research communications

Crystal structure and Hirshfeld surface analysis of 6-((E)-2-{4-[2-(4-chlorophenyl)-2-oxoethoxy]phenyl}ethenyl)-4,5-dihydropyridazin-3(2H)-one

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The pyridazine ring in the title compound, $C_{20}H_{17}ClN_2O_3$, adopts a screw-boat conformation. The whole molecule is flattened, the dihedral angles subtended by the least-squares plane of the central aromatic ring with those of the terminal benzene and pyridazine rings being 15.18 (19) and 11.23 (19)°, respectively. In the crystal, the molecules are linked by pairs of N—H···O bonds into centrosymmetric dimers and by C—H···π contacts into columns. The results of the Hirshfeld surface analysis show that the most prominent interactions are H···H, accounting for 36.5% of overall crystal packing, and H···O/O···H (18.6% contribution) contacts.

1. Chemical context

Pyridazinone derivatives are a class of nitrogenous hetero-cyclic compounds that have attracted considerable attention because of their prospective pharmacological and medicinal properties as anti-inflammatory (Boukharsa et al., 2018), antitumor (Bouchmaa et al., 2018, 2019), antifungal (Rozada et al., 2020), antidepressant (Boukharsa et al., 2016), anti-tubercular, anticonvulsant (Asif et al., 2020) and antiviral (El-Shanbaky et al., 2021) agents. In addition, pyridazinones demonstrate some interesting physicochemical properties (Daoui et al., 2020a; El Kalai et al., 2021a,b) and some studies have shown that these compounds are good corrosion inhibitors (Chelfi et al., 2020). Encouraged by the bioactivity of these compounds and in a continuation of our studies in the field of the synthesis, molecular structures and Hirshfeld surfaces analyses of new pyridazin-3(2H)-one derivatives (Daoui et al., 2020b, 2021), we report herein the crystal structure and the results of the Hirshfeld surface analysis of 6-((E)-2-{4-[2-(4-chlorophenyl)-2-oxoethoxy]phenyl}ethenyl)-4,5-dihydropyridazin-3(2H)-one.
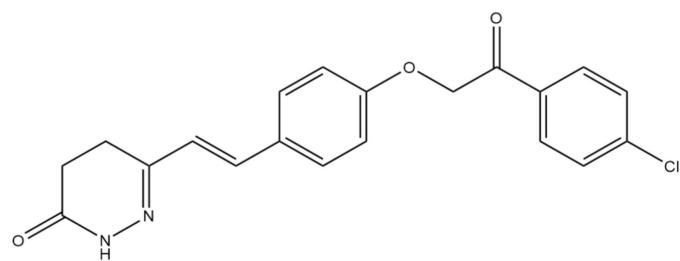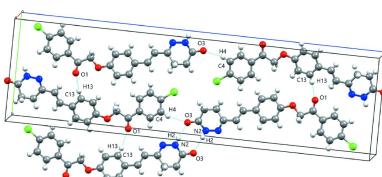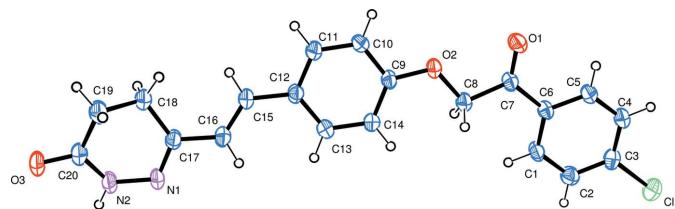
Figure 1
Molecular structure of the title compound showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The molecular structure of the title compound is presented in Fig. 1. The bond lengths in the N1—C15 chain (Table 1) are consistent with an alternation of double and single bonds while those in the amide fragment indicate strong π-conjugation. The N1—N2 distance of 1.406 (4) Å agrees well with the values for related pyridazinones (Daoui, Çınar *et al.*, 2019; Daoui, Baydere *et al.*, 2019). The conformation of the dihydropyridazine ring is close to a screw-boat [$\Theta = 111.9$ (6)°, $\varphi = 34.6$ (6)°]. The whole molecule is flattened with the largest deviations from the least-squares plane of 0.356 (4) and 0.339 (5) Å being observed for atoms C18 and C19, respectively. The central benzene ring forms dihedral angles of 11.23 (19) and 15.18 (19)° with the planes of the terminal dihydropyridazine and benzene rings, respectively.

3. Supramolecular features

In the crystal, the molecules are linked into centrosymmetric dimers by pairs of N—H···O hydrogen bonds, giving rise to an

Table 1
Selected bond lengths (Å).

C20—O3	1.241 (4)	C16—C17	1.459 (4)
N2—C20	1.333 (5)	C15—C16	1.329 (5)
N1—N2	1.406 (4)	C12—C15	1.470 (4)
N1—C17	1.292 (4)	C7—O1	1.219 (4)

Table 2
Hydrogen-bond geometry (Å, °).

$Cg3$ is the centroid of the C9–C14 ring.

| D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.86	2.11	2.891 (4)	151
C4—H4···O3^{ii}	0.93	2.44	3.327 (4)	160
C13—H13···O1^{iii}	0.93	2.53	3.421 (4)	161
C18—H18A···Cl1^{iv}	0.97	2.94	3.737 (3)	140
C8—H8B···$Cg3^{v}$	0.97	2.73	3.514 (3)	138

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

$R_2^2(8)$ graph-set motif (Fig. 2*a*, Table 2). No π–π interactions are present in this structure, but the molecules are connected by weak C—H···π contacts into stacks running along the *a*-axis direction (Fig. 2*b*,*c*, Table 2). Other contacts of the C—H···O and C—H···Cl types further stabilize the crystal structure (Table 2).

4. Hirshfeld surface analysis

In order to visualize and study the intermolecular contacts, a Hirshfeld surface analysis of the title compound was undertaken using *Crystal Explorer 17.5* (Turner *et al.*, 2017). Fig. 3*a* shows the 3D surface mapped over d_{norm} over the range −0.484 (red) to 1.403 (blue) a.u. The pale-red spots on the surface represent short N—H···O and C—H···O interactions (Table 2). The surfaces mapped over d_e and d_i are presented in Fig. 3*b* and 3*c*.

The overall two-dimensional fingerprint plot and those delineated into H···H, H···C/C···H, H···O/O···H, H···Cl/Cl···H and C···C contacts are presented in Fig. 4. H···H

Figure 2
(*a*) A view of the crystal packing of the title compound along the *c* axis. Dashed lines indicate hydrogen bonds. (*b*) C—H···π interactions. (*c*) A view of the molecular stacks running along the *a* axis.
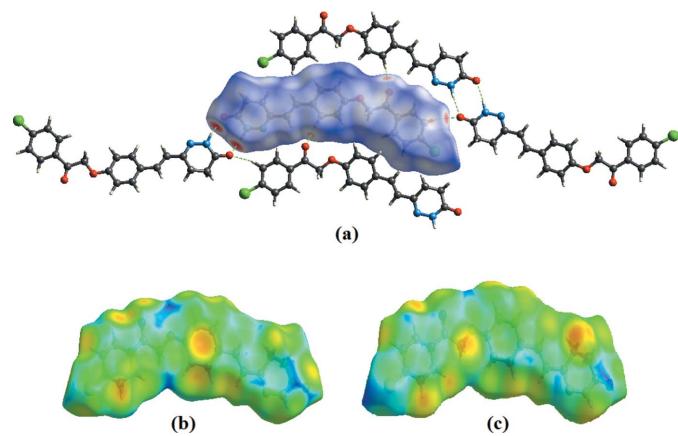
Figure 3
(*a*) Hirshfeld surfaces of the title molecule mapped over (*a*) d_{norm}, (*b*) d_e and (*c*) d_i.
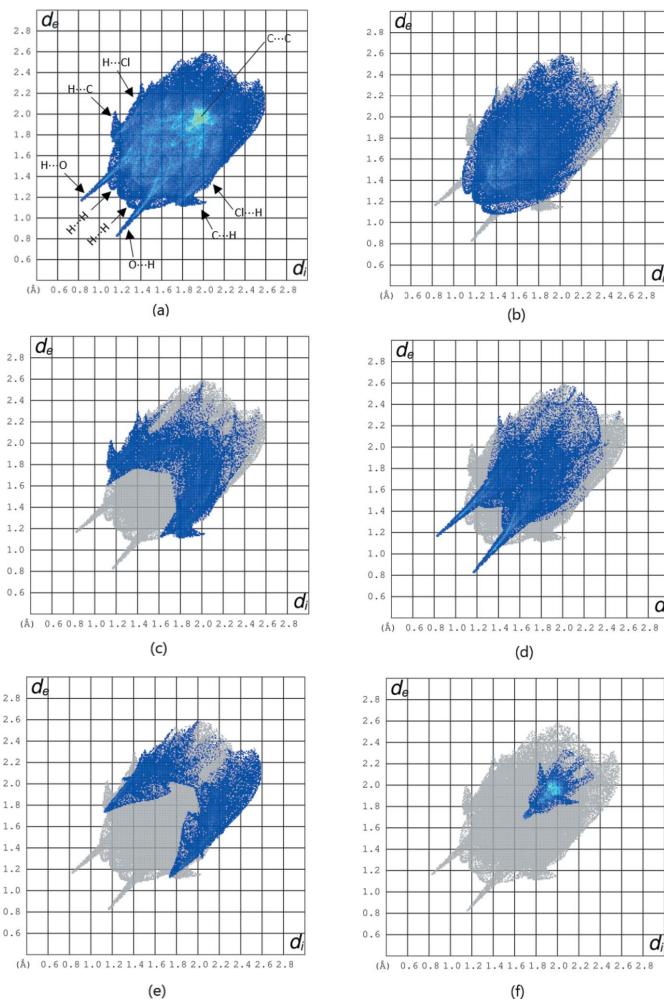
Figure 4
(a) The overall two-dimensional fingerprint plot, and those delineated into (b) H···H, (c) H···C/C···H, (d) H···O/O···H, (e) H···Cl/Cl···H and (f) C···C interactions.

interactions are the most prominent, accounting for 36.5% of the overall crystal packing. H···O/O···H contacts, including intermolecular C—H···O and N—H···O hydrogen bonding, make a 18.6% contribution to the Hirshfeld surface. H···C/C···H contacts add a 15.4% contribution. The contributions from H···Cl/Cl···H and C···C contacts are 11.2% and 7.6%, respectively.

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update March 2020; Groom et al., 2016) revealed two structures containing the same pyridazinone fragments as in the title structure but with different substituents, viz. 6-[(E)-2-(thiophen-2-yl)ethenyl]-4,5-dihydropyridazin-3(2H)-one (MUCLEE; Daoui, Çınar et al., 2019) and (E)-6-(4-hydroxy-3-methoxyphenyl)ethenyl-4,5-dihydropyridazin-3(2H)-one (LOSSOE; Daoui, Baydere et al., 2019). Both these structures exhibit bond lengths in the pyridazine ring and N—H···O

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{17}ClN_2O_3$
M_r	368.80
Crystal system, space group	Orthorhombic, Pbca
Temperature (K)	296
a, b, c (Å)	7.3514 (4), 11.5539 (7), 41.397 (3)
V (Å^3)	3516.2 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.24
Crystal size (mm)	0.45 × 0.20 × 0.05
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (X-RED32; Stoe & Cie, 2002)
T_{min}, T_{max}	0.925, 0.994
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19519, 2913, 1682
R_{int}	0.113
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.584
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.128, 0.99
No. of reflections	2913
No. of parameters	235
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.34, −0.22

Computer programs: X-AREA and X-RED32 (Stoe & Cie, 2002), SHELXT2018/3 (Sheldrick, 2015a), SHELXL2018/3 (Sheldrick, 2015b), OLEX2 (Dolomanov et al., 2009), Mercury (Macrae et al., 2020), WinGX (Farrugia, 2012), PLATON (Spek, 2020) and publCIF (Westrip, 2010).

hydrogen-bonding parameters that are very similar to those observed in the title structure.

6. Synthesis and crystallization

A mixture of (E)-6-(4-hydroxystyryl)-4,5-dihydropyridazin-3(2H)-one (0.5 g, 2.3 mmol), K_2CO_3 (0.79 g, 5.7 mmol) and 2-chloro-1-(4-chlorophenyl)ethan-1-one (0.47 g, 2.5 mmol) in acetone (50 ml) was refluxed overnight. After cooling, the solution was filtered and the solvent removed under reduced pressure. The residue was purified by recrystallization from ethanol to afford single crystals (yield 72%).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were positioned geometrically and treated as riding, with C—H = 0.96 Å for methylene [$U_{iso}(H) = 1.5\ U_{eq}(C)$], C—H = 0.93 Å for aromatic [$U_{iso}(H) = 1.2\ U_{eq}(C)$] and C—H = 0.98 Å for methine [$U_{iso}(H) = 1.2\ U_{eq}(C)$] H atoms.

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supporting information

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT2018/3* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *SHELXL2018/3* (Sheldrick, 2015b), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

6-((*E*)-2-{4-[2-(4-Chlorophenyl)-2-oxoethoxy]phenyl}ethenyl)-4,5-dihydropyridazin-3(2*H*)-one

Crystal data

$C_{20}H_{17}ClN_2O_3$	$D_x = 1.393$ Mg m^{-3}
$M_r = 368.80$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 13252 reflections
$a = 7.3514$ (4) Å	$\theta = 1.0–25.1°$
$b = 11.5539$ (7) Å	$\mu = 0.24$ mm^{-1}
$c = 41.397$ (3) Å	$T = 296$ K
$V = 3516.2$ (4) Å^3	Needle, colorless
$Z = 8$	$0.45 \times 0.20 \times 0.05$ mm
$F(000) = 1536$	

Data collection

STOE IPDS 2 diffractometer	$T_{min} = 0.925$, $T_{max} = 0.994$
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	19519 measured reflections
	2913 independent reflections
Plane graphite monochromator	1682 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.113$
rotation method scans	$\theta_{max} = 24.5°$, $\theta_{min} = 2.0°$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -8 \rightarrow 8$
	$k = -13 \rightarrow 13$
	$l = -48 \rightarrow 48$

Refinement

Refinement on F^2	235 parameters
Least-squares matrix: full	0 restraints
$R[F^2 > 2\sigma(F^2)] = 0.060$	Primary atom site location: structure-invariant direct methods
$wR(F^2) = 0.128$	
$S = 0.99$	Secondary atom site location: difference Fourier map
2913 reflections	

Hydrogen site location: inferred from
  neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.40565 (17)	0.91913 (10)	0.94188 (2)	0.0775 (4)
O2	0.3849 (3)	0.58839 (19)	0.76710 (5)	0.0548 (6)
O1	0.3725 (4)	0.5145 (2)	0.82642 (5)	0.0652 (7)
O3	0.4691 (5)	0.8576 (2)	0.48754 (6)	0.0901 (11)
N1	0.4362 (5)	0.9053 (3)	0.57229 (6)	0.0583 (9)
N2	0.4339 (5)	0.9186 (3)	0.53853 (6)	0.0627 (9)
H2	0.420683	0.987853	0.531280	0.075*
C9	0.3861 (5)	0.6229 (3)	0.73520 (7)	0.0446 (8)
C12	0.3776 (5)	0.6716 (3)	0.66888 (7)	0.0450 (8)
C7	0.3875 (5)	0.6191 (3)	0.82384 (7)	0.0459 (8)
C14	0.4262 (5)	0.7332 (3)	0.72432 (7)	0.0460 (9)
H14	0.455198	0.791510	0.738937	0.055*
C15	0.3713 (5)	0.6918 (3)	0.63384 (7)	0.0485 (9)
H15	0.336983	0.628939	0.621208	0.058*
C8	0.4077 (5)	0.6746 (3)	0.79090 (7)	0.0463 (8)
H8A	0.316866	0.734746	0.788149	0.056*
H8B	0.527120	0.709594	0.788902	0.056*
C10	0.3420 (5)	0.5366 (3)	0.71335 (8)	0.0493 (9)
H10	0.315275	0.462357	0.720621	0.059*
C6	0.3939 (5)	0.6959 (3)	0.85261 (7)	0.0442 (8)
C13	0.4229 (4)	0.7563 (3)	0.69135 (8)	0.0480 (9)
H13	0.451610	0.830326	0.684145	0.058*
C11	0.3378 (5)	0.5613 (3)	0.68064 (8)	0.0495 (9)
H11	0.307759	0.502891	0.666138	0.059*
C17	0.4022 (5)	0.8025 (3)	0.58300 (7)	0.0480 (9)
C16	0.4088 (5)	0.7891 (3)	0.61803 (8)	0.0513 (9)
H16	0.441662	0.853378	0.630205	0.062*
C5	0.3951 (5)	0.6460 (3)	0.88335 (7)	0.0505 (9)
H5	0.395053	0.565786	0.885305	0.061*
C1	0.3956 (5)	0.8158 (3)	0.85007 (8)	0.0507 (9)
H1	0.393722	0.850303	0.829780	0.061*
C4	0.3965 (5)	0.7130 (3)	0.91071 (8)	0.0546 (10)
H4	0.394802	0.678837	0.931046	0.066*
C3	0.4005 (5)	0.8324 (3)	0.90763 (8)	0.0542 (9)

C2	0.4002 (5)	0.8843 (3)	0.87751 (8)	0.0560 (10)
H2A	0.403021	0.964539	0.875701	0.067*
C18	0.3570 (6)	0.7050 (3)	0.56077 (8)	0.0638 (11)
H18A	0.388487	0.632317	0.571073	0.077*
H18B	0.227071	0.704664	0.556707	0.077*
C20	0.4501 (6)	0.8347 (4)	0.51664 (9)	0.0667 (12)
C19	0.4555 (7)	0.7143 (3)	0.52951 (9)	0.0770 (14)
H19A	0.400668	0.662153	0.513941	0.092*
H19B	0.581099	0.690928	0.532538	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1050 (9)	0.0789 (7)	0.0487 (5)	−0.0053 (7)	−0.0003 (6)	−0.0147 (5)
O2	0.0842 (18)	0.0491 (13)	0.0311 (12)	−0.0041 (14)	−0.0035 (13)	0.0037 (11)
O1	0.102 (2)	0.0493 (16)	0.0440 (14)	−0.0081 (15)	0.0098 (15)	0.0043 (12)
O3	0.168 (3)	0.0733 (19)	0.0293 (15)	−0.019 (2)	0.0040 (16)	0.0027 (13)
N1	0.089 (3)	0.058 (2)	0.0279 (14)	−0.0069 (18)	0.0018 (15)	0.0022 (14)
N2	0.101 (3)	0.0548 (18)	0.0319 (15)	−0.0002 (18)	−0.0013 (16)	0.0067 (15)
C9	0.051 (2)	0.052 (2)	0.0315 (17)	−0.0038 (18)	0.0023 (17)	0.0030 (16)
C12	0.050 (2)	0.051 (2)	0.0340 (17)	−0.0002 (18)	0.0026 (16)	−0.0011 (16)
C7	0.051 (2)	0.050 (2)	0.0368 (18)	−0.0005 (18)	0.0030 (18)	0.0056 (15)
C14	0.054 (2)	0.048 (2)	0.0361 (18)	−0.0049 (18)	−0.0008 (16)	0.0006 (16)
C15	0.057 (2)	0.056 (2)	0.0321 (17)	−0.0005 (19)	0.0012 (18)	−0.0004 (16)
C8	0.056 (2)	0.048 (2)	0.0347 (17)	−0.0009 (19)	0.0018 (17)	0.0015 (16)
C10	0.066 (3)	0.0399 (19)	0.0417 (19)	−0.0040 (17)	0.0017 (17)	0.0058 (16)
C6	0.049 (2)	0.049 (2)	0.0346 (17)	0.0001 (18)	0.0049 (17)	0.0051 (15)
C13	0.054 (2)	0.048 (2)	0.0414 (19)	−0.0020 (19)	0.0011 (17)	0.0063 (16)
C11	0.064 (2)	0.049 (2)	0.0351 (18)	−0.0017 (18)	0.0034 (16)	−0.0031 (17)
C17	0.057 (2)	0.053 (2)	0.0349 (17)	0.0009 (19)	−0.0002 (18)	−0.0021 (16)
C16	0.060 (2)	0.059 (2)	0.0347 (18)	−0.004 (2)	0.0018 (19)	−0.0018 (16)
C5	0.063 (2)	0.047 (2)	0.0409 (19)	−0.0010 (19)	−0.0006 (19)	0.0083 (16)
C1	0.070 (3)	0.047 (2)	0.0348 (18)	0.005 (2)	0.0027 (19)	0.0076 (16)
C4	0.069 (3)	0.058 (2)	0.0367 (19)	−0.003 (2)	−0.0005 (19)	0.0076 (16)
C3	0.060 (2)	0.063 (2)	0.0389 (19)	0.002 (2)	0.0005 (19)	−0.0031 (18)
C2	0.071 (3)	0.047 (2)	0.050 (2)	0.001 (2)	0.002 (2)	0.0007 (18)
C18	0.097 (3)	0.057 (2)	0.037 (2)	−0.008 (2)	0.004 (2)	−0.0009 (18)
C20	0.102 (4)	0.065 (3)	0.034 (2)	−0.011 (2)	0.002 (2)	0.001 (2)
C19	0.126 (4)	0.062 (3)	0.043 (2)	−0.006 (3)	0.011 (2)	−0.001 (2)

Geometric parameters (Å, °)

C20—O3	1.241 (4)	C10—C11	1.384 (5)
N2—C20	1.333 (5)	C10—H10	0.9300
N1—N2	1.406 (4)	C6—C1	1.389 (5)
N1—C17	1.292 (4)	C6—C5	1.397 (4)
C16—C17	1.459 (4)	C13—H13	0.9300
C15—C16	1.329 (5)	C11—H11	0.9300

C12—C15	1.470 (4)	C17—C18	1.492 (5)
C7—O1	1.219 (4)	C16—H16	0.9300
Cl1—C3	1.737 (3)	C5—C4	1.373 (5)
O2—C9	1.379 (4)	C5—H5	0.9300
O2—C8	1.411 (4)	C1—C2	1.385 (5)
N2—H2	0.8600	C1—H1	0.9300
C9—C14	1.384 (4)	C4—C3	1.386 (5)
C9—C10	1.385 (4)	C4—H4	0.9300
C12—C13	1.391 (4)	C3—C2	1.383 (5)
C12—C11	1.395 (5)	C2—H2A	0.9300
C7—C6	1.486 (4)	C18—C19	1.487 (5)
C7—C8	1.514 (4)	C18—H18A	0.9700
C14—C13	1.391 (4)	C18—H18B	0.9700
C14—H14	0.9300	C20—C19	1.490 (5)
C15—H15	0.9300	C19—H19A	0.9700
C8—H8A	0.9700	C19—H19B	0.9700
C8—H8B	0.9700		
C9—O2—C8	117.6 (2)	C12—C11—H11	119.2
C17—N1—N2	116.0 (3)	N1—C17—C16	115.6 (3)
C20—N2—N1	126.5 (3)	N1—C17—C18	121.7 (3)
C20—N2—H2	116.7	C16—C17—C18	122.7 (3)
N1—N2—H2	116.7	C15—C16—C17	124.9 (3)
O2—C9—C14	125.4 (3)	C15—C16—H16	117.5
O2—C9—C10	114.6 (3)	C17—C16—H16	117.5
C14—C9—C10	120.0 (3)	C4—C5—C6	121.2 (3)
C13—C12—C11	117.4 (3)	C4—C5—H5	119.4
C13—C12—C15	123.8 (3)	C6—C5—H5	119.4
C11—C12—C15	118.9 (3)	C2—C1—C6	120.5 (3)
O1—C7—C6	121.7 (3)	C2—C1—H1	119.7
O1—C7—C8	120.5 (3)	C6—C1—H1	119.7
C6—C7—C8	117.8 (3)	C5—C4—C3	119.1 (3)
C9—C14—C13	119.5 (3)	C5—C4—H4	120.5
C9—C14—H14	120.3	C3—C4—H4	120.5
C13—C14—H14	120.3	C2—C3—C4	121.0 (3)
C16—C15—C12	127.9 (3)	C2—C3—Cl1	119.1 (3)
C16—C15—H15	116.1	C4—C3—Cl1	120.0 (3)
C12—C15—H15	116.1	C3—C2—C1	119.4 (3)
O2—C8—C7	108.5 (3)	C3—C2—H2A	120.3
O2—C8—H8A	110.0	C1—C2—H2A	120.3
C7—C8—H8A	110.0	C19—C18—C17	112.0 (3)
O2—C8—H8B	110.0	C19—C18—H18A	109.2
C7—C8—H8B	110.0	C17—C18—H18A	109.2
H8A—C8—H8B	108.4	C19—C18—H18B	109.2
C11—C10—C9	119.7 (3)	C17—C18—H18B	109.2
C11—C10—H10	120.1	H18A—C18—H18B	107.9
C9—C10—H10	120.1	O3—C20—N2	121.0 (4)
C1—C6—C5	118.7 (3)	O3—C20—C19	122.9 (4)

C1—C6—C7	122.4 (3)	N2—C20—C19	116.0 (3)
C5—C6—C7	118.9 (3)	C18—C19—C20	111.4 (3)
C12—C13—C14	121.7 (3)	C18—C19—H19A	109.3
C12—C13—H13	119.1	C20—C19—H19A	109.3
C14—C13—H13	119.1	C18—C19—H19B	109.3
C10—C11—C12	121.7 (3)	C20—C19—H19B	109.3
C10—C11—H11	119.2	H19A—C19—H19B	108.0
C17—N1—N2—C20	−19.7 (6)	N2—N1—C17—C16	178.7 (3)
C8—O2—C9—C14	7.0 (5)	N2—N1—C17—C18	−2.0 (5)
C8—O2—C9—C10	−172.8 (3)	C12—C15—C16—C17	179.1 (4)
O2—C9—C14—C13	179.9 (3)	N1—C17—C16—C15	177.3 (4)
C10—C9—C14—C13	−0.4 (5)	C18—C17—C16—C15	−1.9 (6)
C13—C12—C15—C16	1.2 (6)	C1—C6—C5—C4	0.5 (6)
C11—C12—C15—C16	−178.2 (4)	C7—C6—C5—C4	−178.4 (3)
C9—O2—C8—C7	175.7 (3)	C5—C6—C1—C2	0.6 (6)
O1—C7—C8—O2	6.4 (5)	C7—C6—C1—C2	179.5 (3)
C6—C7—C8—O2	−175.9 (3)	C6—C5—C4—C3	−1.3 (6)
O2—C9—C10—C11	179.6 (3)	C5—C4—C3—C2	1.0 (6)
C14—C9—C10—C11	−0.1 (5)	C5—C4—C3—Cl1	−179.1 (3)
O1—C7—C6—C1	−174.5 (4)	C4—C3—C2—C1	0.1 (6)
C8—C7—C6—C1	7.8 (5)	Cl1—C3—C2—C1	−179.8 (3)
O1—C7—C6—C5	4.4 (6)	C6—C1—C2—C3	−0.9 (6)
C8—C7—C6—C5	−173.3 (3)	N1—C17—C18—C19	33.8 (6)
C11—C12—C13—C14	−0.9 (5)	C16—C17—C18—C19	−147.0 (4)
C15—C12—C13—C14	179.7 (3)	N1—N2—C20—O3	−170.9 (4)
C9—C14—C13—C12	0.9 (5)	N1—N2—C20—C19	5.5 (6)
C9—C10—C11—C12	0.2 (6)	C17—C18—C19—C20	−44.6 (5)
C13—C12—C11—C10	0.3 (5)	O3—C20—C19—C18	−156.4 (4)
C15—C12—C11—C10	179.8 (3)	N2—C20—C19—C18	27.3 (6)

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the C9–C14 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H2⋯O3[i]	0.86	2.11	2.891 (4)	151
C4—H4⋯O3[ii]	0.93	2.44	3.327 (4)	160
C13—H13⋯O1[iii]	0.93	2.53	3.421 (4)	161
C18—H18*A*⋯Cl1[iv]	0.97	2.94	3.737 (3)	140
C8—H8*B*⋯*Cg*3[v]	0.97	2.73	3.514 (3)	138

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