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5-(7-Methanesulfonyl-2-morpholin-4-yl-6,7-dihydro-5*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-pyrimidin-2-ylamine mesylate

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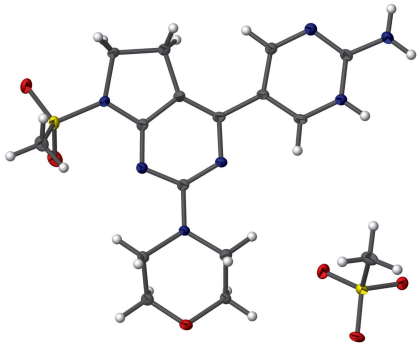
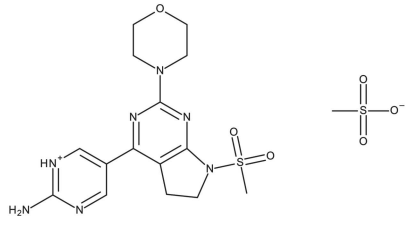
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{15}H_{20}N_7O_3S^+\cdot CH_3O_3S^-$ (CH5132799 mesylate), two molecular entities form a salt with proton transfer from methanesulfonic acid to the aminopyrimidine moiety of CH5132799. In the crystal, methanesulfonate is retained by bifurcated O···H—N hydrogen bonds and an N^+—H···O^- charge-assisted hydrogen bond.

3D view



Chemical scheme



Structure description

5-(7-Methanesulfonyl-2-morpholin-4-yl-6,7-dihydro-5*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-pyrimidin-2-ylamine (CH5132799) was synthesized as an antitumor PI3K inhibitor (Ohwada *et al.*, 2011; Tanaka *et al.*, 2011) and crystallized with methanesulfonic acid to improve its aqueous solubility. Single crystal X-ray structure analysis revealed that the three S—O bond lengths of methanesulfonate to be 1.444 (2), 1.473 (2), and 1.475 (2) Å, and it was confirmed that CH5132799 and methanesulfonic acid form a molecular salt with proton transfer from methanesulfonic acid to the aminopyrimidine moiety of CH5132799. In the crystal, methanesulfonate is retained by bifurcated O30···H19*B*(H19*A*#)—N19(N19#) hydrogen bonds and an N^+17—H17···O^-28 charge-assisted hydrogen bond (Figs. 1 and 2, and Table 1).

Synthesis and crystallization

CH5132799 was synthesized according to the patented process (Shimma *et al.*, 2008; Ebiike *et al.*, 2009). CH5132799 (1.0 eq.) was added to a stirred solution of methane-

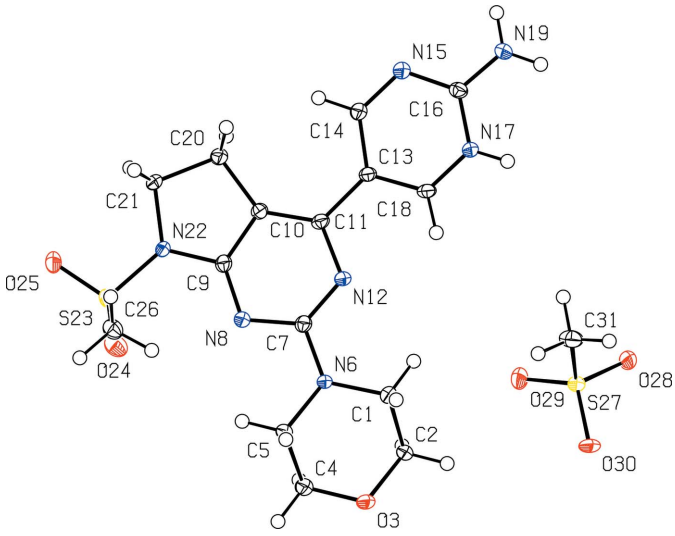


Figure 1
The molecular structure of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

sulfonic acid (2.3 weq.) and water (2.5 weq.). L-Cysteine (0.058 weq.) was then added to the solution and the mixture was continuously stirred for an additional 3 h. The resulting solution was filtered, and the equipment was rinsed with a solution of methanesulfonic acid (0.22 weq.) and water (2.1 weq.). The filtrate and the rinse were combined, and acetone (6.2 veq.) was added slowly to this stirred solution at room temperature. Stirring was continued for at least 2 h and the presence of the solids was confirmed. Further acetone (19 veq.) was added to the mixture, which was stirred for an additional hour at the same temperature. This mixture was then filtered, and the solids were washed twice with acetone (each 4.0 veq). The solids were collected and dried under reduced pressure to afford CH5132799 mesylate as yellow crystals (typical yield 90%).

Refinement

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

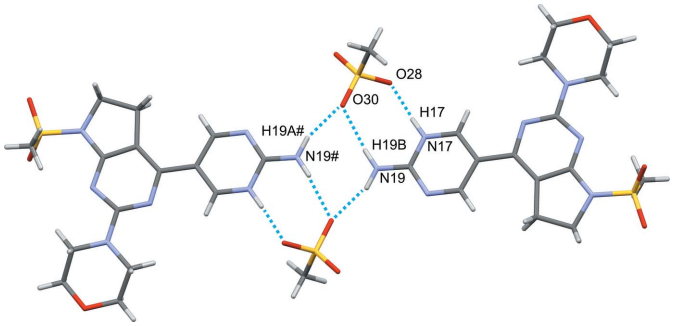


Figure 2
Hydrogen bonds in the crystal structure of the title compound (dashed lines). The suffix # in atom labels indicates atoms related by an inversion center.

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

D—H···A	D—H	H···A	D···A	D—H···A
N17—H17···O28^{i}	0.88	1.80	2.678 (3)	176
N19—H19A···O30^{ii}	0.88	2.00	2.850 (2)	161
N19—H19B···O30^{i}	0.88	2.11	2.906 (3)	150

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{20}N_7O_3S^+\cdot CH_3O_3S^-$
M_r	473.52
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	93
a, b, c (Å)	9.45151 (17), 10.7942 (2), 11.3964 (2)
α, β, γ (°)	63.3450 (7), 76.7692 (8), 88.1338 (8)
V (Å^3)	1008.24 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.86
Crystal size (mm)	0.29 × 0.08 × 0.04
Data collection	
Diffractometer	Rigaku R-AXIS RAPID-II
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.588, 0.884
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	17410, 3621, 2942
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.112, 1.09
No. of reflections	3621
No. of parameters	280
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.52

Computer programs: *RAPID-AUTO* (Rigaku, 1999), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008), *CrystalStructure* (Rigaku, 2016) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2017). **2**, x171292 [https://doi.org/10.1107/S2414314617012925]

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Crystal data

$C_{15}H_{20}N_7O_3S^+·CH_3O_3S^-$
M_r = 473.52
Triclinic, $P\overline{1}$
a = 9.45151 (17) Å
b = 10.7942 (2) Å
c = 11.3964 (2) Å
α = 63.3450 (7)°
β = 76.7692 (8)°
γ = 88.1338 (8)°
V = 1008.24 (3) Å^3
Z = 2
$F(000)$ = 496.00
D_x = 1.560 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 9509 reflections
θ = 4.5–68.2°
μ = 2.86 mm^{-1}
T = 93 K
Block, yellow
0.29 × 0.08 × 0.04 mm

Data collection

Rigaku R-AXIS RAPID-II diffractometer
Radiation source: fine-focus rotating anode x-ray, RIGAKU
Detector resolution: 10.000 pixels mm^{-1}
ω–scan
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
T_{min} = 0.588, T_{max} = 0.884
17410 measured reflections
3621 independent reflections
2942 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.061
θ_{max} = 68.2°, θ_{min} = 4.5°
h = −10→10
k = −12→12
l = −13→13

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.09
3621 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.250P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 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 was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8116 (3)	0.3631 (2)	0.1438 (2)	0.0190 (5)
H1A	0.9127	0.3646	0.0938	0.023*
H1B	0.8142	0.3500	0.2350	0.023*
C2	0.7479 (3)	0.4990 (2)	0.0693 (2)	0.0179 (5)
H2A	0.6521	0.5012	0.1257	0.021*
H2B	0.8130	0.5771	0.0549	0.021*
O3	0.72976 (18)	0.51726 (16)	−0.05928 (15)	0.0208 (4)
C4	0.6381 (3)	0.4043 (2)	−0.0418 (2)	0.0197 (5)
H4A	0.6267	0.4188	−0.1313	0.024*
H4B	0.5403	0.4028	0.0137	0.024*
C5	0.6999 (3)	0.2665 (2)	0.0255 (2)	0.0169 (5)
H5A	0.6319	0.1901	0.0405	0.020*
H5B	0.7941	0.2638	−0.0328	0.020*
N6	0.7213 (2)	0.24915 (19)	0.15512 (18)	0.0173 (4)
C7	0.6958 (2)	0.1218 (2)	0.2668 (2)	0.0148 (5)
N8	0.6153 (2)	0.02500 (19)	0.25782 (18)	0.0167 (4)
C9	0.5905 (3)	−0.0948 (2)	0.3679 (2)	0.0154 (5)
C10	0.6395 (2)	−0.1294 (2)	0.4856 (2)	0.0148 (5)
C11	0.7197 (2)	−0.0231 (2)	0.4821 (2)	0.0144 (5)
N12	0.7487 (2)	0.10429 (18)	0.37118 (18)	0.0151 (4)
C13	0.7882 (2)	−0.0333 (2)	0.5906 (2)	0.0141 (5)
C14	0.7765 (3)	−0.1507 (2)	0.7171 (2)	0.0184 (5)
H14	0.7199	−0.2312	0.7352	0.022*
N15	0.8385 (2)	−0.15666 (19)	0.81191 (19)	0.0194 (5)
C16	0.9182 (2)	−0.0421 (2)	0.7856 (2)	0.0157 (5)
N17	0.9382 (2)	0.07316 (19)	0.66444 (17)	0.0147 (4)
H17	0.9948	0.1450	0.6481	0.018*
C18	0.8733 (2)	0.0790 (2)	0.5699 (2)	0.0151 (5)
H18	0.8859	0.1619	0.4871	0.018*
N19	0.9806 (2)	−0.0410 (2)	0.87759 (19)	0.0213 (5)
H19A	0.9700	−0.1152	0.9562	0.026*
H19B	1.0327	0.0339	0.8603	0.026*
C20	0.5912 (3)	−0.2799 (2)	0.5840 (2)	0.0172 (5)
H20A	0.5197	−0.2874	0.6658	0.021*
H20B	0.6755	−0.3324	0.6115	0.021*
C21	0.5209 (3)	−0.3350 (2)	0.5051 (2)	0.0188 (5)

H21A	0.5823	−0.4013	0.4830	0.023*
H21B	0.4228	−0.3820	0.5581	0.023*
N22	0.5113 (2)	−0.20763 (19)	0.37949 (18)	0.0190 (5)
S23	0.45298 (6)	−0.21101 (6)	0.25455 (6)	0.01767 (17)
O24	0.36279 (17)	−0.09916 (17)	0.20638 (16)	0.0233 (4)
O25	0.39192 (19)	−0.35083 (17)	0.30865 (16)	0.0270 (4)
C26	0.6083 (3)	−0.1798 (2)	0.1241 (2)	0.0204 (5)
H26A	0.5800	−0.1838	0.0483	0.024*
H26B	0.6764	−0.2505	0.1572	0.024*
H26C	0.6554	−0.0874	0.0938	0.024*
S27	0.91174 (6)	0.64832 (6)	0.29026 (5)	0.01677 (17)
O28	0.89847 (17)	0.70007 (16)	0.39179 (15)	0.0195 (4)
O29	0.78257 (18)	0.56674 (16)	0.30994 (16)	0.0232 (4)
O30	0.95755 (18)	0.76462 (16)	0.15328 (15)	0.0203 (4)
C31	1.0534 (3)	0.5373 (3)	0.3124 (2)	0.0234 (6)
H31A	1.1433	0.5887	0.3007	0.028*
H31B	1.0682	0.5019	0.2453	0.028*
H31C	1.0279	0.4592	0.4035	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0256 (14)	0.0140 (12)	0.0164 (12)	−0.0030 (10)	−0.0070 (11)	−0.0048 (10)
C2	0.0268 (14)	0.0143 (12)	0.0130 (12)	−0.0005 (10)	−0.0081 (10)	−0.0050 (10)
O3	0.0354 (10)	0.0132 (8)	0.0119 (8)	−0.0009 (7)	−0.0081 (7)	−0.0027 (7)
C4	0.0292 (15)	0.0151 (12)	0.0164 (12)	0.0017 (10)	−0.0085 (11)	−0.0069 (10)
C5	0.0250 (14)	0.0136 (12)	0.0125 (11)	0.0006 (10)	−0.0073 (10)	−0.0049 (10)
N6	0.0283 (12)	0.0109 (10)	0.0116 (10)	−0.0025 (8)	−0.0087 (9)	−0.0022 (8)
C7	0.0187 (13)	0.0123 (11)	0.0146 (11)	0.0029 (9)	−0.0041 (10)	−0.0072 (10)
N8	0.0234 (11)	0.0133 (10)	0.0134 (10)	−0.0009 (8)	−0.0066 (8)	−0.0049 (8)
C9	0.0197 (13)	0.0134 (12)	0.0148 (12)	0.0018 (9)	−0.0037 (10)	−0.0081 (10)
C10	0.0207 (13)	0.0123 (11)	0.0110 (11)	0.0007 (9)	−0.0021 (9)	−0.0059 (10)
C11	0.0188 (13)	0.0115 (11)	0.0111 (11)	0.0014 (9)	−0.0017 (9)	−0.0043 (9)
N12	0.0213 (11)	0.0112 (10)	0.0120 (10)	0.0008 (8)	−0.0059 (8)	−0.0036 (8)
C13	0.0192 (13)	0.0112 (11)	0.0108 (11)	0.0021 (9)	−0.0037 (9)	−0.0039 (9)
C14	0.0271 (14)	0.0133 (12)	0.0162 (12)	0.0007 (10)	−0.0073 (10)	−0.0067 (10)
N15	0.0276 (12)	0.0151 (10)	0.0154 (10)	−0.0015 (9)	−0.0072 (9)	−0.0056 (9)
C16	0.0199 (13)	0.0155 (12)	0.0130 (12)	0.0047 (10)	−0.0054 (10)	−0.0071 (10)
N17	0.0186 (11)	0.0124 (10)	0.0116 (9)	−0.0012 (8)	−0.0039 (8)	−0.0038 (8)
C18	0.0199 (13)	0.0122 (11)	0.0106 (11)	0.0032 (9)	−0.0037 (10)	−0.0031 (9)
N19	0.0310 (12)	0.0176 (11)	0.0139 (10)	−0.0041 (9)	−0.0096 (9)	−0.0036 (9)
C20	0.0236 (13)	0.0142 (12)	0.0131 (12)	−0.0006 (10)	−0.0041 (10)	−0.0057 (10)
C21	0.0289 (14)	0.0113 (11)	0.0132 (11)	−0.0047 (10)	−0.0059 (10)	−0.0023 (10)
N22	0.0323 (12)	0.0111 (10)	0.0130 (10)	−0.0045 (9)	−0.0077 (9)	−0.0036 (8)
S23	0.0216 (3)	0.0183 (3)	0.0151 (3)	−0.0021 (2)	−0.0055 (2)	−0.0086 (3)
O24	0.0204 (10)	0.0291 (10)	0.0245 (9)	0.0087 (8)	−0.0091 (8)	−0.0144 (8)
O25	0.0385 (11)	0.0221 (10)	0.0209 (9)	−0.0109 (8)	−0.0086 (8)	−0.0086 (8)
C26	0.0221 (14)	0.0231 (13)	0.0184 (12)	0.0030 (10)	−0.0054 (10)	−0.0114 (11)

S27	0.0218 (3)	0.0146 (3)	0.0124 (3)	−0.0011 (2)	−0.0053 (2)	−0.0041 (2)
O28	0.0260 (10)	0.0174 (9)	0.0153 (8)	−0.0024 (7)	−0.0040 (7)	−0.0079 (7)
O29	0.0257 (10)	0.0213 (9)	0.0227 (9)	−0.0069 (8)	−0.0057 (8)	−0.0094 (8)
O30	0.0278 (10)	0.0161 (8)	0.0107 (8)	0.0006 (7)	−0.0054 (7)	−0.0004 (7)
C31	0.0291 (15)	0.0218 (13)	0.0177 (13)	0.0072 (11)	−0.0090 (11)	−0.0063 (11)

Geometric parameters (Å, º)

C1—N6	1.461 (3)	N15—C16	1.345 (3)
C1—C2	1.514 (3)	C16—N19	1.320 (3)
C1—H1A	0.9900	C16—N17	1.358 (3)
C1—H1B	0.9900	N17—C18	1.335 (3)
C2—O3	1.438 (3)	N17—H17	0.8800
C2—H2A	0.9900	C18—H18	0.9500
C2—H2B	0.9900	N19—H19A	0.8800
O3—C4	1.432 (3)	N19—H19B	0.8800
C4—C5	1.506 (3)	C20—C21	1.544 (3)
C4—H4A	0.9900	C20—H20A	0.9900
C4—H4B	0.9900	C20—H20B	0.9900
C5—N6	1.464 (3)	C21—N22	1.495 (3)
C5—H5A	0.9900	C21—H21A	0.9900
C5—H5B	0.9900	C21—H21B	0.9900
N6—C7	1.371 (3)	N22—S23	1.6553 (19)
C7—N12	1.329 (3)	S23—O24	1.4276 (17)
C7—N8	1.365 (3)	S23—O25	1.4318 (16)
N8—C9	1.315 (3)	S23—C26	1.750 (2)
C9—N22	1.390 (3)	C26—H26A	0.9800
C9—C10	1.407 (3)	C26—H26B	0.9800
C10—C11	1.377 (3)	C26—H26C	0.9800
C10—C20	1.511 (3)	S27—O29	1.4435 (16)
C11—N12	1.368 (3)	S27—O30	1.4725 (15)
C11—C13	1.483 (3)	S27—O28	1.4750 (15)
C13—C18	1.375 (3)	S27—C31	1.752 (2)
C13—C14	1.411 (3)	C31—H31A	0.9800
C14—N15	1.319 (3)	C31—H31B	0.9800
C14—H14	0.9500	C31—H31C	0.9800
N6—C1—C2	108.83 (19)	N19—C16—N17	118.7 (2)
N6—C1—H1A	109.9	N15—C16—N17	121.3 (2)
C2—C1—H1A	109.9	C18—N17—C16	120.96 (19)
N6—C1—H1B	109.9	C18—N17—H17	119.5
C2—C1—H1B	109.9	C16—N17—H17	119.5
H1A—C1—H1B	108.3	N17—C18—C13	120.9 (2)
O3—C2—C1	112.14 (18)	N17—C18—H18	119.6
O3—C2—H2A	109.2	C13—C18—H18	119.6
C1—C2—H2A	109.2	C16—N19—H19A	120.0
O3—C2—H2B	109.2	C16—N19—H19B	120.0
C1—C2—H2B	109.2	H19A—N19—H19B	120.0

H2A—C2—H2B	107.9	C10—C20—C21	104.50 (18)
C4—O3—C2	110.46 (16)	C10—C20—H20A	110.9
O3—C4—C5	111.80 (19)	C21—C20—H20A	110.9
O3—C4—H4A	109.3	C10—C20—H20B	110.9
C5—C4—H4A	109.3	C21—C20—H20B	110.9
O3—C4—H4B	109.3	H20A—C20—H20B	108.9
C5—C4—H4B	109.3	N22—C21—C20	104.18 (17)
H4A—C4—H4B	107.9	N22—C21—H21A	110.9
N6—C5—C4	108.52 (18)	C20—C21—H21A	110.9
N6—C5—H5A	110.0	N22—C21—H21B	110.9
C4—C5—H5A	110.0	C20—C21—H21B	110.9
N6—C5—H5B	110.0	H21A—C21—H21B	108.9
C4—C5—H5B	110.0	C9—N22—C21	110.30 (18)
H5A—C5—H5B	108.4	C9—N22—S23	124.24 (16)
C7—N6—C1	122.34 (18)	C21—N22—S23	123.60 (14)
C7—N6—C5	121.21 (18)	O24—S23—O25	119.02 (10)
C1—N6—C5	113.79 (17)	O24—S23—N22	109.06 (10)
N12—C7—N8	126.7 (2)	O25—S23—N22	104.35 (9)
N12—C7—N6	118.56 (19)	O24—S23—C26	107.77 (11)
N8—C7—N6	114.72 (19)	O25—S23—C26	109.78 (11)
C9—N8—C7	112.93 (19)	N22—S23—C26	106.15 (11)
N8—C9—N22	122.2 (2)	S23—C26—H26A	109.5
N8—C9—C10	127.0 (2)	S23—C26—H26B	109.5
N22—C9—C10	110.79 (19)	H26A—C26—H26B	109.5
C11—C10—C9	114.5 (2)	S23—C26—H26C	109.5
C11—C10—C20	136.4 (2)	H26A—C26—H26C	109.5
C9—C10—C20	109.09 (18)	H26B—C26—H26C	109.5
N12—C11—C10	121.5 (2)	O29—S27—O30	113.43 (10)
N12—C11—C13	113.04 (19)	O29—S27—O28	112.91 (10)
C10—C11—C13	125.4 (2)	O30—S27—O28	109.83 (9)
C7—N12—C11	117.37 (19)	O29—S27—C31	106.91 (11)
C18—C13—C14	114.8 (2)	O30—S27—C31	106.96 (11)
C18—C13—C11	119.2 (2)	O28—S27—C31	106.35 (11)
C14—C13—C11	126.0 (2)	S27—C31—H31A	109.5
N15—C14—C13	124.7 (2)	S27—C31—H31B	109.5
N15—C14—H14	117.6	H31A—C31—H31B	109.5
C13—C14—H14	117.6	S27—C31—H31C	109.5
C14—N15—C16	117.3 (2)	H31A—C31—H31C	109.5
N19—C16—N15	120.0 (2)	H31B—C31—H31C	109.5

N6—C1—C2—O3	−54.4 (3)	C10—C11—C13—C18	175.9 (2)
C1—C2—O3—C4	57.8 (2)	N12—C11—C13—C14	179.2 (2)
C2—O3—C4—C5	−59.1 (2)	C10—C11—C13—C14	−3.3 (4)
O3—C4—C5—N6	56.8 (2)	C18—C13—C14—N15	0.9 (3)
C2—C1—N6—C7	−144.2 (2)	C11—C13—C14—N15	−179.9 (2)
C2—C1—N6—C5	54.1 (2)	C13—C14—N15—C16	0.1 (4)
C4—C5—N6—C7	142.8 (2)	C14—N15—C16—N19	178.7 (2)
C4—C5—N6—C1	−55.3 (3)	C14—N15—C16—N17	−2.3 (3)

C1—N6—C7—N12	3.9 (3)	N19—C16—N17—C18	−177.6 (2)
C5—N6—C7—N12	164.3 (2)	N15—C16—N17—C18	3.4 (3)
C1—N6—C7—N8	−176.77 (19)	C16—N17—C18—C13	−2.3 (3)
C5—N6—C7—N8	−16.4 (3)	C14—C13—C18—N17	0.2 (3)
N12—C7—N8—C9	0.7 (3)	C11—C13—C18—N17	−179.11 (19)
N6—C7—N8—C9	−178.6 (2)	C11—C10—C20—C21	−172.6 (3)
C7—N8—C9—N22	−179.6 (2)	C9—C10—C20—C21	5.5 (3)
C7—N8—C9—C10	−1.1 (3)	C10—C20—C21—N22	−9.5 (2)
N8—C9—C10—C11	1.1 (3)	N8—C9—N22—C21	170.9 (2)
N22—C9—C10—C11	179.73 (19)	C10—C9—N22—C21	−7.8 (3)
N8—C9—C10—C20	−177.5 (2)	N8—C9—N22—S23	6.1 (3)
N22—C9—C10—C20	1.1 (3)	C10—C9—N22—S23	−172.67 (16)
C9—C10—C11—N12	−0.6 (3)	C20—C21—N22—C9	10.8 (2)
C20—C10—C11—N12	177.5 (2)	C20—C21—N22—S23	175.83 (16)
C9—C10—C11—C13	−177.8 (2)	C9—N22—S23—O24	−57.8 (2)
C20—C10—C11—C13	0.2 (4)	C21—N22—S23—O24	139.25 (19)
N8—C7—N12—C11	−0.3 (3)	C9—N22—S23—O25	174.00 (19)
N6—C7—N12—C11	179.0 (2)	C21—N22—S23—O25	11.1 (2)
C10—C11—N12—C7	0.2 (3)	C9—N22—S23—C26	58.0 (2)
C13—C11—N12—C7	177.82 (19)	C21—N22—S23—C26	−104.9 (2)
N12—C11—C13—C18	−1.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N17—H17···O28^{i}	0.88	1.80	2.678 (3)	176
N19—H19*A*···O30^{ii}	0.88	2.00	2.850 (2)	161
N19—H19*B*···O30^{i}	0.88	2.11	2.906 (3)	150

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