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5-(2,3-Dichlorophenyl)-3-(4-methoxyphenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

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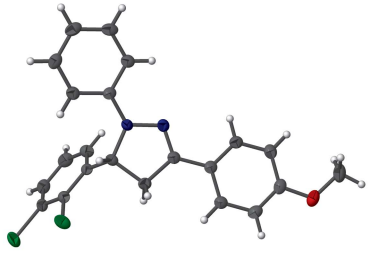
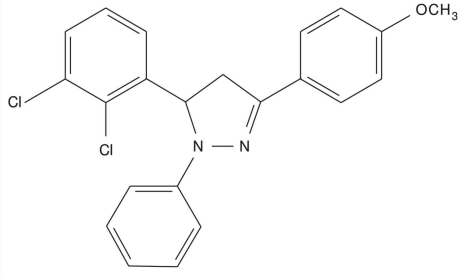
Structural data: full structural data are available from iucrdata.iucr.org

In the racemic title compound, $C_{22}H_{18}Cl_2N_2O$, the dihedral angles between the central dihydropyrazole ring (r.m.s. deviation = 0.018 Å) and the pendant methoxyphenyl, phenyl and dichlorophenyl rings are 3.96 (9), 15.90 (9) and 66.65 (9)° respectively. Weak aromatic π–π stacking [shortest centroid–centroid separation = 3.8476 (11) Å] occurs in the crystal.

3D view



Chemical scheme



Structure description

In continuation of our work on pyrazoline derivatives (Assem *et al.*, 2016), we report herein on the synthesis and crystal structure of the title compound. The title molecule is shown in Fig. 1. The pyrazole ring is nearly planar with atom C1 deviating by 0.017 (2) Å from the mean plane defined by atoms N1, N2, C2 and C3. The dihedral angle between the pyrazole ring and the methoxyphenyl ring is 3.96 (9)°, indicating their near coplanarity, whereas those between the pyrazole ring and the phenyl and dichlorophenyl rings are 15.90 (9) and 66.65 (9)°, respectively. In the arbitrarily chosen asymmetric molecule, the compound possess a chiral center at C3 with *R* conformation. Since the compound crystallizes in a centrosymmetric space group, we can surmise that the compound is a racemic mixture. The torsion angle value of 6.2 (3)° for C10—O1—C—C6 indicates that the methoxy group lies almost in the plane of the phenyl ring. No hydrogen bonds were observed in the crystal but weak aromatic π–π stacking [shortest centroid–centroid separation = 3.8476 (11) Å] is observed.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}Cl_2N_2O$
M_r	397.28
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	13.8255 (5), 11.0655 (4), 13.3583 (5)
β (°)	112.972 (1)
V (Å^3)	1881.57 (12)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.21
Crystal size (mm)	0.29 × 0.26 × 0.23
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.456, 0.525
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19112, 3089, 2996
R_{int}	0.055
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.116, 1.07
No. of reflections	3089
No. of parameters	246
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.31

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS* and *SHELXL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Synthesis and crystallization

To a solution of (*E*)-3-(2,3-dichlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one, (3 mmol) and phenylhydrazine hydrochloride (3 mmol) in methyl alcohol (25 ml), 4–5 drops of conc. hydrochloric acid were added. The mixture was refluxed on a water bath for 4 h. The progress of the reaction was monitored by TLC. After completion, the mixture was poured into ice-cold water and stirred. The solid that separated was filtered and washed with ice-cold water. The product was crystallized from methyl alcohol solution with 2–3 drops of acetonitrile added to get the title compound in the form of yellow blocks in 88% yield, m.p. 134–136°C.

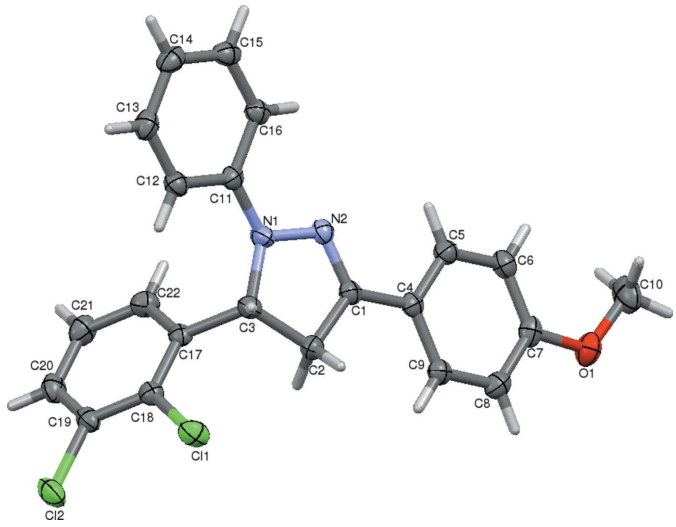


Figure 1
The molecular structure of the title compound with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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References

Assem, B., Naveen, S., Nagamallu, R., Ajay Kumar, K., Abdoh, M., Warad, I. & Lokanath, N. K. (2016). *Z. Kristallogr*, **231**, 267–269.
Bruker (2013). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

full crystallographic data

IUCrData (2017). **2**, x162013 [https://doi.org/10.1107/S2414314616020137]

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Crystal data

$C_{22}H_{18}Cl_2N_2O$
M_r = 397.28
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 13.8255 (5) Å
b = 11.0655 (4) Å
c = 13.3583 (5) Å
β = 112.972 (1)°
V = 1881.57 (12) Å^3
Z = 4
$F(000)$ = 824
D_x = 1.403 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2996 reflections
θ = 5.3–64.6°
μ = 3.21 mm^{-1}
T = 296 K
Block, yellow
0.29 × 0.26 × 0.23 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.456, T_{max} = 0.525
19112 measured reflections
3089 independent reflections
2996 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 64.6°, θ_{min} = 5.3°
h = −15→15
k = −12→12
l = −13→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.07
3089 reflections
246 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.6657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: shelxl, FC*=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.0044 (5)

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 esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.87473 (3)	0.71246 (4)	0.68752 (3)	0.0315 (2)
Cl2	0.99910 (3)	0.94868 (5)	0.68003 (4)	0.0380 (2)
O1	0.13280 (10)	0.71402 (12)	0.56282 (11)	0.0338 (4)
N1	0.59658 (11)	0.63158 (14)	0.38384 (11)	0.0255 (4)
N2	0.49511 (11)	0.62782 (12)	0.37995 (11)	0.0230 (4)
C1	0.49661 (14)	0.65881 (15)	0.47377 (13)	0.0220 (5)
C2	0.60554 (13)	0.68189 (16)	0.55786 (14)	0.0254 (5)
C3	0.67436 (13)	0.66381 (15)	0.49192 (13)	0.0225 (5)
C4	0.40026 (14)	0.67089 (14)	0.49382 (14)	0.0222 (5)
C5	0.30163 (14)	0.64888 (16)	0.41333 (14)	0.0259 (5)
C6	0.21047 (14)	0.66298 (16)	0.43247 (15)	0.0279 (5)
C7	0.21773 (14)	0.69931 (16)	0.53491 (15)	0.0264 (5)
C8	0.31531 (15)	0.72286 (15)	0.61613 (15)	0.0275 (5)
C9	0.40538 (14)	0.70892 (15)	0.59615 (14)	0.0241 (5)
C10	0.03301 (16)	0.6789 (2)	0.4851 (2)	0.0456 (8)
C11	0.62138 (13)	0.57251 (15)	0.30494 (13)	0.0225 (5)
C12	0.72612 (14)	0.56432 (16)	0.31559 (14)	0.0261 (5)
C13	0.75027 (15)	0.50561 (16)	0.23657 (15)	0.0298 (6)
C14	0.67259 (17)	0.45529 (16)	0.14630 (15)	0.0318 (6)
C15	0.56912 (15)	0.46328 (16)	0.13576 (15)	0.0290 (5)
C16	0.54263 (14)	0.52186 (16)	0.21336 (14)	0.0247 (5)
C17	0.73547 (13)	0.77685 (14)	0.48744 (13)	0.0206 (5)
C18	0.82811 (13)	0.80672 (15)	0.57467 (13)	0.0220 (5)
C19	0.88385 (13)	0.91101 (16)	0.57130 (15)	0.0256 (5)
C20	0.84742 (15)	0.98622 (17)	0.48206 (16)	0.0303 (6)
C21	0.75577 (16)	0.95706 (17)	0.39570 (16)	0.0322 (6)
C22	0.70052 (14)	0.85391 (16)	0.39824 (14)	0.0276 (5)
H2A	0.62370	0.62460	0.61740	0.0300*
H2B	0.61210	0.76340	0.58660	0.0300*
H3	0.72290	0.59630	0.52210	0.0270*
H5	0.29650	0.62410	0.34490	0.0310*
H6	0.14520	0.64830	0.37730	0.0330*
H8	0.32010	0.74810	0.68430	0.0330*
H9	0.47040	0.72490	0.65120	0.0290*
H10A	0.01390	0.73050	0.42250	0.0680*

H10B	−0.01850	0.68590	0.51650	0.0680*
H10C	0.03610	0.59670	0.46380	0.0680*
H12	0.77940	0.59820	0.37560	0.0310*
H13	0.82000	0.50000	0.24450	0.0360*
H14	0.68950	0.41670	0.09340	0.0380*
H15	0.51640	0.42880	0.07560	0.0350*
H16	0.47260	0.52740	0.20450	0.0300*
H20	0.88430	1.05590	0.48010	0.0360*
H21	0.73090	1.00730	0.33510	0.0390*
H22	0.63880	0.83570	0.33920	0.0330*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0323 (3)	0.0271 (3)	0.0258 (3)	−0.0009 (2)	0.0012 (2)	0.0050 (2)
Cl2	0.0264 (3)	0.0396 (3)	0.0438 (3)	−0.0121 (2)	0.0092 (2)	−0.0092 (2)
O1	0.0319 (7)	0.0344 (8)	0.0418 (8)	0.0067 (5)	0.0217 (6)	0.0055 (6)
N1	0.0209 (7)	0.0304 (8)	0.0248 (8)	−0.0046 (6)	0.0084 (6)	−0.0078 (6)
N2	0.0233 (7)	0.0196 (8)	0.0266 (8)	−0.0024 (5)	0.0102 (6)	−0.0008 (6)
C1	0.0264 (9)	0.0153 (8)	0.0244 (9)	−0.0016 (6)	0.0100 (7)	0.0012 (6)
C2	0.0289 (9)	0.0245 (9)	0.0238 (9)	−0.0039 (7)	0.0114 (7)	−0.0021 (7)
C3	0.0227 (8)	0.0208 (9)	0.0216 (8)	−0.0020 (7)	0.0059 (7)	−0.0015 (6)
C4	0.0277 (9)	0.0141 (8)	0.0256 (9)	−0.0017 (6)	0.0112 (7)	0.0023 (6)
C5	0.0303 (9)	0.0229 (9)	0.0252 (9)	−0.0025 (7)	0.0117 (7)	−0.0011 (7)
C6	0.0259 (9)	0.0238 (9)	0.0332 (10)	−0.0023 (7)	0.0108 (7)	0.0014 (7)
C7	0.0297 (9)	0.0180 (9)	0.0357 (10)	0.0045 (7)	0.0175 (8)	0.0071 (7)
C8	0.0375 (10)	0.0211 (9)	0.0272 (9)	0.0037 (7)	0.0162 (8)	0.0027 (7)
C9	0.0283 (9)	0.0191 (9)	0.0240 (9)	−0.0005 (7)	0.0094 (7)	0.0024 (6)
C10	0.0312 (11)	0.0472 (13)	0.0647 (15)	−0.0029 (9)	0.0257 (10)	−0.0080 (11)
C11	0.0296 (9)	0.0157 (8)	0.0241 (9)	−0.0016 (6)	0.0125 (7)	0.0008 (6)
C12	0.0287 (9)	0.0208 (9)	0.0285 (9)	−0.0032 (7)	0.0109 (7)	−0.0015 (7)
C13	0.0353 (10)	0.0230 (9)	0.0376 (10)	0.0020 (7)	0.0214 (8)	0.0031 (8)
C14	0.0483 (11)	0.0225 (10)	0.0316 (10)	0.0017 (8)	0.0231 (9)	−0.0003 (7)
C15	0.0415 (10)	0.0197 (9)	0.0235 (9)	−0.0034 (7)	0.0103 (8)	−0.0008 (7)
C16	0.0287 (9)	0.0188 (9)	0.0255 (9)	−0.0014 (7)	0.0093 (7)	0.0011 (7)
C17	0.0224 (8)	0.0167 (8)	0.0236 (9)	0.0008 (6)	0.0101 (7)	−0.0022 (6)
C18	0.0230 (8)	0.0188 (8)	0.0245 (9)	0.0018 (7)	0.0095 (7)	−0.0003 (7)
C19	0.0220 (8)	0.0233 (9)	0.0326 (9)	−0.0024 (7)	0.0119 (7)	−0.0063 (7)
C20	0.0363 (10)	0.0192 (9)	0.0410 (11)	−0.0041 (7)	0.0211 (9)	−0.0012 (8)
C21	0.0437 (11)	0.0233 (10)	0.0330 (10)	0.0041 (8)	0.0188 (9)	0.0071 (7)
C22	0.0296 (9)	0.0248 (9)	0.0254 (9)	0.0034 (7)	0.0074 (7)	0.0012 (7)

Geometric parameters (Å, º)

Cl1—C18	1.7371 (17)	C17—C18	1.394 (2)
Cl2—C19	1.7366 (19)	C17—C22	1.390 (2)
O1—C7	1.373 (3)	C18—C19	1.398 (3)
O1—C10	1.419 (3)	C19—C20	1.378 (3)

N1—N2	1.384 (2)	C20—C21	1.378 (3)
N1—C3	1.468 (2)	C21—C22	1.381 (3)
N1—C11	1.392 (2)	C2—H2A	0.9700
N2—C1	1.292 (2)	C2—H2B	0.9700
C1—C2	1.508 (3)	C3—H3	0.9800
C1—C4	1.464 (3)	C5—H5	0.9300
C2—C3	1.541 (3)	C6—H6	0.9300
C3—C17	1.524 (2)	C8—H8	0.9300
C4—C5	1.389 (3)	C9—H9	0.9300
C4—C9	1.405 (2)	C10—H10A	0.9600
C5—C6	1.389 (3)	C10—H10B	0.9600
C6—C7	1.392 (3)	C10—H10C	0.9600
C7—C8	1.387 (3)	C12—H12	0.9300
C8—C9	1.380 (3)	C13—H13	0.9300
C11—C12	1.402 (3)	C14—H14	0.9300
C11—C16	1.399 (2)	C15—H15	0.9300
C12—C13	1.387 (3)	C16—H16	0.9300
C13—C14	1.381 (3)	C20—H20	0.9300
C14—C15	1.385 (3)	C21—H21	0.9300
C15—C16	1.388 (3)	C22—H22	0.9300

C7—O1—C10	117.32 (16)	C20—C21—C22	120.63 (18)
N2—N1—C3	112.76 (13)	C17—C22—C21	121.17 (17)
N2—N1—C11	120.20 (14)	C1—C2—H2A	111.00
C3—N1—C11	123.80 (15)	C1—C2—H2B	111.00
N1—N2—C1	108.87 (15)	C3—C2—H2A	111.00
N2—C1—C2	113.63 (17)	C3—C2—H2B	111.00
N2—C1—C4	122.05 (16)	H2A—C2—H2B	109.00
C2—C1—C4	124.32 (15)	N1—C3—H3	110.00
C1—C2—C3	102.25 (14)	C2—C3—H3	110.00
N1—C3—C2	102.41 (14)	C17—C3—H3	110.00
N1—C3—C17	111.43 (13)	C4—C5—H5	119.00
C2—C3—C17	113.04 (14)	C6—C5—H5	119.00
C1—C4—C5	122.06 (16)	C5—C6—H6	120.00
C1—C4—C9	120.09 (17)	C7—C6—H6	120.00
C5—C4—C9	117.83 (18)	C7—C8—H8	120.00
C4—C5—C6	121.66 (17)	C9—C8—H8	120.00
C5—C6—C7	119.40 (18)	C4—C9—H9	120.00
O1—C7—C6	124.05 (18)	C8—C9—H9	120.00
O1—C7—C8	116.05 (17)	O1—C10—H10A	109.00
C6—C7—C8	119.90 (19)	O1—C10—H10B	109.00
C7—C8—C9	120.23 (17)	O1—C10—H10C	109.00
C4—C9—C8	120.98 (18)	H10A—C10—H10B	109.00
N1—C11—C12	120.23 (15)	H10A—C10—H10C	110.00
N1—C11—C16	120.84 (17)	H10B—C10—H10C	109.00
C12—C11—C16	118.92 (16)	C11—C12—H12	120.00
C11—C12—C13	119.95 (17)	C13—C12—H12	120.00
C12—C13—C14	121.2 (2)	C12—C13—H13	119.00

C13—C14—C15	118.93 (19)	C14—C13—H13	119.00
C14—C15—C16	121.16 (18)	C13—C14—H14	121.00
C11—C16—C15	119.89 (19)	C15—C14—H14	121.00
C3—C17—C18	120.30 (14)	C14—C15—H15	119.00
C3—C17—C22	121.66 (16)	C16—C15—H15	119.00
C18—C17—C22	118.03 (16)	C11—C16—H16	120.00
Cl1—C18—C17	119.46 (13)	C15—C16—H16	120.00
Cl1—C18—C19	120.07 (13)	C19—C20—H20	120.00
C17—C18—C19	120.47 (15)	C21—C20—H20	120.00
Cl2—C19—C18	120.57 (14)	C20—C21—H21	120.00
Cl2—C19—C20	119.00 (15)	C22—C21—H21	120.00
C18—C19—C20	120.43 (17)	C17—C22—H22	119.00
C19—C20—C21	119.27 (18)	C21—C22—H22	119.00

C10—O1—C7—C6	6.2 (3)	C5—C4—C9—C8	0.6 (2)
C10—O1—C7—C8	−173.76 (16)	C4—C5—C6—C7	−0.4 (3)
C3—N1—N2—C1	2.39 (19)	C5—C6—C7—O1	−178.90 (16)
C11—N1—N2—C1	162.79 (15)	C5—C6—C7—C8	1.0 (3)
N2—N1—C3—C2	−0.60 (17)	O1—C7—C8—C9	179.10 (15)
N2—N1—C3—C17	−121.72 (16)	C6—C7—C8—C9	−0.8 (3)
C11—N1—C3—C2	−160.19 (15)	C7—C8—C9—C4	0.0 (3)
C11—N1—C3—C17	78.7 (2)	N1—C11—C12—C13	−179.84 (16)
N2—N1—C11—C12	−172.59 (15)	C16—C11—C12—C13	−0.7 (3)
N2—N1—C11—C16	8.2 (2)	N1—C11—C16—C15	−179.93 (16)
C3—N1—C11—C12	−14.4 (2)	C12—C11—C16—C15	0.9 (3)
C3—N1—C11—C16	166.39 (16)	C11—C12—C13—C14	0.5 (3)
N1—N2—C1—C2	−3.22 (19)	C12—C13—C14—C15	−0.5 (3)
N1—N2—C1—C4	176.18 (14)	C13—C14—C15—C16	0.8 (3)
N2—C1—C2—C3	2.73 (19)	C14—C15—C16—C11	−0.9 (3)
C4—C1—C2—C3	−176.64 (15)	C3—C17—C18—Cl1	1.2 (2)
N2—C1—C4—C5	0.5 (3)	C3—C17—C18—C19	−179.37 (17)
N2—C1—C4—C9	−177.78 (16)	C22—C17—C18—Cl1	−179.76 (14)
C2—C1—C4—C5	179.80 (16)	C22—C17—C18—C19	−0.4 (3)
C2—C1—C4—C9	1.6 (2)	C3—C17—C22—C21	179.07 (18)
C1—C2—C3—N1	−1.10 (16)	C18—C17—C22—C21	0.1 (3)
C1—C2—C3—C17	118.90 (15)	Cl1—C18—C19—Cl2	−0.8 (2)
N1—C3—C17—C18	−165.11 (16)	Cl1—C18—C19—C20	179.97 (15)
N1—C3—C17—C22	15.9 (2)	C17—C18—C19—Cl2	179.82 (14)
C2—C3—C17—C18	80.2 (2)	C17—C18—C19—C20	0.6 (3)
C2—C3—C17—C22	−98.77 (19)	Cl2—C19—C20—C21	−179.74 (16)
C1—C4—C5—C6	−178.66 (16)	C18—C19—C20—C21	−0.5 (3)
C9—C4—C5—C6	−0.4 (3)	C19—C20—C21—C22	0.2 (3)
C1—C4—C9—C8	178.89 (15)	C20—C21—C22—C17	0.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···N2	0.93	2.50	2.811 (2)	100

C22—H22···N1	0.93	2.46	2.818 (2)	103