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2-(1*H*-Benzotriazol-1-yl)-1-(3-chlorobenzoyl)ethyl 2,4-dichlorobenzoate

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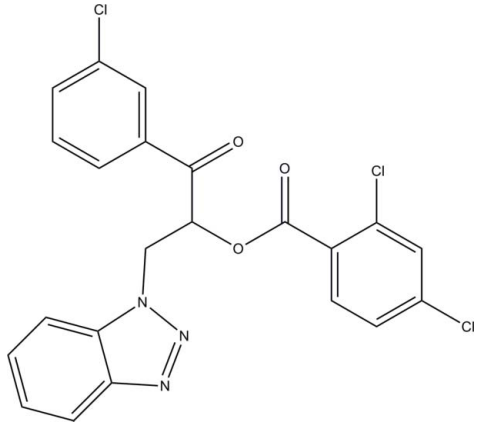
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.151; data-to-parameter ratio = 15.0.

In the crystal structure of the title compound, $C_{22}H_{13}Cl_3N_3O_3$, weak intermolecular C—H···Cl hydrogen bonds link the molecules into chains extending along the c axis. The packing is further stabilized by weak C—H···O interactions.

Related literature

For related literature, see: Chen & Wu (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{13}Cl_3N_3O_3$
M_r = 473.70
Monoclinic, $P2_1/c$
a = 10.9182 (2) Å
b = 19.6123 (3) Å
c = 10.0124 (2) Å
β = 92.096 (1)°
V = 2142.53 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 273 K
0.28 × 0.06 × 0.04 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.960, T_{max} = 0.980
27918 measured reflections
4212 independent reflections
3192 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.151
S = 1.05
4212 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.93	2.41	3.198 (4)	142
C6—H6···Cl3^{ii}	0.93	2.83	3.719 (3)	161
C7—H7*B*···O3^{iii}	0.97	2.55	3.520 (3)	176
C18—H18···O1	0.93	2.28	2.643 (3)	102

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{5}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2324).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
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supplementary materials

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2-(1*H*-Benzotriazol-1-yl)-1-(3-chlorobenzoyl)ethyl 2,4-dichlorobenzoate

W.-L. Zeng, X.-Z. Sun and H.-Q. Wang

Comment

1*H*-Benzotriazoles and its derivatives are an important class of compounds because they exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). We report here the synthesis and structure of the title compound, (I) (Fig. 1), as part of our ongoing studies on new benzotriazole compounds with higher bioactivity.

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The benzotriazole ring system is essentially planar, with a dihedral angle of 1.02 (14) ° between the triazole ring (N1—N3/C1/C2) and the benzene ring (C1—C6). The dihedral angles between the mean planes of the benzotriazole system and rings (C17—C22) and rings (C10—C15) are 50.89 (14) and 44.97 (14) °, respectively. The dihedral angle between rings (C17—C22) and rings (C10—C15) is 84.40 (14)°. In the crystal structure, weak inter molecular C—H···Cl hydrogen bonds (Table1) link the molecules into chains extended along the C axis. The packing (Fig. 2) is further stabilized by weak C—H···O interactions (Table 2).

Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)-1-(3-chlorophenyl)propan-1-one (5.7 g,0.02 mol)and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml). The reaction proceeded for 7 h. Water (50 ml) and chloroform (20 ml) were then added. The organic layer was washed successively with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate and the chloroform solution filtered. It was cooled with ice-water, and then an acetone solution (10 ml) of 2,4-dichlorobenzoic acid (3.8 g, 0.02 mol) and tri ethylamine (2.8 ml) was added. The mixture was stirred with ice-water for about 6 h. The solution was then filtered and concentrated. Single crystals were obtained by slow evaporation of ethanol solution at room temperature over a period of one week.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) and 1.5 U_{eq}(methyl C) H atoms.

Figures

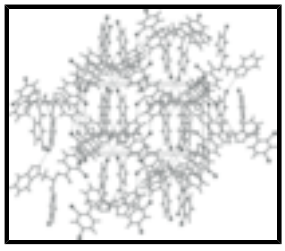


Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids.

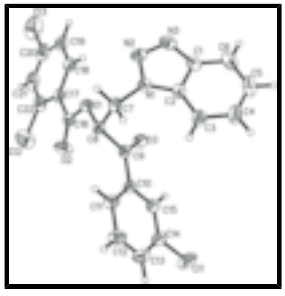


Fig. 2. The crystal packing of (I), viewed along *c* axis. Hydrogen bonding interactions are indicated by dashed lines.

2-(1*H*-Benzotriazol-1-yl)-1-(3-chlorobenzoyl)ethyl 2,4-dichlorobenzoate

Crystal data

$C_{22}H_{13}Cl_3N_3O_3$	F_{000} = 964
M_r = 473.70	D_x = 1.469 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3223 reflections
a = 10.9182 (2) Å	θ = 1.9–26.0º
b = 19.6123 (3) Å	μ = 0.46 mm^{-1}
c = 10.0124 (2) Å	T = 273 K
β = 92.096 (1)º	Prism, colourless
V = 2142.53 (7) Å^3	0.28 × 0.06 × 0.04 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	4212 independent reflections
Radiation source: fine-focus sealed tube	3192 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 273(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −13→12
T_{min} = 0.960, T_{max} = 0.980	k = −24→24
27918 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.151$	$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 1.3064P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
4212 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
280 parameters	$\Delta\rho_{min} = -0.46$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: ?

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *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	0.08295 (7)	0.21406 (6)	0.75068 (11)	0.0959 (4)
Cl2	0.70830 (11)	−0.05478 (5)	1.02091 (11)	0.1040 (4)
Cl3	1.09105 (14)	0.01904 (8)	1.32415 (11)	0.1447 (6)
O1	0.75829 (15)	0.14993 (8)	0.83033 (16)	0.0468 (5)
O2	0.6409 (2)	0.05810 (10)	0.8437 (2)	0.0793 (8)
O3	0.54692 (17)	0.20882 (10)	0.89673 (17)	0.0562 (6)
N1	0.75249 (17)	0.29201 (10)	0.75969 (18)	0.0413 (6)
N2	0.84951 (19)	0.29393 (12)	0.8493 (2)	0.0527 (7)
N3	0.8438 (2)	0.35025 (12)	0.9182 (2)	0.0594 (8)
C1	0.7421 (3)	0.38627 (13)	0.8729 (2)	0.0510 (8)
C2	0.6831 (2)	0.34902 (11)	0.7716 (2)	0.0420 (7)
C3	0.5776 (3)	0.37220 (14)	0.7044 (3)	0.0555 (9)
C4	0.5353 (3)	0.43447 (16)	0.7439 (3)	0.0740 (11)
C5	0.5931 (4)	0.47225 (16)	0.8448 (4)	0.0810 (13)
C6	0.6956 (3)	0.44969 (15)	0.9115 (3)	0.0713 (13)
C7	0.7376 (2)	0.23588 (12)	0.6664 (2)	0.0436 (7)
C8	0.6763 (2)	0.17327 (12)	0.7247 (2)	0.0424 (7)
C9	0.5515 (2)	0.18976 (11)	0.7819 (2)	0.0406 (7)

C10	0.4383 (2)	0.18335 (11)	0.6947 (2)	0.0414 (7)
C11	0.4378 (2)	0.16088 (14)	0.5633 (2)	0.0523 (8)
C12	0.3277 (3)	0.15362 (17)	0.4908 (3)	0.0659 (10)
C13	0.2185 (3)	0.16959 (17)	0.5473 (3)	0.0673 (11)
C14	0.2202 (2)	0.19297 (15)	0.6776 (3)	0.0599 (10)
C15	0.3280 (2)	0.19972 (13)	0.7513 (3)	0.0520 (8)
C16	0.7286 (2)	0.08918 (12)	0.8832 (3)	0.0484 (8)
C17	0.8177 (2)	0.07003 (13)	0.9928 (2)	0.0487 (8)
C18	0.9089 (2)	0.11622 (15)	1.0323 (3)	0.0564 (9)
C19	0.9930 (3)	0.10150 (19)	1.1342 (3)	0.0730 (11)
C20	0.9870 (3)	0.0400 (2)	1.1963 (3)	0.0781 (13)
C21	0.8994 (4)	−0.00732 (18)	1.1621 (3)	0.0806 (13)
C22	0.8140 (3)	0.00766 (14)	1.0588 (3)	0.0629 (10)
H3	0.53820	0.34700	0.63690	0.0670*
H4	0.46510	0.45210	0.70140	0.0890*
H5	0.56050	0.51430	0.86750	0.0970*
H6	0.73340	0.47510	0.97970	0.0850*
H7A	0.81760	0.22290	0.63590	0.0520*
H7B	0.68910	0.25130	0.58910	0.0520*
H11	0.51130	0.15070	0.52370	0.0630*
H12	0.32780	0.13780	0.40330	0.0790*
H13	0.14480	0.16480	0.49870	0.0810*
H15	0.32710	0.21520	0.83900	0.0620*
H18	0.91310	0.15800	0.98890	0.0680*
H19	1.05280	0.13310	1.16010	0.0870*
H21	0.89670	−0.04880	1.20690	0.0970*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0421 (4)	0.1304 (8)	0.1155 (8)	0.0145 (5)	0.0062 (4)	−0.0038 (6)
Cl2	0.1360 (9)	0.0568 (5)	0.1168 (8)	−0.0154 (5)	−0.0278 (7)	0.0304 (5)
Cl3	0.1632 (12)	0.1765 (13)	0.0890 (7)	0.0837 (10)	−0.0691 (8)	−0.0215 (8)
O1	0.0430 (9)	0.0391 (9)	0.0573 (10)	0.0023 (7)	−0.0099 (7)	0.0053 (7)
O2	0.0795 (15)	0.0546 (12)	0.1007 (16)	−0.0224 (11)	−0.0391 (12)	0.0201 (11)
O3	0.0517 (11)	0.0731 (12)	0.0435 (10)	0.0066 (9)	−0.0009 (7)	−0.0078 (9)
N1	0.0394 (10)	0.0443 (10)	0.0401 (10)	0.0010 (8)	0.0010 (8)	0.0055 (8)
N2	0.0447 (12)	0.0611 (14)	0.0518 (12)	−0.0035 (10)	−0.0058 (9)	0.0133 (10)
N3	0.0653 (15)	0.0611 (14)	0.0509 (12)	−0.0160 (11)	−0.0094 (11)	0.0063 (11)
C1	0.0632 (16)	0.0491 (14)	0.0407 (12)	−0.0118 (12)	0.0031 (11)	0.0031 (11)
C2	0.0504 (14)	0.0388 (12)	0.0371 (11)	−0.0001 (10)	0.0061 (10)	0.0041 (9)
C3	0.0603 (17)	0.0520 (15)	0.0536 (14)	0.0104 (12)	−0.0057 (12)	−0.0003 (12)
C4	0.081 (2)	0.0582 (18)	0.082 (2)	0.0245 (16)	−0.0064 (17)	−0.0012 (16)
C5	0.111 (3)	0.0496 (17)	0.083 (2)	0.0168 (17)	0.010 (2)	−0.0103 (16)
C6	0.103 (3)	0.0523 (16)	0.0588 (17)	−0.0130 (17)	0.0054 (17)	−0.0121 (14)
C7	0.0452 (13)	0.0471 (13)	0.0388 (11)	0.0063 (10)	0.0054 (10)	0.0012 (10)
C8	0.0410 (13)	0.0413 (12)	0.0446 (12)	0.0068 (10)	−0.0039 (10)	0.0022 (10)
C9	0.0434 (13)	0.0374 (11)	0.0408 (12)	0.0028 (9)	−0.0002 (9)	0.0038 (9)

C10	0.0406 (13)	0.0388 (12)	0.0446 (12)	0.0009 (10)	−0.0021 (10)	0.0060 (9)
C11	0.0482 (14)	0.0610 (16)	0.0476 (14)	0.0007 (12)	−0.0008 (11)	0.0016 (12)
C12	0.0608 (18)	0.083 (2)	0.0528 (16)	−0.0025 (15)	−0.0127 (13)	−0.0021 (14)
C13	0.0495 (17)	0.079 (2)	0.0721 (19)	−0.0019 (14)	−0.0169 (14)	0.0088 (16)
C14	0.0389 (14)	0.0645 (17)	0.0761 (19)	0.0040 (12)	0.0008 (12)	0.0085 (14)
C15	0.0456 (14)	0.0548 (15)	0.0554 (14)	0.0029 (11)	0.0011 (11)	0.0000 (12)
C16	0.0492 (15)	0.0380 (12)	0.0575 (14)	0.0043 (11)	−0.0062 (11)	0.0013 (11)
C17	0.0512 (14)	0.0448 (13)	0.0499 (14)	0.0141 (11)	−0.0023 (11)	−0.0034 (11)
C18	0.0491 (15)	0.0614 (16)	0.0582 (15)	0.0127 (12)	−0.0048 (12)	−0.0113 (12)
C19	0.0615 (19)	0.087 (2)	0.0691 (19)	0.0222 (16)	−0.0185 (15)	−0.0238 (17)
C20	0.083 (2)	0.094 (3)	0.0555 (17)	0.043 (2)	−0.0218 (16)	−0.0217 (17)
C21	0.114 (3)	0.072 (2)	0.0552 (17)	0.042 (2)	−0.0043 (18)	0.0082 (15)
C22	0.080 (2)	0.0494 (15)	0.0586 (16)	0.0167 (14)	−0.0050 (14)	0.0024 (12)

Geometric parameters (Å, °)

Cl1—C14	1.741 (3)	C12—C13	1.374 (5)
Cl2—C22	1.716 (3)	C13—C14	1.382 (4)
Cl3—C20	1.730 (3)	C14—C15	1.373 (3)
O1—C8	1.435 (3)	C16—C17	1.488 (3)
O1—C16	1.348 (3)	C17—C18	1.393 (3)
O2—C16	1.190 (3)	C17—C22	1.392 (4)
O3—C9	1.212 (3)	C18—C19	1.378 (4)
N1—N2	1.363 (3)	C19—C20	1.360 (5)
N1—C2	1.358 (3)	C20—C21	1.367 (5)
N1—C7	1.449 (3)	C21—C22	1.398 (5)
N2—N3	1.305 (3)	C3—H3	0.9300
N3—C1	1.379 (4)	C4—H4	0.9300
C1—C2	1.389 (3)	C5—H5	0.9300
C1—C6	1.403 (4)	C6—H6	0.9300
C2—C3	1.389 (4)	C7—H7A	0.9700
C3—C4	1.369 (4)	C7—H7B	0.9700
C4—C5	1.386 (5)	C11—H11	0.9300
C5—C6	1.356 (5)	C12—H12	0.9300
C7—C8	1.525 (3)	C13—H13	0.9300
C8—C9	1.532 (3)	C15—H15	0.9300
C9—C10	1.492 (3)	C18—H18	0.9300
C10—C11	1.387 (3)	C19—H19	0.9300
C10—C15	1.387 (3)	C21—H21	0.9300
C11—C12	1.389 (4)		
Cl1···N2^{i}	3.180 (2)	C7···N3^{vii}	3.253 (3)
Cl2···O2	2.915 (2)	C9···O2	2.821 (3)
Cl3···C16^{ii}	3.604 (3)	C9···C2	3.441 (3)
Cl1···H7A^{i}	3.0800	C11···O3^{vii}	3.298 (3)
Cl1···H19^{iii}	3.1500	C16···Cl3^{ii}	3.604 (3)
Cl2···H4^{iv}	2.8700	C16···O3	3.079 (3)
Cl3···H6^{v}	2.8300	C17···C2^{vi}	3.574 (3)

O1···O3	2.686 (2)	C18···C2^{vi}	3.566 (3)
O1···N1	2.875 (3)	C18···N1^{vi}	3.409 (3)
O1···N2	2.998 (3)	C19···N2^{vi}	3.398 (4)
O2···C9	2.821 (3)	C20···C1^{vi}	3.566 (4)
O2···Cl2	2.915 (2)	C20···C22^{ii}	3.539 (4)
O2···O3	3.180 (3)	C21···C6^{vi}	3.588 (5)
O2···C4^{iv}	3.198 (4)	C22···C20^{ii}	3.539 (4)
O3···O2	3.180 (3)	C1···H11^{vi}	3.0700
O3···C11^{vi}	3.298 (3)	C3···H7B	2.9200
O3···O1	2.686 (2)	C6···H11^{vi}	3.0600
O3···C16	3.079 (3)	C7···H3	3.0900
O3···N1	3.132 (3)	C8···H11	2.6900
O3···C2	3.388 (3)	C11···H5^{iv}	2.9600
O1···H18	2.2800	C12···H15^{vii}	2.9900
O2···H4^{iv}	2.4100	H3···C7	3.0900
O3···H15	2.4500	H3···H7B	2.5500
O3···H3^{vi}	2.6500	H3···O3^{vii}	2.6500
O3···H7B^{vi}	2.5500	H4···Cl2^{ix}	2.8700
N1···O1	2.875 (3)	H4···O2^{ix}	2.4100
N1···O3	3.132 (3)	H5···C11^{ix}	2.9600
N1···C18^{vii}	3.409 (3)	H6···Cl3^{x}	2.8300
N2···Cl1^{viii}	3.180 (2)	H7A···Cl1^{viii}	3.0800
N2···O1	2.998 (3)	H7A···N2^{vii}	2.9200
N2···C19^{vii}	3.398 (4)	H7A···N3^{vii}	2.6300
N3···C7^{vi}	3.253 (3)	H7B···C3	2.9200
N2···H7A^{vi}	2.9200	H7B···H3	2.5500
N3···H7A^{vi}	2.6300	H7B···O3^{vii}	2.5500
C1···C20^{vii}	3.566 (4)	H11···C8	2.6900
C2···C17^{vii}	3.574 (3)	H11···C1^{vii}	3.0700
C2···O3	3.388 (3)	H11···C6^{vii}	3.0600
C2···C9	3.441 (3)	H15···O3	2.4500
C2···C18^{vii}	3.566 (3)	H15···C12^{vi}	2.9900
C4···O2^{ix}	3.198 (4)	H18···O1	2.2800
C6···C21^{vii}	3.588 (5)	H19···Cl1^{xi}	3.1500
C8—O1—C16	114.76 (18)	C18—C17—C22	118.0 (2)
N2—N1—C2	109.99 (18)	C17—C18—C19	121.6 (3)
N2—N1—C7	120.75 (19)	C18—C19—C20	118.9 (3)
C2—N1—C7	129.21 (18)	Cl3—C20—C19	120.5 (3)
N1—N2—N3	108.7 (2)	Cl3—C20—C21	117.3 (3)
N2—N3—C1	108.3 (2)	C19—C20—C21	122.2 (3)
N3—C1—C2	108.5 (2)	C20—C21—C22	119.0 (3)
N3—C1—C6	131.2 (2)	Cl2—C22—C17	123.6 (2)
C2—C1—C6	120.3 (3)	Cl2—C22—C21	116.0 (2)

N1—C2—C1	104.6 (2)	C17—C22—C21	120.4 (3)
N1—C2—C3	133.0 (2)	C2—C3—H3	122.00
C1—C2—C3	122.4 (2)	C4—C3—H3	122.00
C2—C3—C4	115.8 (3)	C3—C4—H4	119.00
C3—C4—C5	122.6 (3)	C5—C4—H4	119.00
C4—C5—C6	122.0 (3)	C4—C5—H5	119.00
C1—C6—C5	117.0 (3)	C6—C5—H5	119.00
N1—C7—C8	113.92 (17)	C1—C6—H6	121.00
O1—C8—C7	105.56 (17)	C5—C6—H6	122.00
O1—C8—C9	109.34 (16)	N1—C7—H7A	109.00
C7—C8—C9	112.46 (19)	N1—C7—H7B	109.00
O3—C9—C8	119.2 (2)	C8—C7—H7A	109.00
O3—C9—C10	121.3 (2)	C8—C7—H7B	109.00
C8—C9—C10	119.51 (17)	H7A—C7—H7B	108.00
C9—C10—C11	123.79 (19)	C10—C11—H11	120.00
C9—C10—C15	117.0 (2)	C12—C11—H11	120.00
C11—C10—C15	119.2 (2)	C11—C12—H12	120.00
C10—C11—C12	120.1 (2)	C13—C12—H12	120.00
C11—C12—C13	120.6 (3)	C12—C13—H13	121.00
C12—C13—C14	118.8 (3)	C14—C13—H13	121.00
Cl1—C14—C13	119.6 (2)	C10—C15—H15	120.00
Cl1—C14—C15	119.0 (2)	C14—C15—H15	120.00
C13—C14—C15	121.4 (2)	C17—C18—H18	119.00
C10—C15—C14	119.9 (3)	C19—C18—H18	119.00
O1—C16—O2	121.6 (2)	C18—C19—H19	121.00
O1—C16—C17	110.65 (19)	C20—C19—H19	121.00
O2—C16—C17	127.7 (2)	C20—C21—H21	120.00
C16—C17—C18	119.1 (2)	C22—C21—H21	121.00
C16—C17—C22	122.9 (2)		
C8—O1—C16—C17	−179.15 (18)	C8—C9—C10—C11	2.2 (3)
C16—O1—C8—C7	−171.37 (19)	C8—C9—C10—C15	−179.3 (2)
C16—O1—C8—C9	67.4 (2)	O3—C9—C10—C15	−0.4 (3)
C8—O1—C16—O2	0.1 (3)	O3—C9—C10—C11	−179.0 (2)
C7—N1—N2—N3	178.03 (19)	C9—C10—C15—C14	−178.1 (2)
N2—N1—C2—C1	0.1 (2)	C9—C10—C11—C12	177.2 (2)
N2—N1—C7—C8	83.0 (2)	C15—C10—C11—C12	−1.3 (4)
C2—N1—N2—N3	0.2 (3)	C11—C10—C15—C14	0.6 (4)
C7—N1—C2—C3	1.4 (4)	C10—C11—C12—C13	1.1 (5)
C7—N1—C2—C1	−177.5 (2)	C11—C12—C13—C14	0.0 (5)
C2—N1—C7—C8	−99.7 (3)	C12—C13—C14—Cl1	179.6 (3)
N2—N1—C2—C3	179.0 (3)	C12—C13—C14—C15	−0.7 (5)
N1—N2—N3—C1	−0.4 (3)	C13—C14—C15—C10	0.5 (4)
N2—N3—C1—C6	−179.1 (3)	Cl1—C14—C15—C10	−179.8 (2)
N2—N3—C1—C2	0.5 (3)	O1—C16—C17—C18	4.8 (3)
C6—C1—C2—N1	179.3 (2)	O1—C16—C17—C22	−175.5 (2)
C6—C1—C2—C3	0.2 (4)	O2—C16—C17—C18	−174.4 (3)
N3—C1—C6—C5	178.8 (3)	O2—C16—C17—C22	5.3 (4)
C2—C1—C6—C5	−0.7 (4)	C16—C17—C18—C19	179.3 (3)
N3—C1—C2—N1	−0.3 (3)	C22—C17—C18—C19	−0.5 (4)

N3—C1—C2—C3	−179.4 (2)	C16—C17—C22—Cl2	0.8 (4)
C1—C2—C3—C4	0.3 (4)	C16—C17—C22—C21	−179.3 (3)
N1—C2—C3—C4	−178.5 (3)	C18—C17—C22—Cl2	−179.4 (2)
C2—C3—C4—C5	−0.3 (5)	C18—C17—C22—C21	0.4 (4)
C3—C4—C5—C6	−0.2 (6)	C17—C18—C19—C20	0.7 (4)
C4—C5—C6—C1	0.7 (5)	C18—C19—C20—Cl3	179.7 (2)
N1—C7—C8—O1	−63.4 (2)	C18—C19—C20—C21	−0.8 (5)
N1—C7—C8—C9	55.7 (2)	Cl3—C20—C21—C22	−179.7 (3)
C7—C8—C9—O3	−87.3 (2)	C19—C20—C21—C22	0.8 (5)
O1—C8—C9—O3	29.6 (3)	C20—C21—C22—Cl2	179.3 (3)
O1—C8—C9—C10	−151.55 (19)	C20—C21—C22—C17	−0.6 (5)
C7—C8—C9—C10	91.5 (2)		

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+2, −*y*, −*z*+2; (iii) *x*−1, −*y*+1/2, *z*−1/2; (iv) −*x*+1, *y*−1/2, −*z*+3/2; (v) −*x*+2, *y*−1/2, −*z*+5/2; (vi) *x*, −*y*+1/2, *z*+1/2; (vii) *x*, −*y*+1/2, *z*−1/2; (viii) *x*+1, *y*, *z*; (ix) −*x*+1, *y*+1/2, −*z*+3/2; (x) −*x*+2, *y*+1/2, −*z*+5/2; (xi) *x*+1, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{ix}	0.93	2.41	3.198 (4)	142
C6—H6···Cl3^{x}	0.93	2.83	3.719 (3)	161
C7—H7B···O3^{vii}	0.97	2.55	3.520 (3)	176
C18—H18···O1	0.93	2.28	2.643 (3)	102

Symmetry codes: (ix) −*x*+1, *y*+1/2, −*z*+3/2; (x) −*x*+2, *y*+1/2, −*z*+5/2; (vii) *x*, −*y*+1/2, *z*−1/2.

Fig. 1

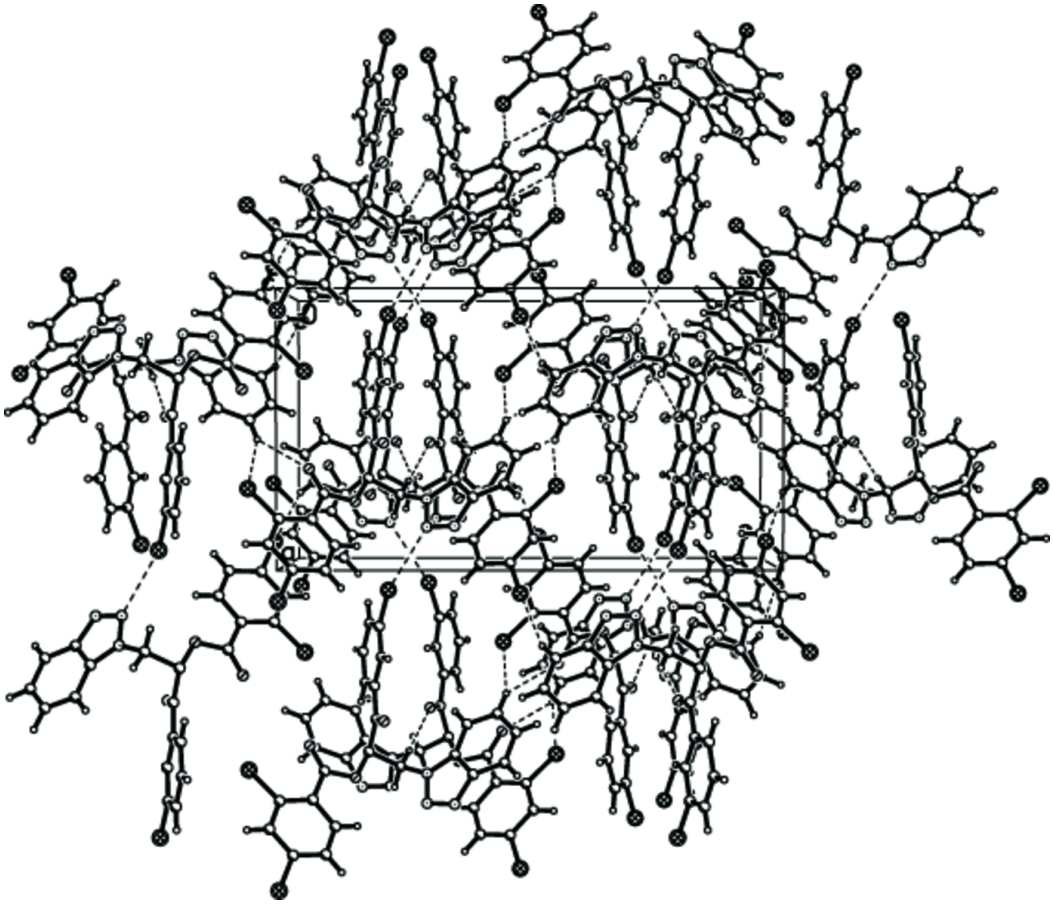
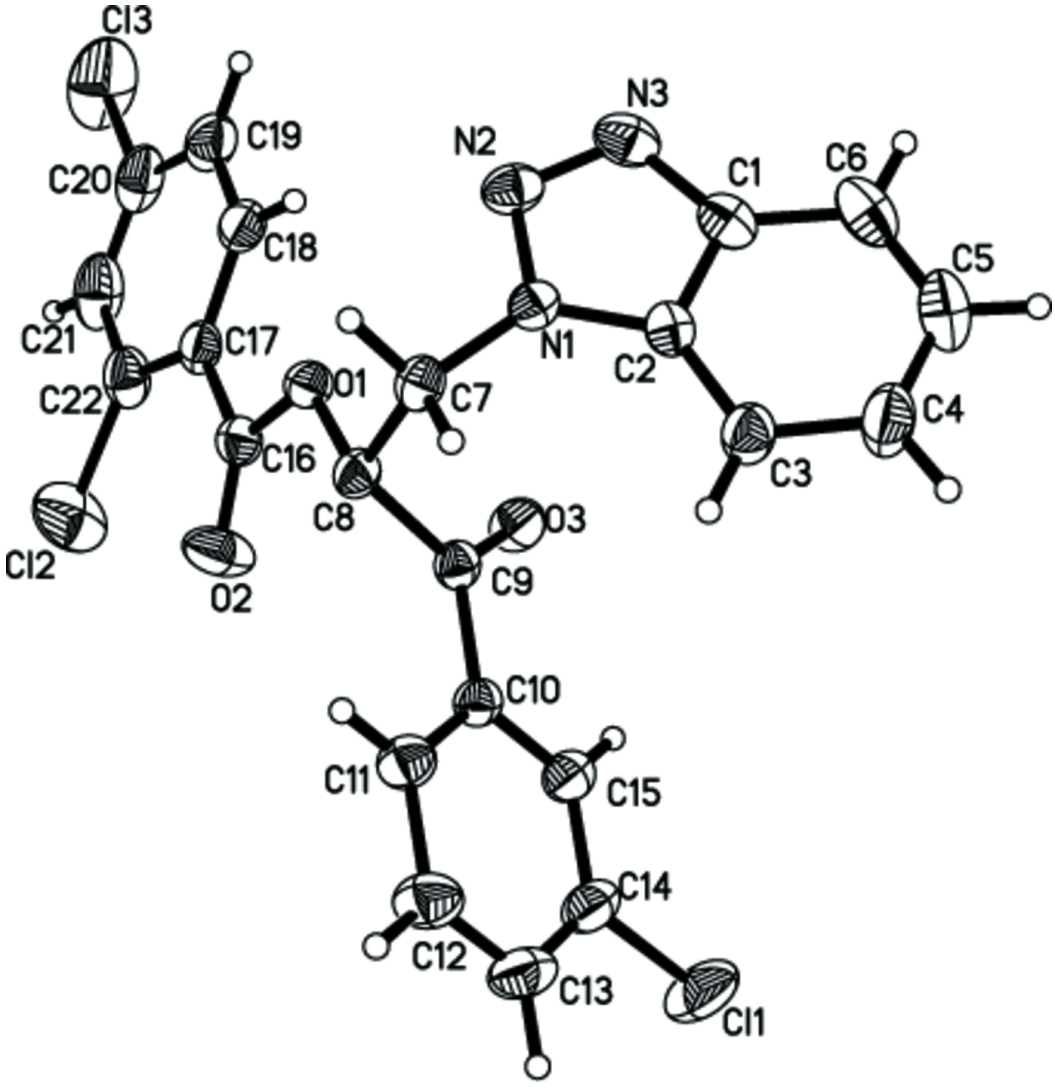


Fig. 2


Cl3
C19
C20
C18
C21
C17
C22
O1
C16
Cl2
O2
C8
C7
N3
N2
C1
C6
C5
N1
C2
C4
C3
O3
C9
C10
C11
C15
C14
C12
C13
Cl1