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3-(3-Chloro-4-methylphenyl)-2-(4-fluorophenyl)thiazolidin-4-one

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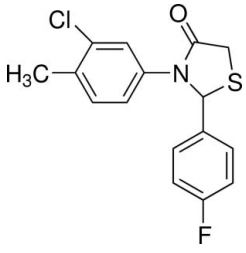
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.048; wR factor = 0.125; data-to-parameter ratio = 14.4.

The title compound, $C_{16}H_{13}ClFNOS$, possesses potent antibacterial activity. The overall molecular conformation is described by the dihedral angles of 43.0 (1)° between the 3-chloro-4-methylbenzene and thiazolidinone rings, and 88.8 (5)° between the thiazolidinone and 4-fluorobenzene rings. The 3-chloro-4-methylbenzene ring is disordered over two positions with occupancy factors approximately 3:1.

Related literature

For related literature, see: Tumul Srivastava *et al.* (2002).



Experimental

Crystal data

$C_{16}H_{13}ClFNOS$
M_r = 321.78
Orthorhombic, *Pbca*
a = 12.265 (3) Å
b = 12.994 (3) Å
c = 18.192 (4) Å
V = 2899.3 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 113 (2) K
0.16 × 0.14 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.937, T_{max} = 0.960
34208 measured reflections
3445 independent reflections
2796 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.125
S = 1.12
3445 reflections
240 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2144).

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supplementary materials

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3-(3-Chloro-4-methylphenyl)-2-(4-fluorophenyl)thiazolidin-4-one

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Comment

In recent years, 4-thiazolidinones are the most extensively investigated class of compounds, which exhibits various biological activities, such as anticancer, antitubercular, antibacterial and herbicidal activities. In view of these properties and in a continuation of our interest in the chemistry of 4-thiazolidinones, we have attempted to synthesize a series of 4-thiazolidinone derivatives, some of which have comparatively high antibacterial activity·The crystal structure determination of the title compound, (I), was undertaken to investigate the relationship between structure and antibacterial activity (Fig. 1). The molecular conformation is described by the dihedral angle between 3-chloro-4-methylbenzene ring and thiazolidinone ring of 43.0 (1)° and the dihedral angle between thiazolidinone ring and 4-fluorobenzene ring of 88.8 (5)°.

Experimental

Compound (I) was synthesized according to the procedure of Tumul Srivastava *et al.* (2002). A crystal of (I) suitable for X-ray analysis was grown from an ethanol solution by slow evaporation at room temperature.

Refinement

The 3-chloro-4-methylbenzene ring shows positional disorder. At the final stage of the refinement, the occupancy factors of two possible sites were fixed at 0.737 (2) and 0.263 (2), respectively. H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic), 0.99 (methylene), 1.00 (methylidyne) and 0.98 Å(methyl), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

Figures

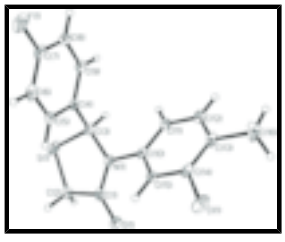


Fig. 1. The molecular structure of (I) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Only the major component of the disorder is shown.

3-(3-Chloro-4-methylphenyl)-2-(4-fluorophenyl)thiazolidin-4-one

Crystal data

$C_{16}H_{13}ClFNOS$

M_r = 321.78

D_x = 1.474 Mg m^{-3}

Mo $K\alpha$ radiation

λ = 0.71070 Å

Orthorhombic, *Pbca*	Cell parameters from 6992 reflections
a = 12.265 (3) Å	θ = 2.0–27.9º
b = 12.994 (3) Å	μ = 0.42 mm^{-1}
c = 18.192 (4) Å	T = 113 (2) K
V = 2899.3 (10) $Å^3$	Block, colourless
Z = 8	0.16 × 0.14 × 0.10 mm
F_{000} = 1328	

Data collection

Rigaku Saturn diffractometer	2796 reflections with $I > 2\sigma(I)$
Radiation source: Rotating anode	R_{int} = 0.056
Monochromator: confocal	θ_{max} = 27.9º
T = 113(2) K	θ_{min} = 2.5º
ω scans	h = −16→15
Absorption correction: multi-scan (Jacobson, 1998)	k = −17→17
T_{min} = 0.937, T_{max} = 0.960	l = −23→23
34208 measured reflections	Standard reflections: ?
3445 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.125	$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.3972P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max}$ = 0.001
3445 reflections	$\Delta\rho_{max}$ = 0.38 e $Å^{-3}$
240 parameters	$\Delta\rho_{min}$ = −0.76 e $Å^{-3}$
8 restraints	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0157 (15)

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 calculat-

ing *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}	Occ. (<1)
S1	0.30373 (5)	0.52351 (4)	0.39652 (3)	0.0435 (2)	
F1	0.49210 (13)	0.10913 (11)	0.54723 (7)	0.0612 (4)	
O1	0.09023 (11)	0.42265 (11)	0.25825 (7)	0.0344 (3)	
N1	0.25973 (12)	0.37796 (11)	0.29988 (7)	0.0258 (3)	
C1	0.16844 (15)	0.43791 (14)	0.29819 (9)	0.0265 (4)	
C2	0.17362 (16)	0.52700 (14)	0.35115 (10)	0.0299 (4)	
H2A	0.1142	0.5215	0.3878	0.036*	
H2B	0.1650	0.5928	0.3243	0.036*	
C3	0.35104 (15)	0.40902 (14)	0.34646 (9)	0.0262 (4)	
H3A	0.4140	0.4287	0.3145	0.031*	
C4	0.38717 (14)	0.32583 (13)	0.39887 (8)	0.0226 (4)	
C5	0.31314 (15)	0.27742 (14)	0.44550 (9)	0.0270 (4)	
H5A	0.2380	0.2950	0.4430	0.032*	
C6	0.34782 (18)	0.20378 (14)	0.49557 (10)	0.0342 (4)	
H6A	0.2977	0.1707	0.5276	0.041*	
C7	0.45733 (18)	0.18018 (15)	0.49737 (10)	0.0374 (5)	
C8	0.53130 (18)	0.22326 (18)	0.45151 (10)	0.0408 (5)	
H8A	0.6058	0.2034	0.4535	0.049*	
C9	0.49613 (16)	0.29727 (17)	0.40134 (10)	0.0332 (4)	
H9A	0.5469	0.3283	0.3687	0.040*	
Cl1	0.10556 (6)	0.05302 (5)	0.18509 (4)	0.0425 (3)	0.7369 (16)
C10	0.2796 (3)	0.2928 (2)	0.2516 (2)	0.0241 (9)	0.7369 (16)
C11	0.3781 (2)	0.2805 (2)	0.21479 (19)	0.0251 (7)	0.7369 (16)
H11A	0.4354	0.3287	0.2220	0.030*	0.7369 (16)
C12	0.39283 (18)	0.19757 (18)	0.16753 (13)	0.0284 (7)	0.7369 (16)
H12A	0.4601	0.1891	0.1424	0.034*	0.7369 (16)
C13	0.3091 (2)	0.12703 (14)	0.15704 (10)	0.0273 (7)	0.7369 (16)
C14	0.2106 (2)	0.13939 (18)	0.19381 (13)	0.0285 (7)	0.7369 (16)
C15	0.1959 (2)	0.2223 (2)	0.24107 (18)	0.0259 (7)	0.7369 (16)
H15A	0.1286	0.2307	0.2662	0.031*	0.7369 (16)
C16	0.3251 (3)	0.0370 (2)	0.10336 (15)	0.0426 (8)	0.7369 (16)
H16A	0.3988	0.0398	0.0827	0.064*	0.7369 (16)
H16B	0.2715	0.0420	0.0636	0.064*	0.7369 (16)
H16C	0.3152	−0.0282	0.1296	0.064*	0.7369 (16)
Cl1'	0.46197 (17)	0.13594 (14)	0.12449 (10)	0.0381 (6)	0.2631 (16)
C10'	0.2546 (8)	0.2828 (6)	0.2566 (6)	0.023 (2)	0.2631 (16)
C11'	0.1642 (6)	0.2184 (6)	0.2549 (5)	0.0210 (18)	0.2631 (16)
H11B	0.1016	0.2344	0.2834	0.025*	0.2631 (16)
C12'	0.1654 (5)	0.1304 (5)	0.2114 (4)	0.032 (2)	0.2631 (16)
H12B	0.1036	0.0864	0.2102	0.039*	0.2631 (16)
C13'	0.2570 (6)	0.1070 (4)	0.1696 (3)	0.0234 (17)	0.2631 (16)
C14'	0.3474 (5)	0.1714 (5)	0.1714 (3)	0.0197 (16)	0.2631 (16)

C15'	0.3462 (6)	0.2594 (6)	0.2149 (5)	0.025 (2)	0.2631 (16)
H15B	0.4080	0.3034	0.2161	0.030*	0.2631 (16)
C16'	0.2502 (9)	0.0116 (6)	0.1187 (4)	0.0398 (19)	0.2631 (16)
H16D	0.1796	−0.0224	0.1256	0.060*	0.2631 (16)
H16E	0.3090	−0.0364	0.1310	0.060*	0.2631 (16)
H16F	0.2576	0.0334	0.0674	0.060*	0.2631 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0665 (4)	0.0283 (3)	0.0359 (3)	0.0119 (2)	−0.0239 (2)	−0.0098 (2)
F1	0.1027 (12)	0.0462 (8)	0.0347 (7)	0.0305 (8)	−0.0128 (7)	0.0098 (6)
O1	0.0335 (8)	0.0393 (8)	0.0304 (7)	0.0034 (6)	−0.0069 (6)	−0.0027 (6)
N1	0.0324 (8)	0.0268 (8)	0.0182 (7)	0.0040 (6)	−0.0049 (6)	−0.0040 (6)
C1	0.0331 (10)	0.0275 (9)	0.0189 (8)	0.0015 (7)	0.0007 (7)	0.0017 (7)
C2	0.0391 (11)	0.0276 (9)	0.0231 (9)	0.0023 (8)	0.0050 (8)	−0.0024 (7)
C3	0.0309 (10)	0.0275 (9)	0.0203 (8)	−0.0011 (7)	−0.0025 (7)	−0.0002 (7)
C4	0.0276 (9)	0.0239 (9)	0.0162 (8)	−0.0001 (7)	−0.0035 (6)	−0.0031 (6)
C5	0.0311 (10)	0.0287 (9)	0.0214 (8)	−0.0012 (7)	0.0002 (7)	−0.0020 (7)
C6	0.0544 (13)	0.0268 (10)	0.0215 (9)	−0.0049 (9)	0.0008 (8)	0.0008 (7)
C7	0.0608 (13)	0.0305 (10)	0.0208 (8)	0.0152 (9)	−0.0100 (9)	−0.0014 (7)
C8	0.0393 (11)	0.0550 (13)	0.0282 (10)	0.0179 (10)	−0.0080 (9)	−0.0035 (9)
C9	0.0302 (10)	0.0452 (12)	0.0241 (9)	0.0022 (8)	−0.0018 (7)	−0.0011 (8)
Cl1	0.0535 (5)	0.0304 (4)	0.0437 (4)	−0.0209 (3)	−0.0178 (3)	0.0066 (3)
C10	0.032 (2)	0.0235 (16)	0.0173 (16)	−0.0010 (13)	−0.0065 (14)	−0.0009 (13)
C11	0.0264 (18)	0.0251 (15)	0.0238 (14)	−0.0027 (13)	−0.0027 (13)	−0.0022 (11)
C12	0.0331 (18)	0.0302 (16)	0.0220 (13)	−0.0030 (13)	0.0025 (13)	−0.0013 (11)
C13	0.044 (2)	0.0207 (16)	0.0173 (13)	−0.0017 (14)	−0.0014 (14)	0.0039 (11)
C14	0.036 (2)	0.0262 (15)	0.0233 (16)	−0.0052 (15)	−0.0077 (14)	0.0044 (12)
C15	0.024 (2)	0.0317 (15)	0.0223 (16)	−0.0002 (13)	−0.0019 (13)	0.0028 (11)
C16	0.073 (2)	0.0288 (15)	0.0263 (14)	0.0019 (15)	−0.0060 (14)	−0.0073 (11)
Cl1'	0.0519 (12)	0.0304 (10)	0.0321 (10)	0.0123 (8)	0.0154 (8)	0.0041 (7)
C10'	0.014 (4)	0.037 (6)	0.018 (4)	0.015 (4)	−0.003 (3)	−0.004 (4)
C11'	0.020 (4)	0.026 (4)	0.018 (4)	0.006 (3)	0.000 (3)	−0.011 (3)
C12'	0.037 (6)	0.034 (5)	0.026 (4)	0.008 (4)	0.000 (4)	−0.008 (3)
C13'	0.027 (5)	0.021 (4)	0.023 (4)	−0.005 (4)	−0.004 (4)	0.009 (3)
C14'	0.023 (5)	0.016 (4)	0.020 (3)	0.000 (3)	0.008 (3)	0.001 (3)
C15'	0.020 (5)	0.036 (5)	0.018 (4)	−0.004 (4)	0.001 (3)	0.009 (3)
C16'	0.060 (6)	0.032 (4)	0.027 (4)	0.005 (4)	−0.014 (4)	−0.009 (3)

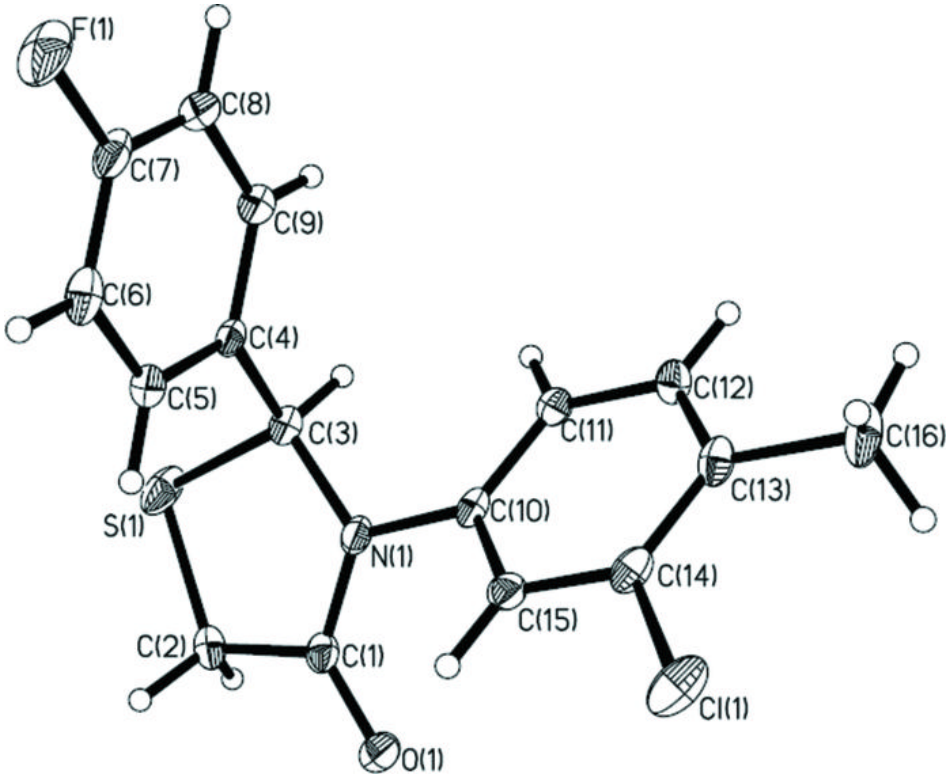
Geometric parameters (Å, °)

S1—C2	1.797 (2)	C11—C12	1.3900
S1—C3	1.8382 (19)	C11—H11A	0.9500
F1—C7	1.363 (2)	C12—C13	1.3900
O1—C1	1.220 (2)	C12—H12A	0.9500
N1—C1	1.364 (2)	C13—C14	1.3900
N1—C10	1.434 (2)	C13—C16	1.537 (3)
N1—C3	1.461 (2)	C14—C15	1.3900

N1—C10'	1.467 (4)	C15—H15A	0.9500
C1—C2	1.507 (2)	C16—H16A	0.9800
C2—H2A	0.9900	C16—H16B	0.9800
C2—H2B	0.9900	C16—H16C	0.9800
C3—C4	1.508 (2)	Cl1'—C14'	1.707 (5)
C3—H3A	1.0000	C10'—C11'	1.3900
C4—C9	1.388 (3)	C10'—C15'	1.3900
C4—C5	1.393 (2)	C11'—C12'	1.3900
C5—C6	1.388 (3)	C11'—H11B	0.9500
C5—H5A	0.9500	C12'—C13'	1.3900
C6—C7	1.378 (3)	C12'—H12B	0.9500
C6—H6A	0.9500	C13'—C14'	1.3900
C7—C8	1.354 (3)	C13'—C16'	1.549 (7)
C8—C9	1.394 (3)	C14'—C15'	1.3900
C8—H8A	0.9500	C15'—H15B	0.9500
C9—H9A	0.9500	C16'—H16D	0.9800
Cl1—C14	1.716 (2)	C16'—H16E	0.9800
C10—C11	1.3900	C16'—H16F	0.9800
C10—C15	1.3900		
C2—S1—C3	94.20 (8)	C12—C11—H11A	120.0
C1—N1—C10	124.5 (2)	C10—C11—H11A	120.0
C1—N1—C3	118.97 (14)	C11—C12—C13	120.0
C10—N1—C3	116.0 (2)	C11—C12—H12A	120.0
C1—N1—C10'	115.7 (5)	C13—C12—H12A	120.0
C10—N1—C10'	13.6 (4)	C12—C13—C14	120.0
C3—N1—C10'	125.2 (5)	C12—C13—C16	119.7 (2)
O1—C1—N1	124.48 (16)	C14—C13—C16	120.3 (2)
O1—C1—C2	122.60 (16)	C15—C14—C13	120.0
N1—C1—C2	112.92 (15)	C15—C14—Cl1	117.82 (16)
C1—C2—S1	108.15 (13)	C13—C14—Cl1	122.16 (16)
C1—C2—H2A	110.1	C14—C15—C10	120.0
S1—C2—H2A	110.1	C14—C15—H15A	120.0
C1—C2—H2B	110.1	C10—C15—H15A	120.0
S1—C2—H2B	110.1	C13—C16—H16A	109.5
H2A—C2—H2B	108.4	C13—C16—H16B	109.5
N1—C3—C4	113.20 (14)	H16A—C16—H16B	109.5
N1—C3—S1	105.60 (12)	C13—C16—H16C	109.5
C4—C3—S1	111.08 (11)	H16A—C16—H16C	109.5
N1—C3—H3A	108.9	H16B—C16—H16C	109.5
C4—C3—H3A	108.9	C11'—C10'—C15'	120.0
S1—C3—H3A	108.9	C11'—C10'—N1	123.7 (5)
C9—C4—C5	119.17 (16)	C15'—C10'—N1	116.3 (5)
C9—C4—C3	119.69 (16)	C10'—C11'—C12'	120.0
C5—C4—C3	121.14 (16)	C10'—C11'—H11B	120.0
C6—C5—C4	120.75 (18)	C12'—C11'—H11B	120.0
C6—C5—H5A	119.6	C11'—C12'—C13'	120.0
C4—C5—H5A	119.6	C11'—C12'—H12B	120.0
C7—C6—C5	117.89 (18)	C13'—C12'—H12B	120.0
C7—C6—H6A	121.1	C12'—C13'—C14'	120.0

C5—C6—H6A	121.1	C12'—C13'—C16'	117.3 (6)
C8—C7—F1	118.72 (19)	C14'—C13'—C16'	122.6 (6)
C8—C7—C6	123.13 (18)	C13'—C14'—C15'	120.0
F1—C7—C6	118.14 (19)	C13'—C14'—Cl1'	118.8 (4)
C7—C8—C9	118.77 (19)	C15'—C14'—Cl1'	121.0 (4)
C7—C8—H8A	120.6	C14'—C15'—C10'	120.0
C9—C8—H8A	120.6	C14'—C15'—H15B	120.0
C4—C9—C8	120.24 (19)	C10'—C15'—H15B	120.0
C4—C9—H9A	119.9	C13'—C16'—H16D	109.5
C8—C9—H9A	119.9	C13'—C16'—H16E	109.5
C11—C10—C15	120.0	H16D—C16'—H16E	109.5
C11—C10—N1	122.16 (19)	C13'—C16'—H16F	109.5
C15—C10—N1	117.83 (19)	H16D—C16'—H16F	109.5
C12—C11—C10	120.0	H16E—C16'—H16F	109.5
C10—N1—C1—O1	4.4 (3)	C3—N1—C10—C15	141.68 (18)
C3—N1—C1—O1	175.57 (17)	C10'—N1—C10—C15	6(3)
C10'—N1—C1—O1	−7.7 (5)	C15—C10—C11—C12	0.0
C10—N1—C1—C2	−175.3 (2)	N1—C10—C11—C12	−178.9 (4)
C3—N1—C1—C2	−4.1 (2)	C10—C11—C12—C13	0.0
C10'—N1—C1—C2	172.6 (5)	C11—C12—C13—C14	0.0
O1—C1—C2—S1	−178.03 (15)	C11—C12—C13—C16	178.6 (2)
N1—C1—C2—S1	1.69 (19)	C12—C13—C14—C15	0.0
C3—S1—C2—C1	0.67 (13)	C16—C13—C14—C15	−178.6 (2)
C1—N1—C3—C4	126.12 (17)	C12—C13—C14—Cl1	−178.2 (2)
C10—N1—C3—C4	−62.0 (3)	C16—C13—C14—Cl1	3.2 (3)
C10'—N1—C3—C4	−50.3 (5)	C13—C14—C15—C10	0.0
C1—N1—C3—S1	4.38 (19)	Cl1—C14—C15—C10	178.24 (19)
C10—N1—C3—S1	176.3 (2)	C11—C10—C15—C14	0.0
C10'—N1—C3—S1	−172.0 (5)	N1—C10—C15—C14	178.9 (4)
C2—S1—C3—N1	−2.61 (13)	C1—N1—C10'—C11'	−42.6 (8)
C2—S1—C3—C4	−125.71 (13)	C10—N1—C10'—C11'	−176 (4)
N1—C3—C4—C9	127.67 (17)	C3—N1—C10'—C11'	133.9 (4)
S1—C3—C4—C9	−113.73 (16)	C1—N1—C10'—C15'	136.3 (4)
N1—C3—C4—C5	−52.9 (2)	C10—N1—C10'—C15'	3(3)
S1—C3—C4—C5	65.75 (18)	C3—N1—C10'—C15'	−47.2 (8)
C9—C4—C5—C6	2.0 (3)	C15'—C10'—C11'—C12'	0.0
C3—C4—C5—C6	−177.47 (16)	N1—C10'—C11'—C12'	178.9 (10)
C4—C5—C6—C7	−0.2 (3)	C10'—C11'—C12'—C13'	0.0
C5—C6—C7—C8	−1.8 (3)	C11'—C12'—C13'—C14'	0.0
C5—C6—C7—F1	178.96 (16)	C11'—C12'—C13'—C16'	−176.3 (7)
F1—C7—C8—C9	−178.89 (17)	C12'—C13'—C14'—C15'	0.0
C6—C7—C8—C9	1.9 (3)	C16'—C13'—C14'—C15'	176.1 (7)
C5—C4—C9—C8	−1.9 (3)	C12'—C13'—C14'—Cl1'	175.6 (5)
C3—C4—C9—C8	177.55 (17)	C16'—C13'—C14'—Cl1'	−8.4 (7)
C7—C8—C9—C4	0.0 (3)	C13'—C14'—C15'—C10'	0.0
C1—N1—C10—C11	132.0 (2)	Cl1'—C14'—C15'—C10'	−175.5 (5)
C3—N1—C10—C11	−39.4 (3)	C11'—C10'—C15'—C14'	0.0
C10'—N1—C10—C11	−175 (3)	N1—C10'—C15'—C14'	−179.0 (10)
C1—N1—C10—C15	−46.9 (3)		

Fig. 1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