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Ethyl 2-cyano-2-{(*Z*)-2-[2,2-dicyano-1-(4-methylphenyl)ethyl]cyclohexylidene}acetate

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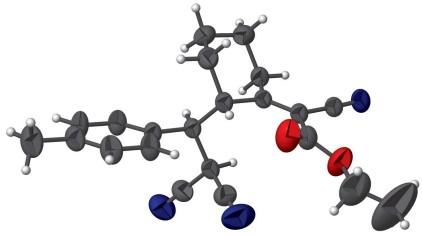
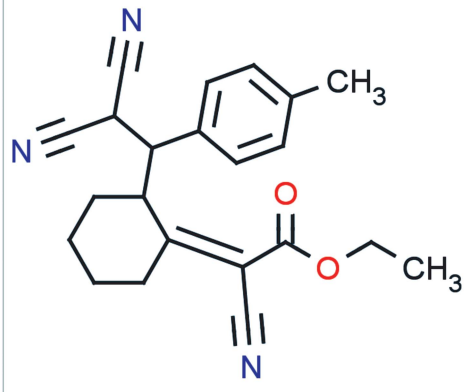
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{23}N_3O_2$, the cyclohexane ring adopts a chair conformation. The methylphenyl ring is oriented at an angle of 36.2 (1)° with respect to the best plane of cyclohexane moiety. In the crystal, molecules associate *via* C—H···N hydrogen bonds, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Cyclohexylidene derivatives possess a wide range of biological activities including antibacterial (Gupta & Narayana, 1997), antiviral (Ulusoy Guzeldemirci *et al.*, 2016), antituberculatic and anti-inflammatory (Kabir *et al.*, 2008). As part of our studies in this area, we have undertaken a single-crystal X-ray diffraction study for the title compound, and the results are presented here.

The methylphenyl ring is oriented at an angle of 36.2 (1)° with respect to the best plane of cyclohexane moiety. The cyclohexane ring adopts a chair conformation, the puckering parameters (Cremer & Pople, 1975) are: q_2 = 0.001 (1) Å, q_3 = −0.562 (2) Å, Q_T = 0.562 (2) Å and θ = 179.0 (1)°. Atoms C1 and C4 deviate by 0.681 (1) and −0.652 (1) Å, respectively, from the least-squares plane through the remaining four atoms. An intramolecular C—H···O hydrogen bond is observed (Table 1), which generates an $S(6)$ ring (Fig. 1).

In the crystal, molecules associate *via* pairwise C5—H5*A*···N1^{i} hydrogen bonds into inversion dimers with an $R_2^2(16)$ loop motif. In addition, C8—H8···N3^{ii} hydrogen bonds form a $R_2^2(16)$ graph-set motif (Fig. 2).

The two-dimensional fingerprint plots (Spackman & Jayatilaka, 2009) of the molecule, created using *Crystal Explorer 17* (Turner *et al.*, 2017) for the contacts contributing to the Hirshfeld surface are shown in Figs. 3–5. The analysis reveals that H···H contacts

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1	0.98	2.23	3.001 (2)	135
C5—H5A···N1^{i}	0.97	2.57	3.536 (3)	172
C8—H8···N3^{ii}	0.98	2.27	3.221 (2)	163

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

(45.7%) and N···H/H···N contacts (29.8%) are the main contributors to the crystal packing, followed by C···H/H···C (14%) and O···H/H···O (7.8%) contacts.

Synthesis and crystallization

A mixture of 2-amino-4-(*p*-tolyl)octahydronaphthalene-1,3,3(2*H*)-tricarbonitrile (0.01 mol), formic acid (5 mL) and a catalytic amount of concentrated HCl was refluxed for 16 h and the reaction mixture was allowed to cool. The reaction mixture was poured onto crushed ice and the solid that separated was filtered, dried and recrystallized using ethanol and water as mixed solvents.

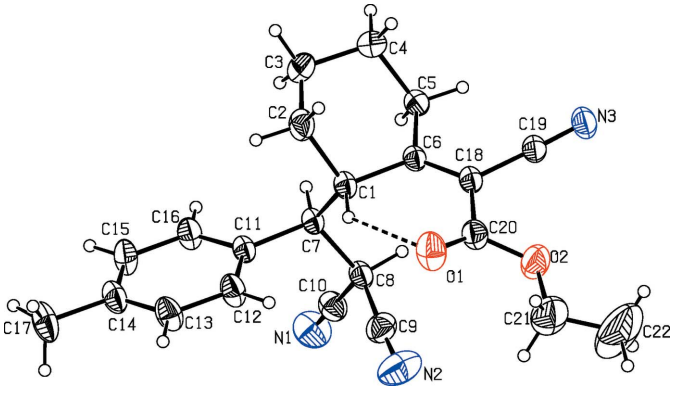


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular C—H···O hydrogen bond is shown as a dashed line.

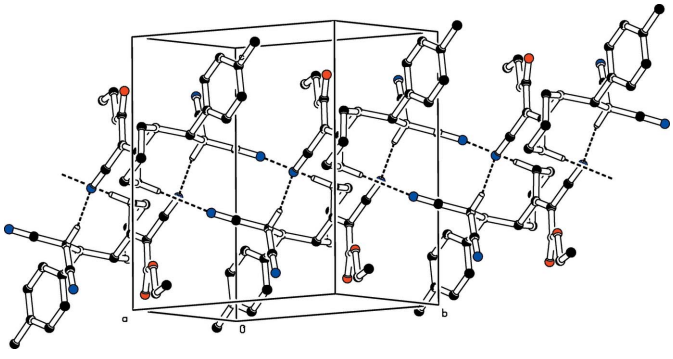


Figure 2
The crystal packing of the title compound viewed down the *a* axis. The C—H···N hydrogen bonds (see Table 1) are shown as dashed lines. For clarity, H atoms not involved in these interactions have been omitted.

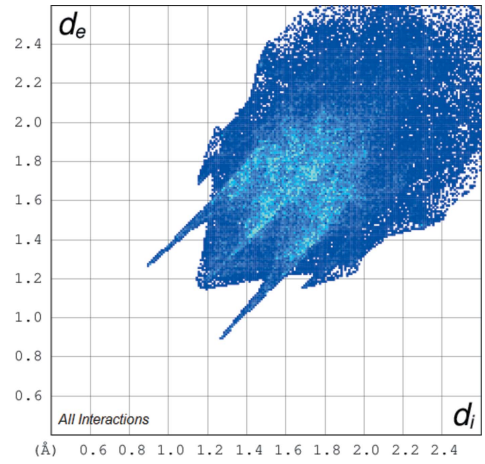


Figure 3
The two-dimensional fingerprint plot for the title compound depicting the overall contribution by the various contacts.

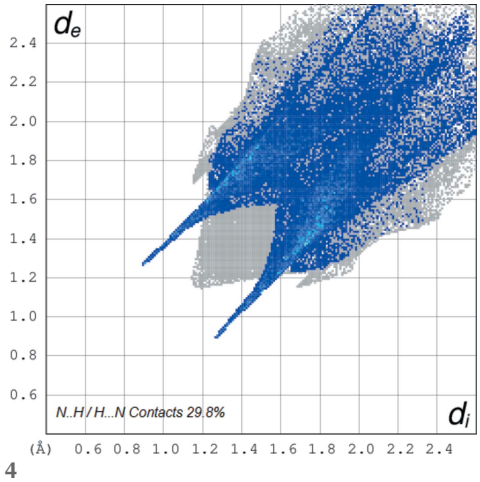


Figure 4
The two-dimensional fingerprint plot for the title compound depicting the contribution of the N···H contacts.

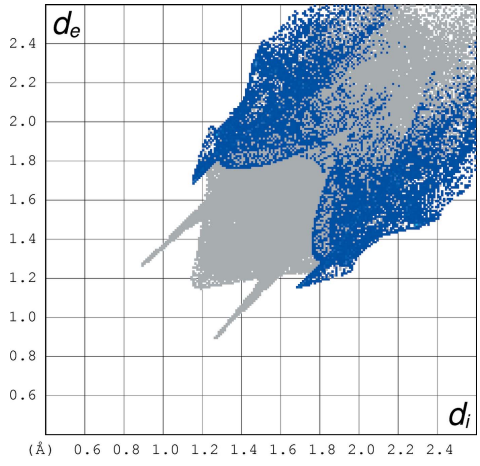


Figure 5
The two-dimensional fingerprint plot for the title compound depicting the contribution of the C···H contacts.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{23}N_3O_2$
M_r	361.43
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.4465 (3), 10.2960 (4), 12.1699 (4)
α, β, γ (°)	91.240 (1), 95.072 (1), 92.102 (1)
V (Å^3)	1053.17 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.24 × 0.21 × 0.19
Data collection	
Diffractometer	Bruker SMART APEX CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28133, 6098, 4212
R_{int}	0.033
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.211, 0.97
No. of reflections	6098
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.31

Computer programs: *SMART* and, *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

Refinement

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

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full crystallographic data

IUCrData (2021). **6**, x210500 [https://doi.org/10.1107/S2414314621005009]

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Ethyl 2-cyano-2-{(*Z*)-2-[2,2-dicyano-1-(4-methylphenyl)ethyl]cyclohexylidene}acetate

Crystal data

$C_{22}H_{23}N_3O_2$
M_r = 361.43
Triclinic, $P\overline{1}$
a = 8.4465 (3) Å
b = 10.2960 (4) Å
c = 12.1699 (4) Å
α = 91.240 (1)°
β = 95.072 (1)°
γ = 92.102 (1)°
V = 1053.17 (7) Å^3
Z = 2
$F(000)$ = 384
D_x = 1.140 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 18428 reflections
θ = 2.8–28.2°
μ = 0.07 mm^{-1}
T = 296 K
Block, colourless
0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
28133 measured reflections
6098 independent reflections
4212 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 30.0°, θ_{min} = 2.6°
h = −11→11
k = −14→14
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.211
S = 0.97
6098 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1037P)^2 + 0.3202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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.

Refinement. H atoms were placed in idealized positions and allowed to ride on their parent atoms: C—H = 0.93–0.98 Å, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.2013 (2)	0.55320 (15)	0.86132 (11)	0.0772 (4)
O2	0.0185 (2)	0.42057 (16)	0.77154 (13)	0.0819 (5)
N1	−0.1230 (3)	1.0587 (2)	0.60489 (18)	0.0857 (6)
N2	−0.0870 (3)	0.7604 (3)	0.8407 (2)	0.1067 (8)
N3	0.11934 (19)	0.34667 (15)	0.52121 (14)	0.0616 (4)
C1	0.30484 (18)	0.75924 (14)	0.70937 (13)	0.0443 (3)
H1	0.285441	0.734845	0.784544	0.053*
C2	0.4861 (2)	0.78324 (19)	0.70392 (18)	0.0628 (5)
H2A	0.521171	0.859385	0.749172	0.075*
H2B	0.541326	0.709455	0.734562	0.075*
C3	0.5315 (2)	0.8033 (2)	0.5874 (2)	0.0732 (6)
H3A	0.486124	0.882452	0.559229	0.088*
H3B	0.646316	0.813127	0.588507	0.088*
C4	0.4726 (2)	0.6896 (2)	0.5118 (2)	0.0700 (5)
H4A	0.528715	0.612669	0.534317	0.084*
H4B	0.495422	0.708172	0.436902	0.084*
C5	0.2929 (2)	0.66303 (15)	0.51486 (13)	0.0489 (4)
H5A	0.235573	0.735033	0.482858	0.059*
H5B	0.260103	0.585006	0.471424	0.059*
C6	0.25320 (16)	0.64621 (13)	0.63136 (12)	0.0411 (3)
C7	0.21454 (17)	0.88396 (13)	0.68062 (12)	0.0417 (3)
H7	0.244434	0.910752	0.608248	0.050*
C8	0.03147 (19)	0.85589 (15)	0.66844 (14)	0.0488 (4)
H8	0.009240	0.789898	0.609301	0.059*
C9	−0.0339 (2)	0.8042 (2)	0.76680 (19)	0.0646 (5)
C10	−0.0551 (2)	0.97122 (18)	0.63408 (15)	0.0576 (4)
C11	0.26493 (18)	0.99501 (14)	0.76145 (12)	0.0440 (3)
C12	0.2656 (3)	0.98255 (17)	0.87475 (14)	0.0602 (5)
H12	0.231616	0.904205	0.903138	0.072*
C13	0.3163 (3)	1.08555 (19)	0.94631 (15)	0.0662 (5)
H13	0.315364	1.074856	1.021940	0.079*
C14	0.3677 (2)	1.20274 (18)	0.90808 (16)	0.0602 (5)
C15	0.3642 (3)	1.21591 (18)	0.79527 (17)	0.0660 (5)
H15	0.397002	1.294798	0.767239	0.079*
C16	0.3129 (2)	1.11375 (16)	0.72261 (15)	0.0563 (4)
H16	0.310842	1.125603	0.646965	0.068*
C17	0.4252 (3)	1.3131 (2)	0.9871 (2)	0.0852 (7)
H17A	0.456292	1.387009	0.946141	0.128*
H17B	0.341186	1.335986	1.031229	0.128*
H17C	0.514778	1.286442	1.034240	0.128*
C18	0.18375 (18)	0.53484 (14)	0.66384 (12)	0.0437 (3)
C19	0.14525 (18)	0.43040 (14)	0.58413 (13)	0.0461 (3)
C20	0.1382 (2)	0.50714 (16)	0.77718 (15)	0.0548 (4)
C21	−0.0385 (4)	0.3775 (3)	0.8773 (3)	0.1121 (11)
H21A	0.051164	0.353762	0.927149	0.135*

H21B	−0.090609	0.448219	0.911649	0.135*
C22	−0.1466 (7)	0.2695 (6)	0.8578 (4)	0.230 (4)
H22A	−0.182981	0.242201	0.926523	0.345*
H22B	−0.235819	0.293629	0.809141	0.345*
H22C	−0.094368	0.199386	0.824606	0.345*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1095 (12)	0.0724 (9)	0.0462 (7)	−0.0169 (8)	−0.0038 (7)	0.0028 (6)
O2	0.0936 (11)	0.0866 (10)	0.0649 (9)	−0.0352 (9)	0.0220 (8)	−0.0082 (7)
N1	0.0845 (13)	0.0805 (12)	0.0916 (14)	0.0291 (10)	−0.0066 (10)	0.0086 (10)
N2	0.0828 (14)	0.1213 (19)	0.122 (2)	0.0053 (13)	0.0354 (14)	0.0376 (16)
N3	0.0638 (9)	0.0504 (8)	0.0681 (10)	−0.0032 (6)	−0.0017 (7)	−0.0148 (7)
C1	0.0461 (7)	0.0394 (7)	0.0454 (7)	−0.0001 (5)	−0.0041 (6)	−0.0053 (6)
C2	0.0452 (8)	0.0555 (9)	0.0841 (13)	0.0001 (7)	−0.0095 (8)	−0.0148 (9)
C3	0.0482 (9)	0.0661 (11)	0.1056 (17)	−0.0106 (8)	0.0168 (10)	−0.0112 (11)
C4	0.0612 (11)	0.0656 (11)	0.0858 (14)	−0.0039 (9)	0.0272 (10)	−0.0125 (10)
C5	0.0544 (9)	0.0440 (7)	0.0484 (8)	−0.0004 (6)	0.0087 (6)	−0.0049 (6)
C6	0.0386 (7)	0.0381 (6)	0.0454 (7)	0.0034 (5)	−0.0021 (5)	−0.0044 (5)
C7	0.0458 (7)	0.0383 (7)	0.0396 (7)	−0.0001 (5)	−0.0014 (5)	−0.0057 (5)
C8	0.0475 (8)	0.0433 (7)	0.0537 (9)	0.0030 (6)	−0.0040 (6)	−0.0112 (6)
C9	0.0506 (9)	0.0612 (10)	0.0824 (13)	0.0027 (8)	0.0066 (9)	0.0061 (10)
C10	0.0557 (9)	0.0585 (10)	0.0568 (10)	0.0076 (8)	−0.0053 (7)	−0.0078 (8)
C11	0.0475 (8)	0.0391 (7)	0.0439 (7)	0.0001 (6)	−0.0020 (6)	−0.0071 (6)
C12	0.0866 (13)	0.0476 (8)	0.0446 (8)	−0.0081 (8)	0.0010 (8)	−0.0054 (7)
C13	0.0893 (14)	0.0608 (10)	0.0457 (9)	−0.0025 (9)	−0.0044 (9)	−0.0133 (8)
C14	0.0635 (10)	0.0509 (9)	0.0621 (10)	0.0011 (7)	−0.0111 (8)	−0.0184 (8)
C15	0.0853 (13)	0.0431 (8)	0.0664 (11)	−0.0135 (8)	−0.0021 (10)	−0.0064 (8)
C16	0.0739 (11)	0.0453 (8)	0.0480 (8)	−0.0082 (7)	0.0008 (8)	−0.0031 (7)
C17	0.1015 (17)	0.0665 (12)	0.0806 (15)	−0.0079 (12)	−0.0192 (12)	−0.0301 (11)
C18	0.0449 (7)	0.0394 (7)	0.0454 (7)	0.0007 (5)	−0.0015 (6)	−0.0044 (6)
C19	0.0447 (7)	0.0409 (7)	0.0515 (8)	0.0009 (6)	−0.0005 (6)	−0.0028 (6)
C20	0.0654 (10)	0.0459 (8)	0.0528 (9)	−0.0025 (7)	0.0055 (8)	−0.0002 (7)
C21	0.133 (3)	0.122 (2)	0.0823 (18)	−0.037 (2)	0.0367 (17)	0.0020 (16)
C22	0.243 (6)	0.294 (8)	0.152 (4)	−0.161 (6)	0.090 (4)	−0.004 (4)

Geometric parameters (Å, º)

O1—C20	1.192 (2)	C8—C10	1.466 (2)
O2—C20	1.320 (2)	C8—C9	1.465 (3)
O2—C21	1.484 (3)	C8—H8	0.9800
N1—C10	1.132 (2)	C11—C16	1.380 (2)
N2—C9	1.135 (3)	C11—C12	1.387 (2)
N3—C19	1.143 (2)	C12—C13	1.388 (2)
C1—C6	1.5125 (19)	C12—H12	0.9300
C1—C7	1.548 (2)	C13—C14	1.372 (3)
C1—C2	1.550 (2)	C13—H13	0.9300

C1—H1	0.9800	C14—C15	1.380 (3)
C2—C3	1.518 (3)	C14—C17	1.511 (2)
C2—H2A	0.9700	C15—C16	1.391 (2)
C2—H2B	0.9700	C15—H15	0.9300
C3—C4	1.514 (3)	C16—H16	0.9300
C3—H3A	0.9700	C17—H17A	0.9600
C3—H3B	0.9700	C17—H17B	0.9600
C4—C5	1.537 (3)	C17—H17C	0.9600
C4—H4A	0.9700	C18—C19	1.441 (2)
C4—H4B	0.9700	C18—C20	1.495 (2)
C5—C6	1.498 (2)	C21—C22	1.415 (5)
C5—H5A	0.9700	C21—H21A	0.9700
C5—H5B	0.9700	C21—H21B	0.9700
C6—C18	1.351 (2)	C22—H22A	0.9600
C7—C11	1.5158 (18)	C22—H22B	0.9600
C7—C8	1.556 (2)	C22—H22C	0.9600
C7—H7	0.9800		

C20—O2—C21	117.29 (18)	N2—C9—C8	177.5 (3)
C6—C1—C7	112.65 (11)	N1—C10—C8	178.2 (2)
C6—C1—C2	107.22 (13)	C16—C11—C12	117.76 (14)
C7—C1—C2	110.65 (13)	C16—C11—C7	119.73 (14)
C6—C1—H1	108.7	C12—C11—C7	122.51 (14)
C7—C1—H1	108.7	C11—C12—C13	120.84 (17)
C2—C1—H1	108.7	C11—C12—H12	119.6
C3—C2—C1	113.00 (15)	C13—C12—H12	119.6
C3—C2—H2A	109.0	C14—C13—C12	121.55 (18)
C1—C2—H2A	109.0	C14—C13—H13	119.2
C3—C2—H2B	109.0	C12—C13—H13	119.2
C1—C2—H2B	109.0	C13—C14—C15	117.60 (15)
H2A—C2—H2B	107.8	C13—C14—C17	120.90 (19)
C4—C3—C2	111.15 (17)	C15—C14—C17	121.50 (19)
C4—C3—H3A	109.4	C14—C15—C16	121.44 (17)
C2—C3—H3A	109.4	C14—C15—H15	119.3
C4—C3—H3B	109.4	C16—C15—H15	119.3
C2—C3—H3B	109.4	C11—C16—C15	120.78 (16)
H3A—C3—H3B	108.0	C11—C16—H16	119.6
C3—C4—C5	111.29 (15)	C15—C16—H16	119.6
C3—C4—H4A	109.4	C14—C17—H17A	109.5
C5—C4—H4A	109.4	C14—C17—H17B	109.5
C3—C4—H4B	109.4	H17A—C17—H17B	109.5
C5—C4—H4B	109.4	C14—C17—H17C	109.5
H4A—C4—H4B	108.0	H17A—C17—H17C	109.5
C6—C5—C4	110.22 (15)	H17B—C17—H17C	109.5
C6—C5—H5A	109.6	C6—C18—C19	119.19 (14)
C4—C5—H5A	109.6	C6—C18—C20	126.34 (13)
C6—C5—H5B	109.6	C19—C18—C20	114.46 (13)
C4—C5—H5B	109.6	N3—C19—C18	177.98 (17)

H5A—C5—H5B	108.1	O1—C20—O2	124.07 (18)
C18—C6—C5	121.57 (13)	O1—C20—C18	125.98 (17)
C18—C6—C1	123.37 (14)	O2—C20—C18	109.94 (15)
C5—C6—C1	114.98 (12)	C22—C21—O2	109.9 (3)
C11—C7—C1	111.82 (11)	C22—C21—H21A	109.7
C11—C7—C8	112.83 (12)	O2—C21—H21A	109.7
C1—C7—C8	111.14 (12)	C22—C21—H21B	109.7
C11—C7—H7	106.9	O2—C21—H21B	109.7
C1—C7—H7	106.9	H21A—C21—H21B	108.2
C8—C7—H7	106.9	C21—C22—H22A	109.5
C10—C8—C9	108.96 (15)	C21—C22—H22B	109.5
C10—C8—C7	111.69 (14)	H22A—C22—H22B	109.5
C9—C8—C7	114.82 (14)	C21—C22—H22C	109.5
C10—C8—H8	107.0	H22A—C22—H22C	109.5
C9—C8—H8	107.0	H22B—C22—H22C	109.5
C7—C8—H8	107.0		

C6—C1—C2—C3	54.57 (19)	C8—C7—C11—C12	74.0 (2)
C7—C1—C2—C3	−68.63 (18)	C16—C11—C12—C13	−1.4 (3)
C1—C2—C3—C4	−56.0 (2)	C7—C11—C12—C13	178.39 (17)
C2—C3—C4—C5	54.3 (2)	C11—C12—C13—C14	−0.1 (3)
C3—C4—C5—C6	−53.9 (2)	C12—C13—C14—C15	1.3 (3)
C4—C5—C6—C18	−120.06 (16)	C12—C13—C14—C17	−178.9 (2)
C4—C5—C6—C1	56.71 (17)	C13—C14—C15—C16	−0.9 (3)
C7—C1—C6—C18	−117.15 (16)	C17—C14—C15—C16	179.3 (2)
C2—C1—C6—C18	120.89 (16)	C12—C11—C16—C15	1.8 (3)
C7—C1—C6—C5	66.15 (17)	C7—C11—C16—C15	−178.03 (16)
C2—C1—C6—C5	−55.82 (17)	C14—C15—C16—C11	−0.6 (3)
C6—C1—C7—C11	178.52 (12)	C5—C6—C18—C19	−0.8 (2)
C2—C1—C7—C11	−61.47 (17)	C1—C6—C18—C19	−177.25 (13)
C6—C1—C7—C8	51.44 (17)	C5—C6—C18—C20	−179.74 (15)
C2—C1—C7—C8	171.45 (13)	C1—C6—C18—C20	3.8 (2)
C11—C7—C8—C10	57.22 (18)	C21—O2—C20—O1	−0.9 (3)
C1—C7—C8—C10	−176.25 (13)	C21—O2—C20—C18	177.7 (2)
C11—C7—C8—C9	−67.48 (17)	C6—C18—C20—O1	−28.4 (3)
C1—C7—C8—C9	59.05 (17)	C19—C18—C20—O1	152.57 (19)
C1—C7—C11—C16	127.58 (17)	C6—C18—C20—O2	153.07 (17)
C8—C7—C11—C16	−106.25 (18)	C19—C18—C20—O2	−26.0 (2)
C1—C7—C11—C12	−52.2 (2)	C20—O2—C21—C22	−169.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1	0.98	2.23	3.001 (2)	135
C5—H5*A*···N1^{i}	0.97	2.57	3.536 (3)	172
C8—H8···N3^{ii}	0.98	2.27	3.221 (2)	163

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