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Ethyl 2-(4-cyanophenyl)-1-(4-fluorobenzyl)-1*H*-benzo[*d*]imidazole-5-carboxylate

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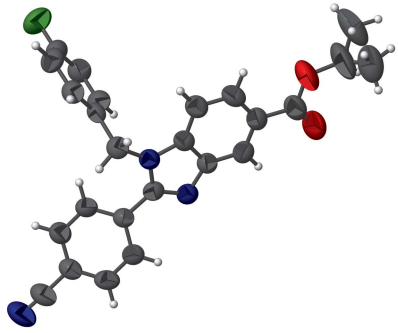
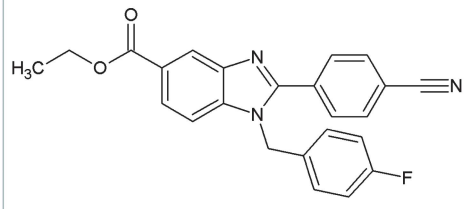
Structural data: full structural data are available from iucrdata.iucr.org

The title benzimidazole derivative, $C_{24}H_{18}FN_3O_2$, is T-shaped, with the 4-cyanobenzene and 4-fluorobenzyl rings inclined to the imidazole ring system by 32.89 (10) and 83.63 (10)°, respectively, and by 89.00 (12)° to one another. The terminal methyl group of the ethylcarboxylate group is disordered over three sites and was refined with a fixed occupancy ratio of 1/3:1/3:1/3. In the crystal, molecules are essentially linked by offset π–π interactions, involving inversion-related imidazole rings [inter-centroid distance = 3.763 (1) Å], and stack along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Having an interest in the synthesis of benzimidazole derivatives, we present herein the synthesis and crystal structure of the title compound, Fig. 1. The molecule is T-shaped, with the 4-cyanobenzene ring (C1–C6) and the 4-fluorobenzyl ring (C10–C15) inclined to imidazole ring system (N1/N2/C8/C16–C21) by 32.89 (10) and 83.63 (10)°, respectively, and by 89.00 (12)° to one another.

In the crystal, Fig. 2, molecules are essentially linked by offset π–π interactions, involving inversion-related imidazole ring systems, and stack along the *b*-axis direction [$Cg1\cdots Cg4^{i}$ = 3.763 (1) Å, interplanar distance = 3.556 (1) Å, slippage 1.277 Å, *Cg*1 and *Cg*4 are the centroids of rings N1/N2/C8/C16/C17 and C16–C21, respectively; symmetry code (i) $-x+1, -y+1, -z+1$].

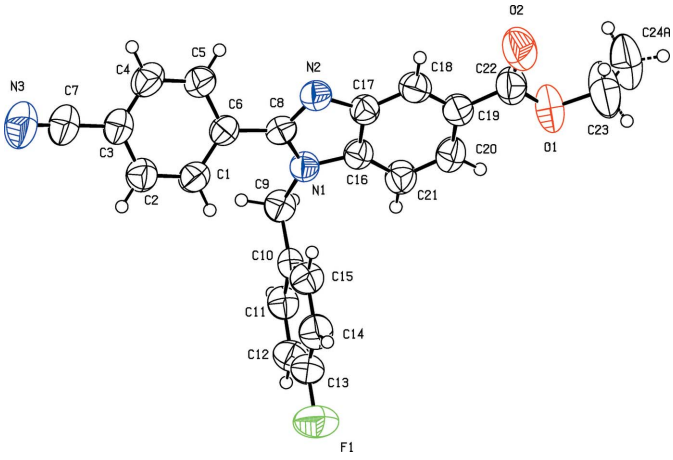


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

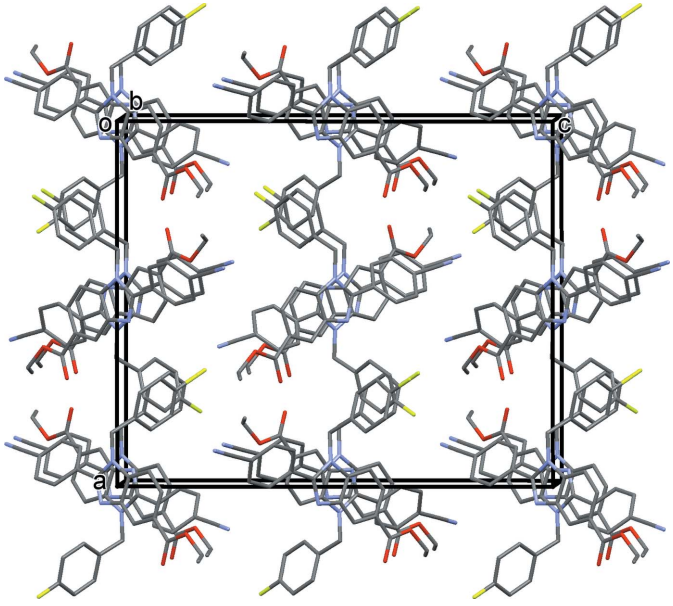


Figure 2
A view along the *b* axis of the crystal packing of the title compound. For clarity, the H atoms and the minor component of the disordered methyl C atom have been omitted.

Synthesis and crystallization

Sodium dithionite (3.0 equiv) was added to a stirred solution of ethyl 4-(4-fluorobenzylamino)-3-nitrobenzoate (0.01 mol; 1.0 equiv) and 4-cyanobenzaldehyde (0.01 mol; 1.0 equiv) in DMSO (20 ml). The reaction mixture was stirred at 363 K for 3 h. After the completion of reaction (monitored by TLC hexane:ethyl acetate (7:3, *v*/*v*)), it was poured onto crushed ice. The solid that separated was filtered off, washed with water and dried. The product was recrystallized from *N*,*N*-dimethylformamide giving crystals suitable for X-ray diffraction analysis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{18}FN_3O_2$
M_r	399.41
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	18.4827 (12), 9.8467 (6), 22.0681 (15)
V (Å^3)	4016.3 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.43 × 0.28 × 0.13
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.970, 0.988
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37377, 3631, 2276
R_{int}	0.078
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.121, 1.06
No. of reflections	3631
No. of parameters	281
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.11, −0.15

Computer programs: *CrystalClear* (Rigaku, 2011), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The terminal methyl group (C24*A*, C24*B* and C24*C*) of the ethylcarboxylate moiety is disordered over three sites and was refined with a fixed occupancy ratio of 1/3:1/3:1/3.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161124 [doi:10.1107/S241431461601124X]

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Crystal data

$C_{24}H_{18}FN_3O_2$
M_r = 399.41
Orthorhombic, *Pbca*
a = 18.4827 (12) Å
b = 9.8467 (6) Å
c = 22.0681 (15) Å
V = 4016.3 (4) Å^3
Z = 8
F(000) = 1664
D_x = 1.321 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71075 Å
Cell parameters from 4608 reflections
θ = 27.5–3.0°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.43 × 0.28 × 0.13 mm

Data collection

Rigaku Saturn724+ diffractometer
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.970, T_{max} = 0.988
37377 measured reflections
3631 independent reflections
2276 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 25.3°, θ_{min} = 3.0°
h = −22→22
k = −11→10
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.121
S = 1.06
3631 reflections
281 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 1.0958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0018 (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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
F1	0.80220 (9)	0.00408 (18)	0.68055 (7)	0.1111 (6)	
N1	0.57339 (10)	0.24922 (19)	0.49515 (8)	0.0573 (5)	
N2	0.45818 (10)	0.2120 (2)	0.46754 (8)	0.0636 (5)	
N3	0.61148 (16)	−0.2833 (3)	0.23995 (11)	0.1117 (9)	
C1	0.60741 (14)	0.0001 (2)	0.41557 (11)	0.0674 (7)	
H1	0.6361	0.0050	0.4501	0.081*	
C2	0.62374 (14)	−0.0929 (3)	0.37106 (11)	0.0708 (7)	
H2	0.6636	−0.1496	0.3755	0.085*	
C3	0.58132 (14)	−0.1023 (3)	0.32020 (11)	0.0655 (7)	
C4	0.52266 (15)	−0.0168 (3)	0.31341 (11)	0.0758 (8)	
H4	0.4939	−0.0227	0.2790	0.091*	
C5	0.50686 (13)	0.0770 (3)	0.35759 (10)	0.0680 (7)	
H5	0.4676	0.1350	0.3526	0.082*	
C6	0.54866 (12)	0.0864 (2)	0.40949 (10)	0.0556 (6)	
C7	0.59760 (16)	−0.2023 (3)	0.27484 (13)	0.0817 (8)	
C8	0.52664 (13)	0.1830 (2)	0.45663 (10)	0.0569 (6)	
C9	0.65188 (11)	0.2605 (2)	0.49315 (10)	0.0608 (6)	
H9A	0.6649	0.3559	0.4939	0.073*	
H9B	0.6689	0.2229	0.4551	0.073*	
C10	0.69001 (12)	0.1895 (2)	0.54441 (9)	0.0508 (6)	
C11	0.76027 (12)	0.2258 (2)	0.55708 (11)	0.0622 (6)	
H11	0.7824	0.2936	0.5344	0.075*	
C12	0.79824 (14)	0.1634 (3)	0.60266 (12)	0.0758 (8)	
H12	0.8458	0.1879	0.6109	0.091*	
C13	0.76507 (16)	0.0659 (3)	0.63530 (11)	0.0717 (7)	
C14	0.69539 (15)	0.0273 (3)	0.62490 (12)	0.0724 (7)	
H14	0.6736	−0.0395	0.6484	0.087*	
C15	0.65808 (13)	0.0898 (2)	0.57864 (11)	0.0661 (7)	
H15	0.6106	0.0641	0.5705	0.079*	
C16	0.53115 (13)	0.3252 (2)	0.53371 (10)	0.0563 (6)	
C17	0.45998 (13)	0.3020 (2)	0.51577 (10)	0.0576 (6)	
C18	0.40424 (13)	0.3651 (3)	0.54635 (11)	0.0673 (7)	
H18	0.3564	0.3507	0.5348	0.081*	
C19	0.42048 (14)	0.4497 (3)	0.59418 (11)	0.0636 (7)	
C20	0.49223 (15)	0.4708 (3)	0.61153 (11)	0.0696 (7)	
H20	0.5022	0.5278	0.6441	0.084*	
C21	0.54850 (14)	0.4090 (3)	0.58150 (11)	0.0691 (7)	
H21	0.5963	0.4233	0.5930	0.083*	
O1	0.38006 (11)	0.5953 (2)	0.67054 (10)	0.1065 (7)	

O2	0.29671 (13)	0.4915 (3)	0.61495 (10)	0.1189 (9)	
C22	0.3591 (2)	0.5116 (3)	0.62677 (13)	0.0830 (9)	
C23	0.3227 (2)	0.6538 (5)	0.7078 (2)	0.1504 (17)	
H23A	0.2788	0.6025	0.7002	0.181*	0.3333
H23B	0.3356	0.6393	0.7499	0.181*	0.3333
H23C	0.2914	0.7123	0.6841	0.181*	0.3333
H23D	0.2938	0.5835	0.7268	0.181*	0.3333
H23E	0.2863	0.6916	0.6811	0.181*	0.3333
H23F	0.3000	0.5809	0.7305	0.181*	0.3333
C24A	0.3082 (7)	0.7746 (12)	0.7016 (6)	0.127 (4)	0.3333
H24A	0.3516	0.8275	0.7058	0.191*	0.3333
H24B	0.2739	0.8016	0.7319	0.191*	0.3333
H24C	0.2879	0.7893	0.6621	0.191*	0.3333
C24B	0.3638 (13)	0.733 (2)	0.7536 (12)	0.127 (4)	0.3333
H24D	0.3898	0.6715	0.7796	0.191*	0.3333
H24E	0.3308	0.7859	0.7774	0.191*	0.3333
H24F	0.3974	0.7918	0.7335	0.191*	0.3333
C24C	0.3433 (12)	0.753 (2)	0.7480 (13)	0.127 (4)	0.3333
H24G	0.3720	0.7132	0.7796	0.191*	0.3333
H24H	0.3011	0.7944	0.7652	0.191*	0.3333
H24I	0.3713	0.8205	0.7271	0.191*	0.3333

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1119 (13)	0.1166 (14)	0.1048 (12)	0.0200 (11)	−0.0263 (11)	0.0256 (11)
N1	0.0539 (11)	0.0617 (12)	0.0562 (11)	−0.0022 (11)	0.0002 (10)	−0.0038 (10)
N2	0.0593 (13)	0.0698 (14)	0.0617 (13)	−0.0004 (11)	−0.0042 (10)	−0.0023 (11)
N3	0.127 (2)	0.116 (2)	0.0915 (19)	−0.0095 (18)	0.0115 (16)	−0.0401 (17)
C1	0.0764 (18)	0.0696 (18)	0.0562 (14)	0.0054 (15)	−0.0087 (13)	−0.0041 (13)
C2	0.0790 (18)	0.0679 (18)	0.0656 (16)	0.0045 (14)	0.0008 (14)	−0.0041 (14)
C3	0.0704 (17)	0.0663 (18)	0.0598 (16)	−0.0126 (14)	0.0080 (13)	−0.0070 (13)
C4	0.0740 (18)	0.094 (2)	0.0593 (16)	−0.0140 (16)	−0.0077 (14)	−0.0109 (16)
C5	0.0638 (16)	0.0791 (18)	0.0611 (15)	0.0006 (14)	−0.0044 (13)	−0.0043 (15)
C6	0.0590 (14)	0.0560 (16)	0.0520 (14)	−0.0051 (13)	0.0000 (12)	0.0008 (12)
C7	0.089 (2)	0.087 (2)	0.0694 (17)	−0.0167 (17)	0.0108 (15)	−0.0171 (17)
C8	0.0608 (16)	0.0571 (16)	0.0527 (14)	−0.0017 (13)	−0.0045 (12)	0.0043 (12)
C9	0.0550 (15)	0.0632 (16)	0.0642 (15)	−0.0093 (12)	0.0044 (12)	0.0008 (13)
C10	0.0501 (14)	0.0511 (14)	0.0513 (13)	−0.0018 (11)	0.0067 (11)	−0.0067 (11)
C11	0.0560 (15)	0.0618 (16)	0.0687 (15)	−0.0083 (13)	0.0041 (13)	−0.0036 (13)
C12	0.0558 (16)	0.082 (2)	0.0895 (19)	−0.0015 (15)	−0.0086 (15)	0.0005 (17)
C13	0.077 (2)	0.0712 (19)	0.0669 (16)	0.0156 (16)	−0.0055 (15)	0.0065 (15)
C14	0.081 (2)	0.0649 (18)	0.0718 (17)	−0.0027 (15)	0.0073 (15)	0.0087 (14)
C15	0.0594 (15)	0.0704 (18)	0.0684 (16)	−0.0092 (14)	−0.0012 (13)	0.0031 (14)
C16	0.0609 (16)	0.0543 (16)	0.0539 (14)	−0.0019 (13)	0.0018 (12)	0.0018 (13)
C17	0.0590 (16)	0.0574 (16)	0.0563 (14)	0.0011 (13)	0.0019 (12)	0.0011 (12)
C18	0.0620 (16)	0.0724 (18)	0.0674 (16)	0.0034 (14)	−0.0003 (13)	0.0047 (14)
C19	0.0699 (17)	0.0595 (16)	0.0615 (15)	0.0059 (14)	0.0080 (13)	0.0090 (13)

C20	0.086 (2)	0.0636 (17)	0.0593 (15)	−0.0017 (15)	0.0043 (14)	−0.0079 (13)
C21	0.0655 (16)	0.0726 (18)	0.0690 (16)	−0.0041 (14)	0.0003 (13)	−0.0104 (15)
O1	0.1117 (16)	0.1008 (16)	0.1070 (15)	0.0137 (13)	0.0386 (13)	−0.0309 (14)
O2	0.0819 (15)	0.161 (2)	0.1135 (17)	0.0187 (15)	0.0192 (14)	−0.0283 (15)
C22	0.094 (2)	0.084 (2)	0.0708 (19)	0.014 (2)	0.0188 (18)	0.0010 (17)
C23	0.135 (3)	0.159 (4)	0.157 (3)	0.020 (3)	0.054 (3)	−0.062 (3)
C24A	0.163 (10)	0.085 (5)	0.134 (6)	0.013 (5)	0.067 (7)	−0.017 (5)
C24B	0.163 (10)	0.085 (5)	0.134 (6)	0.013 (5)	0.067 (7)	−0.017 (5)
C24C	0.163 (10)	0.085 (5)	0.134 (6)	0.013 (5)	0.067 (7)	−0.017 (5)

Geometric parameters (Å, º)

F1—C13	1.356 (3)	C16—C21	1.377 (3)
N1—C16	1.376 (3)	C16—C17	1.393 (3)
N1—C8	1.376 (3)	C17—C18	1.379 (3)
N1—C9	1.456 (3)	C18—C19	1.378 (3)
N2—C8	1.319 (3)	C18—H18	0.9300
N2—C17	1.385 (3)	C19—C20	1.396 (3)
N3—C7	1.138 (3)	C19—C22	1.476 (4)
C1—C2	1.376 (3)	C20—C21	1.375 (3)
C1—C6	1.386 (3)	C20—H20	0.9300
C1—H1	0.9300	C21—H21	0.9300
C2—C3	1.372 (3)	O1—C22	1.328 (3)
C2—H2	0.9300	O1—C23	1.460 (4)
C3—C4	1.381 (3)	O2—C22	1.198 (3)
C3—C7	1.436 (4)	C23—C24A	1.227 (10)
C4—C5	1.375 (3)	C23—C24C	1.37 (2)
C4—H4	0.9300	C23—C24B	1.48 (2)
C5—C6	1.385 (3)	C23—H23A	0.9700
C5—H5	0.9300	C23—H23B	0.9700
C6—C8	1.467 (3)	C23—H23C	0.9700
C9—C10	1.505 (3)	C23—H23D	0.9700
C9—H9A	0.9700	C23—H23E	0.9700
C9—H9B	0.9700	C23—H23F	0.9700
C10—C15	1.372 (3)	C24A—H24A	0.9600
C10—C11	1.375 (3)	C24A—H24B	0.9600
C11—C12	1.371 (3)	C24A—H24C	0.9600
C11—H11	0.9300	C24B—H24D	0.9600
C12—C13	1.348 (3)	C24B—H24E	0.9600
C12—H12	0.9300	C24B—H24F	0.9600
C13—C14	1.362 (3)	C24C—H24G	0.9600
C14—C15	1.377 (3)	C24C—H24H	0.9600
C14—H14	0.9300	C24C—H24I	0.9600
C15—H15	0.9300		
C16—N1—C8	106.45 (18)	C18—C17—C16	119.5 (2)
C16—N1—C9	122.88 (19)	N2—C17—C16	110.2 (2)
C8—N1—C9	130.0 (2)	C19—C18—C17	119.0 (2)

C8—N2—C17	104.81 (19)	C19—C18—H18	120.5
C2—C1—C6	120.7 (2)	C17—C18—H18	120.5
C2—C1—H1	119.6	C18—C19—C20	120.5 (2)
C6—C1—H1	119.6	C18—C19—C22	117.1 (3)
C3—C2—C1	120.2 (2)	C20—C19—C22	122.4 (3)
C3—C2—H2	119.9	C21—C20—C19	121.4 (2)
C1—C2—H2	119.9	C21—C20—H20	119.3
C2—C3—C4	119.8 (2)	C19—C20—H20	119.3
C2—C3—C7	119.8 (3)	C20—C21—C16	117.3 (2)
C4—C3—C7	120.5 (2)	C20—C21—H21	121.4
C5—C4—C3	120.0 (2)	C16—C21—H21	121.4
C5—C4—H4	120.0	C22—O1—C23	116.3 (3)
C3—C4—H4	120.0	O2—C22—O1	122.8 (3)
C4—C5—C6	120.9 (2)	O2—C22—C19	124.5 (3)
C4—C5—H5	119.6	O1—C22—C19	112.7 (3)
C6—C5—H5	119.6	C24A—C23—O1	118.5 (7)
C5—C6—C1	118.5 (2)	C24C—C23—O1	116.3 (10)
C5—C6—C8	118.4 (2)	C24B—C23—O1	102.6 (10)
C1—C6—C8	123.1 (2)	C24A—C23—H23A	107.7
N3—C7—C3	178.3 (4)	O1—C23—H23A	107.7
N2—C8—N1	112.8 (2)	C24A—C23—H23B	107.7
N2—C8—C6	122.4 (2)	O1—C23—H23B	107.7
N1—C8—C6	124.8 (2)	H23A—C23—H23B	107.1
N1—C9—C10	114.12 (18)	C24B—C23—H23C	111.2
N1—C9—H9A	108.7	O1—C23—H23C	111.2
C10—C9—H9A	108.7	C24B—C23—H23D	111.2
N1—C9—H9B	108.7	O1—C23—H23D	111.2
C10—C9—H9B	108.7	H23C—C23—H23D	109.2
H9A—C9—H9B	107.6	C24C—C23—H23E	108.2
C15—C10—C11	118.7 (2)	O1—C23—H23E	108.2
C15—C10—C9	123.0 (2)	C24C—C23—H23F	108.2
C11—C10—C9	118.3 (2)	O1—C23—H23F	108.2
C12—C11—C10	121.1 (2)	H23E—C23—H23F	107.4
C12—C11—H11	119.5	C23—C24A—H24A	109.5
C10—C11—H11	119.5	C23—C24A—H24B	109.5
C13—C12—C11	118.6 (2)	H24A—C24A—H24B	109.5
C13—C12—H12	120.7	C23—C24A—H24C	109.5
C11—C12—H12	120.7	H24A—C24A—H24C	109.5
C12—C13—F1	118.9 (3)	H24B—C24A—H24C	109.5
C12—C13—C14	122.6 (2)	C23—C24B—H24D	109.5
F1—C13—C14	118.5 (3)	C23—C24B—H24E	109.5
C13—C14—C15	118.3 (2)	H24D—C24B—H24E	109.5
C13—C14—H14	120.9	C23—C24B—H24F	109.5
C15—C14—H14	120.9	H24D—C24B—H24F	109.5
C10—C15—C14	120.8 (2)	H24E—C24B—H24F	109.5
C10—C15—H15	119.6	C23—C24C—H24G	109.5
C14—C15—H15	119.6	C23—C24C—H24H	109.5
N1—C16—C21	131.9 (2)	H24G—C24C—H24H	109.5

N1—C16—C17	105.7 (2)	C23—C24C—H24I	109.5
C21—C16—C17	122.4 (2)	H24G—C24C—H24I	109.5
C18—C17—N2	130.3 (2)	H24H—C24C—H24I	109.5
C6—C1—C2—C3	−0.7 (4)	C11—C10—C15—C14	0.2 (3)
C1—C2—C3—C4	0.8 (4)	C9—C10—C15—C14	179.6 (2)
C1—C2—C3—C7	−178.2 (2)	C13—C14—C15—C10	−0.8 (4)
C2—C3—C4—C5	−0.1 (4)	C8—N1—C16—C21	178.9 (2)
C7—C3—C4—C5	178.9 (2)	C9—N1—C16—C21	−9.5 (4)
C3—C4—C5—C6	−0.7 (4)	C8—N1—C16—C17	−0.7 (2)
C4—C5—C6—C1	0.8 (4)	C9—N1—C16—C17	170.88 (19)
C4—C5—C6—C8	−176.5 (2)	C8—N2—C17—C18	−179.6 (2)
C2—C1—C6—C5	−0.1 (3)	C8—N2—C17—C16	−0.5 (2)
C2—C1—C6—C8	177.0 (2)	N1—C16—C17—C18	180.0 (2)
C17—N2—C8—N1	0.0 (2)	C21—C16—C17—C18	0.3 (3)
C17—N2—C8—C6	178.0 (2)	N1—C16—C17—N2	0.8 (3)
C16—N1—C8—N2	0.5 (3)	C21—C16—C17—N2	−178.9 (2)
C9—N1—C8—N2	−170.3 (2)	N2—C17—C18—C19	178.9 (2)
C16—N1—C8—C6	−177.5 (2)	C16—C17—C18—C19	−0.1 (3)
C9—N1—C8—C6	11.7 (4)	C17—C18—C19—C20	−0.2 (4)
C5—C6—C8—N2	32.9 (3)	C17—C18—C19—C22	−178.1 (2)
C1—C6—C8—N2	−144.3 (2)	C18—C19—C20—C21	0.4 (4)
C5—C6—C8—N1	−149.4 (2)	C22—C19—C20—C21	178.2 (2)
C1—C6—C8—N1	33.5 (3)	C19—C20—C21—C16	−0.2 (4)
C16—N1—C9—C10	77.3 (3)	N1—C16—C21—C20	−179.7 (2)
C8—N1—C9—C10	−113.2 (3)	C17—C16—C21—C20	−0.2 (4)
N1—C9—C10—C15	19.3 (3)	C23—O1—C22—O2	5.3 (5)
N1—C9—C10—C11	−161.2 (2)	C23—O1—C22—C19	−175.9 (3)
C15—C10—C11—C12	0.4 (3)	C18—C19—C22—O2	1.2 (4)
C9—C10—C11—C12	−179.1 (2)	C20—C19—C22—O2	−176.7 (3)
C10—C11—C12—C13	−0.4 (4)	C18—C19—C22—O1	−177.6 (2)
C11—C12—C13—F1	−179.8 (2)	C20—C19—C22—O1	4.5 (4)
C11—C12—C13—C14	−0.2 (4)	C22—O1—C23—C24A	−108.1 (10)
C12—C13—C14—C15	0.8 (4)	C22—O1—C23—C24C	−172.1 (14)
F1—C13—C14—C15	−179.6 (2)	C22—O1—C23—C24B	176.4 (12)