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N′-[(*E*)-4-Chlorobenzylidene]-2-(2,3-dimethylanilino)benzohydrazide

Jerry P. Jasinski,[a] Mehmet Akkurt,[b] Shaaban K. Mohamed,[c,d] Evan M. Dunkley[a] and Mustafa R. Albayati[e]*

[a]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [b]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [c]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [d]Chemistry Department, Faculty of Science, Mini University, 61519 El-Minia, Egypt, and [e]Department of Chemistry, College of Education, Kirkuk University, Kirkuk, Iraq. *Correspondence e-mail: shaabankamel@yahoo.com

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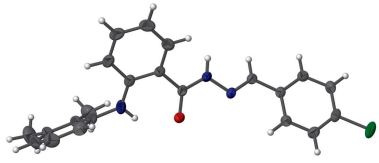
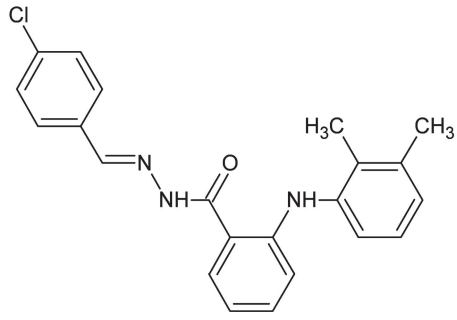
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{20}ClN_3O$, the dihedral angle between the planes of the chlorophenyl and dimethylphenyl rings is 66.50 (9)°. These rings make dihedral angles 47.79 (8) and 69.24 (9)°, respectively, with the central benzene ring. In the crystal, molecules are linked into a three-dimensional supramolecular network by N—H···O, C—H···O hydrogen bonds and weak C—H···π interactions.

3D view



Chemical scheme



Structure description

Mefenamic acid (MA) is a non-steroidal anti-inflammatory drug (NSAID), which has analgesic, anti-inflammatory and antipyretic actions (Idowu *et al.*, 2002). In addition, it can be indicated for the treatment of primary dysmenorrhea (Zhang & Wan, 1998) and periodontitis (Corry & Moran, 1998). The main side effects of MA include peptic ulceration and gastric bleeding, which can be attributed to the combination of local irritation produced by the direct contact of the free carboxylic group (Arun & Ashok, 2009; Tegeli & More, 2014). It has also been reported that compounds containing the hydrazide-hydrazone or imide moiety possess good analgesic and anti-inflammatory activity (Mohamed *et al.*, 2012). A number of hydrazidehydrazones have been demonstrated to possess interesting antidepressant, antibacterial, antifungal, anticonvulsant, anti-inflammatory, antimalarial and antituberculosis activities (Mohamed *et al.*, 2015*a*,*b*). Based on these findings and further to our previous interest in the synthesis of hydrazone NSAIDs, we report herein the synthesis and crystal structure determination of the title compound.

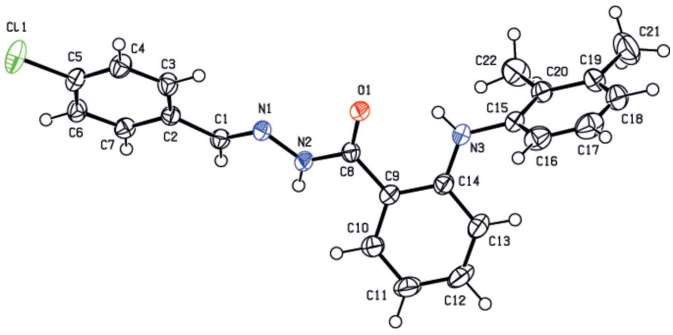


Figure 1
The structure of the title compound, with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

The title molecule (Fig. 1) is twisted with a dihedral angle of 66.50 (9)° between the chlorophenyl and dimethylphenyl rings. The chlorophenyl and dimethylphenyl rings make dihedral angles 47.79 (8) of and 69.24 (9)°, respectively, with the central benzene ring. The methyl groups of the 2,3-dimethylphenyl unit are co-planar with its bound benzene ring [C21—C19—C20—C22 = −1.9 (3)°]. The middle bridging fragment (C1/N1/N2/O1/C8) is not planar with the torsion angle N1—N2—C8—O1 = 16.3 (2)°. All bond lengths and angles are within normal ranges and are comparable with those in related structures (Zhen & Han, 2005; Chantrapromma *et al.*, 2014; Fun *et al.*, 2011; Horkaew *et al.*, 2012).

In the crystal (Fig. 2), the molecules are linked by N—H···O, and C—H···O hydrogen bonds (Table 1) into a three dimensional network. A weak C—H···π interaction (Table 1) is also observed.

Synthesis and crystallization

The title compound was synthesized according to our previously reported procedure (Mohamed *et al.*, 2015*b*). The crystals were collected and recrystallized from ethanol to afford pure crystals suitable for X-ray analysis with m.p. = 473 − 477 K.

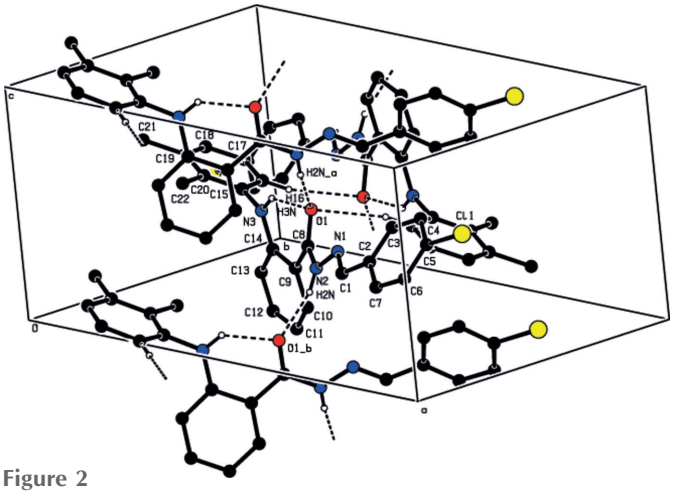


Figure 2
A part of packing diagram for the title compound, with hydrogen bonds drawn as dashed lines.

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

Cg3 is the centroid of the C15–C20 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O1^{i}	0.84 (2)	2.01 (2)	2.8195 (18)	161 (2)
N3—H3*N*···O1	0.85 (2)	2.02 (2)	2.708 (2)	137 (2)
C16—H16···O1^{ii}	0.95	2.59	3.518 (2)	166
C12—H12···*Cg3*^{iii}	0.95	2.81	3.6466 (19)	147

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{20}ClN_3O$
M_r	377.86
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	171
a, b, c (Å)	15.6759 (5), 15.7743 (5), 8.0115 (3)
β (°)	100.530 (3)
V (Å^3)	1947.69 (12)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.86
Crystal size (mm)	0.4 × 0.4 × 0.3
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.833, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7282, 3703, 3188
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.132, 1.04
No. of reflections	3703
No. of parameters	252
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.32

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171187 [https://doi.org/10.1107/S2414314617011877]

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Crystal data

$C_{22}H_{20}ClN_3O$
M_r = 377.86
Monoclinic, $P2_1/c$
a = 15.6759 (5) Å
b = 15.7743 (5) Å
c = 8.0115 (3) Å
β = 100.530 (3)°
V = 1947.69 (12) Å^3
Z = 4
$F(000)$ = 792
D_x = 1.289 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2873 reflections
θ = 4.0–71.1°
μ = 1.86 mm^{-1}
T = 171 K
Prism, colourless
0.4 × 0.4 × 0.3 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.833, T_{max} = 1.000
7282 measured reflections
3703 independent reflections
3188 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 71.3°, θ_{min} = 4.0°
h = −11→19
k = −11→19
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.04
3703 reflections
252 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2 + 0.2369P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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. The C-bound H atoms were placed in calculated positions and allowed to ride on their carrier atoms: aromatic C—H = 0.95 Å, with U_{iso}(H) = 1.2U_{eq}(C), *C*—H_{methyl} = 0.98 Å with U_{iso}(H) = 1.5U_{eq}(C). The H atom of the NH group was found in a difference Fourier map and refined with N—H = 0.87 (2) Å, with U_{iso}(H) = 1.2U_{eq}(N).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.70836 (10)	0.18574 (10)	0.3822 (2)	0.0263 (3)
H1	0.6838	0.1555	0.2825	0.032*
C2	0.79706 (10)	0.16644 (10)	0.4687 (2)	0.0248 (3)
C3	0.83570 (11)	0.21061 (11)	0.6143 (2)	0.0315 (4)
H3A	0.8025	0.2506	0.6640	0.038*
C4	0.92144 (11)	0.19700 (11)	0.6868 (2)	0.0337 (4)
H4	0.9470	0.2266	0.7867	0.040*
C5	0.96965 (11)	0.13950 (10)	0.6119 (2)	0.0302 (4)
C6	0.93316 (11)	0.09513 (10)	0.4677 (2)	0.0307 (4)
H6	0.9669	0.0560	0.4173	0.037*
C7	0.84679 (11)	0.10853 (10)	0.3977 (2)	0.0279 (3)
H7	0.8211	0.0776	0.2995	0.033*
C8	0.53377 (10)	0.32116 (10)	0.3908 (2)	0.0253 (3)
C9	0.46765 (10)	0.36110 (10)	0.2587 (2)	0.0267 (3)
C10	0.48285 (13)	0.36930 (12)	0.0929 (2)	0.0371 (4)
H10	0.5355	0.3481	0.0662	0.045*
C11	0.42359 (16)	0.40722 (14)	−0.0327 (2)	0.0483 (5)
H11	0.4354	0.4131	−0.1443	0.058*
C12	0.34591 (14)	0.43681 (13)	0.0065 (2)	0.0456 (5)
H12	0.3038	0.4617	−0.0801	0.055*
C13	0.32920 (12)	0.43061 (12)	0.1687 (2)	0.0368 (4)
H13	0.2755	0.4509	0.1921	0.044*
C14	0.39028 (11)	0.39477 (11)	0.3009 (2)	0.0293 (4)
C15	0.30223 (11)	0.42961 (12)	0.5171 (2)	0.0311 (4)
C16	0.29755 (13)	0.51764 (13)	0.5204 (3)	0.0414 (4)
H16	0.3419	0.5508	0.4862	0.050*
C17	0.22818 (15)	0.55678 (13)	0.5735 (3)	0.0480 (5)
H17	0.2247	0.6169	0.5764	0.058*
C18	0.16424 (14)	0.50783 (14)	0.6223 (3)	0.0452 (5)
H18	0.1161	0.5348	0.6568	0.054*
C19	0.16843 (12)	0.42067 (13)	0.6221 (2)	0.0375 (4)
C20	0.23916 (11)	0.37978 (11)	0.5699 (2)	0.0315 (4)
C21	0.09662 (17)	0.36903 (19)	0.6768 (4)	0.0660 (7)
H21A	0.0783	0.3240	0.5938	0.099*
H21B	0.0472	0.4060	0.6838	0.099*
H21C	0.1180	0.3437	0.7884	0.099*
C22	0.24639 (16)	0.28469 (13)	0.5726 (3)	0.0508 (5)
H22A	0.2962	0.2675	0.5224	0.076*
H22B	0.1933	0.2601	0.5070	0.076*
H22C	0.2544	0.2645	0.6901	0.076*
Cl1	1.07800 (3)	0.12222 (3)	0.70239 (7)	0.04846 (18)

N1	0.66402 (8)	0.24281 (9)	0.43998 (17)	0.0265 (3)
N2	0.58792 (8)	0.26525 (9)	0.33423 (18)	0.0277 (3)
H2N	0.5781 (13)	0.2445 (13)	0.236 (2)	0.033*
N3	0.37413 (10)	0.39047 (12)	0.4626 (2)	0.0417 (4)
H3N	0.4163 (13)	0.3735 (15)	0.537 (3)	0.050*
O1	0.54090 (7)	0.33759 (8)	0.54416 (14)	0.0299 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0240 (7)	0.0287 (8)	0.0257 (7)	−0.0011 (6)	0.0032 (6)	0.0006 (6)
C2	0.0233 (7)	0.0239 (7)	0.0272 (8)	−0.0004 (6)	0.0047 (6)	0.0034 (6)
C3	0.0296 (8)	0.0324 (8)	0.0321 (8)	0.0043 (7)	0.0042 (7)	−0.0058 (7)
C4	0.0316 (8)	0.0329 (9)	0.0339 (8)	0.0008 (7)	−0.0014 (7)	−0.0046 (7)
C5	0.0226 (7)	0.0262 (8)	0.0400 (9)	0.0006 (6)	0.0006 (6)	0.0064 (7)
C6	0.0304 (8)	0.0238 (7)	0.0385 (9)	0.0059 (6)	0.0079 (7)	0.0024 (7)
C7	0.0303 (8)	0.0243 (7)	0.0286 (8)	0.0004 (6)	0.0041 (6)	−0.0002 (6)
C8	0.0198 (7)	0.0287 (7)	0.0273 (8)	−0.0010 (6)	0.0038 (6)	0.0015 (6)
C9	0.0256 (8)	0.0275 (7)	0.0257 (7)	0.0010 (6)	0.0010 (6)	0.0014 (6)
C10	0.0424 (10)	0.0393 (9)	0.0299 (9)	0.0101 (8)	0.0075 (7)	0.0023 (7)
C11	0.0655 (14)	0.0534 (12)	0.0248 (9)	0.0192 (11)	0.0050 (9)	0.0050 (8)
C12	0.0550 (12)	0.0445 (11)	0.0309 (9)	0.0191 (9)	−0.0092 (8)	0.0018 (8)
C13	0.0336 (9)	0.0368 (9)	0.0366 (9)	0.0093 (7)	−0.0032 (7)	−0.0008 (7)
C14	0.0256 (8)	0.0311 (8)	0.0301 (8)	0.0014 (6)	0.0019 (6)	0.0029 (7)
C15	0.0259 (8)	0.0379 (9)	0.0285 (8)	0.0065 (7)	0.0026 (6)	0.0045 (7)
C16	0.0432 (10)	0.0367 (10)	0.0423 (10)	−0.0058 (8)	0.0026 (8)	0.0058 (8)
C17	0.0661 (14)	0.0301 (9)	0.0455 (11)	0.0111 (9)	0.0039 (10)	−0.0010 (8)
C18	0.0495 (11)	0.0475 (11)	0.0401 (10)	0.0195 (9)	0.0125 (8)	−0.0032 (8)
C19	0.0338 (9)	0.0460 (10)	0.0345 (9)	0.0040 (8)	0.0111 (7)	−0.0005 (8)
C20	0.0330 (9)	0.0322 (9)	0.0292 (8)	0.0040 (7)	0.0057 (7)	−0.0002 (6)
C21	0.0525 (14)	0.0758 (17)	0.0790 (18)	0.0007 (12)	0.0363 (13)	0.0073 (14)
C22	0.0660 (14)	0.0329 (10)	0.0581 (13)	0.0035 (9)	0.0237 (11)	0.0012 (9)
Cl1	0.0259 (2)	0.0426 (3)	0.0702 (4)	0.00625 (17)	−0.0086 (2)	−0.0052 (2)
N1	0.0202 (6)	0.0328 (7)	0.0256 (7)	0.0014 (5)	0.0017 (5)	0.0011 (5)
N2	0.0222 (6)	0.0360 (7)	0.0232 (7)	0.0039 (5)	−0.0001 (5)	−0.0011 (6)
N3	0.0281 (8)	0.0637 (11)	0.0339 (8)	0.0181 (7)	0.0075 (6)	0.0143 (7)
O1	0.0263 (6)	0.0389 (6)	0.0235 (5)	0.0050 (5)	0.0021 (4)	0.0003 (5)

Geometric parameters (Å, º)

C1—N1	1.275 (2)	C13—C14	1.410 (2)
C1—C2	1.468 (2)	C13—H13	0.9500
C1—H1	0.9500	C14—N3	1.367 (2)
C2—C7	1.388 (2)	C15—C20	1.388 (2)
C2—C3	1.398 (2)	C15—C16	1.391 (3)
C3—C4	1.380 (2)	C15—N3	1.422 (2)
C3—H3A	0.9500	C16—C17	1.384 (3)
C4—C5	1.385 (3)	C16—H16	0.9500

C4—H4	0.9500	C17—C18	1.377 (3)
C5—C6	1.382 (3)	C17—H17	0.9500
C5—Cl1	1.7419 (16)	C18—C19	1.377 (3)
C6—C7	1.384 (2)	C18—H18	0.9500
C6—H6	0.9500	C19—C20	1.411 (2)
C7—H7	0.9500	C19—C21	1.518 (3)
C8—O1	1.241 (2)	C20—C22	1.504 (3)
C8—N2	1.358 (2)	C21—H21A	0.9800
C8—C9	1.480 (2)	C21—H21B	0.9800
C9—C10	1.398 (2)	C21—H21C	0.9800
C9—C14	1.420 (2)	C22—H22A	0.9800
C10—C11	1.375 (3)	C22—H22B	0.9800
C10—H10	0.9500	C22—H22C	0.9800
C11—C12	1.393 (3)	N1—N2	1.3772 (18)
C11—H11	0.9500	N2—H2N	0.843 (16)
C12—C13	1.375 (3)	N3—H3N	0.846 (16)
C12—H12	0.9500		

N1—C1—C2	120.50 (15)	N3—C14—C9	121.42 (15)
N1—C1—H1	119.7	C13—C14—C9	117.62 (16)
C2—C1—H1	119.7	C20—C15—C16	121.10 (17)
C7—C2—C3	118.65 (15)	C20—C15—N3	119.75 (17)
C7—C2—C1	119.84 (15)	C16—C15—N3	119.13 (17)
C3—C2—C1	121.27 (15)	C17—C16—C15	119.90 (18)
C4—C3—C2	120.92 (16)	C17—C16—H16	120.0
C4—C3—H3A	119.5	C15—C16—H16	120.1
C2—C3—H3A	119.5	C18—C17—C16	119.39 (18)
C3—C4—C5	119.07 (16)	C18—C17—H17	120.3
C3—C4—H4	120.5	C16—C17—H17	120.3
C5—C4—H4	120.5	C19—C18—C17	121.49 (18)
C6—C5—C4	121.22 (15)	C19—C18—H18	119.3
C6—C5—Cl1	119.45 (13)	C17—C18—H18	119.3
C4—C5—Cl1	119.32 (14)	C18—C19—C20	119.83 (18)
C5—C6—C7	119.09 (16)	C18—C19—C21	119.84 (19)
C5—C6—H6	120.5	C20—C19—C21	120.33 (19)
C7—C6—H6	120.5	C15—C20—C19	118.26 (16)
C6—C7—C2	121.04 (15)	C15—C20—C22	120.87 (17)
C6—C7—H7	119.5	C19—C20—C22	120.86 (18)
C2—C7—H7	119.5	C19—C21—H21A	109.5
O1—C8—N2	121.16 (14)	C19—C21—H21B	109.5
O1—C8—C9	122.94 (15)	H21A—C21—H21B	109.5
N2—C8—C9	115.90 (14)	C19—C21—H21C	109.5
C10—C9—C14	119.52 (15)	H21A—C21—H21C	109.5
C10—C9—C8	120.00 (15)	H21B—C21—H21C	109.5
C14—C9—C8	120.41 (15)	C20—C22—H22A	109.5
C11—C10—C9	121.73 (18)	C20—C22—H22B	109.5
C11—C10—H10	119.1	H22A—C22—H22B	109.5
C9—C10—H10	119.1	C20—C22—H22C	109.5

C10—C11—C12	118.82 (18)	H22A—C22—H22C	109.5
C10—C11—H11	120.6	H22B—C22—H22C	109.5
C12—C11—H11	120.6	C1—N1—N2	115.25 (14)
C13—C12—C11	120.98 (17)	C8—N2—N1	119.05 (14)
C13—C12—H12	119.5	C8—N2—H2N	123.1 (14)
C11—C12—H12	119.5	N1—N2—H2N	117.8 (14)
C12—C13—C14	121.20 (17)	C14—N3—C15	124.34 (15)
C12—C13—H13	119.4	C14—N3—H3N	115.0 (18)
C14—C13—H13	119.4	C15—N3—H3N	118.9 (18)
N3—C14—C13	120.93 (16)		

N1—C1—C2—C7	−175.36 (15)	C10—C9—C14—C13	4.0 (3)
N1—C1—C2—C3	−1.0 (2)	C8—C9—C14—C13	−178.89 (15)
C7—C2—C3—C4	−0.2 (3)	C20—C15—C16—C17	−1.4 (3)
C1—C2—C3—C4	−174.63 (16)	N3—C15—C16—C17	−179.80 (17)
C2—C3—C4—C5	0.9 (3)	C15—C16—C17—C18	−0.2 (3)
C3—C4—C5—C6	−0.7 (3)	C16—C17—C18—C19	1.1 (3)
C3—C4—C5—Cl1	179.80 (14)	C17—C18—C19—C20	−0.5 (3)
C4—C5—C6—C7	−0.2 (3)	C17—C18—C19—C21	179.9 (2)
Cl1—C5—C6—C7	179.30 (13)	C16—C15—C20—C19	2.0 (3)
C5—C6—C7—C2	0.9 (3)	N3—C15—C20—C19	−179.61 (16)
C3—C2—C7—C6	−0.7 (2)	C16—C15—C20—C22	−177.56 (19)
C1—C2—C7—C6	173.79 (15)	N3—C15—C20—C22	0.8 (3)
O1—C8—C9—C10	153.40 (17)	C18—C19—C20—C15	−1.1 (3)
N2—C8—C9—C10	−25.9 (2)	C21—C19—C20—C15	178.51 (19)
O1—C8—C9—C14	−23.7 (2)	C18—C19—C20—C22	178.48 (19)
N2—C8—C9—C14	157.00 (15)	C21—C19—C20—C22	−1.9 (3)
C14—C9—C10—C11	−1.8 (3)	C2—C1—N1—N2	169.64 (14)
C8—C9—C10—C11	−178.97 (19)	O1—C8—N2—N1	−16.3 (2)
C9—C10—C11—C12	−1.1 (3)	C9—C8—N2—N1	162.97 (14)
C10—C11—C12—C13	1.8 (3)	C1—N1—N2—C8	175.36 (14)
C11—C12—C13—C14	0.5 (3)	C13—C14—N3—C15	−8.1 (3)
C12—C13—C14—N3	178.55 (19)	C9—C14—N3—C15	173.89 (18)
C12—C13—C14—C9	−3.4 (3)	C20—C15—N3—C14	115.0 (2)
C10—C9—C14—N3	−177.95 (17)	C16—C15—N3—C14	−66.6 (3)
C8—C9—C14—N3	−0.8 (3)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C15–C20 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O1^{i}	0.84 (2)	2.01 (2)	2.8195 (18)	161 (2)
N3—H3*N*···O1	0.85 (2)	2.02 (2)	2.708 (2)	137 (2)
C16—H16···O1^{ii}	0.95	2.59	3.518 (2)	166
C12—H12···*Cg*3^{iii}	0.95	2.81	3.6466 (19)	147

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