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Methyl 2-(4-methylphenylsulfonamido)-3-phenylpropanoate

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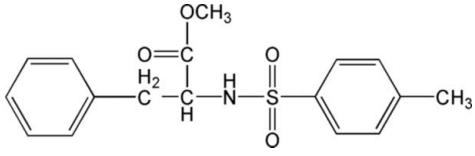
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.078; wR factor = 0.172; data-to-parameter ratio = 13.9.

The title compound, $C_{17}H_{19}NO_4S$, has two independent molecules in the asymmetric unit linked by an N—H···O hydrogen bond. The principal difference between them lies in the relative orientations of the two aromatic rings. These are inclined at an angle of 3.70 (3)° in one molecule but at 58.41 (12)° in the other. N—H···O hydrogen bonds form zigzag chains down the a axis and these chains are further stabilized by weak C—H···O interactions, forming a network structure.

Related literature

For general background, see Patani & Lavoie (1996) and Yan *et al.* (2007). For related structures, see Ziemer *et al.* (2001), Kazak *et al.* (2000), Creaser *et al.* (2001) and Yu (2006).



Experimental

Crystal data

$C_{17}H_{19}NO_4S$
M_r = 333.39
Orthorhombic, $P2_12_12_1$
a = 7.5812 (4) Å
b = 11.6107 (7) Å
c = 37.659 (2) Å
V = 3314.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 298 (2) K
0.29 × 0.24 × 0.09 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.938, T_{max} = 0.979
17577 measured reflections
5844 independent reflections
5517 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.172
S = 1.05
5844 reflections
419 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 2489 Friedel pairs
Flack parameter: −0.03 (1)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O5	0.86	2.04	2.844 (5)	155
N2—H2···O2^{i}	0.86	2.18	2.938 (5)	146
C21—H21···O4	0.93	2.68	3.494 (6)	146
C30—H30···O1^{ii}	0.93	2.68	3.416 (6)	137
C9—H9···O8^{iii}	0.93	2.67	3.521 (7)	153

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2288).

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supplementary materials

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Methyl 2-(4-methylphenylsulfonamido)-3-phenylpropanoate

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Comment

The sulfonamide group is present in many bioactive compounds and has been used as protecting group (Yan *et al.*, 2007; Patani & Lavoie, 1996). In an extension of research on sulfonamide derivatives, we report here the synthesis and structure of the title compound (1), Fig. 1.

The title compound, $C_{17}H_8NO_4S$, has two independent molecules in the asymmetric unit linked by an N—H···O hydrogen bond. The methyl-3-phenyl propanoate residue carries a 4-methylbenzenesulfonamide substituent in the 2-position. The principal difference between the two unique molecules lies in the relative orientations of the two aromatic rings. These are inclined at 3.70 (3)° in one molecule but 58.41 (12)° in the other. N—H···O hydrogen bonds form zigzag rows down the a axis and these rows are further stabilised by weak C—H···O interactions forming a network structure.

Experimental

Aqueous NaOH (20 ml, 10%) was added dropwise to a mixture of 4-methylbenzene-1-sulfonyl chloride (10 mmol, 1.905 g) and methyl 2-amino-3-phenylpropanoate (12 mmol, 2.148 g) with constant stirring for 4 h. The solvent was then evaporated in a vacuum. After column chromatography on silica eluting with petroleum ether/ethyl acetate (5/1 v/v), the purified product was dissolved in ethanol and left for 10 d until single crystals formed.

Refinement

The all H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å with $U_{iso} = 1.2U_{eq}$(parent atom), Csp^3—H = 0.96, 0.97 or 0.98 Å with $U_{iso} = 1.5U_{eq}$(parent atom) and N—H = 0.86 Å with $U_{iso} = 1.2U_{eq}$(parent atom).

Figures

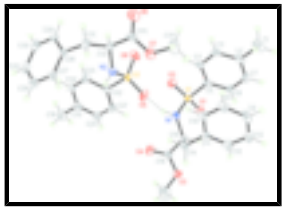

Fig. 1. The asymmetric unit of (I) showing 30% probability displacement ellipsoids and the atomic numbering. The hydrogen bond linking the two unique molecules is shown as a dashed line.

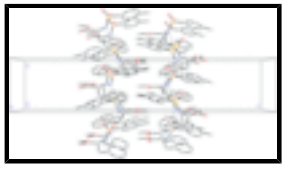

Fig. 2. The crystal packing of (I) viewed down the b axis. Hydrogen bonds are drawn as dashed lines.

Methyl 2-(4-methylphenylsulfonamido)-3-phenylpropanoate

Crystal data

$C_{17}H_{19}NO_4S$	F_{000} = 1408
M_r = 333.39	D_x = 1.336 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3436 reflections
a = 7.5812 (4) Å	θ = 2.2–24.2º
b = 11.6107 (7) Å	μ = 0.22 mm^{-1}
c = 37.659 (2) Å	T = 298 (2) K
V = 3314.8 (3) Å^3	Block, colorless
Z = 8	0.29 × 0.24 × 0.09 mm

Data collection

Bruker APEX area-detector diffractometer	5844 independent reflections
Radiation source: fine-focus sealed tube	5517 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.1º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −8→9
T_{min} = 0.938, T_{max} = 0.979	k = −13→13
17577 measured reflections	l = −44→39

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.078	$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2 + 1.5711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.172	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
5844 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
419 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2489 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.03 (1)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.30565 (15)	0.41714 (9)	0.88519 (3)	0.0308 (3)
S2	0.78670 (15)	0.65352 (10)	0.87955 (3)	0.0332 (3)
O1	0.1703 (4)	0.3475 (3)	0.90049 (9)	0.0436 (8)
O2	0.2899 (5)	0.5393 (3)	0.88534 (10)	0.0485 (9)
O3	0.5169 (5)	0.1975 (3)	0.97873 (9)	0.0509 (10)
O4	0.5427 (7)	0.3860 (3)	0.97724 (10)	0.0735 (14)
O5	0.7735 (5)	0.5321 (3)	0.88491 (10)	0.0526 (10)
O6	0.6695 (4)	0.7071 (3)	0.85494 (9)	0.0485 (9)
O7	0.9814 (6)	0.5722 (3)	0.80681 (9)	0.0555 (10)
O8	1.0416 (8)	0.7242 (5)	0.77332 (11)	0.0972 (19)
N1	0.4871 (5)	0.3878 (3)	0.90489 (10)	0.0357 (9)
H1	0.5673	0.4402	0.9051	0.043*
N2	0.9852 (5)	0.6845 (3)	0.86746 (9)	0.0331 (9)
H2	1.0716	0.6608	0.8803	0.040*
C1	0.4465 (10)	0.2586 (7)	0.73480 (15)	0.077 (2)
H1A	0.4116	0.3152	0.7176	0.115*
H1B	0.3857	0.1876	0.7302	0.115*
H1C	0.5714	0.2462	0.7332	0.115*
C2	0.4004 (8)	0.3011 (5)	0.77176 (13)	0.0469 (13)
C3	0.4548 (8)	0.4083 (5)	0.78334 (14)	0.0509 (14)
H3	0.5141	0.4564	0.7676	0.061*
C4	0.4240 (7)	0.4458 (4)	0.81734 (14)	0.0427 (13)
H4	0.4633	0.5179	0.8247	0.051*
C5	0.3334 (6)	0.3744 (4)	0.84049 (12)	0.0324 (11)
C6	0.2739 (7)	0.2682 (4)	0.82948 (13)	0.0456 (13)
H6	0.2119	0.2205	0.8449	0.055*
C7	0.3082 (8)	0.2343 (5)	0.79527 (14)	0.0550 (15)
H7	0.2670	0.1630	0.7877	0.066*
C8	0.7147 (8)	0.0712 (5)	0.80804 (15)	0.0575 (15)
H8	0.7168	0.0360	0.7859	0.069*
C9	0.7900 (8)	0.1786 (5)	0.81268 (14)	0.0540 (14)
H9	0.8446	0.2154	0.7937	0.065*
C10	0.7839 (7)	0.2306 (4)	0.84540 (13)	0.0422 (12)
H10	0.8338	0.3032	0.8482	0.051*
C11	0.7059 (6)	0.1780 (4)	0.87402 (11)	0.0323 (10)
C12	0.6303 (7)	0.0701 (5)	0.86856 (14)	0.0463 (13)
H12	0.5740	0.0337	0.8874	0.056*
C13	0.6364 (8)	0.0164 (5)	0.83651 (16)	0.0551 (15)

H13	0.5881	−0.0567	0.8338	0.066*
C14	0.7054 (6)	0.2304 (4)	0.91055 (11)	0.0361 (11)
H14A	0.7918	0.2920	0.9112	0.043*
H14B	0.7425	0.1723	0.9275	0.043*
C15	0.5268 (6)	0.2789 (4)	0.92248 (11)	0.0285 (10)
H15	0.4343	0.2231	0.9166	0.034*
C16	0.5283 (6)	0.2975 (4)	0.96227 (13)	0.0358 (11)
C17	0.5214 (9)	0.1996 (6)	1.01749 (14)	0.0658 (17)
H17A	0.6413	0.1932	1.0254	0.099*
H17B	0.4539	0.1362	1.0266	0.099*
H17C	0.4720	0.2707	1.0259	0.099*
C18	0.6813 (9)	0.8776 (5)	1.02333 (15)	0.0652 (17)
H18A	0.5868	0.8395	1.0356	0.098*
H18B	0.6526	0.9575	1.0203	0.098*
H18C	0.7879	0.8708	1.0369	0.098*
C19	0.7072 (7)	0.8225 (4)	0.98741 (13)	0.0427 (12)
C20	0.6593 (6)	0.7100 (5)	0.98159 (13)	0.0460 (13)
H20	0.6089	0.6681	1.0000	0.055*
C21	0.6837 (7)	0.6577 (4)	0.94926 (12)	0.0414 (12)
H21	0.6495	0.5816	0.9459	0.050*
C22	0.7590 (5)	0.7186 (4)	0.92179 (12)	0.0314 (10)
C23	0.8106 (7)	0.8313 (4)	0.92689 (13)	0.0401 (12)
H23	0.8630	0.8725	0.9085	0.048*
C24	0.7836 (7)	0.8820 (4)	0.95953 (14)	0.0444 (12)
H24	0.8176	0.9582	0.9629	0.053*
C25	1.2226 (7)	1.0151 (5)	0.93353 (15)	0.0491 (14)
H25	1.2241	1.0585	0.9543	0.059*
C26	1.3082 (7)	0.9111 (5)	0.93215 (14)	0.0519 (14)
H26	1.3702	0.8849	0.9519	0.062*
C27	1.3029 (7)	0.8457 (4)	0.90196 (14)	0.0421 (12)
H27	1.3591	0.7745	0.9016	0.051*
C28	1.2150 (6)	0.8836 (4)	0.87189 (12)	0.0343 (11)
C29	1.1317 (6)	0.9901 (4)	0.87353 (14)	0.0404 (12)
H29	1.0729	1.0183	0.8537	0.049*
C30	1.1352 (7)	1.0544 (4)	0.90425 (16)	0.0457 (13)
H30	1.0777	1.1251	0.9051	0.055*
C31	1.2030 (7)	0.8098 (4)	0.83955 (13)	0.0439 (12)
H31A	1.2943	0.7513	0.8406	0.053*
H31B	1.2250	0.8569	0.8187	0.053*
C32	1.0244 (6)	0.7511 (4)	0.83555 (12)	0.0385 (12)
H32	0.9350	0.8118	0.8336	0.046*
C33	1.0183 (7)	0.6815 (5)	0.80167 (13)	0.0471 (14)
C34	0.9743 (10)	0.4971 (6)	0.77597 (17)	0.076 (2)
H34A	0.9096	0.5345	0.7573	0.113*
H34B	0.9165	0.4264	0.7822	0.113*
H34C	1.0919	0.4809	0.7680	0.113*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0306 (6)	0.0310 (6)	0.0309 (6)	0.0008 (5)	−0.0019 (5)	0.0014 (5)
S2	0.0268 (5)	0.0380 (6)	0.0347 (6)	−0.0098 (5)	0.0015 (5)	−0.0005 (5)
O1	0.0349 (18)	0.054 (2)	0.0419 (19)	0.0009 (17)	0.0030 (15)	0.0007 (16)
O2	0.053 (2)	0.0405 (19)	0.052 (2)	0.0063 (18)	−0.008 (2)	−0.0012 (16)
O3	0.077 (3)	0.041 (2)	0.0342 (19)	−0.008 (2)	0.0005 (18)	0.0058 (16)
O4	0.139 (4)	0.046 (2)	0.036 (2)	−0.004 (3)	−0.002 (2)	−0.0130 (18)
O5	0.053 (2)	0.041 (2)	0.064 (2)	−0.0175 (17)	0.018 (2)	−0.0087 (18)
O6	0.0319 (19)	0.074 (3)	0.0391 (19)	−0.0033 (19)	−0.0007 (15)	−0.0007 (18)
O7	0.073 (3)	0.050 (2)	0.043 (2)	0.001 (2)	0.005 (2)	−0.0105 (19)
O8	0.152 (5)	0.106 (4)	0.033 (2)	−0.051 (4)	0.012 (3)	−0.001 (2)
N1	0.035 (2)	0.036 (2)	0.035 (2)	−0.0139 (19)	−0.0022 (18)	0.0040 (17)
N2	0.029 (2)	0.037 (2)	0.034 (2)	−0.0010 (17)	−0.0003 (17)	0.0051 (17)
C1	0.088 (5)	0.102 (6)	0.040 (3)	0.008 (4)	0.004 (3)	−0.004 (4)
C2	0.053 (3)	0.056 (4)	0.032 (3)	0.012 (3)	−0.003 (2)	0.002 (3)
C3	0.055 (3)	0.058 (4)	0.040 (3)	−0.006 (3)	0.002 (3)	0.018 (3)
C4	0.048 (3)	0.036 (3)	0.044 (3)	−0.009 (2)	−0.007 (2)	0.011 (2)
C5	0.033 (2)	0.035 (2)	0.030 (2)	0.004 (2)	−0.003 (2)	0.0047 (19)
C6	0.056 (3)	0.045 (3)	0.036 (3)	−0.017 (3)	−0.004 (2)	0.002 (2)
C7	0.069 (4)	0.045 (3)	0.051 (3)	−0.018 (3)	−0.005 (3)	−0.008 (3)
C8	0.055 (3)	0.075 (4)	0.042 (3)	0.005 (3)	−0.002 (3)	−0.028 (3)
C9	0.056 (3)	0.070 (4)	0.037 (3)	0.001 (3)	0.012 (3)	0.000 (3)
C10	0.043 (3)	0.042 (3)	0.041 (3)	−0.001 (3)	0.000 (2)	0.000 (2)
C11	0.027 (2)	0.033 (2)	0.036 (2)	0.007 (2)	−0.001 (2)	0.0027 (19)
C12	0.043 (3)	0.053 (3)	0.043 (3)	0.000 (3)	0.007 (2)	0.004 (3)
C13	0.058 (4)	0.049 (3)	0.058 (4)	−0.005 (3)	0.005 (3)	−0.023 (3)
C14	0.030 (2)	0.044 (3)	0.035 (3)	−0.001 (2)	−0.002 (2)	0.002 (2)
C15	0.029 (2)	0.024 (2)	0.033 (2)	−0.0012 (19)	0.0010 (19)	−0.0007 (19)
C16	0.030 (3)	0.041 (3)	0.037 (3)	−0.002 (2)	−0.002 (2)	0.001 (2)
C17	0.082 (4)	0.079 (4)	0.036 (3)	0.001 (4)	0.011 (3)	0.013 (3)
C18	0.070 (4)	0.075 (4)	0.051 (4)	−0.003 (4)	0.014 (3)	−0.007 (3)
C19	0.033 (3)	0.054 (3)	0.041 (3)	0.004 (3)	0.000 (2)	−0.002 (2)
C20	0.039 (3)	0.059 (3)	0.040 (3)	−0.013 (3)	0.008 (2)	0.013 (3)
C21	0.042 (3)	0.041 (3)	0.042 (3)	−0.011 (3)	0.005 (2)	0.005 (2)
C22	0.022 (2)	0.035 (3)	0.037 (2)	0.0004 (18)	−0.0012 (18)	0.002 (2)
C23	0.044 (3)	0.036 (3)	0.041 (3)	−0.005 (2)	0.015 (2)	0.008 (2)
C24	0.047 (3)	0.034 (3)	0.052 (3)	−0.001 (3)	0.003 (3)	0.000 (2)
C25	0.040 (3)	0.049 (3)	0.059 (3)	−0.010 (3)	0.007 (3)	−0.016 (3)
C26	0.045 (3)	0.063 (4)	0.047 (3)	−0.018 (3)	−0.005 (3)	0.004 (3)
C27	0.033 (3)	0.037 (3)	0.056 (3)	−0.001 (3)	−0.002 (3)	0.006 (2)
C28	0.025 (2)	0.035 (2)	0.043 (3)	−0.011 (2)	0.006 (2)	0.009 (2)
C29	0.036 (3)	0.034 (3)	0.051 (3)	−0.003 (2)	−0.004 (2)	0.014 (2)
C30	0.037 (3)	0.028 (3)	0.071 (4)	0.001 (2)	0.008 (3)	−0.004 (3)
C31	0.040 (3)	0.042 (3)	0.050 (3)	−0.006 (3)	0.010 (3)	0.005 (2)
C32	0.038 (3)	0.041 (3)	0.037 (3)	−0.003 (2)	0.008 (2)	0.006 (2)

C33	0.043 (3)	0.070 (4)	0.029 (3)	−0.009 (3)	0.000 (2)	0.001 (3)
C34	0.090 (5)	0.073 (4)	0.064 (4)	0.002 (4)	0.002 (4)	−0.031 (4)

Geometric parameters (Å, °)

S1—O2	1.423 (3)	C13—H13	0.9300
S1—O1	1.428 (4)	C14—C15	1.534 (6)
S1—N1	1.600 (4)	C14—H14A	0.9700
S1—C5	1.768 (5)	C14—H14B	0.9700
S2—O6	1.427 (4)	C15—C16	1.514 (6)
S2—O5	1.427 (4)	C15—H15	0.9800
S2—N2	1.613 (4)	C17—H17A	0.9600
S2—C22	1.774 (5)	C17—H17B	0.9600
O3—C16	1.318 (6)	C17—H17C	0.9600
O3—C17	1.460 (6)	C18—C19	1.509 (7)
O4—C16	1.178 (6)	C18—H18A	0.9600
O7—C33	1.313 (7)	C18—H18B	0.9600
O7—C34	1.453 (7)	C18—H18C	0.9600
O8—C33	1.190 (6)	C19—C20	1.374 (7)
N1—C15	1.459 (6)	C19—C24	1.384 (7)
N1—H1	0.8600	C20—C21	1.373 (7)
N2—C32	1.459 (6)	C20—H20	0.9300
N2—H2	0.8600	C21—C22	1.377 (6)
C1—C2	1.517 (8)	C21—H21	0.9300
C1—H1A	0.9600	C22—C23	1.378 (6)
C1—H1B	0.9600	C23—C24	1.378 (7)
C1—H1C	0.9600	C23—H23	0.9300
C2—C7	1.368 (8)	C24—H24	0.9300
C2—C3	1.382 (8)	C25—C30	1.365 (8)
C3—C4	1.373 (7)	C25—C26	1.371 (8)
C3—H3	0.9300	C25—H25	0.9300
C4—C5	1.385 (7)	C26—C27	1.368 (7)
C4—H4	0.9300	C26—H26	0.9300
C5—C6	1.377 (7)	C27—C28	1.386 (7)
C6—C7	1.372 (7)	C27—H27	0.9300
C6—H6	0.9300	C28—C29	1.390 (7)
C7—H7	0.9300	C28—C31	1.492 (7)
C8—C13	1.381 (8)	C29—C30	1.377 (7)
C8—C9	1.382 (8)	C29—H29	0.9300
C8—H8	0.9300	C30—H30	0.9300
C9—C10	1.373 (7)	C31—C32	1.523 (7)
C9—H9	0.9300	C31—H31A	0.9700
C10—C11	1.373 (6)	C31—H31B	0.9700
C10—H10	0.9300	C32—C33	1.511 (7)
C11—C12	1.393 (7)	C32—H32	0.9800
C11—C14	1.504 (6)	C34—H34A	0.9600
C12—C13	1.359 (7)	C34—H34B	0.9600
C12—H12	0.9300	C34—H34C	0.9600
O2—S1—O1	120.2 (2)	C14—C15—H15	108.8

O2—S1—N1	106.4 (2)	O4—C16—O3	123.3 (5)
O1—S1—N1	108.1 (2)	O4—C16—C15	126.8 (5)
O2—S1—C5	107.1 (2)	O3—C16—C15	109.8 (4)
O1—S1—C5	108.1 (2)	O3—C17—H17A	109.5
N1—S1—C5	106.2 (2)	O3—C17—H17B	109.5
O6—S2—O5	118.6 (2)	H17A—C17—H17B	109.5
O6—S2—N2	107.5 (2)	O3—C17—H17C	109.5
O5—S2—N2	109.0 (2)	H17A—C17—H17C	109.5
O6—S2—C22	108.9 (2)	H17B—C17—H17C	109.5
O5—S2—C22	106.6 (2)	C19—C18—H18A	109.5
N2—S2—C22	105.6 (2)	C19—C18—H18B	109.5
C16—O3—C17	117.0 (4)	H18A—C18—H18B	109.5
C33—O7—C34	118.0 (5)	C19—C18—H18C	109.5
C15—N1—S1	124.9 (3)	H18A—C18—H18C	109.5
C15—N1—H1	117.5	H18B—C18—H18C	109.5
S1—N1—H1	117.5	C20—C19—C24	117.7 (5)
C32—N2—S2	122.7 (3)	C20—C19—C18	120.8 (5)
C32—N2—H2	118.6	C24—C19—C18	121.5 (5)
S2—N2—H2	118.6	C21—C20—C19	121.7 (5)
C2—C1—H1A	109.5	C21—C20—H20	119.1
C2—C1—H1B	109.5	C19—C20—H20	119.1
H1A—C1—H1B	109.5	C20—C21—C22	119.7 (5)
C2—C1—H1C	109.5	C20—C21—H21	120.2
H1A—C1—H1C	109.5	C22—C21—H21	120.2
H1B—C1—H1C	109.5	C21—C22—C23	120.0 (4)
C7—C2—C3	117.3 (5)	C21—C22—S2	120.2 (4)
C7—C2—C1	121.8 (6)	C23—C22—S2	119.7 (4)
C3—C2—C1	120.9 (6)	C22—C23—C24	119.2 (4)
C4—C3—C2	122.0 (5)	C22—C23—H23	120.4
C4—C3—H3	119.0	C24—C23—H23	120.4
C2—C3—H3	119.0	C23—C24—C19	121.7 (5)
C3—C4—C5	118.7 (5)	C23—C24—H24	119.2
C3—C4—H4	120.6	C19—C24—H24	119.2
C5—C4—H4	120.6	C30—C25—C26	119.6 (5)
C6—C5—C4	120.6 (5)	C30—C25—H25	120.2
C6—C5—S1	119.9 (4)	C26—C25—H25	120.2
C4—C5—S1	119.4 (4)	C27—C26—C25	120.4 (5)
C7—C6—C5	118.5 (5)	C27—C26—H26	119.8
C7—C6—H6	120.7	C25—C26—H26	119.8
C5—C6—H6	120.7	C26—C27—C28	121.1 (5)
C2—C7—C6	122.8 (5)	C26—C27—H27	119.4
C2—C7—H7	118.6	C28—C27—H27	119.4
C6—C7—H7	118.6	C27—C28—C29	117.7 (5)
C13—C8—C9	119.7 (5)	C27—C28—C31	120.9 (4)
C13—C8—H8	120.2	C29—C28—C31	121.3 (4)
C9—C8—H8	120.2	C30—C29—C28	120.7 (5)
C10—C9—C8	119.8 (5)	C30—C29—H29	119.6
C10—C9—H9	120.1	C28—C29—H29	119.6
C8—C9—H9	120.1	C25—C30—C29	120.4 (5)

C11—C10—C9	121.5 (5)	C25—C30—H30	119.8
C11—C10—H10	119.2	C29—C30—H30	119.8
C9—C10—H10	119.2	C28—C31—C32	113.1 (4)
C10—C11—C12	117.5 (4)	C28—C31—H31A	109.0
C10—C11—C14	122.6 (4)	C32—C31—H31A	109.0
C12—C11—C14	119.9 (4)	C28—C31—H31B	109.0
C13—C12—C11	122.0 (5)	C32—C31—H31B	109.0
C13—C12—H12	119.0	H31A—C31—H31B	107.8
C11—C12—H12	119.0	N2—C32—C33	113.9 (4)
C12—C13—C8	119.5 (5)	N2—C32—C31	109.7 (4)
C12—C13—H13	120.2	C33—C32—C31	110.5 (4)
C8—C13—H13	120.2	N2—C32—H32	107.5
C11—C14—C15	114.7 (4)	C33—C32—H32	107.5
C11—C14—H14A	108.6	C31—C32—H32	107.5
C15—C14—H14A	108.6	O8—C33—O7	124.5 (5)
C11—C14—H14B	108.6	O8—C33—C32	122.0 (5)
C15—C14—H14B	108.6	O7—C33—C32	113.5 (4)
H14A—C14—H14B	107.6	O7—C34—H34A	109.5
N1—C15—C16	109.1 (4)	O7—C34—H34B	109.5
N1—C15—C14	111.5 (4)	H34A—C34—H34B	109.5
C16—C15—C14	109.6 (4)	O7—C34—H34C	109.5
N1—C15—H15	108.8	H34A—C34—H34C	109.5
C16—C15—H15	108.8	H34B—C34—H34C	109.5
O2—S1—N1—C15	155.8 (4)	C14—C15—C16—O4	103.6 (6)
O1—S1—N1—C15	25.5 (4)	N1—C15—C16—O3	163.4 (4)
C5—S1—N1—C15	−90.3 (4)	C14—C15—C16—O3	−74.2 (5)
O6—S2—N2—C32	−2.8 (4)	C24—C19—C20—C21	−0.7 (8)
O5—S2—N2—C32	126.9 (4)	C18—C19—C20—C21	−179.2 (5)
C22—S2—N2—C32	−118.9 (4)	C19—C20—C21—C22	0.4 (8)
C7—C2—C3—C4	2.2 (9)	C20—C21—C22—C23	0.4 (7)
C1—C2—C3—C4	−176.0 (6)	C20—C21—C22—S2	−178.5 (4)
C2—C3—C4—C5	−0.9 (8)	O6—S2—C22—C21	110.8 (4)
C3—C4—C5—C6	−0.6 (8)	O5—S2—C22—C21	−18.2 (4)
C3—C4—C5—S1	175.7 (4)	N2—S2—C22—C21	−134.0 (4)
O2—S1—C5—C6	−150.3 (4)	O6—S2—C22—C23	−68.1 (4)
O1—S1—C5—C6	−19.6 (5)	O5—S2—C22—C23	162.9 (4)
N1—S1—C5—C6	96.2 (4)	N2—S2—C22—C23	47.1 (4)
O2—S1—C5—C4	33.4 (4)	C21—C22—C23—C24	−0.8 (7)
O1—S1—C5—C4	164.1 (4)	S2—C22—C23—C24	178.1 (4)
N1—S1—C5—C4	−80.0 (4)	C22—C23—C24—C19	0.5 (8)
C4—C5—C6—C7	0.7 (8)	C20—C19—C24—C23	0.3 (8)
S1—C5—C6—C7	−175.6 (4)	C18—C19—C24—C23	178.7 (5)
C3—C2—C7—C6	−2.1 (9)	C30—C25—C26—C27	−1.5 (8)
C1—C2—C7—C6	176.1 (6)	C25—C26—C27—C28	1.5 (8)
C5—C6—C7—C2	0.7 (9)	C26—C27—C28—C29	−0.4 (7)
C13—C8—C9—C10	−1.0 (9)	C26—C27—C28—C31	−177.4 (4)
C8—C9—C10—C11	0.6 (8)	C27—C28—C29—C30	−0.8 (7)
C9—C10—C11—C12	−0.9 (7)	C31—C28—C29—C30	176.2 (4)
C9—C10—C11—C14	176.8 (5)	C26—C25—C30—C29	0.4 (8)

C10—C11—C12—C13	1.6 (8)	C28—C29—C30—C25	0.8 (8)
C14—C11—C12—C13	−176.2 (5)	C27—C28—C31—C32	102.0 (5)
C11—C12—C13—C8	−2.0 (9)	C29—C28—C31—C32	−74.9 (6)
C9—C8—C13—C12	1.7 (9)	S2—N2—C32—C33	−80.4 (5)
C10—C11—C14—C15	106.8 (5)	S2—N2—C32—C31	155.2 (3)
C12—C11—C14—C15	−75.4 (5)	C28—C31—C32—N2	−55.8 (5)
S1—N1—C15—C16	−108.6 (4)	C28—C31—C32—C33	177.8 (4)
S1—N1—C15—C14	130.1 (4)	C34—O7—C33—O8	2.2 (9)
C11—C14—C15—N1	−75.1 (5)	C34—O7—C33—C32	−179.3 (5)
C11—C14—C15—C16	164.0 (4)	N2—C32—C33—O8	177.5 (5)
C17—O3—C16—O4	0.5 (8)	C31—C32—C33—O8	−58.5 (7)
C17—O3—C16—C15	178.4 (4)	N2—C32—C33—O7	−1.0 (6)
N1—C15—C16—O4	−18.8 (7)	C31—C32—C33—O7	123.0 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O5	0.86	2.04	2.844 (5)	155
N2—H2···O2^{i}	0.86	2.18	2.938 (5)	146
C21—H21···O4	0.93	2.68	3.494 (6)	146
C30—H30···O1^{ii}	0.93	2.68	3.416 (6)	137
C9—H9···O8^{iii}	0.93	2.67	3.521 (7)	153

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

Fig. 1

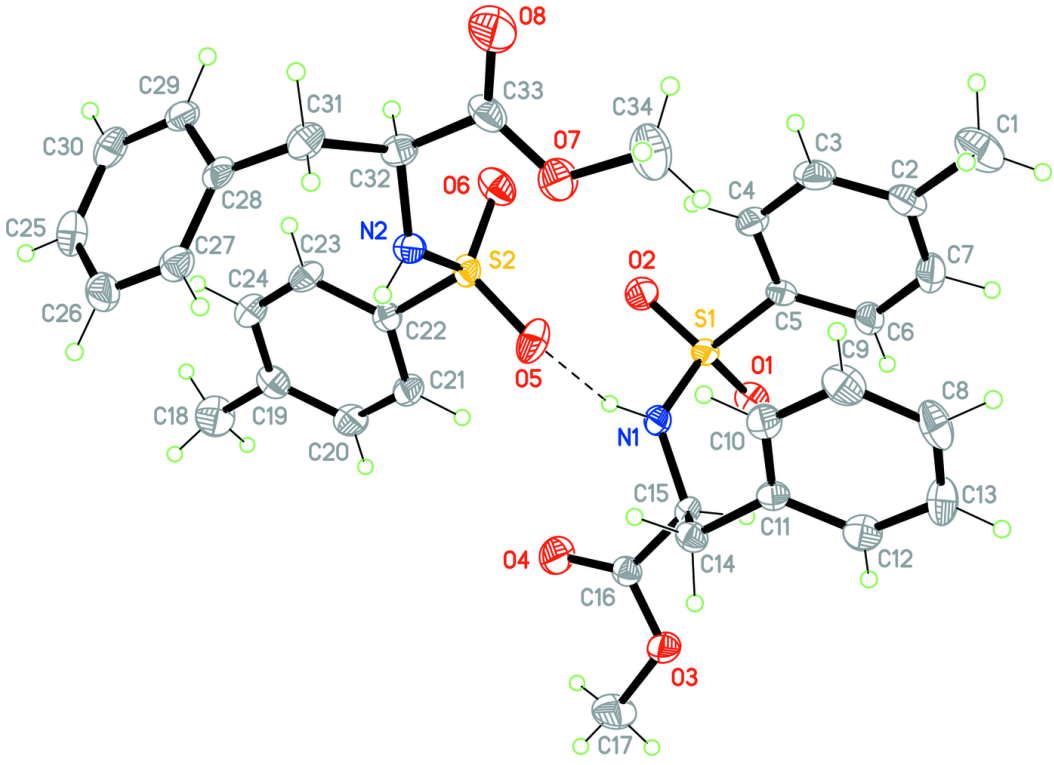
O8
C29
C31
C33
C34
C1
C30
O7
C3
C2
C32
O6
C4
C28
N2
S2
O2
C25
C27
C23
C7
C24
S1
C5
C6
C26
C22
O5
C9
O1
C21
C8
C18
C19
N1
C10
C20
C15
C13
C11
O4
C14
C12
C16
O3
C17

Fig. 2