organic compounds

2-(4-Chlorophenyl)acetic acid–2-{(E)-[(E)-2-(2-pyridylmethylidene)hydrazin-1-ylidene]methyl}pyridine (1/1)

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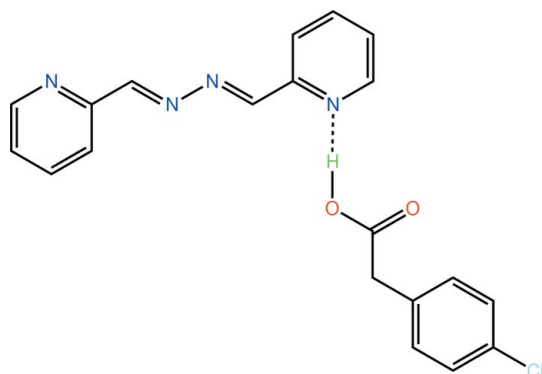Correspondence e-mail: edward.tiekink@gmail.com

In the crystal of the title 1:1 adduct, $C_8H_7ClO_2 \cdot C_{12}H_{10}N_4$, the components are linked by an O—H$\cdots$N hydrogen bond between the carboxylic acid and one of the pyridine N atoms. In the acid, the carboxylic acid group is approximately normal to [dihedral angle = 72.9 (2)°] but twisted with respect to the plane through the benzene ring [C—C—C—O torsion angle = 25.4 (5)°]. The base is roughly planar [dihedral angle between rings = 12.66 (15)°; r.m.s. deviation of the 16 non-H atoms = 0.107 Å] and the conformations about both imine bonds are E. The dimeric aggregates are linked into a supramolecular layer in the ab plane by C—H$\cdots$O interactions.

Related literature

For related studies on co-crystal formation, see: Broker & Tiekink (2007); Broker et al. (2008); Arman et al. (2010).

Experimental

Crystal data

$C_8H_7ClO_2 \cdot C_{12}H_{10}N_4$	V = 1822.6 (15) Å^3
M_r = 380.83	Z = 4
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
a = 11.740 (6) Å	μ = 0.23 mm^{-1}
b = 4.641 (2) Å	T = 98 K
c = 33.451 (15) Å	$0.22 \times 0.19 \times 0.09$ mm

Data collection

Rigaku Saturn724 diffractometer	7554 measured reflections
Absorption correction: multi-scan	4091 independent reflections
(ABSCOR; Higashi, 1995)	3661 reflections with $I > 2\sigma(I)$
T_{min} = 0.625, T_{max} = 1.000	R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057	H atoms treated by a mixture of
$wR(F^2)$ = 0.113	independent and constrained
S = 1.14	refinement
4091 reflections	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
247 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
2 restraints	Absolute structure: Flack (1983),
	1973 Friedel pairs
	Flack parameter: 0.09 (8)

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

D—H$\cdots$A	D—H	H$\cdots$A	$D\cdots$A	D—H$\cdots$A
O1—H1o$\cdots$N1	0.85 (3)	1.89 (3)	2.734 (4)	173 (3)
C9—H9$\cdots$O2	0.95	2.51	3.215 (4)	131
C10—H10$\cdots$O1^i	0.95	2.57	3.493 (4)	164

Symmetry code: (i) $x - \frac{1}{2}, -y + 2, z$.

Data collection: CrystalClear (Molecular Structure Corporation & Rigaku, 2005); cell refinement: CrystalClear; data reduction: CrystalClear; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5608).

References

Arman, H. D., Kaulgud, T. & Tiekink, E. R. T. (2010). Acta Cryst. E**66**, o2117.
Brandenburg, K. (2006). DIAMOND. Crystal Impact GbR, Bonn, Germany.
Broker, G. A., Bettens, R. P. A. & Tiekink, E. R. T. (2008). CrystEngComm, **10**, 879–887.
Broker, G. A. & Tiekink, E. R. T. (2007). CrystEngComm, **9**, 1096–1109.
Farrugia, L. J. (1997). J. Appl. Cryst. **30**, 565.
Flack, H. D. (1983). Acta Cryst. A**39**, 876–881.
Higashi, T. (1995). ABSCOR. Rigaku Corporation, Tokyo, Japan.
Molecular Structure Corporation & Rigaku (2005). CrystalClear. MSC, The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). Acta Cryst. A**64**, 112–122.
Westrip, S. P. (2010). J. Appl. Cryst. **43**, 920–925.

supplementary materials

2-(4-Chlorophenyl)acetic acid-2-{(*E*)-[(*E*)-2-(2-pyridylmethylidene)hydrazin-1-ylidene]methyl}pyridine (1/1)

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Comment

Co-crystallization of carboxylic acids with pyridine-containing bases has led to several structural motifs as well as salts (Broker & Tiekink, 2007; Broker *et al.*, 2008; Arman *et al.*, 2010). In continuation of these studies, the co-crystallization experiment between 2-(4-chlorophenyl)acetic acid and 2-[(1*E*)-[(*E*)-2-(pyridin-2-ylmethylidene)hydrazin-1-ylidene] methyl]pyridine in a 1:1 ratio in their methanol solution was investigated. This lead to the isolation of the title 1:1 co-crystal, (I).

The constituents of (I), Fig. 1, are connected by a O–H⋯N hydrogen bond where the N is a pyridine-N, rather than an imine-N, as usually seen in co-crystals of this type (Broker *et al.*, 2008), Table 1. In the acid, the dihedral angle formed between the carboxylic acid group and the benzene ring is 72.9 (2) ° and the former is twisted with respect to the plane of the benzene ring as seen in the value of the C1–C7–C8–O2 torsion angle of 25.4 (5) °. In the base, the 16 non-hydrogen atoms are almost co-planar with the r.m.s. deviation being 0.107 Å [max. deviations are 0.132 (3) Å for atom C18 and -0.153 (2) Å for the N1 atom]. The greatest twist in the base is found about the C15–C16 bond as seen in the N3–C15–C16–C17 torsion angle of 6.0 (5) °. The pyridine-N atoms are *anti* with respect to each other and the conformation about each imine bond [N2═C14 = 1.276 (4) Å and N3═C15 = 1.280 (4) Å] is *E*, again observations normally seen in related systems (Broker *et al.*, 2008).

In the crystal packing, the dimeric aggregates held together by the O–H⋯N hydrogen bonds are linked into a supramolecular array in the *ab* plane *via* C–H⋯O contacts, Fig. 2 and Table 1. The resulting layers stack along the *c* direction, Fig. 3.

Experimental

Yellow crystals of (I) were isolated from the 1/1 co-crystallization of 2-[(1*E*)-[(*E*)-2-(pyridin-2-ylmethylidene)hydrazin-1-ylidene]methyl]pyridine (Sigma-Aldrich; 0.095 mmol) and 2-(4-chlorophenyl)acetic acid (Sigma-Aldrich; 0.094 mmol) in a methanol solution, m. pt. 370 - 373 K.

Refinement

C-bound H-atoms were placed in calculated positions (C–H 0.95–0.99 Å) and were included in the refinement in the riding model approximation with $U_{iso}(H)$ set to $1.2U_{eq}(C)$. The O-bound H-atom was located in a difference Fourier map and was refined with a distance restraint of O–H = 0.84±0.01 Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.
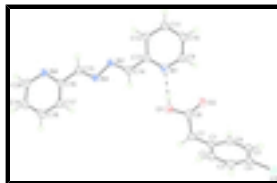
supplementary materials

Figures

Fig. 1. Molecular structure of the constituents of co-crystal (I) showing displacement ellipsoids at the 50% probability level. The O–H⋯N hydrogen bond is shown as a dashed line.
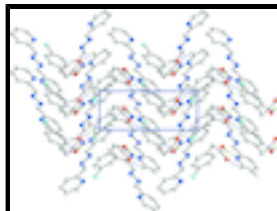
Fig. 2. Supramolecular layer formation in the *ab* plane in (I). Dimeric aggregates, connected by an O–H⋯N hydrogen bond (orange dashed lines) are connected *via* C–H⋯O contacts (blue dashed lines). Hydrogen atoms not involved in the aforementioned interactions have been omitted for reasons of clarity.
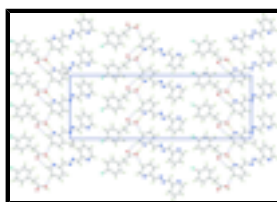
Fig. 3. Stacking of layers along the *c* axis in (I). The O–H⋯N (orange) and C–H⋯O (blue) contacts are shown as dashed lines.

2-(4-Chlorophenyl)acetic acid–2-{(*E*)-[(*E*)-2-(2-pyridylmethylidene)hydrazin-1- ylidene]methyl}pyridine (1/1)

Crystal data

$C_8H_7ClO_2 \cdot C_{12}H_{10}N_4$	$F(000) = 792$
$M_r = 380.83$	$D_x = 1.388$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2ac	Cell parameters from 4996 reflections
$a = 11.740$ (6) Å	$\theta = 2.1$–$40.3°$
$b = 4.641$ (2) Å	$\mu = 0.23$ mm^{-1}
$c = 33.451$ (15) Å	$T = 98$ K
$V = 1822.6$ (15) Å^3	Prism, yellow
$Z = 4$	$0.22 \times 0.19 \times 0.09$ mm

Data collection

Rigaku Saturn724 diffractometer	4091 independent reflections
Radiation source: sealed tube	3661 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.046$
Detector resolution: 28.5714 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
ω scans	$h = -4 \rightarrow 15$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$k = -4 \rightarrow 6$
$T_{min} = 0.625$, $T_{max} = 1.000$	$l = -43 \rightarrow 42$
7554 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.113$	$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 0.6335P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{max} = 0.001$
4091 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
247 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
2 restraints	Absolute structure: Flack (1983), 1973 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.09 (8)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.54028 (7)	1.20255 (16)	0.67877 (3)	0.03461 (19)
O1	0.2462 (2)	0.4385 (5)	0.86536 (7)	0.0339 (6)
H1o	0.201 (3)	0.542 (7)	0.8788 (10)	0.051*
O2	0.2010 (2)	0.7655 (5)	0.81878 (7)	0.0349 (6)
N1	0.0916 (2)	0.7320 (5)	0.91096 (8)	0.0273 (6)
N2	0.0996 (2)	0.3341 (5)	1.00194 (8)	0.0256 (6)
N3	0.1807 (2)	0.1275 (5)	1.01538 (8)	0.0249 (6)
N4	0.1708 (2)	−0.3295 (6)	1.10056 (8)	0.0278 (6)
C1	0.3916 (3)	0.5966 (7)	0.77127 (10)	0.0273 (7)
C2	0.4965 (3)	0.7262 (7)	0.77713 (10)	0.0311 (7)
H2	0.5380	0.6864	0.8009	0.037*
C3	0.5427 (3)	0.9140 (7)	0.74890 (10)	0.0308 (7)
H3	0.6146	1.0022	0.7533	0.037*
C4	0.4823 (3)	0.9690 (6)	0.71456 (10)	0.0261 (7)
C5	0.3768 (3)	0.8454 (7)	0.70749 (10)	0.0291 (7)
H5	0.3354	0.8872	0.6838	0.035*

C6	0.3332 (3)	0.6583 (7)	0.73615 (10)	0.0297 (7)
H6	0.2613	0.5701	0.7316	0.036*
C7	0.3417 (3)	0.4012 (7)	0.80335 (10)	0.0319 (8)
H7A	0.3044	0.2341	0.7904	0.038*
H7B	0.4040	0.3272	0.8204	0.038*
C8	0.2559 (3)	0.5567 (7)	0.82911 (10)	0.0276 (7)
C9	0.0329 (3)	0.9348 (7)	0.89091 (10)	0.0284 (7)
H9	0.0593	0.9934	0.8653	0.034*
C10	−0.0646 (3)	1.0608 (7)	0.90619 (10)	0.0302 (7)
H10	−0.1038	1.2045	0.8914	0.036*
C11	−0.1048 (3)	0.9744 (7)	0.94373 (10)	0.0263 (7)
H11	−0.1721	1.0564	0.9547	0.032*
C12	−0.0443 (3)	0.7666 (6)	0.96461 (10)	0.0255 (6)
H12	−0.0696	0.7024	0.9901	0.031*
C13	0.0548 (3)	0.6533 (6)	0.94746 (10)	0.0245 (6)
C14	0.1254 (3)	0.4354 (6)	0.96765 (9)	0.0252 (7)
H14	0.1924	0.3680	0.9547	0.030*
C15	0.1501 (3)	0.0090 (6)	1.04822 (9)	0.0250 (7)
H15	0.0799	0.0642	1.0601	0.030*
C16	0.2202 (3)	−0.2089 (6)	1.06803 (9)	0.0220 (6)
C17	0.3292 (3)	−0.2836 (6)	1.05470 (10)	0.0265 (7)
H17	0.3609	−0.1966	1.0315	0.032*
C18	0.3902 (3)	−0.4885 (7)	1.07626 (10)	0.0287 (7)
H18	0.4648	−0.5416	1.0682	0.034*
C19	0.3413 (3)	−0.6131 (7)	1.10929 (10)	0.0306 (7)
H19	0.3815	−0.7537	1.1244	0.037*
C20	0.2316 (3)	−0.5292 (7)	1.12030 (10)	0.0299 (7)
H20	0.1980	−0.6182	1.1430	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0384 (4)	0.0313 (4)	0.0342 (4)	−0.0011 (3)	0.0090 (4)	0.0029 (4)
O1	0.0357 (14)	0.0361 (13)	0.0299 (14)	0.0045 (10)	0.0061 (10)	0.0038 (10)
O2	0.0357 (14)	0.0371 (13)	0.0320 (14)	0.0084 (11)	0.0047 (11)	0.0067 (11)
N1	0.0269 (14)	0.0267 (13)	0.0281 (14)	−0.0008 (11)	−0.0003 (11)	−0.0001 (12)
N2	0.0238 (13)	0.0274 (13)	0.0255 (14)	0.0036 (10)	−0.0027 (11)	0.0004 (11)
N3	0.0215 (13)	0.0276 (13)	0.0256 (14)	0.0015 (11)	−0.0025 (10)	−0.0002 (11)
N4	0.0273 (14)	0.0276 (14)	0.0285 (15)	−0.0005 (12)	−0.0004 (12)	0.0022 (11)
C1	0.0304 (17)	0.0263 (16)	0.0254 (16)	0.0081 (13)	0.0056 (13)	0.0002 (13)
C2	0.0298 (17)	0.0371 (18)	0.0263 (17)	0.0060 (14)	−0.0028 (13)	0.0000 (14)
C3	0.0238 (16)	0.0304 (16)	0.038 (2)	−0.0023 (13)	0.0010 (14)	−0.0014 (15)
C4	0.0313 (16)	0.0210 (14)	0.0259 (16)	0.0018 (13)	0.0058 (14)	−0.0032 (12)
C5	0.0296 (17)	0.0312 (16)	0.0266 (17)	0.0036 (13)	−0.0031 (13)	−0.0024 (14)
C6	0.0268 (16)	0.0287 (16)	0.0337 (19)	−0.0007 (13)	0.0005 (14)	−0.0039 (14)
C7	0.0338 (18)	0.0256 (16)	0.036 (2)	0.0058 (14)	0.0059 (15)	0.0021 (14)
C8	0.0264 (16)	0.0275 (16)	0.0288 (17)	−0.0079 (13)	−0.0023 (14)	0.0020 (14)
C9	0.0296 (17)	0.0298 (17)	0.0256 (17)	0.0004 (13)	−0.0025 (13)	0.0038 (14)

C10	0.0327 (17)	0.0265 (15)	0.0313 (19)	0.0019 (14)	−0.0106 (15)	0.0006 (14)
C11	0.0220 (16)	0.0257 (15)	0.0314 (17)	0.0007 (12)	−0.0035 (13)	0.0005 (14)
C12	0.0244 (15)	0.0250 (15)	0.0270 (16)	−0.0056 (12)	0.0015 (13)	0.0003 (13)
C13	0.0235 (15)	0.0226 (14)	0.0273 (17)	−0.0033 (12)	−0.0025 (13)	−0.0032 (12)
C14	0.0212 (15)	0.0249 (16)	0.0294 (17)	−0.0006 (12)	−0.0001 (13)	−0.0020 (13)
C15	0.0244 (16)	0.0244 (15)	0.0263 (16)	0.0006 (12)	−0.0038 (13)	−0.0026 (12)
C16	0.0243 (15)	0.0193 (13)	0.0223 (15)	−0.0027 (12)	−0.0019 (12)	−0.0013 (12)
C17	0.0253 (17)	0.0273 (16)	0.0269 (17)	−0.0021 (13)	0.0002 (13)	0.0018 (14)
C18	0.0193 (15)	0.0299 (16)	0.037 (2)	−0.0005 (13)	−0.0029 (13)	−0.0037 (14)
C19	0.0378 (18)	0.0256 (16)	0.0283 (18)	0.0004 (14)	−0.0123 (14)	0.0019 (14)
C20	0.0383 (19)	0.0292 (16)	0.0222 (16)	−0.0014 (14)	−0.0031 (14)	0.0020 (13)

Geometric parameters (Å, °)

Cl1—C4	1.753 (3)	C7—H7A	0.9900
O1—C8	1.336 (4)	C7—H7B	0.9900
O1—H1o	0.85 (3)	C9—C10	1.383 (5)
O2—C8	1.214 (4)	C9—H9	0.9500
N1—C13	1.346 (4)	C10—C11	1.400 (5)
N1—C9	1.346 (4)	C10—H10	0.9500
N2—C14	1.276 (4)	C11—C12	1.387 (4)
N2—N3	1.424 (3)	C11—H11	0.9500
N3—C15	1.280 (4)	C12—C13	1.399 (4)
N4—C20	1.343 (4)	C12—H12	0.9500
N4—C16	1.354 (4)	C13—C14	1.472 (4)
C1—C2	1.385 (5)	C14—H14	0.9500
C1—C6	1.391 (5)	C15—C16	1.463 (4)
C1—C7	1.522 (4)	C15—H15	0.9500
C2—C3	1.394 (5)	C16—C17	1.399 (4)
C2—H2	0.9500	C17—C18	1.391 (4)
C3—C4	1.373 (5)	C17—H17	0.9500
C3—H3	0.9500	C18—C19	1.373 (5)
C4—C5	1.386 (4)	C18—H18	0.9500
C5—C6	1.391 (5)	C19—C20	1.396 (5)
C5—H5	0.9500	C19—H19	0.9500
C6—H6	0.9500	C20—H20	0.9500
C7—C8	1.509 (4)		
C8—O1—H1o	108 (3)	C10—C9—H9	118.8
C13—N1—C9	118.5 (3)	C9—C10—C11	119.3 (3)
C14—N2—N3	111.9 (3)	C9—C10—H10	120.4
C15—N3—N2	111.9 (3)	C11—C10—H10	120.4
C20—N4—C16	116.9 (3)	C12—C11—C10	118.6 (3)
C2—C1—C6	118.0 (3)	C12—C11—H11	120.7
C2—C1—C7	120.1 (3)	C10—C11—H11	120.7
C6—C1—C7	121.9 (3)	C11—C12—C13	118.7 (3)
C1—C2—C3	121.4 (3)	C11—C12—H12	120.6
C1—C2—H2	119.3	C13—C12—H12	120.6
C3—C2—H2	119.3	N1—C13—C12	122.5 (3)
C4—C3—C2	118.8 (3)	N1—C13—C14	115.0 (3)

C4—C3—H3	120.6	C12—C13—C14	122.5 (3)
C2—C3—H3	120.6	N2—C14—C13	122.1 (3)
C3—C4—C5	121.8 (3)	N2—C14—H14	118.9
C3—C4—Cl1	119.1 (2)	C13—C14—H14	118.9
C5—C4—Cl1	119.1 (3)	N3—C15—C16	121.9 (3)
C4—C5—C6	118.0 (3)	N3—C15—H15	119.1
C4—C5—H5	121.0	C16—C15—H15	119.1
C6—C5—H5	121.0	N4—C16—C17	123.1 (3)
C1—C6—C5	122.0 (3)	N4—C16—C15	114.1 (3)
C1—C6—H6	119.0	C17—C16—C15	122.8 (3)
C5—C6—H6	119.0	C18—C17—C16	118.3 (3)
C8—C7—C1	112.0 (3)	C18—C17—H17	120.8
C8—C7—H7A	109.2	C16—C17—H17	120.8
C1—C7—H7A	109.2	C19—C18—C17	119.4 (3)
C8—C7—H7B	109.2	C19—C18—H18	120.3
C1—C7—H7B	109.2	C17—C18—H18	120.3
H7A—C7—H7B	107.9	C18—C19—C20	118.7 (3)
O2—C8—O1	122.7 (3)	C18—C19—H19	120.6
O2—C8—C7	125.0 (3)	C20—C19—H19	120.6
O1—C8—C7	112.3 (3)	N4—C20—C19	123.6 (3)
N1—C9—C10	122.4 (3)	N4—C20—H20	118.2
N1—C9—H9	118.8	C19—C20—H20	118.2
C14—N2—N3—C15	−174.8 (3)	C9—N1—C13—C12	2.4 (5)
C6—C1—C2—C3	0.2 (5)	C9—N1—C13—C14	−178.6 (3)
C7—C1—C2—C3	−177.8 (3)	C11—C12—C13—N1	−2.1 (5)
C1—C2—C3—C4	−0.3 (5)	C11—C12—C13—C14	179.0 (3)
C2—C3—C4—C5	0.6 (5)	N3—N2—C14—C13	−179.8 (2)
C2—C3—C4—Cl1	−179.5 (2)	N1—C13—C14—N2	−178.1 (3)
C3—C4—C5—C6	−0.9 (5)	C12—C13—C14—N2	0.9 (5)
Cl1—C4—C5—C6	179.3 (2)	N2—N3—C15—C16	−179.6 (3)
C2—C1—C6—C5	−0.4 (5)	C20—N4—C16—C17	0.0 (4)
C7—C1—C6—C5	177.5 (3)	C20—N4—C16—C15	−179.3 (3)
C4—C5—C6—C1	0.7 (5)	N3—C15—C16—N4	−174.6 (3)
C2—C1—C7—C8	98.4 (4)	N3—C15—C16—C17	6.0 (5)
C6—C1—C7—C8	−79.5 (4)	N4—C16—C17—C18	−0.9 (5)
C1—C7—C8—O2	25.4 (5)	C15—C16—C17—C18	178.4 (3)
C1—C7—C8—O1	−154.6 (3)	C16—C17—C18—C19	0.9 (5)
C13—N1—C9—C10	−1.1 (5)	C17—C18—C19—C20	−0.1 (5)
N1—C9—C10—C11	−0.5 (5)	C16—N4—C20—C19	0.8 (5)
C9—C10—C11—C12	0.8 (5)	C18—C19—C20—N4	−0.8 (5)
C10—C11—C12—C13	0.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···N1	0.85 (3)	1.89 (3)	2.734 (4)	173 (3)
C9—H9···O2	0.95	2.51	3.215 (4)	131
C10—H10···O1[i]	0.95	2.57	3.493 (4)	164

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

Fig. 1

Fig. 2

Fig. 3