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{(3*S*,5*R*)-5-(2,4-Difluorophenyl)-5-[(1*H*-1,2,4-triazol-1-yl)methyl]tetrahydrofuran-3-yl}methyl 4-methylbenzenesulfonate

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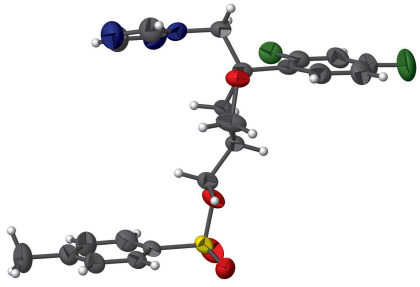
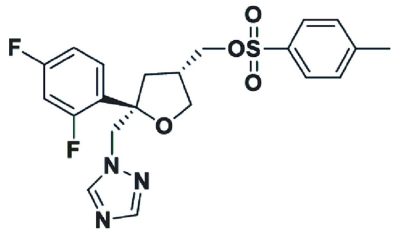
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{21}H_{21}F_2N_3O_4S$, the tetrahydrofuran ring adopts an envelope conformation with the β-C atom positioned at the flap. The triazole, difluorophenyl and tolyl rings of the various substituents on the tetrahydrofuran ring are inclined at 77.88 (12), 83.81 (10) and 81.00 (10)°, respectively, to the best-fit mean plane through the five atoms of the tetrahydrofuran ring. In the crystal, weak C—H···O and C—H···F hydrogen bonds link the molecules into a three-dimensional structure, with molecules stacked along the *a*-axis direction.

3D view



Chemical scheme



Structure description

Derivatives of triazole exhibit a broad spectrum of pharmaceutical applications, particularly as antifungal agents (Sheehan *et al.*, 1999). The title compound is a key intermediate in the synthesis of the antifungal agent Posaconazole. Compared with the existing antifungal drugs, it has a higher potency against a broad range of fungal pathogens including *Asperigillus*, *Candida* and *Cryptococcus* (Oakley *et al.*, 1997; Koltin & Hitchcock, 1997). We report herein the synthesis and crystal structure of the title compound (Fig. 1).

The molecule contains a central tetrahydrofuran ring with a 2–4-difluorophenyl ring in an *R*-configuration and a methyl 1,2,4-triazole substituent at C8 with a methyl 4-methylbenzenesulfonate substituent in an *S*-configuration at C10. The tetrahydrofuran ring O1/C8–C11 adopts an envelope conformation with the C9 atom at the flap. The best-fit mean plane through atoms O1,C8–C11 of the tetrahydrofuran ring is inclined at 77.88 (12)° to the triazole ring, 83.81 (10)° to the difluorophenyl ring and 81.00 (10)° to

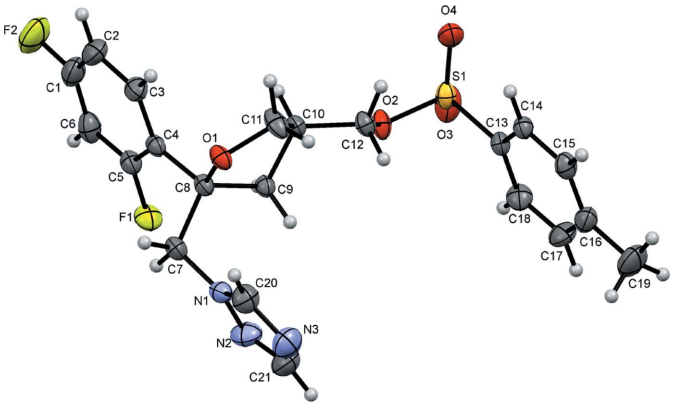


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

the tolyl ring. The triazole ring is inclined at angles of 14.32 (7) and 17.73 (9)° to the tolyl and fluorobenzene rings, respectively. The tolyl and fluorobenzene rings are almost parallel, as indicated by the interplanar angle of 3.89 (9)°. Bond lengths and angles in the molecule are generally within the normal ranges and are similar to those observed in the related compounds *N*′-[(*E*)-(1*S*,3*R*)-(3-isopropyl-1-methyl-2-oxo cyclopentyl)methylidene]-4-methylbenzenesulfonohydrazide (Tymann *et al.*, 2015) and 3-*O*-benzyl-4(*R*)-*C*-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-1,2-*O*- isopropylidene-α-D-erythrofuranose (Semjonovs *et al.*, 2015).

In the crystal, weak C—H···O and C—H···F hydrogen bonds generate a three-dimensional structure, with molecules stacked along the *a*-axis direction (Table 1, Fig. 2).

Synthesis and crystallization

The title compound was prepared according to a literature procedure (Saksena *et al.*, 1995). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature over a period of 10 d.

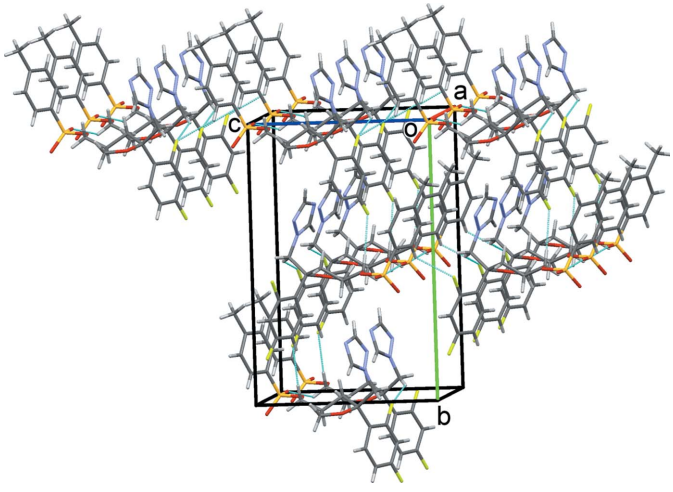


Figure 2
Packing of the title compound viewed along the *a* axis, with hydrogen bonds drawn as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···O3^{i}	0.97	2.48	3.128 (3)	124
C14—H14···F1^{ii}	0.93	2.60	3.222 (3)	125
C12—H12*B*···F2^{iii}	0.97	2.54	3.492 (4)	168

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{21}F_2N_3O_4S$
M_r	449.47
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	293
a, *b*, *c* (Å)	5.93718 (11), 16.9484 (3), 10.8841 (2)
β (°)	103.7973 (19)
V (Å^3)	1063.62 (3)
Z	2
Radiation type	Cu *Kα*
μ (mm^{-1})	1.81
Crystal size (mm)	0.36 × 0.12 × 0.02
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.721, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11514, 3732, 3465
R_{int}	0.036
(sin θ/λ)$_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.085, 1.05
No. of reflections	3732
No. of parameters	281
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.16
Absolute structure	Flack (1983)
Absolute structure parameter	−0.014 (16)

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SUPERFLIP* (Palatinus *et al.*, 2012), *SHELXL96* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170242 [https://doi.org/10.1107/S2414314617002425]

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Crystal data

$C_{21}H_{21}F_2N_3O_4S$
M_r = 449.47
Monoclinic, $P2_1$
a = 5.93718 (11) Å
b = 16.9484 (3) Å
c = 10.8841 (2) Å
β = 103.7973 (19)°
V = 1063.62 (3) Å^3
Z = 2
$F(000)$ = 468
D_x = 1.403 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 5053 reflections
θ = 4.2–72.3°
μ = 1.81 mm^{-1}
T = 293 K
, colourless
0.36 × 0.12 × 0.02 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0355 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.721, T_{max} = 1.000
11514 measured reflections
3732 independent reflections
3465 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 66.6°, θ_{min} = 4.2°
h = −5→7
k = −20→20
l = −12→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.085
S = 1.05
3732 reflections
281 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.0885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983) ???? Friedel pairs
Absolute structure parameter: −0.014 (16)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.56836 (9)	0.48540 (3)	0.07225 (5)	0.04259 (14)
O2	0.7081 (2)	0.48578 (12)	0.21565 (13)	0.0479 (4)
O4	0.6463 (4)	0.54834 (10)	0.00697 (17)	0.0564 (5)
F1	0.8681 (3)	0.51345 (9)	0.72967 (13)	0.0568 (4)
O1	1.4023 (2)	0.51967 (10)	0.52970 (13)	0.0424 (4)
O3	0.3339 (3)	0.48282 (15)	0.08029 (18)	0.0686 (5)
N1	1.3532 (3)	0.36806 (11)	0.65236 (18)	0.0456 (5)
C4	1.1446 (4)	0.58104 (14)	0.64476 (18)	0.0380 (5)
F2	0.9096 (5)	0.78712 (12)	0.7749 (2)	0.1063 (8)
C13	0.6451 (4)	0.39536 (13)	0.01338 (19)	0.0359 (5)
C14	0.8229 (4)	0.39399 (13)	−0.0472 (2)	0.0391 (5)
H14	0.9019	0.4400	−0.0572	0.047*
N2	1.1927 (5)	0.31089 (14)	0.6471 (3)	0.0650 (7)
C5	0.9697 (4)	0.58272 (15)	0.7095 (2)	0.0446 (5)
C15	0.8825 (4)	0.32311 (15)	−0.0929 (2)	0.0490 (6)
H15	1.0031	0.3216	−0.1339	0.059*
C1	0.9917 (6)	0.71952 (18)	0.7334 (3)	0.0690 (8)
C9	1.0182 (3)	0.47417 (13)	0.48126 (17)	0.0377 (4)
H9A	1.0341	0.4181	0.4673	0.045*
H9B	0.8675	0.4842	0.4982	0.045*
C10	1.0532 (4)	0.52271 (13)	0.36911 (18)	0.0384 (5)
H10	0.9879	0.5756	0.3721	0.046*
C12	0.9601 (3)	0.48732 (16)	0.23982 (17)	0.0415 (4)
H12A	1.0079	0.5188	0.1761	0.050*
H12B	1.0196	0.4342	0.2369	0.050*
C8	1.2160 (3)	0.50486 (12)	0.58950 (18)	0.0370 (5)
C16	0.7658 (5)	0.25394 (15)	−0.0789 (3)	0.0571 (7)
C6	0.8899 (5)	0.64998 (19)	0.7559 (3)	0.0608 (7)
H6	0.7736	0.6484	0.7999	0.073*
N3	1.4914 (6)	0.26643 (17)	0.5730 (3)	0.0801 (8)
C2	1.1656 (6)	0.72282 (16)	0.6729 (3)	0.0672 (8)
H2	1.2329	0.7709	0.6612	0.081*
C3	1.2428 (5)	0.65347 (16)	0.6283 (2)	0.0513 (6)
H3	1.3624	0.6556	0.5867	0.062*
C7	1.3139 (4)	0.44595 (14)	0.6970 (2)	0.0424 (5)

H7A	1.4593	0.4663	0.7476	0.051*
H7B	1.2065	0.4420	0.7513	0.051*
C17	0.5868 (6)	0.25747 (16)	−0.0185 (3)	0.0639 (8)
H17	0.5060	0.2117	−0.0095	0.077*
C20	1.5278 (5)	0.33992 (18)	0.6096 (3)	0.0618 (7)
H20	1.6595	0.3686	0.6060	0.074*
C18	0.5253 (5)	0.32757 (17)	0.0289 (3)	0.0540 (6)
H18	0.4056	0.3292	0.0705	0.065*
C11	1.3187 (4)	0.5280 (2)	0.3973 (2)	0.0583 (7)
H11A	1.3800	0.4864	0.3534	0.070*
H11B	1.3657	0.5785	0.3696	0.070*
C21	1.2873 (7)	0.25194 (18)	0.5978 (3)	0.0777 (10)
H21	1.2149	0.2031	0.5813	0.093*
C19	0.8364 (7)	0.1771 (2)	−0.1289 (4)	0.0932 (12)
H19A	0.9298	0.1877	−0.1879	0.140*
H19B	0.7003	0.1484	−0.1706	0.140*
H19C	0.9242	0.1463	−0.0599	0.140*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0350 (2)	0.0537 (3)	0.0381 (2)	0.0052 (3)	0.00674 (19)	−0.0099 (3)
O2	0.0406 (7)	0.0715 (10)	0.0349 (7)	−0.0048 (9)	0.0154 (6)	−0.0128 (8)
O4	0.0672 (12)	0.0452 (9)	0.0538 (10)	0.0087 (8)	0.0083 (9)	0.0000 (8)
F1	0.0528 (8)	0.0663 (9)	0.0574 (8)	−0.0105 (7)	0.0253 (7)	0.0048 (7)
O1	0.0333 (7)	0.0616 (9)	0.0329 (7)	−0.0049 (7)	0.0089 (6)	0.0048 (7)
O3	0.0390 (8)	0.0927 (14)	0.0737 (11)	0.0054 (11)	0.0124 (8)	−0.0275 (12)
N1	0.0479 (11)	0.0454 (11)	0.0422 (10)	−0.0014 (9)	0.0081 (9)	0.0089 (8)
C4	0.0367 (11)	0.0465 (11)	0.0277 (9)	−0.0045 (9)	0.0016 (8)	0.0009 (8)
F2	0.1321 (19)	0.0673 (12)	0.1169 (17)	0.0173 (12)	0.0245 (15)	−0.0368 (12)
C13	0.0339 (11)	0.0440 (12)	0.0290 (10)	−0.0007 (9)	0.0061 (9)	−0.0039 (8)
C14	0.0409 (12)	0.0445 (12)	0.0324 (10)	−0.0029 (9)	0.0099 (9)	−0.0023 (9)
N2	0.0620 (14)	0.0535 (14)	0.0801 (17)	−0.0121 (11)	0.0181 (13)	0.0101 (12)
C5	0.0443 (12)	0.0539 (13)	0.0349 (11)	−0.0048 (11)	0.0078 (10)	−0.0001 (10)
C15	0.0506 (14)	0.0571 (14)	0.0425 (12)	0.0079 (11)	0.0173 (11)	−0.0059 (11)
C1	0.083 (2)	0.0554 (16)	0.0629 (17)	0.0069 (15)	0.0050 (16)	−0.0179 (14)
C9	0.0378 (10)	0.0426 (12)	0.0314 (9)	−0.0059 (9)	0.0059 (8)	−0.0014 (9)
C10	0.0428 (12)	0.0413 (10)	0.0291 (10)	−0.0003 (9)	0.0047 (8)	0.0009 (8)
C12	0.0384 (10)	0.0553 (12)	0.0327 (9)	0.0041 (12)	0.0118 (8)	−0.0017 (11)
C8	0.0358 (10)	0.0453 (12)	0.0298 (9)	−0.0050 (8)	0.0073 (8)	0.0023 (8)
C16	0.0651 (17)	0.0480 (14)	0.0524 (14)	0.0021 (12)	0.0027 (13)	−0.0085 (11)
C6	0.0591 (16)	0.0776 (18)	0.0459 (13)	0.0092 (14)	0.0134 (12)	−0.0115 (13)
N3	0.093 (2)	0.0677 (17)	0.0816 (19)	0.0115 (15)	0.0242 (16)	−0.0104 (14)
C2	0.082 (2)	0.0445 (14)	0.0690 (18)	−0.0134 (14)	0.0069 (16)	−0.0077 (13)
C3	0.0539 (15)	0.0528 (14)	0.0453 (12)	−0.0129 (12)	0.0083 (11)	−0.0014 (11)
C7	0.0446 (13)	0.0501 (12)	0.0316 (10)	0.0009 (10)	0.0071 (9)	0.0039 (9)
C17	0.0707 (18)	0.0439 (14)	0.0751 (18)	−0.0189 (13)	0.0135 (16)	−0.0022 (13)
C20	0.0589 (16)	0.0664 (17)	0.0645 (17)	0.0030 (13)	0.0230 (14)	−0.0023 (14)

C18	0.0477 (14)	0.0624 (15)	0.0550 (15)	−0.0129 (12)	0.0184 (12)	−0.0025 (12)
C11	0.0455 (14)	0.094 (2)	0.0359 (11)	−0.0173 (14)	0.0116 (10)	0.0086 (12)
C21	0.095 (3)	0.0499 (16)	0.081 (2)	−0.0096 (16)	0.006 (2)	−0.0034 (15)
C19	0.121 (3)	0.0553 (19)	0.099 (3)	0.0145 (19)	0.017 (2)	−0.0234 (18)

Geometric parameters (Å, º)

S1—O2	1.5832 (14)	C9—C8	1.542 (3)
S1—O4	1.419 (2)	C10—H10	0.9800
S1—O3	1.4159 (18)	C10—C12	1.508 (3)
S1—C13	1.757 (2)	C10—C11	1.535 (3)
O2—C12	1.456 (2)	C12—H12A	0.9700
F1—C5	1.362 (3)	C12—H12B	0.9700
O1—C8	1.433 (3)	C8—C7	1.542 (3)
O1—C11	1.414 (3)	C16—C17	1.378 (4)
N1—N2	1.351 (3)	C16—C19	1.509 (4)
N1—C7	1.445 (3)	C6—H6	0.9300
N1—C20	1.322 (4)	N3—C20	1.310 (4)
C4—C5	1.388 (3)	N3—C21	1.326 (5)
C4—C8	1.526 (3)	C2—H2	0.9300
C4—C3	1.389 (3)	C2—C3	1.390 (4)
F2—C1	1.363 (3)	C3—H3	0.9300
C13—C14	1.372 (3)	C7—H7A	0.9700
C13—C18	1.382 (3)	C7—H7B	0.9700
C14—H14	0.9300	C17—H17	0.9300
C14—C15	1.378 (3)	C17—C18	1.378 (4)
N2—C21	1.322 (4)	C20—H20	0.9300
C5—C6	1.376 (4)	C18—H18	0.9300
C15—H15	0.9300	C11—H11A	0.9700
C15—C16	1.389 (4)	C11—H11B	0.9700
C1—C6	1.373 (5)	C21—H21	0.9300
C1—C2	1.352 (5)	C19—H19A	0.9600
C9—H9A	0.9700	C19—H19B	0.9600
C9—H9B	0.9700	C19—H19C	0.9600
C9—C10	1.527 (3)		

O2—S1—C13	104.04 (10)	O1—C8—C9	104.00 (15)
O4—S1—O2	109.50 (11)	O1—C8—C7	105.41 (16)
O4—S1—C13	109.05 (11)	C4—C8—C9	110.73 (17)
O3—S1—O2	103.35 (10)	C4—C8—C7	109.78 (17)
O3—S1—O4	119.81 (13)	C9—C8—C7	116.22 (18)
O3—S1—C13	109.87 (12)	C15—C16—C19	120.0 (3)
C12—O2—S1	116.90 (11)	C17—C16—C15	118.5 (2)
C11—O1—C8	111.00 (16)	C17—C16—C19	121.5 (3)
N2—N1—C7	120.0 (2)	C5—C6—H6	121.9
C20—N1—N2	109.3 (2)	C1—C6—C5	116.2 (3)
C20—N1—C7	130.6 (2)	C1—C6—H6	121.9
C5—C4—C8	122.0 (2)	C20—N3—C21	101.9 (3)

C5—C4—C3	115.8 (2)	C1—C2—H2	120.4
C3—C4—C8	122.2 (2)	C1—C2—C3	119.3 (3)
C14—C13—S1	119.09 (17)	C3—C2—H2	120.4
C14—C13—C18	121.5 (2)	C4—C3—C2	121.3 (3)
C18—C13—S1	119.45 (18)	C4—C3—H3	119.4
C13—C14—H14	120.6	C2—C3—H3	119.4
C13—C14—C15	118.8 (2)	N1—C7—C8	113.47 (18)
C15—C14—H14	120.6	N1—C7—H7A	108.9
C21—N2—N1	101.2 (3)	N1—C7—H7B	108.9
F1—C5—C4	118.6 (2)	C8—C7—H7A	108.9
F1—C5—C6	116.8 (2)	C8—C7—H7B	108.9
C6—C5—C4	124.6 (3)	H7A—C7—H7B	107.7
C14—C15—H15	119.4	C16—C17—H17	119.4
C14—C15—C16	121.2 (2)	C16—C17—C18	121.3 (2)
C16—C15—H15	119.4	C18—C17—H17	119.4
F2—C1—C6	117.1 (3)	N1—C20—H20	124.3
C2—C1—F2	120.1 (3)	N3—C20—N1	111.3 (3)
C2—C1—C6	122.8 (3)	N3—C20—H20	124.3
H9A—C9—H9B	109.3	C13—C18—H18	120.6
C10—C9—H9A	111.4	C17—C18—C13	118.7 (2)
C10—C9—H9B	111.4	C17—C18—H18	120.6
C10—C9—C8	101.83 (16)	O1—C11—C10	107.01 (18)
C8—C9—H9A	111.4	O1—C11—H11A	110.3
C8—C9—H9B	111.4	O1—C11—H11B	110.3
C9—C10—H10	109.6	C10—C11—H11A	110.3
C9—C10—C11	101.56 (17)	C10—C11—H11B	110.3
C12—C10—C9	116.25 (19)	H11A—C11—H11B	108.6
C12—C10—H10	109.6	N2—C21—N3	116.1 (3)
C12—C10—C11	109.89 (19)	N2—C21—H21	121.9
C11—C10—H10	109.6	N3—C21—H21	121.9
O2—C12—C10	107.92 (16)	C16—C19—H19A	109.5
O2—C12—H12A	110.1	C16—C19—H19B	109.5
O2—C12—H12B	110.1	C16—C19—H19C	109.5
C10—C12—H12A	110.1	H19A—C19—H19B	109.5
C10—C12—H12B	110.1	H19A—C19—H19C	109.5
H12A—C12—H12B	108.4	H19B—C19—H19C	109.5
O1—C8—C4	110.35 (17)		

S1—O2—C12—C10	155.39 (17)	C9—C10—C11—O1	−25.6 (3)
S1—C13—C14—C15	179.88 (17)	C9—C8—C7—N1	44.5 (3)
S1—C13—C18—C17	179.6 (2)	C10—C9—C8—O1	−35.4 (2)
O2—S1—C13—C14	−94.97 (18)	C10—C9—C8—C4	83.1 (2)
O2—S1—C13—C18	85.1 (2)	C10—C9—C8—C7	−150.75 (19)
O4—S1—O2—C12	−52.0 (2)	C12—C10—C11—O1	−149.2 (2)
O4—S1—C13—C14	21.8 (2)	C8—O1—C11—C10	3.4 (3)
O4—S1—C13—C18	−158.2 (2)	C8—C4—C5—F1	3.5 (3)
F1—C5—C6—C1	−179.2 (2)	C8—C4—C5—C6	−176.6 (2)
O1—C8—C7—N1	−70.0 (2)	C8—C4—C3—C2	176.1 (2)

O3—S1—O2—C12	179.3 (2)	C8—C9—C10—C12	155.55 (19)
O3—S1—C13—C14	154.94 (18)	C8—C9—C10—C11	36.3 (2)
O3—S1—C13—C18	−25.0 (2)	C16—C17—C18—C13	0.8 (4)
N1—N2—C21—N3	0.7 (4)	C6—C1—C2—C3	1.5 (5)
C4—C5—C6—C1	1.0 (4)	C2—C1—C6—C5	−2.0 (5)
C4—C8—C7—N1	171.16 (18)	C3—C4—C5—F1	−179.39 (19)
F2—C1—C6—C5	177.8 (2)	C3—C4—C5—C6	0.5 (3)
F2—C1—C2—C3	−178.3 (3)	C3—C4—C8—O1	4.0 (3)
C13—S1—O2—C12	64.5 (2)	C3—C4—C8—C9	−110.6 (2)
C13—C14—C15—C16	0.2 (4)	C3—C4—C8—C7	119.8 (2)
C14—C13—C18—C17	−0.3 (4)	C7—N1—N2—C21	177.5 (2)
C14—C15—C16—C17	0.3 (4)	C7—N1—C20—N3	−177.1 (2)
C14—C15—C16—C19	−179.4 (3)	C20—N1—N2—C21	−1.1 (3)
N2—N1—C7—C8	−97.1 (3)	C20—N1—C7—C8	81.1 (3)
N2—N1—C20—N3	1.2 (3)	C20—N3—C21—N2	0.0 (4)
C5—C4—C8—O1	−179.07 (17)	C18—C13—C14—C15	−0.2 (3)
C5—C4—C8—C9	66.3 (2)	C11—O1—C8—C4	−98.5 (2)
C5—C4—C8—C7	−63.3 (2)	C11—O1—C8—C9	20.3 (2)
C5—C4—C3—C2	−1.0 (3)	C11—O1—C8—C7	143.0 (2)
C15—C16—C17—C18	−0.8 (4)	C11—C10—C12—O2	−178.2 (2)
C1—C2—C3—C4	0.0 (4)	C21—N3—C20—N1	−0.8 (4)
C9—C10—C12—O2	67.2 (3)	C19—C16—C17—C18	178.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···O3^{i}	0.97	2.48	3.128 (3)	124
C14—H14···F1^{ii}	0.93	2.60	3.222 (3)	125
C12—H12*B*···F2^{iii}	0.97	2.54	3.492 (4)	168

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