | 0.8700 | C15—H15 | 0.9400 |
| C5—C10 | 1.397 (2) | C16—O3 | 1.3704 (17) |
| C5—C6 | 1.406 (2) | C16—C17 | 1.382 (2) |
| C6—O1 | 1.3675 (19) | C17—H17 | 0.9400 |
| C6—C7 | 1.390 (2) | O2—C18 | 1.4246 (18) |
| C7—C8 | 1.375 (2) | C18—H18A | 0.9700 |

| | | | |
|---|---|---|---|
| C7—H7 | 0.9400 | C18—H18B | 0.9700 |
| C8—C9 | 1.374 (3) | C18—H18C | 0.9700 |
| C8—H8 | 0.9400 | O3—C19 | 1.4199 (19) |
| C9—C10 | 1.378 (2) | C19—H19A | 0.9700 |
| C9—H9 | 0.9400 | C19—H19B | 0.9700 |
| C10—H10 | 0.9400 | C19—H19C | 0.9700 |

| | | | |
|---|---|---|---|
| N1—C1—N3 | 116.69 (13) | O1—C11—H11B | 109.5 |
| N1—C1—N2 | 126.16 (14) | H11A—C11—H11B | 109.5 |
| N3—C1—N2 | 117.15 (13) | O1—C11—H11C | 109.5 |
| C2—N1—C1 | 117.58 (13) | H11A—C11—H11C | 109.5 |
| N1—C2—C3 | 120.33 (13) | H11B—C11—H11C | 109.5 |
| N1—C2—C5 | 114.92 (13) | C13—C12—C17 | 120.67 (14) |
| C3—C2—C5 | 124.63 (14) | C13—C12—C4 | 120.77 (13) |
| C4—C3—C2 | 117.65 (14) | C17—C12—C4 | 118.48 (14) |
| C4—C3—H3 | 121.2 | C12—C13—C14 | 119.40 (14) |
| C2—C3—H3 | 121.2 | C12—C13—H13 | 120.3 |
| N2—C4—C3 | 122.85 (14) | C14—C13—H13 | 120.3 |
| N2—C4—C12 | 116.92 (13) | O2—C14—C15 | 123.43 (13) |
| C3—C4—C12 | 120.12 (13) | O2—C14—C13 | 115.83 (13) |
| C4—N2—C1 | 115.26 (13) | C15—C14—C13 | 120.73 (14) |
| C1—N3—H3A | 120.0 | C14—C15—C16 | 119.08 (14) |
| C1—N3—H3B | 120.0 | C14—C15—H15 | 120.5 |
| H3A—N3—H3B | 120.0 | C16—C15—H15 | 120.5 |
| C10—C5—C6 | 117.11 (14) | O3—C16—C17 | 124.54 (14) |
| C10—C5—C2 | 117.29 (14) | O3—C16—C15 | 114.35 (13) |
| C6—C5—C2 | 125.53 (14) | C17—C16—C15 | 121.11 (13) |
| O1—C6—C7 | 121.48 (14) | C16—C17—C12 | 118.91 (14) |
| O1—C6—C5 | 118.28 (13) | C16—C17—H17 | 120.5 |
| C7—C6—C5 | 120.23 (15) | C12—C17—H17 | 120.5 |
| C8—C7—C6 | 120.64 (16) | C14—O2—C18 | 116.94 (12) |
| C8—C7—H7 | 119.7 | O2—C18—H18A | 109.5 |
| C6—C7—H7 | 119.7 | O2—C18—H18B | 109.5 |
| C9—C8—C7 | 120.26 (16) | H18A—C18—H18B | 109.5 |
| C9—C8—H8 | 119.9 | O2—C18—H18C | 109.5 |
| C7—C8—H8 | 119.9 | H18A—C18—H18C | 109.5 |
| C8—C9—C10 | 119.40 (16) | H18B—C18—H18C | 109.5 |
| C8—C9—H9 | 120.3 | C16—O3—C19 | 117.23 (12) |
| C10—C9—H9 | 120.3 | O3—C19—H19A | 109.5 |
| C9—C10—C5 | 122.32 (16) | O3—C19—H19B | 109.5 |
| C9—C10—H10 | 118.8 | H19A—C19—H19B | 109.5 |
| C5—C10—H10 | 118.8 | O3—C19—H19C | 109.5 |
| C6—O1—C11 | 117.68 (13) | H19A—C19—H19C | 109.5 |
| O1—C11—H11A | 109.5 | H19B—C19—H19C | 109.5 |

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|---|---|---|---|
| N3—C1—N1—C2 | 178.82 (14) | C6—C5—C10—C9 | 0.8 (2) |
| N2—C1—N1—C2 | −1.4 (2) | C2—C5—C10—C9 | −176.38 (15) |
| C1—N1—C2—C3 | −2.6 (2) | C7—C6—O1—C11 | 3.7 (2) |

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|---|---|---|---|
| C1—N1—C2—C5 | 173.46 (13) | C5—C6—O1—C11 | −175.69 (15) |
| N1—C2—C3—C4 | 4.4 (2) | N2—C4—C12—C13 | −140.95 (15) |
| C5—C2—C3—C4 | −171.27 (14) | C3—C4—C12—C13 | 42.5 (2) |
| C2—C3—C4—N2 | −2.4 (2) | N2—C4—C12—C17 | 42.3 (2) |
| C2—C3—C4—C12 | 173.89 (14) | C3—C4—C12—C17 | −134.23 (16) |
| C3—C4—N2—C1 | −1.2 (2) | C17—C12—C13—C14 | 0.9 (2) |
| C12—C4—N2—C1 | −177.64 (13) | C4—C12—C13—C14 | −175.80 (14) |
| N1—C1—N2—C4 | 3.3 (2) | C12—C13—C14—O2 | −177.38 (13) |
| N3—C1—N2—C4 | −176.92 (14) | C12—C13—C14—C15 | 2.2 (2) |
| N1—C2—C5—C10 | −13.77 (19) | O2—C14—C15—C16 | 175.90 (14) |
| C3—C2—C5—C10 | 162.12 (14) | C13—C14—C15—C16 | −3.6 (2) |
| N1—C2—C5—C6 | 169.36 (14) | C14—C15—C16—O3 | −177.70 (14) |
| C3—C2—C5—C6 | −14.8 (2) | C14—C15—C16—C17 | 2.1 (2) |
| C10—C5—C6—O1 | 177.62 (14) | O3—C16—C17—C12 | −179.36 (14) |
| C2—C5—C6—O1 | −5.5 (2) | C15—C16—C17—C12 | 0.9 (2) |
| C10—C5—C6—C7 | −1.8 (2) | C13—C12—C17—C16 | −2.4 (2) |
| C2—C5—C6—C7 | 175.08 (15) | C4—C12—C17—C16 | 174.36 (14) |
| O1—C6—C7—C8 | −178.07 (16) | C15—C14—O2—C18 | −4.5 (2) |
| C5—C6—C7—C8 | 1.3 (3) | C13—C14—O2—C18 | 175.04 (14) |
| C6—C7—C8—C9 | 0.3 (3) | C17—C16—O3—C19 | −4.9 (2) |
| C7—C8—C9—C10 | −1.3 (3) | C15—C16—O3—C19 | 174.89 (13) |
| C8—C9—C10—C5 | 0.8 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*B*···N2$^{i}$ | 0.87 | 2.28 | 3.1374 (19) | 167 |
| N3—H3*A*···O3$^{ii}$ | 0.87 | 2.39 | 3.2545 (17) | 175 |

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