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N-(4-Chlorophenyl)-*N*′-(3-methylphenyl)succinamide monohydrate

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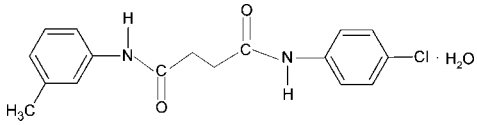
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.127; data-to-parameter ratio = 14.9.

In the title hydrate, $C_{17}H_{17}ClN_2O_2\cdot H_2O$, the dihedral angles formed by the aromatic rings of the chlorobenzene and methylbenzene groups with the mean planes of their attached NH—C(O)—CH_2 fragments are 16.6 (2) and 22.8 (2)°, respectively. In the crystal, O—H···O and N—H···O hydrogen bonds link the components into a two-dimensional network parallel to the *ab* plane.

Related literature

For studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Arjunan *et al.* (2004); Gowda *et al.* (2000); Saraswathi *et al.* (2011), on *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007) and on *N*-chloro-arylsulfonamides, see: Gowda & Kumar (2003).



Experimental

Crystal data

$C_{17}H_{17}ClN_2O_2\cdot H_2O$
M_r = 334.79
Monoclinic, $P2_1/n$
a = 12.210 (1) Å
b = 4.9111 (5) Å
c = 27.078 (3) Å
β = 93.104 (9)°
V = 1621.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 K
0.36 × 0.28 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.915, T_{max} = 0.980
5592 measured reflections
3297 independent reflections
2047 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.127
S = 1.02
3297 reflections
221 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O3^{i}	0.85 (2)	2.14 (2)	2.971 (3)	166 (3)
N2—H2*N*···O1^{ii}	0.85 (2)	2.10 (2)	2.949 (3)	172 (3)
O3—H31···O2^{iii}	0.88 (3)	1.86 (3)	2.730 (3)	177 (3)
O3—H32···O3^{i}	0.83 (3)	1.97 (3)	2.802 (2)	175 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2132).

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supporting information

Acta Cryst. (2011). E**67**, o2418 [doi:10.1107/S1600536811032685]

N-(4-Chlorophenyl)-*N*′-(3-methylphenyl)succinamide monohydrate

B. S. Saraswathi, Sabine Foro and B. Thimme Gowda

S1. Comment

The amide and sulfonamide moieties are important constituents of many biologically important compounds. As part of our studies on the effects of substitutions on the structures and other aspects of *N*-(aryl)-amides (Arjunan *et al.*, 2004; Gowda *et al.*, 2000; Saraswathi *et al.*, 2011); *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007) and on *N*-chloro-aryl-sulfonamides (Gowda & Kumar, 2003), in the present work, the structure of *N*-(4-Chlorophenyl),*N*-(3-methylphenyl)-succinamide monohydrate has been determined (Fig.1). In the C—NH—C(O)—C—C—C(O)—NH—C segment of the structure, all the N—H, C=O and C—H bonds in the amide and aliphatic fragments are *anti* to the adjacent bonds, similar to that observed in *N*-(3-chlorophenyl),*N*-(3-methylphenyl)- succinamide (II) (Saraswathi *et al.*, 2011).

Further, conformations of the N—H bond in the amide fragment is *anti* to the *meta*-methyl group in the adjacent benzene ring, similar to that observed in (II). Further, the dihedral angle between the 4-chlorophenyl ring and the adjacent NH—C(O)—CH_2 segment is 16.6 (2)° and that between the 3-methylphenyl ring and the adjacent NH—C(O)—CH_2 segment is 22.8 (2)°.

The crystal packing of (I) through N1—H1N···O3, N2—H2N···O1, O3—H31O···O2 and O3—H32O···O3 hydrogen bonding (Table 1) is shown in Fig.2.

S2. Experimental

Succinic anhydride (0.01 mol) in toluene (25 ml) was treated drop wise with *m*-toluidine (0.01 mol) also in toluene (20 ml) with constant stirring. The resulting mixture was stirred for one hour and set aside for an additional hour at room temperature for completion of the reaction. The mixture was then treated with dilute hydrochloric acid to remove unreacted *m*-toluidine. The resultant solid *N*-(3-methylphenyl)-succinamic acid was filtered under suction and washed thoroughly with water to remove the unreacted succinic anhydride and succinic acid. The compound was recrystallized to constant melting point from ethanol. The purity of the compound was checked and characterized by its infrared and NMR spectra.

The *N*-(3-methylphenyl)-succinamic acid obtained was then treated with phosphorous oxychloride and excess of 4-chloroaniline at room temperature with constant stirring. The resultant mixture was stirred for 4 h, kept aside for additional 6 h for completion of the reaction and poured slowly into crushed ice with constant stirring. It was kept aside for a day. The resultant solid, *N*-(4-Chlorophenyl), *N*-(3-methylphenyl)-succinamide monohydrate was filtered under suction, washed thoroughly with water, dilute sodium hydroxide solution and finally with water. It was recrystallized to constant melting point from a mixture of acetone and chloroform. The purity of the compound was checked and characterized by its infrared and NMR spectra.

Prism like colorless single crystals used in the X-ray diffraction studies were grown in 1:1 mixture of acetone and chloroform at room temperature.

S3. Refinement

The H atoms of the NH groups and the H atoms of the water molecule were located in a difference map and later restrained to the distance N—H = 0.86 (2) Å and O—H = 0.85 (2) Å, respectively. The other H atoms were positioned with idealized geometry using a riding model with the aromatic C—H = 0.93 Å, the methyl C—H = 0.96Å and the methylene C—H = 0.97 Å.

All H atoms were refined with isotropic displacement parameters. The U_{iso}(H) values were set at 1.2U_{eq}(C-aromatic, N) and 1.5U_{eq}(*C*-methyl).

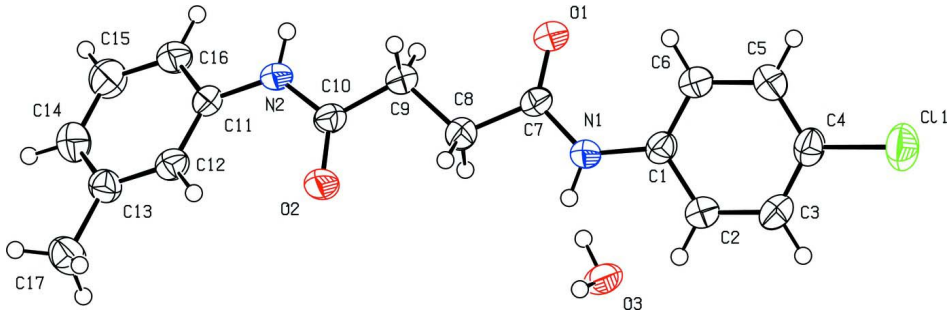

Figure 1

The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level. The intermolecular O—H···O hydrogen bond involving the water molecule is drawn as a dashed line.

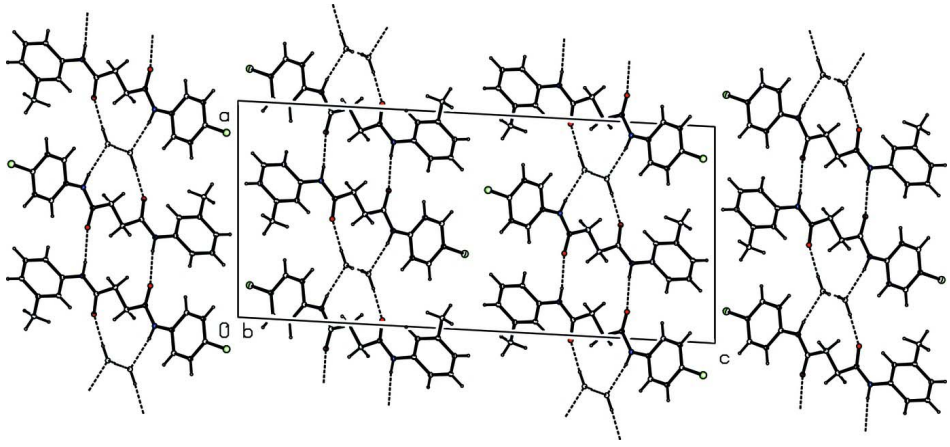

Figure 2

A partial packing diagram of the title compound viewed along the *b* axis, showing the hydrogen-bonding scheme with dashed lines.

N-(4-Chlorophenyl)-*N*′-(3-methylphenyl)succinamide monohydrate

Crystal data

$C_{17}H_{17}ClN_2O_2·H_2O$
M_r = 334.79
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 12.210 (1) Å
b = 4.9111 (5) Å
c = 27.078 (3) Å
β = 93.104 (9)°
V = 1621.3 (3) Å^3
Z = 4
F(000) = 704
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1575 reflections
θ = 2.9–27.9°
μ = 0.25 mm^{-1}

T = 293 K
Prism, colourless

0.36 × 0.28 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur Single Crystal X-ray Diffractometer with Sapphire CCD Detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω scans.
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.915, T_{max} = 0.980

5592 measured reflections
3297 independent reflections
2047 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.4°, θ_{min} = 2.9°
h = −15→12
k = −6→4
l = −33→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.127
S = 1.02
3297 reflections
221 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.9732P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.34943 (7)	−0.42307 (17)	0.47553 (3)	0.0622 (3)
O1	0.62296 (14)	0.4094 (4)	0.31577 (7)	0.0451 (5)
O2	0.47762 (15)	1.1220 (4)	0.19755 (8)	0.0554 (6)
N1	0.43883 (17)	0.4107 (5)	0.32510 (8)	0.0380 (5)
H1N	0.3799 (17)	0.487 (5)	0.3143 (10)	0.046*
N2	0.65157 (17)	1.1254 (5)	0.17399 (8)	0.0373 (6)
H2N	0.7152 (16)	1.057 (5)	0.1796 (10)	0.045*
C1	0.4245 (2)	0.2068 (5)	0.36099 (9)	0.0351 (6)
C2	0.3184 (2)	0.1093 (6)	0.36530 (11)	0.0457 (7)
H2	0.2618	0.1769	0.3444	0.055*
C3	0.2956 (2)	−0.0856 (6)	0.39993 (11)	0.0480 (8)
H3	0.2246	−0.1509	0.4021	0.058*
C4	0.3790 (2)	−0.1817 (6)	0.43102 (10)	0.0410 (7)

C5	0.4841 (2)	−0.0908 (6)	0.42698 (11)	0.0510 (8)
H5	0.5402	−0.1603	0.4479	0.061*
C6	0.5079 (2)	0.1033 (6)	0.39211 (11)	0.0469 (7)
H6	0.5796	0.1638	0.3896	0.056*
C7	0.5316 (2)	0.4993 (5)	0.30498 (9)	0.0322 (6)
C8	0.5080 (2)	0.7174 (6)	0.26629 (10)	0.0398 (7)
H8A	0.4700	0.8660	0.2816	0.048*
H8B	0.4585	0.6421	0.2406	0.048*
C9	0.6068 (2)	0.8327 (6)	0.24219 (10)	0.0379 (6)
H9A	0.6470	0.6861	0.2274	0.046*
H9B	0.6552	0.9190	0.2671	0.046*
C10	0.5724 (2)	1.0393 (5)	0.20277 (10)	0.0356 (6)
C11	0.6394 (2)	1.2938 (5)	0.13128 (9)	0.0336 (6)
C12	0.5546 (2)	1.4811 (5)	0.12350 (10)	0.0371 (6)
H12	0.5030	1.5018	0.1473	0.044*
C13	0.5460 (2)	1.6381 (5)	0.08064 (10)	0.0400 (7)
C14	0.6241 (2)	1.6058 (6)	0.04607 (11)	0.0515 (8)
H14	0.6194	1.7083	0.0172	0.062*
C15	0.7089 (3)	1.4234 (7)	0.05399 (11)	0.0536 (8)
H15	0.7611	1.4055	0.0304	0.064*
C16	0.7176 (2)	1.2668 (6)	0.09629 (10)	0.0436 (7)
H16	0.7752	1.1444	0.1013	0.052*
C17	0.4529 (3)	1.8381 (6)	0.07173 (12)	0.0548 (8)
H17A	0.4172	1.8673	0.1020	0.066*
H17B	0.4011	1.7662	0.0472	0.066*
H17C	0.4814	2.0078	0.0603	0.066*
O3	0.26720 (16)	0.1047 (4)	0.22674 (8)	0.0468 (5)
H31	0.334 (3)	0.112 (6)	0.2162 (11)	0.056*
H32	0.255 (3)	0.256 (7)	0.2390 (12)	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0730 (6)	0.0536 (5)	0.0616 (5)	−0.0016 (4)	0.0197 (4)	0.0174 (4)
O1	0.0285 (10)	0.0509 (12)	0.0559 (12)	−0.0002 (9)	0.0033 (8)	0.0104 (10)
O2	0.0303 (10)	0.0670 (15)	0.0701 (14)	0.0120 (10)	0.0148 (9)	0.0289 (12)
N1	0.0273 (11)	0.0412 (13)	0.0457 (13)	0.0033 (11)	0.0043 (10)	0.0110 (11)
N2	0.0237 (11)	0.0434 (14)	0.0452 (13)	0.0038 (10)	0.0050 (10)	0.0084 (11)
C1	0.0330 (14)	0.0361 (15)	0.0368 (14)	−0.0021 (12)	0.0066 (11)	0.0001 (12)
C2	0.0331 (14)	0.0499 (18)	0.0541 (18)	−0.0007 (14)	0.0023 (13)	0.0109 (15)
C3	0.0371 (15)	0.0505 (19)	0.0575 (18)	−0.0076 (14)	0.0113 (14)	0.0078 (16)
C4	0.0469 (17)	0.0359 (15)	0.0415 (16)	−0.0018 (13)	0.0133 (13)	0.0021 (13)
C5	0.0460 (17)	0.0529 (19)	0.0538 (18)	0.0040 (15)	0.0008 (14)	0.0168 (16)
C6	0.0322 (14)	0.0548 (19)	0.0536 (17)	−0.0029 (14)	0.0000 (13)	0.0136 (15)
C7	0.0278 (13)	0.0325 (14)	0.0364 (14)	−0.0034 (11)	0.0025 (11)	−0.0036 (11)
C8	0.0350 (14)	0.0384 (15)	0.0465 (16)	0.0006 (13)	0.0072 (12)	0.0058 (13)
C9	0.0300 (13)	0.0387 (15)	0.0452 (16)	−0.0001 (12)	0.0032 (12)	0.0049 (13)
C10	0.0282 (13)	0.0363 (15)	0.0426 (15)	0.0008 (12)	0.0057 (11)	0.0002 (12)

C11	0.0305 (13)	0.0323 (14)	0.0380 (14)	−0.0048 (12)	0.0012 (11)	0.0014 (12)
C12	0.0329 (14)	0.0377 (15)	0.0410 (15)	−0.0004 (12)	0.0058 (12)	−0.0033 (12)
C13	0.0401 (15)	0.0326 (15)	0.0465 (16)	−0.0006 (12)	−0.0044 (12)	0.0007 (13)
C14	0.0543 (18)	0.0526 (19)	0.0479 (17)	0.0000 (16)	0.0051 (15)	0.0115 (15)
C15	0.0505 (18)	0.064 (2)	0.0482 (18)	0.0066 (17)	0.0172 (14)	0.0094 (17)
C16	0.0334 (14)	0.0494 (18)	0.0487 (17)	0.0051 (13)	0.0077 (13)	0.0059 (14)
C17	0.0543 (19)	0.0449 (18)	0.064 (2)	0.0063 (16)	−0.0041 (16)	0.0057 (16)
O3	0.0288 (10)	0.0451 (12)	0.0670 (14)	−0.0026 (10)	0.0065 (9)	−0.0049 (11)

Geometric parameters (Å, º)

Cl1—C4	1.742 (3)	C8—H8A	0.9700
O1—C7	1.220 (3)	C8—H8B	0.9700
O2—C10	1.227 (3)	C9—C10	1.516 (4)
N1—C7	1.355 (3)	C9—H9A	0.9700
N1—C1	1.413 (3)	C9—H9B	0.9700
N1—H1N	0.849 (17)	C11—C16	1.388 (3)
N2—C10	1.343 (3)	C11—C12	1.392 (4)
N2—C11	1.423 (3)	C12—C13	1.392 (4)
N2—H2N	0.852 (17)	C12—H12	0.9300
C1—C6	1.382 (4)	C13—C14	1.381 (4)
C1—C2	1.393 (3)	C13—C17	1.512 (4)
C2—C3	1.379 (4)	C14—C15	1.377 (4)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.369 (4)	C15—C16	1.379 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.369 (4)	C16—H16	0.9300
C5—C6	1.384 (4)	C17—H17A	0.9600
C5—H5	0.9300	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
C7—C8	1.515 (4)	O3—H31	0.88 (3)
C8—C9	1.513 (3)	O3—H32	0.83 (3)
C7—N1—C1	129.9 (2)	C8—C9—H9A	109.5
C7—N1—H1N	115.5 (19)	C10—C9—H9A	109.5
C1—N1—H1N	114.6 (19)	C8—C9—H9B	109.5
C10—N2—C11	127.4 (2)	C10—C9—H9B	109.5
C10—N2—H2N	116.8 (19)	H9A—C9—H9B	108.0
C11—N2—H2N	115.4 (19)	O2—C10—N2	122.2 (3)
C6—C1—C2	118.7 (2)	O2—C10—C9	121.8 (2)
C6—C1—N1	124.4 (2)	N2—C10—C9	116.0 (2)
C2—C1—N1	116.8 (2)	C16—C11—C12	119.6 (2)
C3—C2—C1	121.2 (3)	C16—C11—N2	117.0 (2)
C3—C2—H2	119.4	C12—C11—N2	123.5 (2)
C1—C2—H2	119.4	C11—C12—C13	120.9 (2)
C4—C3—C2	119.1 (3)	C11—C12—H12	119.5
C4—C3—H3	120.4	C13—C12—H12	119.5
C2—C3—H3	120.4	C14—C13—C12	118.5 (3)

C3—C4—C5	120.5 (3)	C14—C13—C17	120.5 (3)
C3—C4—Cl1	119.0 (2)	C12—C13—C17	121.0 (2)
C5—C4—Cl1	120.5 (2)	C15—C14—C13	120.6 (3)
C4—C5—C6	120.8 (3)	C15—C14—H14	119.7
C4—C5—H5	119.6	C13—C14—H14	119.7
C6—C5—H5	119.6	C14—C15—C16	121.0 (3)
C1—C6—C5	119.6 (3)	C14—C15—H15	119.5
C1—C6—H6	120.2	C16—C15—H15	119.5
C5—C6—H6	120.2	C15—C16—C11	119.3 (3)
O1—C7—N1	124.1 (2)	C15—C16—H16	120.4
O1—C7—C8	123.9 (2)	C11—C16—H16	120.4
N1—C7—C8	111.9 (2)	C13—C17—H17A	109.5
C7—C8—C9	115.9 (2)	C13—C17—H17B	109.5
C7—C8—H8A	108.3	H17A—C17—H17B	109.5
C9—C8—H8A	108.3	C13—C17—H17C	109.5
C7—C8—H8B	108.3	H17A—C17—H17C	109.5
C9—C8—H8B	108.3	H17B—C17—H17C	109.5
H8A—C8—H8B	107.4	H31—O3—H32	106 (3)
C8—C9—C10	110.9 (2)		

C7—N1—C1—C6	17.5 (5)	C11—N2—C10—O2	−7.3 (5)
C7—N1—C1—C2	−163.6 (3)	C11—N2—C10—C9	172.6 (2)
C6—C1—C2—C3	0.3 (4)	C8—C9—C10—O2	9.3 (4)
N1—C1—C2—C3	−178.6 (3)	C8—C9—C10—N2	−170.6 (2)
C1—C2—C3—C4	0.9 (5)	C10—N2—C11—C16	−153.7 (3)
C2—C3—C4—C5	−1.7 (5)	C10—N2—C11—C12	26.7 (4)
C2—C3—C4—Cl1	178.8 (2)	C16—C11—C12—C13	1.3 (4)
C3—C4—C5—C6	1.2 (5)	N2—C11—C12—C13	−179.1 (2)
Cl1—C4—C5—C6	−179.2 (2)	C11—C12—C13—C14	−0.6 (4)
C2—C1—C6—C5	−0.8 (4)	C11—C12—C13—C17	178.9 (3)
N1—C1—C6—C5	178.1 (3)	C12—C13—C14—C15	−0.3 (5)
C4—C5—C6—C1	0.0 (5)	C17—C13—C14—C15	−179.9 (3)
C1—N1—C7—O1	−0.1 (5)	C13—C14—C15—C16	0.6 (5)
C1—N1—C7—C8	178.2 (3)	C14—C15—C16—C11	0.1 (5)
O1—C7—C8—C9	−2.7 (4)	C12—C11—C16—C15	−1.0 (4)
N1—C7—C8—C9	179.1 (2)	N2—C11—C16—C15	179.4 (3)
C7—C8—C9—C10	177.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3^{i}	0.85 (2)	2.14 (2)	2.971 (3)	166 (3)
N2—H2*N*···O1^{ii}	0.85 (2)	2.10 (2)	2.949 (3)	172 (3)
O3—H31···O2^{iii}	0.88 (3)	1.86 (3)	2.730 (3)	177 (3)
O3—H32···O3^{i}	0.83 (3)	1.97 (3)	2.802 (2)	175 (3)

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