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5-{[5-(4-Chlorophenyl)-3-methyl-1*H*-pyrazol-1-yl]-methyl}-1,3,4-oxadiazole-2(3*H*)-thione

Joel T. Mague,[a] Shaaban K. Mohamed,[b,c] Mehmet Akkurt,[d] Adel A. Marzouk,[e] Farouq E. Hawaiz[f]* and Hamdy M. Abdel-Rahman[g]

[a]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA, [b]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [c]Chemistry Department, Faculty of Science, Minia University, 61519 El-Minia, Egypt, [d]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [e]Pharmaceutical Chemistry Department, Faculty of Pharmacy, Al Azhar University, 71515 Assiut, Egypt, [f]Chemistry Department, College of Education, Salahaddin University-Hawler, Erbil, Kurdistan Region, Iraq, and [g]Faculty of Pharmacy, Medicinal Chemistry Department, Assiut University, Assiut 71526, Egypt. *Correspondence e-mail: shaabankamel@yahoo.com

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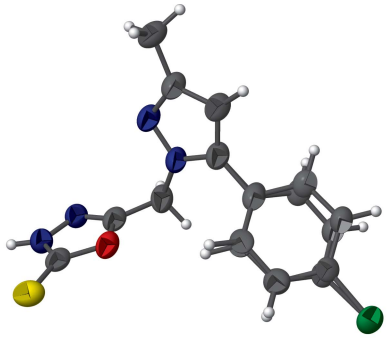
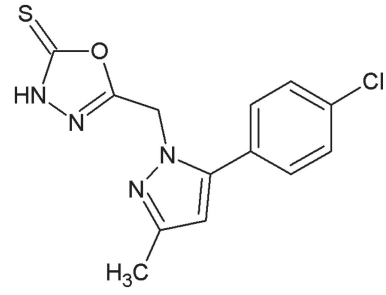
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{13}H_{11}ClN_4OS$, the oxadiazolethione ring is inclined to the pyrazole ring by 79.2 (2)°. The 4-chlorophenyl ring is rotationally disordered, with the two fragments inclined to one another by 27.1 (4)°, and to the pyrazole ring by 43.1 (3) and 68.6 (3)°. In the crystal, molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers, enclosing an $R_2^2(14)$ ring motif. The dimers are linked by C—H···N hydrogen bonds, forming ribbons propagating along the *a*-axis direction and enclosing $R_2^2(8)$ ring motifs. The ribbons are linked by C—H···Cl hydrogen bonds, forming a three-dimensional supramolecular structure.

3D view



Chemical scheme



Structure description

The pyrazole nucleus is common in a number of biologically active molecules, exhibiting antibacterial (Nada *et al.*, 2009), antitubercular (Pattan *et al.*, 2009), antidepressant (Mathew *et al.*, 2012), anti-inflammatory (El-Moghazy *et al.*, 2012), analgesic (Panneer *et al.*, 2011), anticancer (Mohareb *et al.*, 2012) and antioxidant (Tarun *et al.*, 2012) activities. Our research is directed towards the synthesis of novel pyrazole derivatives with good anti-inflammatory activity in good yield. Herein, we report on the synthesis and crystal structure of the title pyrazole derivative.

In the title compound, Fig. 1, the dihedral angle between the mean planes of the two five-membered rings is 79.2 (2)°, while that between the pyrazole ring and the C8*A*–C13*A*

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N4^{i}	0.88	2.02	2.836 (5)	153
C3—H3B···N2^{ii}	0.99	2.51	3.445 (6)	158
C7—H7C···Cl1B^{iii}	0.98	2.73	3.635 (10)	153

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

orientation of the disordered 4-chlorophenyl ring is 43.1 (3)°. The disorder in the benzene ring involves primarily a rotation about the C4—C8 (*A* or *B*) bond by 27.1 (4)°, with a nearly equal population in both orientations.

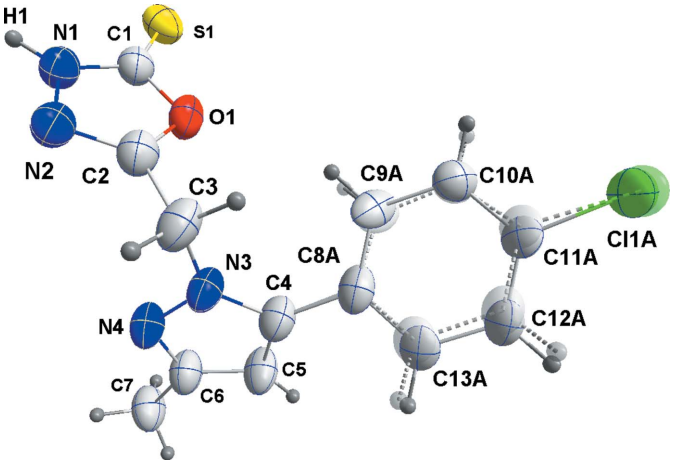


Figure 1
The molecular structure of the title compound, showing the atom labelling and 50% probability displacement ellipsoids. The alternate location of the 4-chlorophenyl ring is shown by pale solid ellipsoids and dotted line bonds.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{11}ClN_4OS$
M_r	306.77
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	4.9309 (2), 17.1173 (8), 16.6517 (7)
β (°)	91.189 (3)
V (Å^3)	1405.16 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.81
Crystal size (mm)	0.20 × 0.05 × 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.63, 0.92
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10669, 2632, 1759
R_{int}	0.080
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.068, 0.195, 1.05
No. of reflections	2632
No. of parameters	180
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.49

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) *Mercury* (Macrae *et al.*, 2008) and *SHELXTL* (Sheldrick, 2008).

In the crystal, pairwise N1—H1···N4^{i} and C3—H3B···N2^{ii} hydrogen bonds (see Table 1) form ribbons running along the *a*-axis direction (Fig. 2). The ribbons are connected by pair-

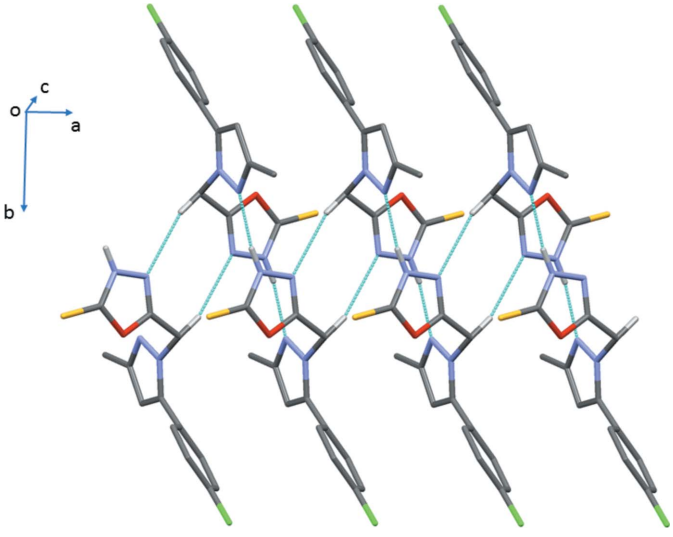


Figure 2
A view of the ribbons formed by N—H···N and C—H···N hydrogen bonds (dashed lines; see Table 1). For clarity, only the H atoms involved in hydrogen bonding have been included.

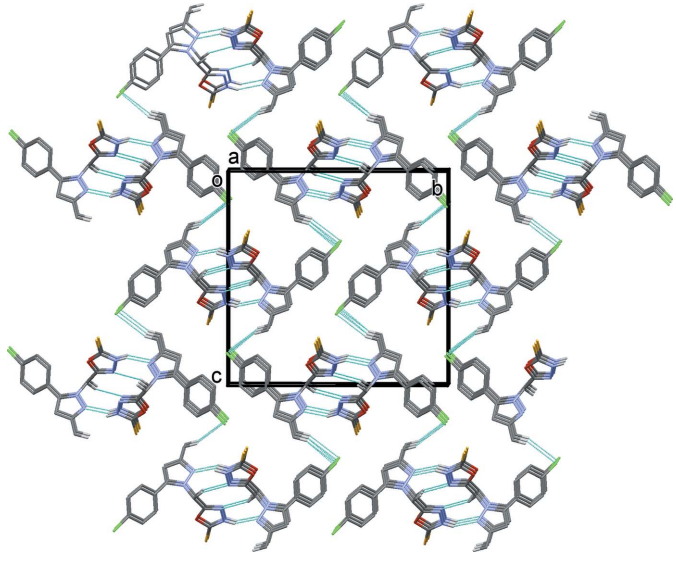


Figure 3
A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only the H atoms involved in hydrogen bonding have been included.

wise C7—H7*C*···Cl1*B*^{iii} hydrogen bonds (see Table 1) to form a three-dimensional supramolecular structure (Fig. 3).

Synthesis and crystallization

A mixture of 2-(5-(4-chlorophenyl)-3-methyl-1*H*-pyrazol-1-yl)acetic acid hydrazide (1.33 g, 5 mmol) and potassium hydroxide (0.2 g, 5 mmol) in carbon disulfide (5 ml) was refluxed in ethanol (25 ml) for 12 h on a steam bath. The reaction mixture was concentrated, cooled and neutralized with hydrochloric acid solution. The separated solid was collected, washed with water, dried and crystallized from ethanol solution to give colourless needle-like crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The benzene ring (C8–C13) is rotationally disordered by 27.1 (4)° in approximately equal amounts; refined occupancy ratio (*A*:*B*) = 0.506 (5): 0.494 (5). The two components of the disordered ring were refined as rigid hexagons.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170176 [https://doi.org/10.1107/S2414314617001766]

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Crystal data

$C_{13}H_{11}ClN_4OS$
M_r = 306.77
Monoclinic, $P2_1/c$
a = 4.9309 (2) Å
b = 17.1173 (8) Å
c = 16.6517 (7) Å
β = 91.189 (3)°
V = 1405.16 (11) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.450 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 4259 reflections
θ = 3.7–69.9°
μ = 3.81 mm^{-1}
T = 150 K
Needles, colourless
0.20 × 0.05 × 0.02 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.63, T_{max} = 0.92
10669 measured reflections
2632 independent reflections
1759 reflections with $I > 2\sigma(I)$
R_{int} = 0.080
θ_{max} = 70.1°, θ_{min} = 3.7°
h = −5→5
k = −20→18
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.195
S = 1.05
2632 reflections
180 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.106P)^2 + 0.4524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-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.

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. The 4-chlorophenyl group is rotationally disordered by 27.1 (4)° in approximately equal amounts. The two components of the disorder were refined as rigid hexagons. H-atoms were placed in calculated positions (C—H = 0.95 - 0.9 Å; N—H = 0.88 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	1.3239 (3)	0.90840 (8)	0.71546 (7)	0.0599 (4)	
O1	0.9335 (6)	0.86722 (16)	0.60987 (18)	0.0498 (7)	
N1	0.9888 (7)	0.9914 (2)	0.6167 (2)	0.0491 (8)	
H1	1.0495	1.0379	0.6307	0.059*	
N2	0.7856 (7)	0.9795 (2)	0.5597 (2)	0.0482 (8)	
N3	0.7160 (7)	0.8117 (2)	0.4491 (2)	0.0489 (9)	
N4	0.8597 (7)	0.8490 (2)	0.3914 (2)	0.0511 (9)	
C1	1.0829 (8)	0.9253 (2)	0.6482 (2)	0.0473 (10)	
C2	0.7581 (8)	0.9051 (2)	0.5581 (3)	0.0476 (10)	
C3	0.5703 (9)	0.8592 (3)	0.5072 (3)	0.0556 (11)	
H3A	0.4608	0.8246	0.5415	0.067*	
H3B	0.4447	0.8950	0.4782	0.067*	
C4	0.7085 (9)	0.7334 (3)	0.4378 (3)	0.0526 (11)	
C5	0.8504 (10)	0.7191 (3)	0.3686 (3)	0.0564 (12)	
H5	0.8798	0.6700	0.3438	0.068*	
C6	0.9417 (9)	0.7919 (3)	0.3426 (3)	0.0527 (11)	
C7	1.1209 (10)	0.8099 (3)	0.2742 (3)	0.0613 (12)	
H7A	1.0721	0.7764	0.2284	0.092*	
H7B	1.3103	0.8004	0.2903	0.092*	
H7C	1.0983	0.8649	0.2588	0.092*	
Cl1A	0.1985 (12)	0.4995 (3)	0.6544 (5)	0.0542 (10)	0.506 (5)
C8A	0.5677 (16)	0.6786 (3)	0.4912 (5)	0.0459 (10)	0.506 (5)
C9A	0.5994 (16)	0.6831 (4)	0.5742 (5)	0.049 (2)	0.506 (5)
H9A	0.6967	0.7255	0.5979	0.059*	0.506 (5)
C10A	0.4886 (18)	0.6258 (5)	0.6227 (3)	0.0514 (17)	0.506 (5)
H10A	0.5102	0.6289	0.6794	0.062*	0.506 (5)
C11A	0.3461 (18)	0.5638 (4)	0.5881 (4)	0.0418 (16)	0.506 (5)
C12A	0.3145 (15)	0.5593 (4)	0.5051 (5)	0.0475 (15)	0.506 (5)
H12A	0.2171	0.5169	0.4815	0.057*	0.506 (5)
C13A	0.4252 (16)	0.6167 (4)	0.4567 (3)	0.0433 (18)	0.506 (5)
H13A	0.4036	0.6136	0.3999	0.052*	0.506 (5)
Cl1B	0.1220 (12)	0.5135 (4)	0.6530 (5)	0.0542 (10)	0.494 (5)

C8B	0.5833 (15)	0.6771 (4)	0.4934 (5)	0.0459 (10)	0.494 (5)
C9B	0.6805 (13)	0.6650 (5)	0.5714 (6)	0.049 (2)	0.494 (5)
H9B	0.8412	0.6906	0.5897	0.059*	0.494 (5)
C10B	0.5427 (17)	0.6154 (5)	0.6226 (4)	0.0514 (17)	0.494 (5)
H10B	0.6091	0.6072	0.6759	0.062*	0.494 (5)
C11B	0.3076 (16)	0.5780 (4)	0.5958 (4)	0.0418 (16)	0.494 (5)
C12B	0.2104 (13)	0.5901 (4)	0.5178 (5)	0.0475 (15)	0.494 (5)
H12B	0.0498	0.5644	0.4995	0.057*	0.494 (5)
C13B	0.3483 (16)	0.6396 (5)	0.4666 (4)	0.0433 (18)	0.494 (5)
H13B	0.2819	0.6479	0.4134	0.052*	0.494 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0586 (7)	0.0667 (8)	0.0547 (6)	0.0081 (5)	0.0091 (5)	0.0061 (5)
O1	0.0478 (16)	0.0355 (15)	0.0665 (19)	0.0006 (12)	0.0149 (14)	−0.0005 (13)
N1	0.055 (2)	0.041 (2)	0.0515 (19)	−0.0032 (16)	0.0035 (17)	−0.0019 (15)
N2	0.051 (2)	0.042 (2)	0.052 (2)	−0.0013 (15)	0.0075 (16)	−0.0023 (14)
N3	0.049 (2)	0.0377 (19)	0.061 (2)	−0.0072 (15)	0.0139 (17)	−0.0069 (15)
N4	0.051 (2)	0.0371 (19)	0.066 (2)	−0.0013 (15)	0.0133 (17)	0.0025 (15)
C1	0.048 (2)	0.042 (2)	0.053 (2)	0.0021 (17)	0.0185 (19)	0.0016 (17)
C2	0.043 (2)	0.042 (2)	0.058 (2)	0.0014 (17)	0.0153 (19)	−0.0005 (18)
C3	0.052 (3)	0.041 (2)	0.074 (3)	−0.0029 (19)	0.014 (2)	−0.012 (2)
C4	0.050 (2)	0.042 (2)	0.066 (3)	−0.0030 (18)	0.013 (2)	−0.0052 (19)
C5	0.060 (3)	0.038 (2)	0.072 (3)	0.0026 (19)	0.023 (2)	−0.004 (2)
C6	0.051 (3)	0.041 (2)	0.066 (3)	−0.0018 (18)	0.015 (2)	0.0029 (19)
C7	0.066 (3)	0.051 (3)	0.068 (3)	0.002 (2)	0.024 (2)	0.009 (2)
Cl1A	0.069 (3)	0.0373 (19)	0.0567 (7)	0.0002 (16)	0.001 (2)	0.0098 (13)
C8A	0.038 (2)	0.036 (2)	0.064 (3)	0.0009 (16)	0.0118 (19)	−0.0029 (18)
C9A	0.025 (5)	0.070 (5)	0.053 (3)	−0.010 (4)	0.023 (3)	−0.023 (3)
C10A	0.036 (4)	0.069 (4)	0.050 (3)	−0.004 (3)	0.009 (2)	−0.008 (2)
C11A	0.046 (3)	0.028 (3)	0.052 (3)	0.007 (3)	0.009 (2)	−0.006 (2)
C12A	0.045 (4)	0.040 (4)	0.058 (4)	−0.003 (3)	0.002 (3)	0.002 (3)
C13A	0.031 (5)	0.040 (5)	0.058 (3)	0.009 (3)	−0.005 (3)	0.008 (3)
Cl1B	0.069 (3)	0.0373 (19)	0.0567 (7)	0.0002 (16)	0.001 (2)	0.0098 (13)
C8B	0.038 (2)	0.036 (2)	0.064 (3)	0.0009 (16)	0.0118 (19)	−0.0029 (18)
C9B	0.025 (5)	0.070 (5)	0.053 (3)	−0.010 (4)	0.023 (3)	−0.023 (3)
C10B	0.036 (4)	0.069 (4)	0.050 (3)	−0.004 (3)	0.009 (2)	−0.008 (2)
C11B	0.046 (3)	0.028 (3)	0.052 (3)	0.007 (3)	0.009 (2)	−0.006 (2)
C12B	0.045 (4)	0.040 (4)	0.058 (4)	−0.003 (3)	0.002 (3)	0.002 (3)
C13B	0.031 (5)	0.040 (5)	0.058 (3)	0.009 (3)	−0.005 (3)	0.008 (3)

Geometric parameters (Å, º)

S1—C1	1.642 (5)	Cl1A—C11A	1.730 (3)
O1—C2	1.371 (5)	C8A—C9A	1.3900
O1—C1	1.386 (5)	C8A—C13A	1.3900
N1—C1	1.327 (5)	C9A—C10A	1.3900

N1—N2	1.380 (5)	C9A—H9A	0.9500
N1—H1	0.8800	C10A—C11A	1.3900
N2—C2	1.282 (5)	C10A—H10A	0.9500
N3—C4	1.355 (6)	C11A—C12A	1.3900
N3—N4	1.364 (5)	C12A—C13A	1.3900
N3—C3	1.463 (5)	C12A—H12A	0.9500
N4—C6	1.339 (6)	C13A—H13A	0.9500
C2—C3	1.470 (6)	Cl1B—C11B	1.732 (3)
C3—H3A	0.9900	C8B—C9B	1.3900
C3—H3B	0.9900	C8B—C13B	1.3900
C4—C5	1.383 (6)	C9B—C10B	1.3900
C4—C8A	1.476 (5)	C9B—H9B	0.9500
C4—C8B	1.480 (5)	C10B—C11B	1.3900
C5—C6	1.396 (6)	C10B—H10B	0.9500
C5—H5	0.9500	C11B—C12B	1.3900
C6—C7	1.488 (6)	C12B—C13B	1.3900
C7—H7A	0.9800	C12B—H12B	0.9500
C7—H7B	0.9800	C13B—H13B	0.9500
C7—H7C	0.9800		

C2—O1—C1	105.8 (3)	H7B—C7—H7C	109.5
C1—N1—N2	112.8 (4)	C9A—C8A—C13A	120.0
C1—N1—H1	123.6	C9A—C8A—C4	121.3 (7)
N2—N1—H1	123.6	C13A—C8A—C4	118.4 (7)
C2—N2—N1	103.7 (3)	C10A—C9A—C8A	120.0
C4—N3—N4	112.2 (3)	C10A—C9A—H9A	120.0
C4—N3—C3	129.0 (4)	C8A—C9A—H9A	120.0
N4—N3—C3	118.4 (3)	C11A—C10A—C9A	120.0
C6—N4—N3	104.8 (3)	C11A—C10A—H10A	120.0
N1—C1—O1	104.6 (4)	C9A—C10A—H10A	120.0
N1—C1—S1	131.5 (4)	C10A—C11A—C12A	120.0
O1—C1—S1	123.9 (3)	C10A—C11A—Cl1A	115.9 (6)
N2—C2—O1	113.0 (4)	C12A—C11A—Cl1A	123.9 (6)
N2—C2—C3	127.5 (4)	C13A—C12A—C11A	120.0
O1—C2—C3	119.5 (4)	C13A—C12A—H12A	120.0
N3—C3—C2	111.5 (4)	C11A—C12A—H12A	120.0
N3—C3—H3A	109.3	C12A—C13A—C8A	120.0
C2—C3—H3A	109.3	C12A—C13A—H13A	120.0
N3—C3—H3B	109.3	C8A—C13A—H13A	120.0
C2—C3—H3B	109.3	C9B—C8B—C13B	120.0
H3A—C3—H3B	108.0	C9B—C8B—C4	122.8 (7)
N3—C4—C5	106.1 (4)	C13B—C8B—C4	117.1 (7)
N3—C4—C8A	123.8 (5)	C8B—C9B—C10B	120.0
C5—C4—C8A	130.0 (5)	C8B—C9B—H9B	120.0
N3—C4—C8B	124.6 (5)	C10B—C9B—H9B	120.0
C5—C4—C8B	129.2 (5)	C11B—C10B—C9B	120.0
C4—C5—C6	105.9 (4)	C11B—C10B—H10B	120.0
C4—C5—H5	127.1	C9B—C10B—H10B	120.0

C6—C5—H5	127.1	C10B—C11B—C12B	120.0
N4—C6—C5	111.1 (4)	C10B—C11B—Cl1B	124.4 (6)
N4—C6—C7	120.3 (4)	C12B—C11B—Cl1B	115.6 (6)
C5—C6—C7	128.5 (4)	C13B—C12B—C11B	120.0
C6—C7—H7A	109.5	C13B—C12B—H12B	120.0
C6—C7—H7B	109.5	C11B—C12B—H12B	120.0
H7A—C7—H7B	109.5	C12B—C13B—C8B	120.0
C6—C7—H7C	109.5	C12B—C13B—H13B	120.0
H7A—C7—H7C	109.5	C8B—C13B—H13B	120.0
C1—N1—N2—C2	0.5 (5)	N3—C4—C8A—C9A	−46.9 (7)
C4—N3—N4—C6	0.5 (5)	C5—C4—C8A—C9A	134.3 (6)
C3—N3—N4—C6	−172.9 (4)	N3—C4—C8A—C13A	140.1 (5)
N2—N1—C1—O1	0.0 (4)	C5—C4—C8A—C13A	−38.8 (9)
N2—N1—C1—S1	178.6 (3)	C13A—C8A—C9A—C10A	0.0
C2—O1—C1—N1	−0.5 (4)	C4—C8A—C9A—C10A	−173.0 (7)
C2—O1—C1—S1	−179.2 (3)	C8A—C9A—C10A—C11A	0.0
N1—N2—C2—O1	−0.8 (4)	C9A—C10A—C11A—C12A	0.0
N1—N2—C2—C3	−179.3 (4)	C9A—C10A—C11A—Cl1A	−175.9 (7)
C1—O1—C2—N2	0.8 (4)	C10A—C11A—C12A—C13A	0.0
C1—O1—C2—C3	179.5 (3)	Cl1A—C11A—C12A—C13A	175.6 (7)
C4—N3—C3—C2	123.0 (5)	C11A—C12A—C13A—C8A	0.0
N4—N3—C3—C2	−64.9 (5)	C9A—C8A—C13A—C12A	0.0
N2—C2—C3—N3	113.1 (5)	C4—C8A—C13A—C12A	173.2 (7)
O1—C2—C3—N3	−65.3 (5)	N3—C4—C8B—C9B	−64.5 (7)
N4—N3—C4—C5	−1.0 (5)	C5—C4—C8B—C9B	111.6 (7)
C3—N3—C4—C5	171.5 (4)	N3—C4—C8B—C13B	111.0 (6)
N4—N3—C4—C8A	179.9 (6)	C5—C4—C8B—C13B	−72.9 (7)
C3—N3—C4—C8A	−7.6 (9)	C13B—C8B—C9B—C10B	0.0
N4—N3—C4—C8B	175.8 (6)	C4—C8B—C9B—C10B	175.4 (7)
C3—N3—C4—C8B	−11.7 (9)	C8B—C9B—C10B—C11B	0.0
N3—C4—C5—C6	1.1 (6)	C9B—C10B—C11B—C12B	0.0
C8A—C4—C5—C6	−179.9 (7)	C9B—C10B—C11B—Cl1B	178.6 (7)
C8B—C4—C5—C6	−175.5 (6)	C10B—C11B—C12B—C13B	0.0
N3—N4—C6—C5	0.3 (5)	Cl1B—C11B—C12B—C13B	−178.7 (7)
N3—N4—C6—C7	−176.2 (4)	C11B—C12B—C13B—C8B	0.0
C4—C5—C6—N4	−0.9 (6)	C9B—C8B—C13B—C12B	0.0
C4—C5—C6—C7	175.3 (5)	C4—C8B—C13B—C12B	−175.7 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4^{i}	0.88	2.02	2.836 (5)	153
C3—H3*B*···N2^{ii}	0.99	2.51	3.445 (6)	158
C7—H7*C*···Cl1*B*^{iii}	0.98	2.73	3.635 (10)	153

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