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

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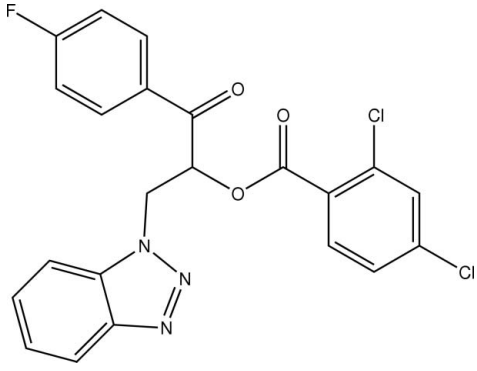
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.060; wR factor = 0.151; data-to-parameter ratio = 14.5.

In the title compound, $C_{22}H_{14}Cl_2FN_3O_3$, the two molecules in the asymmetric unit are linked into infinite chains along the a axis by intermolecular C—H···N and C—H···Cl hydrogen bonds.

Related literature

For related literature, see: Zhang *et al.* (2006); Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{14}Cl_2FN_3O_3$
M_r = 458.26
Monoclinic, $P2_1/c$
a = 11.9859 (7) Å
b = 25.1527 (16) Å
c = 13.8358 (9) Å
β = 98.6470 (10)°
V = 4123.8 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 293 (2) K
0.34 × 0.30 × 0.14 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.889, T_{max} = 0.952
23035 measured reflections
8111 independent reflections
4644 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.151
S = 1.03
8111 reflections
559 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···N3$'^{i}$	0.97	2.46	3.191 (4)	132
C4$'$—H26A···Cl1^{ii}	0.93	2.73	3.632 (5)	164
C9$'$—H31B···N3^{iii}	0.97	2.58	3.323 (4)	134

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2192).

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  doi:10.1107/S1600536807047046

supplementary materials

Acta Cryst. (2007). E**63**, o4192 [**doi:10.1107/S1600536807047046**]

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

S. Bi, J. Li, W.-L. Zeng and J. Wan

Comment

Recently we have reported the structure of 3-(benzotriazol-1-yl)-1-(4-chlorophenyl)-1-oxopropan-2-yl 2-chlorobenzoate (II) (Zhang *et al.*, 2006). As part of our ongoing studies of searching for triazole derivatives with higher pharmacological activities, the title compound, (I), was synthesized and its structure is presented here.

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable with those in the related compound, (II). In the molecule of (I), the asymmetric unit contains two molecules, A and B. The benzotriazole system is essentially planar, with a dihedral of 0.70 (2) and 0.73 (2)/% between the triazole rings (N1—N3/C10/C11 and N1'-N3'/C10'/C11') and benzne rings (C10—C15 and C10'-C15') in A and B, respectively. In A, the mean plane of the benzotriazole group makes dihedral angles of 17.55 (2) and 17.02 (1)/% with the C1—C6 and C17—C22 benzene rings, respectively. The corresponding dihedral angles in B are 26.66 (1) and 11.21 (1)/%. The dihedral angles between the latter two benzene rings are 30.88 (2) and 32.44 (2)/% in A and B, respectively.

In the crystal structure, the intermolecular C9—H9A···N3', C9'-H31B···N3 and C4'-H26A···Cl1 hydrogen bonds link the molecules, forming infinite chains along the *a* axis. The packing is further stabilized by π-π interactions, with *Cg*1···*Cg*7 (*x*, 1/2 − *y*, −1/2 + *z*) and *Cg*2···*Cg*6 (−*x*, 1 − *y*, 2 − *z*) distances of 3.710 (1) and 3.661 (1) /%A, respectively (*Cg*1, *Cg*2, *Cg*6 and *Cg*7 are the centroids of the rings N1—N3/C10/C11, N1'-N3'/C10'/C11', C10'-C15' and C17—C22, respectively).

Experimental

The title compound was prepared according to the literature method of Zhang *et al.* (2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of six days.

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 0.93–0.98 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) H atoms.

Figures

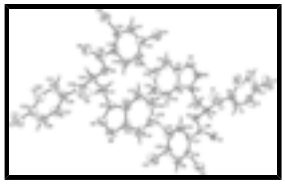

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

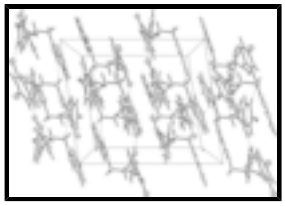

Fig. 2. A packing diagram of (I), viewed down the *b* axis. Hydrogen bonds are indicated by dashed lines.

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Crystal data

$C_{22}H_{14}Cl_2FN_3O_3$	F_{000} = 1872
M_r = 458.26	D_x = 1.476 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.9859 (7) Å	Cell parameters from 3056 reflections
b = 25.1527 (16) Å	θ = 2.4–21.2º
c = 13.8358 (9) Å	μ = 0.35 mm^{-1}
β = 98.6470 (10)º	T = 293 (2) K
V = 4123.8 (4) Å^3	Block, colourless
Z = 8	0.34 × 0.30 × 0.14 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	8111 independent reflections
Radiation source: fine-focus sealed tube	4644 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 1.6º
ω scans	h = −14→8
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −31→31
T_{min} = 0.889, T_{max} = 0.952	l = −16→17
23035 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
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H-atom parameters constrained
$wR(F^2)$ = 0.151	$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 0.2266P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
8111 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
559 parameters	$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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'	0.34033 (7)	0.37234 (3)	0.57244 (7)	0.0729 (3)
Cl1	−0.84381 (7)	0.32434 (3)	0.90731 (7)	0.0769 (3)
Cl2'	0.03377 (9)	0.22597 (3)	0.62058 (7)	0.0860 (3)
Cl2	−0.54316 (9)	0.47425 (3)	0.86955 (8)	0.0875 (3)
O2	−0.63982 (17)	0.22146 (7)	0.75847 (14)	0.0571 (6)
N1	−0.5387 (2)	0.15190 (9)	0.61983 (17)	0.0516 (6)
N2'	−0.0207 (2)	0.59177 (10)	0.86134 (19)	0.0615 (7)
O2'	0.13449 (18)	0.47776 (7)	0.71538 (16)	0.0658 (6)
N1'	0.0338 (2)	0.54473 (9)	0.85562 (17)	0.0496 (6)
O3	−0.7272 (2)	0.22071 (8)	0.89038 (16)	0.0714 (7)
C18	−0.7131 (2)	0.33972 (11)	0.8769 (2)	0.0484 (7)
C17	−0.6439 (3)	0.30175 (11)	0.8436 (2)	0.0483 (7)
C16	−0.6762 (3)	0.24432 (11)	0.8364 (2)	0.0515 (8)
C19	−0.6818 (3)	0.39220 (11)	0.8847 (2)	0.0571 (8)
H19A	−0.7293	0.4172	0.9067	0.068*
N2	−0.4831 (3)	0.10495 (10)	0.6184 (2)	0.0675 (8)
N3'	−0.1209 (2)	0.58228 (11)	0.8810 (2)	0.0672 (8)
C22	−0.5418 (3)	0.31834 (12)	0.8189 (2)	0.0627 (9)
H22A	−0.4944	0.2935	0.7962	0.075*
C8	−0.6625 (3)	0.16534 (10)	0.7475 (2)	0.0527 (8)
H8A	−0.7393	0.1580	0.7601	0.063*
O3'	0.2331 (2)	0.47809 (9)	0.59088 (18)	0.0876 (8)
C9	−0.6533 (2)	0.15132 (12)	0.6422 (2)	0.0579 (8)
H9A	−0.6850	0.1162	0.6282	0.069*
H9B	−0.6984	0.1763	0.5995	0.069*
C19'	0.1745 (3)	0.30608 (12)	0.5972 (2)	0.0557 (8)
H41A	0.2215	0.2800	0.5778	0.067*
C11	−0.3738 (3)	0.16814 (14)	0.5827 (2)	0.0616 (9)
C8'	0.1612 (3)	0.53319 (11)	0.7308 (2)	0.0557 (8)
H30A	0.2394	0.5395	0.7211	0.067*
C10'	−0.0345 (2)	0.50342 (11)	0.8726 (2)	0.0476 (7)

C15	−0.4905 (3)	0.24709 (13)	0.5867 (2)	0.0660 (9)
H15A	−0.5580	0.2631	0.5960	0.079*
C9'	0.1490 (2)	0.54536 (11)	0.8360 (2)	0.0536 (8)
H31A	0.1924	0.5195	0.8781	0.064*
H31B	0.1811	0.5801	0.8528	0.064*
C10	−0.4737 (2)	0.19277 (11)	0.5968 (2)	0.0482 (7)
N3	−0.3843 (3)	0.11433 (12)	0.5964 (2)	0.0741 (8)
C18'	0.2077 (2)	0.35877 (12)	0.6012 (2)	0.0494 (7)
C15'	−0.0207 (3)	0.44841 (12)	0.8769 (2)	0.0601 (8)
H37A	0.0461	0.4322	0.8662	0.072*
C16'	0.1755 (3)	0.45477 (12)	0.6397 (2)	0.0600 (9)
C17'	0.1394 (3)	0.39824 (12)	0.6302 (2)	0.0540 (8)
C20'	0.0719 (3)	0.29273 (12)	0.6219 (2)	0.0615 (9)
C21'	−0.0002 (3)	0.33062 (14)	0.6491 (3)	0.0756 (10)
H43A	−0.0704	0.3213	0.6646	0.091*
C22'	0.0350 (3)	0.38318 (13)	0.6525 (2)	0.0724 (10)
H44A	−0.0130	0.4092	0.6704	0.087*
C21	−0.5089 (3)	0.37078 (13)	0.8271 (2)	0.0675 (9)
H21A	−0.4397	0.3812	0.8107	0.081*
C20	−0.5798 (3)	0.40763 (12)	0.8599 (2)	0.0585 (9)
C1'	0.2164 (3)	0.64490 (13)	0.6779 (2)	0.0706 (10)
H23A	0.2770	0.6217	0.6930	0.085*
C11'	−0.1338 (3)	0.52797 (13)	0.8890 (2)	0.0548 (8)
C7'	0.0830 (3)	0.56708 (14)	0.6600 (2)	0.0637 (9)
C1	−0.7148 (3)	0.05963 (13)	0.8374 (2)	0.0688 (9)
H1A	−0.7747	0.0833	0.8235	0.083*
C6'	0.1092 (3)	0.62478 (13)	0.6561 (2)	0.0573 (8)
C12'	−0.2249 (3)	0.49825 (16)	0.9085 (2)	0.0719 (10)
H34A	−0.2922	0.5143	0.9183	0.086*
C6	−0.6064 (3)	0.07765 (13)	0.8378 (2)	0.0598 (8)
F1'	0.1635 (3)	0.78465 (9)	0.6575 (2)	0.1505 (12)
C13'	−0.2117 (3)	0.44440 (17)	0.9129 (3)	0.0781 (11)
H35A	−0.2715	0.4235	0.9263	0.094*
C7	−0.5786 (3)	0.13398 (12)	0.8188 (2)	0.0582 (8)
C14	−0.4023 (4)	0.27588 (15)	0.5621 (3)	0.0849 (12)
H14A	−0.4098	0.3125	0.5537	0.102*
O1	−0.4902 (2)	0.15392 (10)	0.85322 (19)	0.0873 (8)
C14'	−0.1108 (3)	0.41961 (14)	0.8979 (2)	0.0760 (11)
H36A	−0.1052	0.3828	0.9022	0.091*
C5	−0.5184 (4)	0.04214 (17)	0.8588 (3)	0.0987 (14)
H5B	−0.4446	0.0539	0.8603	0.118*
O1'	−0.0013 (2)	0.54804 (11)	0.6142 (2)	0.1042 (9)
F1	−0.6685 (3)	−0.07828 (10)	0.8933 (2)	0.1785 (14)
C5'	0.0202 (3)	0.65950 (17)	0.6320 (3)	0.0869 (12)
H27A	−0.0525	0.6462	0.6157	0.104*
C12	−0.2841 (3)	0.19776 (18)	0.5579 (3)	0.0869 (12)
H12A	−0.2168	0.1819	0.5478	0.104*
C4'	0.0373 (5)	0.7126 (2)	0.6317 (3)	0.1026 (16)
H26A	−0.0228	0.7359	0.6154	0.123*

C2'	0.2360 (4)	0.69905 (14)	0.6777 (3)	0.0869 (12)
H24A	0.3086	0.7128	0.6919	0.104*
C13	−0.3001 (4)	0.25110 (19)	0.5493 (3)	0.0924 (13)
H13A	−0.2412	0.2721	0.5343	0.111*
C3'	0.1444 (5)	0.73137 (14)	0.6558 (3)	0.0924 (14)
C4	−0.5384 (5)	−0.0103 (2)	0.8775 (4)	0.125 (2)
H4A	−0.4791	−0.0343	0.8915	0.150*
C2	−0.7365 (4)	0.00691 (15)	0.8574 (3)	0.0894 (12)
H2B	−0.8097	−0.0051	0.8586	0.107*
C3	−0.6469 (6)	−0.02618 (16)	0.8751 (3)	0.1099 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1'	0.0613 (6)	0.0613 (5)	0.1003 (7)	−0.0031 (4)	0.0262 (5)	−0.0085 (5)
Cl1	0.0613 (6)	0.0558 (5)	0.1190 (8)	−0.0036 (4)	0.0309 (5)	−0.0132 (5)
Cl2'	0.1007 (8)	0.0586 (5)	0.1043 (8)	−0.0226 (5)	0.0342 (6)	−0.0107 (5)
Cl2	0.0940 (7)	0.0515 (5)	0.1151 (8)	−0.0223 (5)	0.0093 (6)	−0.0061 (5)
O2	0.0615 (14)	0.0436 (11)	0.0705 (14)	−0.0052 (10)	0.0240 (11)	−0.0096 (10)
N1	0.0485 (16)	0.0438 (14)	0.0627 (17)	0.0056 (12)	0.0092 (13)	−0.0101 (11)
N2'	0.0602 (19)	0.0478 (15)	0.0771 (19)	0.0116 (13)	0.0125 (15)	−0.0036 (13)
O2'	0.0745 (16)	0.0463 (12)	0.0844 (16)	−0.0044 (11)	0.0371 (13)	−0.0144 (11)
N1'	0.0458 (16)	0.0407 (13)	0.0635 (16)	0.0066 (12)	0.0115 (12)	−0.0046 (11)
O3	0.0970 (19)	0.0486 (13)	0.0766 (16)	−0.0012 (12)	0.0394 (14)	0.0061 (11)
C18	0.0489 (18)	0.0456 (16)	0.0498 (18)	−0.0025 (14)	0.0044 (14)	−0.0019 (13)
C17	0.0533 (19)	0.0433 (16)	0.0473 (18)	0.0017 (15)	0.0045 (15)	0.0012 (13)
C16	0.055 (2)	0.0447 (17)	0.056 (2)	0.0042 (15)	0.0101 (16)	0.0013 (15)
C19	0.059 (2)	0.0455 (18)	0.066 (2)	0.0005 (16)	0.0071 (17)	−0.0089 (14)
N2	0.070 (2)	0.0490 (16)	0.086 (2)	0.0127 (14)	0.0215 (16)	−0.0113 (14)
N3'	0.0570 (19)	0.0638 (19)	0.082 (2)	0.0165 (15)	0.0132 (15)	0.0005 (14)
C22	0.063 (2)	0.057 (2)	0.071 (2)	0.0001 (17)	0.0187 (18)	−0.0089 (16)
C8	0.0483 (19)	0.0407 (16)	0.071 (2)	−0.0038 (14)	0.0137 (16)	−0.0086 (14)
O3'	0.122 (2)	0.0588 (15)	0.0950 (19)	−0.0115 (15)	0.0602 (18)	−0.0053 (13)
C9	0.0440 (19)	0.0563 (19)	0.072 (2)	−0.0048 (15)	0.0063 (16)	−0.0117 (16)
C19'	0.056 (2)	0.0502 (18)	0.062 (2)	0.0015 (16)	0.0133 (16)	−0.0095 (15)
C11	0.053 (2)	0.072 (2)	0.062 (2)	0.0070 (18)	0.0151 (17)	−0.0054 (17)
C8'	0.051 (2)	0.0437 (17)	0.075 (2)	−0.0029 (14)	0.0180 (17)	−0.0069 (15)
C10'	0.0419 (18)	0.0481 (17)	0.0527 (19)	0.0002 (14)	0.0068 (14)	−0.0047 (14)
C15	0.062 (2)	0.061 (2)	0.075 (2)	0.0047 (18)	0.0107 (19)	0.0041 (17)
C9'	0.0444 (19)	0.0430 (16)	0.073 (2)	−0.0008 (14)	0.0070 (16)	−0.0054 (14)
C10	0.0468 (19)	0.0490 (17)	0.0489 (18)	0.0030 (15)	0.0073 (14)	−0.0020 (14)
N3	0.066 (2)	0.067 (2)	0.093 (2)	0.0230 (16)	0.0239 (17)	−0.0058 (16)
C18'	0.0493 (19)	0.0549 (18)	0.0448 (17)	0.0015 (15)	0.0093 (14)	−0.0021 (14)
C15'	0.063 (2)	0.0461 (18)	0.072 (2)	0.0027 (16)	0.0140 (17)	−0.0036 (15)
C16'	0.068 (2)	0.0528 (19)	0.063 (2)	0.0029 (17)	0.0217 (18)	−0.0043 (16)
C17'	0.060 (2)	0.0523 (18)	0.0528 (19)	−0.0006 (16)	0.0170 (16)	−0.0047 (14)
C20'	0.072 (2)	0.0539 (19)	0.060 (2)	−0.0055 (18)	0.0148 (18)	−0.0073 (15)
C21'	0.072 (3)	0.073 (2)	0.089 (3)	−0.018 (2)	0.035 (2)	−0.018 (2)

C22'	0.072 (3)	0.066 (2)	0.086 (3)	−0.0002 (19)	0.032 (2)	−0.0215 (18)
C21	0.061 (2)	0.065 (2)	0.078 (2)	−0.0186 (18)	0.0159 (19)	−0.0062 (18)
C20	0.072 (2)	0.0439 (17)	0.058 (2)	−0.0110 (17)	0.0012 (18)	−0.0030 (14)
C1'	0.069 (2)	0.052 (2)	0.091 (3)	0.0116 (18)	0.009 (2)	0.0164 (18)
C11'	0.0436 (19)	0.066 (2)	0.054 (2)	0.0038 (17)	0.0053 (15)	0.0008 (15)
C7'	0.055 (2)	0.072 (2)	0.064 (2)	0.0011 (18)	0.0082 (18)	−0.0093 (18)
C1	0.079 (3)	0.052 (2)	0.073 (2)	0.0033 (18)	0.0007 (19)	0.0020 (16)
C6'	0.059 (2)	0.063 (2)	0.0495 (19)	0.0142 (17)	0.0095 (16)	0.0060 (15)
C12'	0.052 (2)	0.090 (3)	0.073 (2)	0.002 (2)	0.0082 (18)	0.003 (2)
C6	0.067 (2)	0.058 (2)	0.056 (2)	0.0123 (18)	0.0129 (17)	−0.0050 (15)
F1'	0.261 (4)	0.0524 (14)	0.151 (2)	0.0348 (18)	0.075 (2)	0.0217 (14)
C13'	0.063 (3)	0.098 (3)	0.075 (3)	−0.022 (2)	0.016 (2)	0.007 (2)
C7	0.057 (2)	0.058 (2)	0.062 (2)	0.0043 (17)	0.0129 (17)	−0.0143 (16)
C14	0.101 (3)	0.067 (2)	0.092 (3)	−0.007 (2)	0.029 (2)	0.012 (2)
O1	0.0586 (16)	0.0885 (18)	0.108 (2)	−0.0064 (14)	−0.0091 (14)	−0.0116 (15)
C14'	0.095 (3)	0.058 (2)	0.078 (3)	−0.017 (2)	0.020 (2)	0.0029 (18)
C5	0.098 (3)	0.088 (3)	0.119 (4)	0.041 (3)	0.045 (3)	0.026 (3)
O1'	0.083 (2)	0.111 (2)	0.109 (2)	−0.0135 (17)	−0.0187 (17)	−0.0123 (17)
F1	0.280 (4)	0.0628 (16)	0.199 (3)	0.014 (2)	0.057 (3)	0.0405 (18)
C5'	0.077 (3)	0.101 (3)	0.084 (3)	0.036 (2)	0.016 (2)	0.025 (2)
C12	0.065 (3)	0.108 (3)	0.095 (3)	0.006 (2)	0.034 (2)	−0.001 (2)
C4'	0.123 (4)	0.088 (3)	0.104 (3)	0.059 (3)	0.039 (3)	0.033 (3)
C2'	0.105 (3)	0.057 (2)	0.096 (3)	−0.001 (2)	0.008 (2)	0.015 (2)
C13	0.086 (3)	0.109 (4)	0.089 (3)	−0.032 (3)	0.033 (2)	0.004 (2)
C3'	0.164 (5)	0.044 (2)	0.077 (3)	0.028 (3)	0.041 (3)	0.0142 (19)
C4	0.144 (5)	0.090 (4)	0.152 (5)	0.065 (4)	0.062 (4)	0.046 (3)
C2	0.115 (3)	0.063 (2)	0.086 (3)	−0.014 (2)	0.002 (3)	0.005 (2)
C3	0.180 (6)	0.053 (3)	0.102 (3)	0.023 (3)	0.039 (4)	0.015 (2)

Geometric parameters (Å, °)

Cl1'—C18'	1.730 (3)	C18'—C17'	1.384 (4)
Cl1—C18	1.726 (3)	C15'—C14'	1.368 (4)
Cl2'—C20'	1.740 (3)	C15'—H37A	0.9300
Cl2—C20	1.732 (3)	C16'—C17'	1.487 (4)
O2—C16	1.351 (3)	C17'—C22'	1.385 (4)
O2—C8	1.441 (3)	C20'—C21'	1.376 (4)
N1—C10	1.357 (3)	C21'—C22'	1.387 (4)
N1—N2	1.358 (3)	C21'—H43A	0.9300
N1—C9	1.453 (3)	C22'—H44A	0.9300
N2'—N3'	1.293 (3)	C21—C20	1.379 (4)
N2'—N1'	1.359 (3)	C21—H21A	0.9300
O2'—C16'	1.352 (3)	C1'—C6'	1.371 (4)
O2'—C8'	1.439 (3)	C1'—C2'	1.382 (4)
N1'—C10'	1.365 (3)	C1'—H23A	0.9300
N1'—C9'	1.447 (3)	C11'—C12'	1.383 (4)
O3—C16	1.192 (3)	C7'—O1'	1.207 (4)
C18—C19	1.372 (4)	C7'—C6'	1.488 (4)
C18—C17	1.389 (4)	C1—C6	1.375 (4)

C17—C22	1.383 (4)	C1—C2	1.387 (4)
C17—C16	1.495 (4)	C1—H1A	0.9300
C19—C20	1.374 (4)	C6'—C5'	1.380 (4)
C19—H19A	0.9300	C12'—C13'	1.364 (5)
N2—N3	1.288 (4)	C12'—H34A	0.9300
N3'—C11'	1.381 (4)	C6—C5	1.379 (5)
C22—C21	1.377 (4)	C6—C7	1.488 (4)
C22—H22A	0.9300	F1'—C3'	1.359 (4)
C8—C9	1.518 (4)	C13'—C14'	1.404 (5)
C8—C7	1.519 (4)	C13'—H35A	0.9300
C8—H8A	0.9800	C7—O1	1.204 (4)
O3'—C16'	1.191 (3)	C14—C13	1.409 (5)
C9—H9A	0.9700	C14—H14A	0.9300
C9—H9B	0.9700	C14'—H36A	0.9300
C19'—C20'	1.368 (4)	C5—C4	1.372 (6)
C19'—C18'	1.382 (4)	C5—H5B	0.9300
C19'—H41A	0.9300	F1—C3	1.366 (5)
C11—N3	1.375 (4)	C5'—C4'	1.353 (6)
C11—C10	1.388 (4)	C5'—H27A	0.9300
C11—C12	1.392 (5)	C12—C13	1.358 (5)
C8'—C7'	1.514 (4)	C12—H12A	0.9300
C8'—C9'	1.515 (4)	C4'—C3'	1.361 (6)
C8'—H30A	0.9800	C4'—H26A	0.9300
C10'—C11'	1.389 (4)	C2'—C3'	1.363 (6)
C10'—C15'	1.394 (4)	C2'—H24A	0.9300
C15—C14	1.365 (5)	C13—H13A	0.9300
C15—C10	1.385 (4)	C4—C3	1.357 (7)
C15—H15A	0.9300	C4—H4A	0.9300
C9'—H31A	0.9700	C2—C3	1.352 (6)
C9'—H31B	0.9700	C2—H2B	0.9300
C16—O2—C8	115.0 (2)	C19'—C20'—C21'	121.6 (3)
C10—N1—N2	110.8 (2)	C19'—C20'—Cl2'	118.6 (2)
C10—N1—C9	130.7 (2)	C21'—C20'—Cl2'	119.8 (3)
N2—N1—C9	118.4 (3)	C20'—C21'—C22'	118.0 (3)
N3'—N2'—N1'	108.7 (2)	C20'—C21'—H43A	121.0
C16'—O2'—C8'	115.5 (2)	C22'—C21'—H43A	121.0
N2'—N1'—C10'	110.3 (2)	C17'—C22'—C21'	122.2 (3)
N2'—N1'—C9'	118.8 (2)	C17'—C22'—H44A	118.9
C10'—N1'—C9'	130.9 (2)	C21'—C22'—H44A	118.9
C19—C18—C17	121.2 (3)	C22—C21—C20	119.2 (3)
C19—C18—Cl1	116.4 (2)	C22—C21—H21A	120.4
C17—C18—Cl1	122.5 (2)	C20—C21—H21A	120.4
C22—C17—C18	118.0 (3)	C19—C20—C21	120.5 (3)
C22—C17—C16	120.3 (3)	C19—C20—Cl2	118.6 (3)
C18—C17—C16	121.7 (3)	C21—C20—Cl2	120.9 (3)
O3—C16—O2	123.1 (3)	C6'—C1'—C2'	121.1 (3)
O3—C16—C17	126.3 (3)	C6'—C1'—H23A	119.4
O2—C16—C17	110.7 (3)	C2'—C1'—H23A	119.4
C18—C19—C20	119.7 (3)	N3'—C11'—C12'	130.7 (3)

C18—C19—H19A	120.2	N3'—C11'—C10'	108.5 (3)
C20—C19—H19A	120.2	C12'—C11'—C10'	120.8 (3)
N3—N2—N1	108.4 (3)	O1'—C7'—C6'	122.2 (3)
N2'—N3'—C11'	108.5 (2)	O1'—C7'—C8'	120.3 (3)
C21—C22—C17	121.5 (3)	C6'—C7'—C8'	117.3 (3)
C21—C22—H22A	119.3	C6—C1—C2	121.4 (4)
C17—C22—H22A	119.3	C6—C1—H1A	119.3
O2—C8—C9	106.8 (2)	C2—C1—H1A	119.3
O2—C8—C7	110.1 (2)	C1'—C6'—C5'	119.0 (3)
C9—C8—C7	111.5 (2)	C1'—C6'—C7'	123.3 (3)
O2—C8—H8A	109.5	C5'—C6'—C7'	117.8 (3)
C9—C8—H8A	109.5	C13'—C12'—C11'	117.2 (3)
C7—C8—H8A	109.5	C13'—C12'—H34A	121.4
N1—C9—C8	114.2 (2)	C11'—C12'—H34A	121.4
N1—C9—H9A	108.7	C1—C6—C5	118.6 (3)
C8—C9—H9A	108.7	C1—C6—C7	123.3 (3)
N1—C9—H9B	108.7	C5—C6—C7	118.0 (4)
C8—C9—H9B	108.7	C12'—C13'—C14'	122.0 (3)
H9A—C9—H9B	107.6	C12'—C13'—H35A	119.0
C20'—C19'—C18'	119.3 (3)	C14'—C13'—H35A	119.0
C20'—C19'—H41A	120.3	O1—C7—C6	122.3 (3)
C18'—C19'—H41A	120.3	O1—C7—C8	119.8 (3)
N3—C11—C10	108.7 (3)	C6—C7—C8	117.7 (3)
N3—C11—C12	130.6 (3)	C15—C14—C13	121.1 (4)
C10—C11—C12	120.7 (3)	C15—C14—H14A	119.4
O2'—C8'—C7'	110.3 (3)	C13—C14—H14A	119.4
O2'—C8'—C9'	106.7 (2)	C15'—C14'—C13'	121.5 (3)
C7'—C8'—C9'	111.6 (3)	C15'—C14'—H36A	119.3
O2'—C8'—H30A	109.4	C13'—C14'—H36A	119.3
C7'—C8'—H30A	109.4	C4—C5—C6	120.8 (4)
C9'—C8'—H30A	109.4	C4—C5—H5B	119.6
N1'—C10'—C11'	103.9 (3)	C6—C5—H5B	119.6
N1'—C10'—C15'	133.8 (3)	C4'—C5'—C6'	120.9 (4)
C11'—C10'—C15'	122.3 (3)	C4'—C5'—H27A	119.5
C14—C15—C10	116.2 (3)	C6'—C5'—H27A	119.5
C14—C15—H15A	121.9	C13—C12—C11	116.5 (4)
C10—C15—H15A	121.9	C13—C12—H12A	121.8
N1'—C9'—C8'	114.3 (2)	C11—C12—H12A	121.8
N1'—C9'—H31A	108.7	C5'—C4'—C3'	118.6 (4)
C8'—C9'—H31A	108.7	C5'—C4'—H26A	120.7
N1'—C9'—H31B	108.7	C3'—C4'—H26A	120.7
C8'—C9'—H31B	108.7	C3'—C2'—C1'	117.2 (4)
H31A—C9'—H31B	107.6	C3'—C2'—H24A	121.4
N1—C10—C15	133.7 (3)	C1'—C2'—H24A	121.4
N1—C10—C11	103.5 (3)	C12—C13—C14	122.7 (4)
C15—C10—C11	122.8 (3)	C12—C13—H13A	118.7
N2—N3—C11	108.6 (3)	C14—C13—H13A	118.7
C19'—C18'—C17'	121.3 (3)	F1'—C3'—C4'	119.7 (5)
C19'—C18'—Cl1'	116.7 (2)	F1'—C3'—C2'	117.2 (5)

C17'—C18'—Cl1'	122.0 (2)	C4'—C3'—C2'	123.1 (4)
C14'—C15'—C10'	116.2 (3)	C3—C4—C5	118.2 (4)
C14'—C15'—H37A	121.9	C3—C4—H4A	120.9
C10'—C15'—H37A	121.9	C5—C4—H4A	120.9
O3'—C16'—O2'	122.6 (3)	C3—C2—C1	117.2 (4)
O3'—C16'—C17'	127.4 (3)	C3—C2—H2B	121.4
O2'—C16'—C17'	110.1 (3)	C1—C2—H2B	121.4
C18'—C17'—C22'	117.5 (3)	C2—C3—C4	123.8 (4)
C18'—C17'—C16'	122.3 (3)	C2—C3—F1	117.2 (5)
C22'—C17'—C16'	120.2 (3)	C4—C3—F1	119.0 (5)
N3'—N2'—N1'—C10'	−0.2 (3)	C18'—C19'—C20'—Cl2'	−177.7 (2)
N3'—N2'—N1'—C9'	−178.9 (2)	C19'—C20'—C21'—C22'	−1.2 (5)
C19—C18—C17—C22	0.3 (4)	Cl2'—C20'—C21'—C22'	177.8 (3)
Cl1—C18—C17—C22	178.4 (2)	C18'—C17'—C22'—C21'	1.7 (5)
C19—C18—C17—C16	178.9 (3)	C16'—C17'—C22'—C21'	−177.0 (3)
Cl1—C18—C17—C16	−2.9 (4)	C20'—C21'—C22'—C17'	−0.3 (5)
C8—O2—C16—O3	−2.9 (4)	C17—C22—C21—C20	−0.6 (5)
C8—O2—C16—C17	177.4 (2)	C18—C19—C20—C21	0.1 (5)
C22—C17—C16—O3	144.0 (3)	C18—C19—C20—Cl2	179.4 (2)
C18—C17—C16—O3	−34.6 (5)	C22—C21—C20—C19	0.4 (5)
C22—C17—C16—O2	−36.3 (4)	C22—C21—C20—Cl2	−178.9 (2)
C18—C17—C16—O2	145.0 (3)	N2'—N3'—C11'—C12'	−179.7 (3)
C17—C18—C19—C20	−0.4 (4)	N2'—N3'—C11'—C10'	−0.2 (3)
Cl1—C18—C19—C20	−178.7 (2)	N1'—C10'—C11'—N3'	0.1 (3)
C10—N1—N2—N3	0.8 (3)	C15'—C10'—C11'—N3'	179.2 (3)
C9—N1—N2—N3	179.5 (2)	N1'—C10'—C11'—C12'	179.6 (3)
N1'—N2'—N3'—C11'	0.3 (3)	C15'—C10'—C11'—C12'	−1.3 (5)
C18—C17—C22—C21	0.3 (5)	O2'—C8'—C7'—O1'	13.7 (4)
C16—C17—C22—C21	−178.4 (3)	C9'—C8'—C7'—O1'	−104.7 (4)
C16—O2—C8—C9	161.2 (2)	O2'—C8'—C7'—C6'	−171.4 (2)
C16—O2—C8—C7	−77.6 (3)	C9'—C8'—C7'—C6'	70.2 (3)
C10—N1—C9—C8	−82.4 (4)	C2'—C1'—C6'—C5'	1.2 (5)
N2—N1—C9—C8	99.1 (3)	C2'—C1'—C6'—C7'	−176.9 (3)
O2—C8—C9—N1	71.7 (3)	O1'—C7'—C6'—C1'	−157.0 (4)
C7—C8—C9—N1	−48.7 (3)	C8'—C7'—C6'—C1'	28.3 (4)
C16'—O2'—C8'—C7'	79.9 (3)	O1'—C7'—C6'—C5'	24.8 (5)
C16'—O2'—C8'—C9'	−158.7 (3)	C8'—C7'—C6'—C5'	−149.9 (3)
N2'—N1'—C10'—C11'	0.1 (3)	N3'—C11'—C12'—C13'	−179.3 (3)
C9'—N1'—C10'—C11'	178.5 (3)	C10'—C11'—C12'—C13'	1.3 (5)
N2'—N1'—C10'—C15'	−178.9 (3)	C2—C1—C6—C5	−0.2 (5)
C9'—N1'—C10'—C15'	−0.4 (5)	C2—C1—C6—C7	−178.7 (3)
N2'—N1'—C9'—C8'	−100.9 (3)	C11'—C12'—C13'—C14'	−0.3 (5)
C10'—N1'—C9'—C8'	80.8 (4)	C1—C6—C7—O1	151.4 (3)
O2'—C8'—C9'—N1'	−70.1 (3)	C5—C6—C7—O1	−27.2 (5)
C7'—C8'—C9'—N1'	50.5 (3)	C1—C6—C7—C8	−33.1 (4)
N2—N1—C10—C15	178.8 (3)	C5—C6—C7—C8	148.3 (3)
C9—N1—C10—C15	0.3 (5)	O2—C8—C7—O1	−20.7 (4)
N2—N1—C10—C11	−1.0 (3)	C9—C8—C7—O1	97.6 (3)
C9—N1—C10—C11	−179.5 (3)	O2—C8—C7—C6	163.7 (2)

C14—C15—C10—N1	180.0 (3)	C9—C8—C7—C6	−77.9 (3)
C14—C15—C10—C11	−0.3 (5)	C10—C15—C14—C13	−0.7 (5)
N3—C11—C10—N1	0.8 (3)	C10'—C15'—C14'—C13'	0.7 (5)
C12—C11—C10—N1	−179.7 (3)	C12'—C13'—C14'—C15'	−0.7 (5)
N3—C11—C10—C15	−179.0 (3)	C1—C6—C5—C4	1.0 (6)
C12—C11—C10—C15	0.5 (5)	C7—C6—C5—C4	179.6 (4)
N1—N2—N3—C11	−0.2 (4)	C1'—C6'—C5'—C4'	−1.5 (5)
C10—C11—N3—N2	−0.4 (4)	C7'—C6'—C5'—C4'	176.8 (3)
C12—C11—N3—N2	−179.8 (3)	N3—C11—C12—C13	179.8 (4)
C20'—C19'—C18'—C17'	0.2 (4)	C10—C11—C12—C13	0.4 (5)
C20'—C19'—C18'—Cl1'	178.1 (2)	C6'—C5'—C4'—C3'	0.0 (6)
N1'—C10'—C15'—C14'	179.0 (3)	C6'—C1'—C2'—C3'	0.5 (5)
C11'—C10'—C15'—C14'	0.2 (4)	C11—C12—C13—C14	−1.5 (6)
C8'—O2'—C16'—O3'	2.5 (5)	C15—C14—C13—C12	1.7 (6)
C8'—O2'—C16'—C17'	−178.4 (3)	C5'—C4'—C3'—F1'	−179.0 (3)
C19'—C18'—C17'—C22'	−1.7 (4)	C5'—C4'—C3'—C2'	1.9 (7)
Cl1'—C18'—C17'—C22'	−179.4 (2)	C1'—C2'—C3'—F1'	178.8 (3)
C19'—C18'—C17'—C16'	177.0 (3)	C1'—C2'—C3'—C4'	−2.1 (6)
Cl1'—C18'—C17'—C16'	−0.8 (4)	C6—C5—C4—C3	−0.2 (7)
O3'—C16'—C17'—C18'	34.4 (5)	C6—C1—C2—C3	−1.4 (6)
O2'—C16'—C17'—C18'	−144.7 (3)	C1—C2—C3—C4	2.3 (7)
O3'—C16'—C17'—C22'	−147.0 (4)	C1—C2—C3—F1	−179.0 (3)
O2'—C16'—C17'—C22'	33.9 (4)	C5—C4—C3—C2	−1.5 (8)
C18'—C19'—C20'—C21'	1.2 (5)	C5—C4—C3—F1	179.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···N3^{i}	0.97	2.46	3.191 (4)	132
C4'—H26A···Cl1^{ii}	0.93	2.73	3.632 (5)	164
C9'—H31B···N3^{iii}	0.97	2.58	3.323 (4)	134

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

Fig. 1

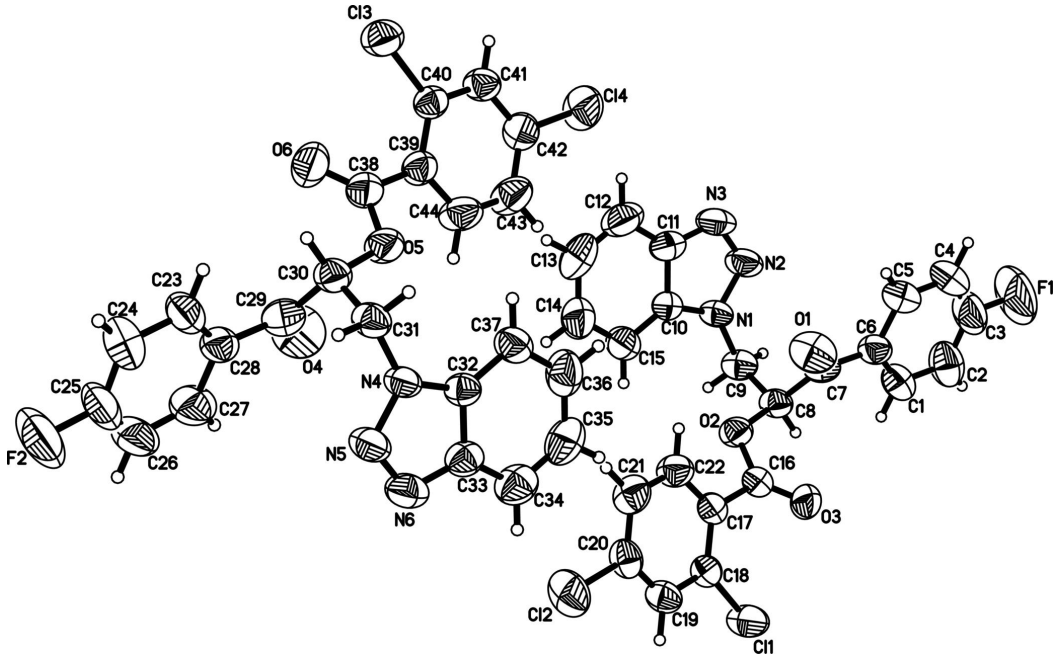
Cl3
C40
C41
Cl4
C42
O6
C38
C39
C44
C43
C12
N3
C11
O5
C13
N2
C4
C5
F1
C23
C30
C29
C24
C14
C10
N1
O1
C6
C3
C31
C37
C15
C28
O4
N4
C32
C36
C9
C7
C2
C25
C27
C8
C1
C35
O2
F2
N5
C21
C22
C16
C26
C33
C34
C17
O3
N6
C20
C18
Cl2
C19
Cl1

Fig. 2