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1-[(4-Methoxyphenyl)sulfonyl]-1*H*-indole-3-carbaldehyde

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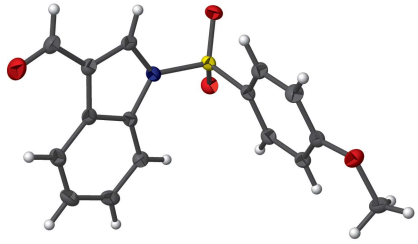
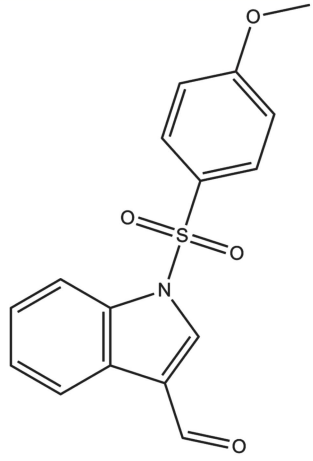
In the molecule of the title compound, $C_{16}H_{13}NO_4S$, the mean plane of the indole ring system and that of the methoxyphenyl ring, which are bridged by a sulfonyl group, are inclined at a dihedral angle of 88.98 (9)°. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Indole is a nitrogen-containing bicyclic heteroaromatic compound comprising a six-membered benzene ring fused to a five-membered pyrrole ring. Indole is one of the most important scaffolds in drug discovery and its derivatives are used as commercial drugs for many clinical applications (Zhang *et al.*, 2015) and as key building blocks for the preparation of biological and pharmaceutical agents. For example, they find use in antibacterial screening (El-Sayed *et al.*, 2016), antiviral studies (El-Sayed *et al.*, 2016) and as antitumour (Ma *et al.*, 2015) or antimalarial agents (Santos *et al.*, 2015). We have synthesized the title indole derivative and present its crystal structure here.

In the molecular structure, the bond lengths (Allen *et al.*, 1987) and angles of the title compound (Fig. 1) are generally within the normal ranges. The indole moiety is bridged by the N-bound sulfonyl group to the methoxyphenyl unit. The planes of the benzene ring and the indole ring system are inclined at 88.98 (9)°. The carbaldehyde and methoxy groups are in antiperiplanar and synperiplanar conformations with respect to the pyrrole and phenyl rings, as indicated by torsion angles of −172.8 (2) (C9—C8—C10—O11) and −1.7 (3)° (C19—C18—C21—C22). A weak intramolecular C3—H3···O14 hydrogen bond also affects the conformation of the molecule (Table 1). In the crystal, intermolecular C3—H3···O21 hydrogen bonds form chains of molecules along *b*. Additional

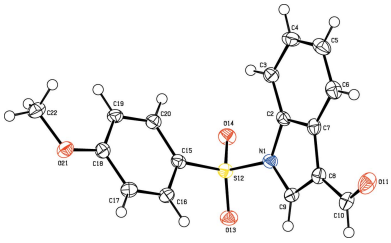


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O14	0.93	2.53	3.095 (3)	119
C3—H3···O21^{i}	0.93	2.59	3.345 (3)	139
C22—H22A···O11^{ii}	0.96	2.45	3.327 (3)	151

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

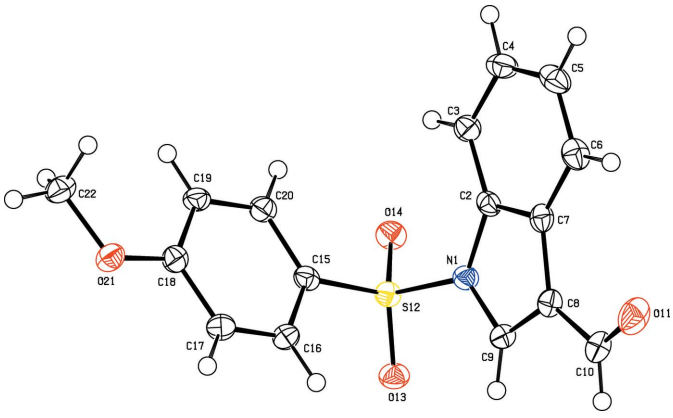


Figure 1
Perspective diagram of the title molecule, shown with 50% probability displacement ellipsoids.

C22—H22A···O11 contacts further stabilize the packing, stacking molecules along the b-axis direction (Fig. 2).

Synthesis and crystallization

1H-Indole-3-carbaldehyde (3.4 mmol) was dissolved in N,N-dimethylformamide (DMF) and K_2CO_3 (4.1 mmol) was added. The solution was stirred for 15 min and then 4-methoxybenzenesulfonyl chloride (3.5 mmol) was added portionwise to the ice-cold solution. The reaction continued for 6 h and was monitored by thin-layer chromatography (TLC). On completion, the reaction mixture was diluted with water (50 ml). The aqueous layer was extracted with ethyl acetate (3 × 20 ml) and the combined ethyl acetate layers were washed with brine (2 × 25 ml). The organic layer was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure to afford the crude product. This was purified by column chromatography over silica gel (60–120 mesh) using hexane–ethyl acetate (8:2 v/v) as eluent. The pure compound was crystallized from ethyl acetate and hexane as colourless single crystals.

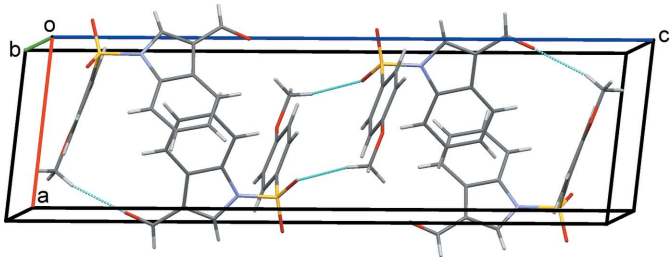


Figure 2
The packing of the title compound, viewed along the b-axis direction.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{13}NO_4S$
M_r	315.34
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	6.9942 (7), 8.2942 (9), 24.598 (3)
β (°)	96.814 (2)
V (Å^3)	1416.9 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.20
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker X8 Proteum
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10500, 2291, 2220
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.584
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.106, 1.10
No. of reflections	2291
No. of parameters	200
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.43

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{16}H_{13}NO_4S$
M_r = 315.34
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.9942 (7) Å
b = 8.2942 (9) Å
c = 24.598 (3) Å
β = 96.814 (2)°
V = 1416.9 (3) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.478 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2291 reflections
θ = 6.4–64.3°
μ = 2.20 mm^{-1}
T = 296 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 10.7 pixels mm^{-1}
φ and ω scans
10500 measured reflections
2291 independent reflections
2220 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 64.3°, θ_{min} = 6.4°
h = −8→8
k = −9→8
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.10
2291 reflections
200 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 1.4084P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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 e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}
S12	0.89891 (7)	0.41020 (6)	0.42187 (2)	0.0189 (2)
O11	0.9913 (2)	0.4522 (2)	0.17498 (6)	0.0352 (5)
O13	1.0955 (2)	0.45093 (19)	0.43860 (6)	0.0244 (5)
O14	0.8108 (2)	0.27610 (18)	0.44527 (6)	0.0242 (5)
O21	0.4462 (2)	1.00075 (18)	0.43282 (6)	0.0245 (5)
N1	0.8930 (2)	0.3701 (2)	0.35443 (7)	0.0194 (5)
C2	0.7317 (3)	0.3124 (2)	0.31978 (8)	0.0187 (6)
C3	0.5632 (3)	0.2421 (3)	0.33293 (9)	0.0218 (6)
C4	0.4314 (3)	0.1927 (3)	0.28930 (9)	0.0263 (7)
C5	0.4673 (3)	0.2143 (3)	0.23517 (9)	0.0278 (7)
C6	0.6348 (3)	0.2847 (3)	0.22240 (9)	0.0253 (7)
C7	0.7704 (3)	0.3354 (3)	0.26557 (8)	0.0200 (6)
C8	0.9589 (3)	0.4099 (3)	0.26807 (8)	0.0210 (6)
C9	1.0265 (3)	0.4299 (3)	0.32206 (8)	0.0202 (6)
C10	1.0620 (3)	0.4573 (3)	0.22269 (9)	0.0252 (7)
C15	0.7541 (3)	0.5802 (3)	0.42364 (8)	0.0187 (6)
C16	0.8295 (3)	0.7300 (3)	0.41079 (8)	0.0219 (6)
C17	0.7212 (3)	0.8668 (3)	0.41341 (8)	0.0232 (6)
C18	0.5359 (3)	0.8571 (3)	0.42915 (8)	0.0209 (6)
C19	0.4582 (3)	0.7078 (3)	0.44049 (8)	0.0211 (6)
C20	0.5677 (3)	0.5690 (3)	0.43757 (8)	0.0214 (6)
C22	0.2546 (3)	1.0020 (3)	0.44815 (9)	0.0264 (7)
H3	0.53960	0.22880	0.36910	0.0260*
H4	0.31700	0.14430	0.29640	0.0320*
H5	0.37590	0.18020	0.20700	0.0330*
H6	0.65720	0.29830	0.18620	0.0300*
H9	1.14400	0.47640	0.33510	0.0240*
H10	1.18830	0.49330	0.23040	0.0300*
H16	0.95290	0.73660	0.40050	0.0260*
H17	0.77100	0.96620	0.40470	0.0280*
H19	0.33360	0.70120	0.45000	0.0250*
H20	0.51650	0.46900	0.44490	0.0260*
H22A	0.16780	0.95410	0.41950	0.0400*
H22B	0.21600	1.11110	0.45390	0.0400*
H22C	0.25190	0.94150	0.48130	0.0400*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S12	0.0204 (3)	0.0209 (3)	0.0153 (3)	−0.0019 (2)	0.0015 (2)	0.0010 (2)

O11	0.0343 (9)	0.0517 (11)	0.0205 (8)	0.0046 (8)	0.0076 (7)	−0.0002 (7)
O13	0.0192 (7)	0.0304 (9)	0.0226 (8)	−0.0017 (6)	−0.0015 (6)	−0.0006 (6)
O14	0.0281 (8)	0.0224 (8)	0.0225 (8)	−0.0041 (6)	0.0050 (6)	0.0042 (6)
O21	0.0222 (8)	0.0228 (9)	0.0297 (8)	0.0008 (6)	0.0077 (6)	0.0027 (6)
N1	0.0191 (8)	0.0217 (9)	0.0175 (8)	−0.0026 (7)	0.0022 (7)	−0.0011 (7)
C2	0.0195 (10)	0.0148 (10)	0.0210 (10)	0.0010 (8)	−0.0006 (8)	−0.0020 (8)
C3	0.0221 (10)	0.0184 (11)	0.0251 (11)	−0.0009 (9)	0.0038 (8)	0.0001 (8)
C4	0.0205 (11)	0.0200 (11)	0.0374 (12)	−0.0030 (9)	−0.0004 (9)	−0.0011 (9)
C5	0.0264 (12)	0.0231 (12)	0.0312 (12)	0.0003 (9)	−0.0076 (9)	−0.0038 (9)
C6	0.0283 (12)	0.0257 (12)	0.0207 (10)	0.0038 (10)	−0.0026 (8)	−0.0012 (9)
C7	0.0219 (10)	0.0170 (11)	0.0210 (10)	0.0045 (9)	0.0021 (8)	−0.0003 (8)
C8	0.0219 (11)	0.0201 (12)	0.0213 (10)	0.0022 (8)	0.0044 (8)	−0.0002 (8)
C9	0.0176 (10)	0.0208 (11)	0.0226 (11)	−0.0010 (8)	0.0040 (8)	−0.0008 (8)
C10	0.0240 (11)	0.0276 (12)	0.0248 (12)	0.0055 (10)	0.0069 (9)	−0.0003 (9)
C15	0.0213 (10)	0.0210 (11)	0.0137 (9)	−0.0039 (8)	0.0013 (8)	−0.0003 (8)
C16	0.0212 (10)	0.0235 (12)	0.0220 (10)	−0.0034 (9)	0.0068 (8)	−0.0005 (8)
C17	0.0246 (11)	0.0204 (11)	0.0257 (11)	−0.0047 (9)	0.0073 (9)	0.0020 (9)
C18	0.0216 (10)	0.0247 (12)	0.0162 (9)	0.0001 (9)	0.0015 (8)	−0.0007 (8)
C19	0.0198 (10)	0.0243 (12)	0.0196 (10)	−0.0061 (9)	0.0046 (8)	−0.0007 (8)
C20	0.0229 (11)	0.0235 (12)	0.0182 (10)	−0.0047 (9)	0.0043 (8)	−0.0005 (8)
C22	0.0180 (10)	0.0339 (13)	0.0273 (11)	0.0008 (9)	0.0028 (8)	0.0009 (9)

Geometric parameters (Å, º)

S12—O13	1.4282 (15)	C15—C20	1.390 (3)
S12—O14	1.4256 (16)	C16—C17	1.370 (3)
S12—N1	1.6875 (18)	C17—C18	1.398 (3)
S12—C15	1.740 (2)	C18—C19	1.394 (3)
O11—C10	1.219 (3)	C19—C20	1.389 (3)
O21—C18	1.355 (3)	C3—H3	0.9300
O21—C22	1.435 (3)	C4—H4	0.9300
N1—C2	1.414 (3)	C5—H5	0.9300
N1—C9	1.389 (3)	C6—H6	0.9300
C2—C3	1.387 (3)	C9—H9	0.9300
C2—C7	1.405 (3)	C10—H10	0.9300
C3—C4	1.391 (3)	C16—H16	0.9300
C4—C5	1.396 (3)	C17—H17	0.9300
C5—C6	1.378 (3)	C19—H19	0.9300
C6—C7	1.402 (3)	C20—H20	0.9300
C7—C8	1.451 (3)	C22—H22A	0.9600
C8—C9	1.366 (3)	C22—H22B	0.9600
C8—C10	1.453 (3)	C22—H22C	0.9600
C15—C16	1.401 (3)		

S12···H3	3.0800	C6···H10^{ii}	2.8900
O11···C6	3.193 (3)	C7···H4^{vi}	3.0100
O11···C22^{i}	3.327 (3)	C7···H10^{ii}	2.8500
O11···C16^{ii}	3.170 (3)	C8···H4^{vi}	3.0500

O11···C17^{ii}	3.211 (3)	C10···H4^{vi}	3.0600
O13···C19^{iii}	3.309 (3)	C16···H22A^{iii}	3.0000
O14···C3	3.095 (3)	C17···H22C^{iv}	3.0300
O21···C22^{iv}	3.391 (3)	C18···H6^{vi}	3.0300
O21···C3^{v}	3.345 (3)	C18···H22C^{iv}	3.0100
O11···H6	2.7100	C19···H22A	2.8800
O11···H22A^{i}	2.4500	C19···H22C	2.6800
O11···H17^{ii}	2.7200	C20···H20^{viii}	3.0300
O11···H16^{ii}	2.6400	C22···H19	2.5500
O11···H4^{vi}	2.8400	H3···S12	3.0800
O13···H9	2.6200	H3···O14	2.5300
O13···H16	2.7000	H3···O21^{vii}	2.5900
O13···H19^{iii}	2.6600	H4···O11^{i}	2.8400
O14···H17^{vii}	2.7600	H4···C6^{i}	3.0400
O14···H19^{viii}	2.8800	H4···C7^{i}	3.0100
O14···H22C^{viii}	2.6300	H4···C8^{i}	3.0500
O14···H20	2.6100	H4···C10^{i}	3.0600
O14···H3	2.5300	H6···O11	2.7100
O21···H3^{v}	2.5900	H6···C18^{i}	3.0300
O21···H22C^{iv}	2.8400	H9···O13	2.6200
C2···C10^{ii}	3.494 (3)	H10···C5^{iii}	3.0200
C3···O14	3.095 (3)	H10···C2^{x}	3.0000
C3···O21^{vii}	3.345 (3)	H10···C5^{x}	3.0700
C4···C6^{i}	3.423 (4)	H10···C6^{x}	2.8900
C4···C7^{i}	3.485 (3)	H10···C7^{x}	2.8500
C5···C7^{i}	3.554 (3)	H16···O13	2.7000
C5···C10^{ix}	3.462 (3)	H16···H22A^{iii}	2.3600
C6···O11	3.193 (3)	H16···O11^{x}	2.6400
C6···C4^{vi}	3.423 (4)	H17···O14^{v}	2.7600
C7···C5^{vi}	3.554 (3)	H17···O11^{x}	2.7200
C7···C4^{vi}	3.485 (3)	H19···O13^{ix}	2.6600
C7···C10^{ii}	3.348 (3)	H19···C22	2.5500
C10···C2^{x}	3.494 (3)	H19···H22A	2.4700
C10···C5^{iii}	3.462 (3)	H19···H22C	2.2400
C10···C7^{x}	3.348 (3)	H19···O14^{viii}	2.8800
C16···O11^{x}	3.170 (3)	H20···O14	2.6100
C17···O11^{x}	3.211 (3)	H20···C20^{viii}	3.0300
C17···C22^{iv}	3.560 (3)	H22A···C16^{ix}	3.0000
C18···C22^{iv}	3.402 (3)	H22A···C19	2.8800
C19···O13^{ix}	3.309 (3)	H22A···H16^{ix}	2.3600
C20···C20^{viii}	3.511 (3)	H22A···H19	2.4700
C22···O21^{iv}	3.391 (3)	H22A···O11^{vi}	2.4500
C22···C18^{iv}	3.402 (3)	H22C···C19	2.6800
C22···C17^{iv}	3.560 (3)	H22C···H19	2.2400
C22···O11^{vi}	3.327 (3)	H22C···O14^{viii}	2.6300
C2···H10^{ii}	3.0000	H22C···O21^{iv}	2.8400
C5···H10^{ii}	3.0700	H22C···C17^{iv}	3.0300
C5···H10^{ix}	3.0200	H22C···C18^{iv}	3.0100

C6···H4^{vi}	3.0400

O13—S12—O14	121.04 (9)	O21—C18—C19	124.99 (19)
O13—S12—N1	103.91 (8)	C17—C18—C19	120.2 (2)
O13—S12—C15	110.15 (10)	C18—C19—C20	119.7 (2)
O14—S12—N1	106.37 (9)	C15—C20—C19	119.8 (2)
O14—S12—C15	109.96 (10)	C2—C3—H3	122.00
N1—S12—C15	103.77 (9)	C4—C3—H3	122.00
C18—O21—C22	118.58 (17)	C3—C4—H4	119.00
S12—N1—C2	125.72 (13)	C5—C4—H4	119.00
S12—N1—C9	123.61 (14)	C4—C5—H5	119.00
C2—N1—C9	108.54 (16)	C6—C5—H5	119.00
N1—C2—C3	129.85 (18)	C5—C6—H6	121.00
N1—C2—C7	107.24 (17)	C7—C6—H6	121.00
C3—C2—C7	122.90 (19)	N1—C9—H9	125.00
C2—C3—C4	116.6 (2)	C8—C9—H9	125.00
C3—C4—C5	121.4 (2)	O11—C10—H10	118.00
C4—C5—C6	121.7 (2)	C8—C10—H10	118.00
C5—C6—C7	118.1 (2)	C15—C16—H16	120.00
C2—C7—C6	119.3 (2)	C17—C16—H16	120.00
C2—C7—C8	107.10 (17)	C16—C17—H17	120.00
C6—C7—C8	133.61 (19)	C18—C17—H17	120.00
C7—C8—C9	107.51 (18)	C18—C19—H19	120.00
C7—C8—C10	127.88 (18)	C20—C19—H19	120.00
C9—C8—C10	124.6 (2)	C15—C20—H20	120.00
N1—C9—C8	109.60 (19)	C19—C20—H20	120.00
O11—C10—C8	123.3 (2)	O21—C22—H22A	109.00
S12—C15—C16	118.52 (16)	O21—C22—H22B	109.00
S12—C15—C20	121.20 (19)	O21—C22—H22C	109.00
C16—C15—C20	120.3 (2)	H22A—C22—H22B	110.00
C15—C16—C17	119.9 (2)	H22A—C22—H22C	109.00
C16—C17—C18	120.1 (2)	H22B—C22—H22C	109.00
O21—C18—C17	114.8 (2)		

O13—S12—N1—C2	175.17 (15)	C3—C2—C7—C8	−179.4 (2)
O14—S12—N1—C2	46.38 (17)	C2—C3—C4—C5	−0.5 (3)
C15—S12—N1—C2	−69.61 (17)	C3—C4—C5—C6	0.3 (4)
O13—S12—N1—C9	−23.36 (19)	C4—C5—C6—C7	−0.2 (4)
O14—S12—N1—C9	−152.15 (17)	C5—C6—C7—C8	178.9 (3)
C15—S12—N1—C9	91.86 (18)	C5—C6—C7—C2	0.3 (3)
N1—S12—C15—C20	103.34 (17)	C2—C7—C8—C10	−180.0 (2)
O14—S12—C15—C16	169.75 (15)	C6—C7—C8—C9	−179.0 (3)
N1—S12—C15—C16	−76.82 (17)	C2—C7—C8—C9	−0.3 (3)
O13—S12—C15—C16	33.89 (19)	C6—C7—C8—C10	1.3 (5)
O14—S12—C15—C20	−10.1 (2)	C7—C8—C9—N1	0.9 (3)
O13—S12—C15—C20	−145.96 (16)	C10—C8—C9—N1	−179.4 (2)
C22—O21—C18—C17	179.34 (17)	C7—C8—C10—O11	6.8 (4)
C22—O21—C18—C19	−1.7 (3)	C9—C8—C10—O11	−172.8 (2)

C9—N1—C2—C3	179.9 (2)	S12—C15—C20—C19	177.73 (15)
C2—N1—C9—C8	−1.2 (2)	C16—C15—C20—C19	−2.1 (3)
C9—N1—C2—C7	1.0 (2)	S12—C15—C16—C17	−178.04 (16)
S12—N1—C2—C7	164.81 (15)	C20—C15—C16—C17	1.8 (3)
S12—N1—C2—C3	−16.3 (3)	C15—C16—C17—C18	0.3 (3)
S12—N1—C9—C8	−165.41 (16)	C16—C17—C18—C19	−2.1 (3)
N1—C2—C3—C4	−178.2 (2)	C16—C17—C18—O21	176.95 (18)
N1—C2—C7—C8	−0.5 (2)	O21—C18—C19—C20	−177.17 (18)
C7—C2—C3—C4	0.6 (3)	C17—C18—C19—C20	1.8 (3)
N1—C2—C7—C6	178.5 (2)	C18—C19—C20—C15	0.3 (3)
C3—C2—C7—C6	−0.5 (3)		

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+2, *y*−1/2, −*z*+1/2; (iii) *x*+1, *y*, *z*; (iv) −*x*+1, −*y*+2, −*z*+1; (v) *x*, *y*+1, *z*; (vi) −*x*+1, *y*+1/2, −*z*+1/2; (vii) *x*, *y*−1, *z*; (viii) −*x*+1, −*y*+1, −*z*+1; (ix) *x*−1, *y*, *z*; (x) −*x*+2, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O14	0.93	2.53	3.095 (3)	119
C3—H3···O21^{vii}	0.93	2.59	3.345 (3)	139
C22—H22*A*···O11^{vi}	0.96	2.45	3.327 (3)	151

Symmetry codes: (vi) −*x*+1, *y*+1/2, −*z*+1/2; (vii) *x*, *y*−1, *z*.