



Synthesis, crystal structure and Hirshfeld surface analysis of [1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl]methyl 2-(4-nitrophenoxy)acetate

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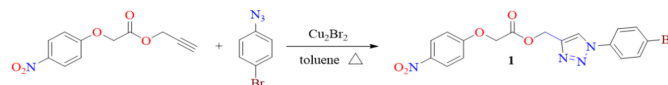
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The title compound, C₁₇H₁₃BrN₄O₅, was synthesized by a Cu₂Br₂-catalysed Meldal–Sharpless reaction between 4-nitrophenoxyacetic acid propargyl ether and *para*-bromophenylazide, and characterized by X-ray structure determination and ¹H NMR spectroscopy. The molecules, with a near-perpendicular orientation of the bromophenyl-triazole and nitrophenoxyacetate fragments, are connected into a three-dimensional network by intermolecular C–H···O and C–H···N hydrogen bonds (confirmed by Hirshfeld surface analysis), π–π and Br–π interactions.

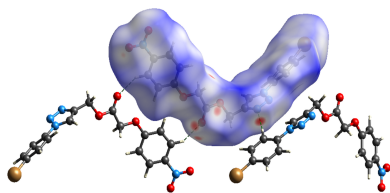
1. Chemical context

1,3-Dipolar cycloaddition, a reaction between a 1,3-dipole and a dipolarophile to generate a five-membered ring, has been known since the early 20th century, following the discovery of 1,3-dipoles; its mechanism was studied and synthetic applications were developed in the 1960s, primarily through the work of Rolf Huisgen (Bertrand *et al.*, 1994; Huisgen, 1963). Meldal and Sharpless independently developed a copper(I)-catalysed version of the Huisgen cycloaddition reaction (Tornøe *et al.*, 2002; Rostovtsev *et al.*, 2002), which earned the name of ‘click chemistry’ for its versatility. They found that only one isomer, 1,4-disubstituted 1,2,3-triazole, was formed from the cycloaddition of terminal alkyne and organic azides under these conditions. The mechanism of the reaction and the role of the Cu^I salt were fully explained. Currently, 1,2,3-triazole derivatives are researched intensively because of their pharmacological and biological activity (Borgati *et al.*, 2013; Bozorov *et al.*, 2019; Faraz *et al.*, 2017; Li *et al.*, 2015). In the course these studies, we prepared the title compound **1** by the cross-ring reaction of 4-nitrophenoxyacetic acid propargyl ether with *para*-bromophenylazide and characterized it by single-crystal X-ray diffraction and NMR spectroscopy.



2. Structural commentary

Compound **1** crystallizes in the monoclinic space group *P*2₁/*n*, the asymmetric unit comprising one molecule (Fig. 1) which contains five planar fragments, namely a bromophenyl group,



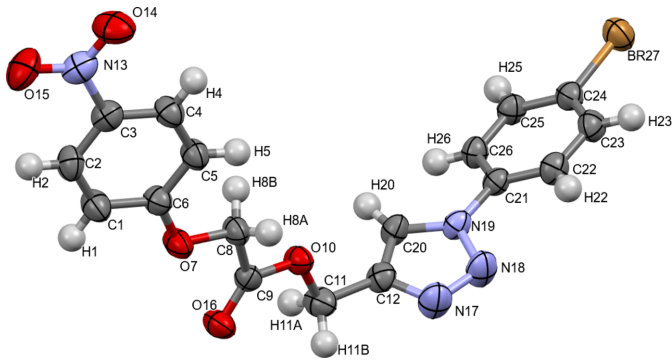


Figure 1
The molecular structure of **1** with displacement ellipsoids drawn at the 50% probability level.

a 1-*H*-1,2,3-triazole ring, a CH₂OC(=O)CH₂O bridge, phenyl and nitro groups. The interplanar angles between adjacent fragments in this succession are 23.5 (1), 80.3 (1), 19.3 (1) and 6.0 (2)[°], respectively. The N17–C12–C11–O10 torsion angle is 97.3 (3)[°].

3. Supramolecular features

Although the structure contains no classical strong hydrogen bonds, some intermolecular C–H···O and C–H···N contacts (Table 1) can be identified as hydrogen bonds by Hirshfeld surface analysis (*vide infra*). They link the molecules into a three-dimensional network (Fig. 2), complemented by π – π stacking between the triazole ring and the brominated phenyl ring [interplanar angle of 8.76 (15)[°], Cg1···Cg2 distance of 3.723 (16) Å and slippage of 0.917 Å], as well as C24–Br27··· π interactions [Br27···Cg2 = 3.787 (11) Å] involving the same phenyl ring.

4. Hirshfeld surface analysis

A Hirshfeld surface analysis was performed using *Crystal-Explorer21* (Spackman *et al.*, 2021). The Hirshfeld surface of

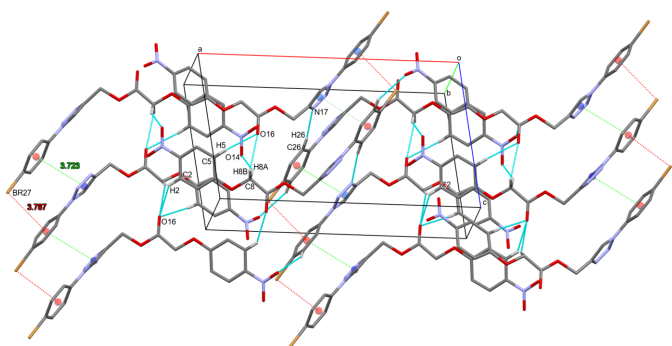


Figure 2
Crystal packing of **1**, showing hydrogen bonds, π – π and Br– π interactions as blue, green and red dotted lines, respectively. The centroids of the triazole (Cg1) and brominated phenyl (Cg2) rings are shown by blue and red circles, respectively. H atoms not participating in hydrogen bonds are omitted.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C26–H26···N17 ⁱ	0.93	2.54	3.463 (3)	173
C5–H5···O16 ⁱⁱ	0.93	2.56	3.493 (3)	176
C8–H8A···O16 ⁱⁱ	0.97	2.51	3.195 (3)	128
C8–H8B···O14 ⁱⁱⁱ	0.97	2.54	3.427 (3)	153
C2–H2···O16 ^{iv}	0.93	2.52	3.287 (3)	140

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

molecule **1** mapped over d_{norm} is shown in Fig. 3. The C–H···O and C–H···N contacts are represented by red spots on the d_{norm} surface, indicating close interactions (hydrogen bonds). The 2D fingerprint plots (McKinnon *et al.*, 2007), show that intermolecular H···H and O···H/H···O contacts make the largest contributions to the total Hirshfeld surface, 23.2% and 25.7%, respectively, other significant contributions being N···H/H···N (11.7%), Br···H/H···Br (5.6%) and C···H/H···C (11.1%) (Fig. 4). The characteristic ‘spikes’ in the N···H/H···N and especially O···H/H···O plots are also indicative of hydrogen bonds.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, last update November 2022; Groom *et al.*, 2016)

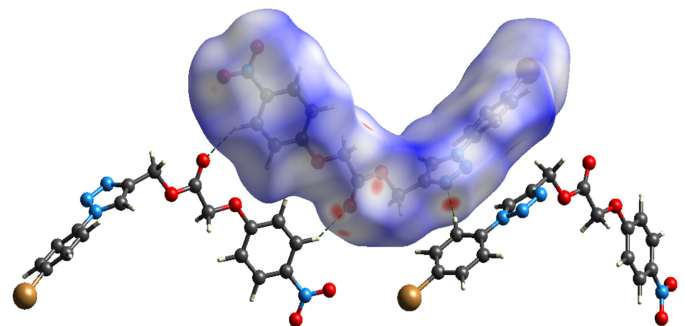


Figure 3
Hirshfeld surface of **1** mapped over d_{norm} and close intermolecular contacts.

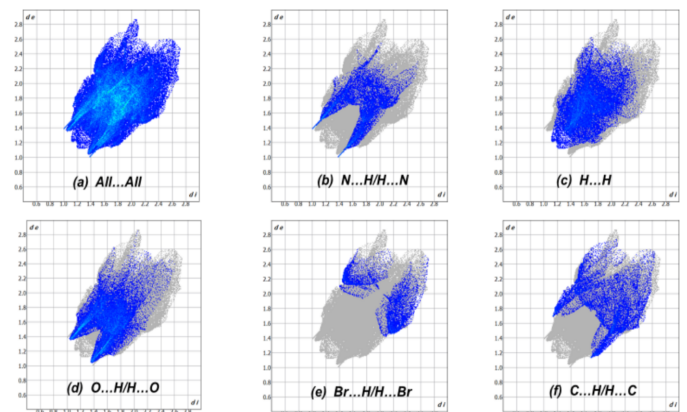


Figure 4
Two-dimensional fingerprint plots of the intermolecular contacts in **1**.

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₇ H ₁₃ BrN ₄ O ₅
<i>M</i> _r	433.22
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	17.3468 (3), 10.40583 (19), 9.87841 (16)
β (°)	99.4243 (16)
<i>V</i> (Å ³)	1759.07 (5)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	3.54
Crystal size (mm)	0.6 × 0.4 × 0.2
Data collection	
Diffraction	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2020)
<i>T</i> _{min} , <i>T</i> _{max}	0.654, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	16655, 3401, 2758
<i>R</i> _{int}	0.044
(sin θ/λ) _{max} (Å ⁻¹)	0.616
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.035, 0.094, 1.06
No. of reflections	3401
No. of parameters	244
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.27, -0.53

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT2014I* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

for the 1-(4-bromophenyl)-1*H*-1,2,3-triazole unit, resulted in four hits, CSD refcodes CEWMID (Tireli *et al.*, 2017), HEHNAL (Boechat *et al.*, 2012), HOHVAD01 (Li *et al.*, 2015) and XABPIC (Singh *et al.*, 2013). In these structures, the dihedral angles between the bromophenyl and triazole rings are comparable to those in the title compound.

6. Synthesis and crystallization

Synthesis of 1.

1.00 g (5 mmol) of *para*-bromophenylazide, 1.175 g (5 mmol) of prop-2-yn-1-yl-2-(4-nitrophenoxy) acetate, 0.10 g (0.32 mmol) of CuBr and 30 ml of toluene were placed into a flask with a reflux condenser, which was heated on an oil bath at the boiling point of toluene (383 K) for 6 h. The progress of the reaction was monitored by thin-layer chromatography. Over time, a precipitate began to form in the reaction mixture. After 6 h, the reaction was stopped and it was left overnight at room temperature. The precipitate was filtered, dried and recrystallized from ethanol, yielding 1.717 g (79.3%) of **1**, m.p. 417–419 K, *R*_f = 0.55 (system benzene:methanol, 10:1). Colourless single crystals suitable for X-ray diffraction analysis were grown from ethanol at room temperature over two weeks.

In the ¹H NMR spectrum (Fig. S1) of **1** in CDCl₃ the protons of the methylene groups C8H₂ and C11H₂ (see atom numbering in Fig. 1) showed as 2H singlets at 4.76 and 5.43 ppm, respectively. Protons H1 and H5 of the 4-nitrophenoxy

group gave a 2H doublet (*J* = 9.35 Hz) at 6.94 ppm, H2 and H4 a 2H doublet at 8.18 ppm (*J* = 9.2 Hz). Protons H22 and H26 of the 4-bromophenyl group give a 2H doublet (*J* = 9.1 Hz) at 7.59 ppm, H23 and H25 a 2H doublet at 7.66 ppm (*J* = 9.0 Hz). The sole proton of the triazole moiety shows a singlet signal at 8.03 ppm.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C were positioned geometrically, with C–H = 0.93 Å for aromatic or C–H = 0.97 Å for methylene C atoms, and were refined as riding with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Acknowledgements

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Synthesis, crystal structure and Hirshfeld surface analysis of [1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl]methyl 2-(4-nitrophenoxy)acetate

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Computing details

[1-(4-Bromophenyl)-1*H*-1,2,3-triazol-4-yl]methyl 2-(4-nitrophenoxy)acetate

Crystal data

$C_{17}H_{13}BrN_4O_5$

$M_r = 433.22$

Monoclinic, $P2_1/c$

$a = 17.3468$ (3) Å

$b = 10.40583$ (19) Å

$c = 9.87841$ (16) Å

$\beta = 99.4243$ (16)°

$V = 1759.07$ (5) Å³

$Z = 4$

$F(000) = 872$

$D_x = 1.636$ Mg m⁻³

Melting point: 419 K

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 5570 reflections

$\theta = 2.6$ – 70.8 °

$\mu = 3.54$ mm⁻¹

$T = 293$ K

Prism, colourless

$0.6 \times 0.4 \times 0.2$ mm

Data collection

XtaLAB Synergy, Single source at home/near,

HyPix3000

diffractometer

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2020)

$T_{\min} = 0.654$, $T_{\max} = 1.000$

16655 measured reflections

3401 independent reflections

2758 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 71.6$ °, $\theta_{\min} = 2.6$ °

$h = -21 \rightarrow 21$

$k = -12 \rightarrow 11$

$l = -11 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.094$

$S = 1.06$

3401 reflections

244 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

$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.3925P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.27$ e Å⁻³

$\Delta\rho_{\min} = -0.53$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br27	0.23315 (2)	0.34083 (3)	0.13747 (3)	0.05876 (13)
C25	0.33490 (14)	0.4068 (2)	0.3824 (3)	0.0435 (5)
H25	0.312633	0.487975	0.368205	0.052*
O10	0.71928 (9)	0.30539 (17)	0.81015 (16)	0.0444 (4)
O7	0.92280 (10)	0.35886 (19)	0.85518 (17)	0.0513 (5)
O16	0.80463 (11)	0.33428 (18)	1.00422 (17)	0.0526 (5)
N19	0.48779 (11)	0.24275 (18)	0.6241 (2)	0.0393 (4)
O14	1.15099 (13)	0.4209 (2)	0.4317 (2)	0.0723 (6)
O15	1.21345 (13)	0.5260 (2)	0.6045 (3)	0.0725 (6)
N18	0.50303 (15)	0.1230 (2)	0.6747 (3)	0.0599 (6)
N13	1.15860 (13)	0.4594 (2)	0.5506 (3)	0.0531 (6)
N17	0.56280 (15)	0.1328 (2)	0.7739 (3)	0.0629 (7)
C24	0.31006 (14)	0.3080 (2)	0.2928 (2)	0.0423 (5)
C21	0.42602 (13)	0.2639 (2)	0.5120 (2)	0.0377 (5)
C26	0.39253 (14)	0.3849 (2)	0.4926 (3)	0.0413 (5)
H26	0.409094	0.450859	0.554001	0.050*
C9	0.79074 (14)	0.3230 (2)	0.8828 (2)	0.0382 (5)
C3	1.09852 (14)	0.4243 (2)	0.6322 (3)	0.0449 (6)
C6	0.97995 (14)	0.3746 (2)	0.7767 (2)	0.0424 (5)
C20	0.53775 (14)	0.3271 (2)	0.6942 (3)	0.0429 (5)
H20	0.538958	0.415583	0.681321	0.052*
C12	0.58587 (14)	0.2570 (2)	0.7874 (3)	0.0434 (6)
C5	0.97409 (15)	0.3327 (3)	0.6420 (3)	0.0463 (6)
H5	0.930095	0.287661	0.600952	0.056*
C8	0.84817 (14)	0.3220 (3)	0.7848 (2)	0.0441 (6)
H8A	0.850981	0.236529	0.746602	0.053*
H8B	0.831325	0.381126	0.709912	0.053*
C22	0.40085 (15)	0.1648 (2)	0.4226 (3)	0.0441 (6)
H22	0.423542	0.083905	0.436396	0.053*
C23	0.34185 (16)	0.1861 (2)	0.3127 (3)	0.0466 (6)
H23	0.323799	0.119527	0.252980	0.056*
C11	0.65520 (15)	0.2966 (3)	0.8875 (3)	0.0505 (6)
H11A	0.646112	0.379063	0.927913	0.061*
H11B	0.666662	0.233527	0.960297	0.061*
C2	1.10697 (15)	0.4614 (3)	0.7680 (3)	0.0503 (6)
H2	1.152186	0.502689	0.809906	0.060*
C4	1.03377 (15)	0.3580 (2)	0.5696 (3)	0.0470 (6)
H4	1.030331	0.330596	0.479185	0.056*
C1	1.04753 (15)	0.4362 (3)	0.8399 (3)	0.0521 (7)

H1 1.052372 0.460485 0.931496 0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br27	0.0594 (2)	0.0613 (2)	0.05047 (19)	-0.00121 (14)	-0.00636 (14)	-0.00058 (13)
C25	0.0436 (13)	0.0356 (12)	0.0504 (14)	0.0032 (10)	0.0049 (11)	0.0015 (11)
O10	0.0324 (8)	0.0594 (11)	0.0399 (9)	-0.0027 (7)	0.0020 (7)	0.0041 (8)
O7	0.0361 (9)	0.0798 (13)	0.0372 (9)	-0.0098 (8)	0.0034 (7)	-0.0045 (8)
O16	0.0471 (10)	0.0738 (13)	0.0352 (9)	-0.0019 (9)	0.0019 (8)	0.0010 (8)
N19	0.0348 (10)	0.0323 (10)	0.0506 (11)	0.0024 (8)	0.0067 (9)	0.0047 (9)
O14	0.0652 (14)	0.1000 (18)	0.0563 (13)	0.0045 (12)	0.0239 (11)	0.0074 (12)
O15	0.0580 (13)	0.0667 (14)	0.0988 (16)	-0.0162 (11)	0.0307 (12)	-0.0042 (12)
N18	0.0595 (15)	0.0357 (11)	0.0773 (17)	-0.0009 (10)	-0.0099 (12)	0.0114 (11)
N13	0.0463 (13)	0.0515 (13)	0.0643 (15)	0.0071 (10)	0.0171 (11)	0.0111 (11)
N17	0.0587 (15)	0.0465 (13)	0.0766 (17)	0.0007 (11)	-0.0093 (13)	0.0150 (12)
C24	0.0385 (13)	0.0472 (14)	0.0414 (13)	-0.0027 (10)	0.0070 (10)	0.0002 (11)
C21	0.0331 (12)	0.0379 (12)	0.0429 (13)	-0.0016 (9)	0.0090 (10)	0.0016 (10)
C26	0.0402 (13)	0.0347 (12)	0.0484 (14)	-0.0008 (10)	0.0057 (10)	-0.0034 (10)
C9	0.0350 (12)	0.0378 (12)	0.0403 (13)	0.0009 (9)	0.0014 (10)	0.0057 (10)
C3	0.0389 (13)	0.0449 (14)	0.0519 (14)	0.0052 (11)	0.0104 (11)	0.0037 (11)
C6	0.0349 (12)	0.0521 (14)	0.0400 (13)	0.0002 (10)	0.0059 (10)	0.0004 (11)
C20	0.0354 (12)	0.0362 (12)	0.0567 (15)	-0.0028 (10)	0.0058 (11)	0.0029 (11)
C12	0.0333 (12)	0.0481 (14)	0.0496 (14)	0.0001 (10)	0.0094 (10)	0.0033 (11)
C5	0.0384 (13)	0.0558 (16)	0.0430 (13)	-0.0045 (11)	0.0020 (10)	-0.0057 (11)
C8	0.0365 (13)	0.0562 (15)	0.0377 (12)	-0.0058 (11)	0.0007 (10)	-0.0024 (11)
C22	0.0446 (13)	0.0359 (13)	0.0529 (14)	0.0034 (10)	0.0115 (11)	-0.0036 (11)
C23	0.0519 (15)	0.0425 (14)	0.0455 (14)	-0.0045 (11)	0.0084 (12)	-0.0093 (11)
C11	0.0380 (13)	0.0693 (17)	0.0448 (14)	0.0007 (12)	0.0086 (11)	0.0038 (13)
C2	0.0368 (13)	0.0553 (16)	0.0576 (16)	-0.0071 (11)	0.0040 (11)	-0.0067 (13)
C4	0.0441 (14)	0.0547 (16)	0.0422 (13)	0.0015 (12)	0.0071 (11)	-0.0054 (11)
C1	0.0438 (14)	0.0692 (18)	0.0430 (14)	-0.0045 (13)	0.0061 (11)	-0.0098 (13)

Geometric parameters (Å, °)

Br27—C24	1.892 (2)	C9—C8	1.498 (3)
C25—H25	0.9300	C3—C2	1.381 (4)
C25—C24	1.379 (3)	C3—C4	1.376 (4)
C25—C26	1.371 (3)	C6—C5	1.388 (3)
O10—C9	1.339 (3)	C6—C1	1.391 (3)
O10—C11	1.451 (3)	C20—H20	0.9300
O7—C6	1.365 (3)	C20—C12	1.351 (3)
O7—C8	1.418 (3)	C12—C11	1.485 (4)
O16—C9	1.190 (3)	C5—H5	0.9300
N19—N18	1.353 (3)	C5—C4	1.377 (4)
N19—C21	1.426 (3)	C8—H8A	0.9700
N19—C20	1.344 (3)	C8—H8B	0.9700
O14—N13	1.228 (3)	C22—H22	0.9300

O15—N13	1.226 (3)	C22—C23	1.383 (4)
N18—N17	1.309 (3)	C23—H23	0.9300
N13—C3	1.464 (3)	C11—H11A	0.9700
N17—C12	1.353 (3)	C11—H11B	0.9700
C24—C23	1.385 (4)	C2—H2	0.9300
C21—C26	1.387 (3)	C2—C1	1.370 (3)
C21—C22	1.381 (3)	C4—H4	0.9300
C26—H26	0.9300	C1—H1	0.9300
C24—C25—H25	120.1	N17—C12—C11	121.7 (2)
C26—C25—H25	120.1	C20—C12—N17	108.0 (2)
C26—C25—C24	119.8 (2)	C20—C12—C11	130.3 (2)
C9—O10—C11	116.63 (19)	C6—C5—H5	120.2
C6—O7—C8	116.33 (18)	C4—C5—C6	119.6 (2)
N18—N19—C21	120.4 (2)	C4—C5—H5	120.2
C20—N19—N18	109.9 (2)	O7—C8—C9	109.35 (19)
C20—N19—C21	129.7 (2)	O7—C8—H8A	109.8
N17—N18—N19	106.7 (2)	O7—C8—H8B	109.8
O14—N13—C3	118.1 (2)	C9—C8—H8A	109.8
O15—N13—O14	123.6 (2)	C9—C8—H8B	109.8
O15—N13—C3	118.3 (2)	H8A—C8—H8B	108.3
N18—N17—C12	109.5 (2)	C21—C22—H22	120.0
C25—C24—Br27	119.41 (19)	C21—C22—C23	119.9 (2)
C25—C24—C23	121.1 (2)	C23—C22—H22	120.0
C23—C24—Br27	119.47 (19)	C24—C23—H23	120.5
C26—C21—N19	119.5 (2)	C22—C23—C24	119.0 (2)
C22—C21—N19	120.0 (2)	C22—C23—H23	120.5
C22—C21—C26	120.5 (2)	O10—C11—C12	105.9 (2)
C25—C26—C21	119.7 (2)	O10—C11—H11A	110.6
C25—C26—H26	120.2	O10—C11—H11B	110.6
C21—C26—H26	120.2	C12—C11—H11A	110.6
O10—C9—C8	107.9 (2)	C12—C11—H11B	110.6
O16—C9—O10	124.8 (2)	H11A—C11—H11B	108.7
O16—C9—C8	127.3 (2)	C3—C2—H2	120.6
C2—C3—N13	119.6 (2)	C1—C2—C3	118.8 (2)
C4—C3—N13	118.7 (2)	C1—C2—H2	120.6
C4—C3—C2	121.7 (2)	C3—C4—C5	119.4 (2)
O7—C6—C5	124.1 (2)	C3—C4—H4	120.3
O7—C6—C1	115.9 (2)	C5—C4—H4	120.3
C5—C6—C1	120.0 (2)	C6—C1—H1	119.8
N19—C20—H20	127.1	C2—C1—C6	120.4 (2)
N19—C20—C12	105.8 (2)	C2—C1—H1	119.8
C12—C20—H20	127.1		
Br27—C24—C23—C22	176.72 (19)	C21—N19—N18—N17	178.9 (2)
C25—C24—C23—C22	-1.7 (4)	C21—N19—C20—C12	-178.4 (2)
O10—C9—C8—O7	171.6 (2)	C21—C22—C23—C24	1.3 (4)
O7—C6—C5—C4	177.3 (2)	C26—C25—C24—Br27	-177.75 (18)

O7—C6—C1—C2	-177.3 (2)	C26—C25—C24—C23	0.6 (4)
O16—C9—C8—O7	-10.0 (4)	C26—C21—C22—C23	0.1 (4)
N19—N18—N17—C12	0.1 (3)	C9—O10—C11—C12	-171.2 (2)
N19—C21—C26—C25	177.9 (2)	C3—C2—C1—C6	-0.1 (4)
N19—C21—C22—C23	-178.9 (2)	C6—O7—C8—C9	-173.9 (2)
N19—C20—C12—N17	-1.5 (3)	C6—C5—C4—C3	0.2 (4)
N19—C20—C12—C11	176.0 (2)	C20—N19—N18—N17	-1.0 (3)
O14—N13—C3—C2	177.3 (3)	C20—N19—C21—C26	-23.2 (4)
O14—N13—C3—C4	-4.5 (4)	C20—N19—C21—C22	155.8 (2)
O15—N13—C3—C2	-3.1 (4)	C20—C12—C11—O10	-79.9 (3)
O15—N13—C3—C4	175.0 (2)	C5—C6—C1—C2	3.2 (4)
N18—N19—C21—C26	156.9 (2)	C8—O7—C6—C5	-13.6 (4)
N18—N19—C21—C22	-24.1 (3)	C8—O7—C6—C1	166.9 (2)
N18—N19—C20—C12	1.6 (3)	C22—C21—C26—C25	-1.1 (3)
N18—N17—C12—C20	0.9 (3)	C11—O10—C9—O16	-1.6 (4)
N18—N17—C12—C11	-176.8 (2)	C11—O10—C9—C8	176.9 (2)
N13—C3—C2—C1	175.2 (2)	C2—C3—C4—C5	2.9 (4)
N13—C3—C4—C5	-175.2 (2)	C4—C3—C2—C1	-3.0 (4)
N17—C12—C11—O10	97.3 (3)	C1—C6—C5—C4	-3.2 (4)
C24—C25—C26—C21	0.8 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C26—H26...N17 ⁱ	0.93	2.54	3.463 (3)	173
C5—H5...O16 ⁱⁱ	0.93	2.56	3.493 (3)	176
C8—H8 <i>A</i> ...O16 ⁱⁱ	0.97	2.51	3.195 (3)	128
C8—H8 <i>B</i> ...O14 ⁱⁱⁱ	0.97	2.54	3.427 (3)	153
C2—H2...O16 ^{iv}	0.93	2.52	3.287 (3)	140

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