



# Crystal structure of bis(1,10-phenanthroline- $\kappa^2N,N'$ )(1,3-thiazole-2-thiolato- $\kappa^2S^2,N$ )nickel(II) hexafluoridophosphate 1,4-dioxane sesquisolvate

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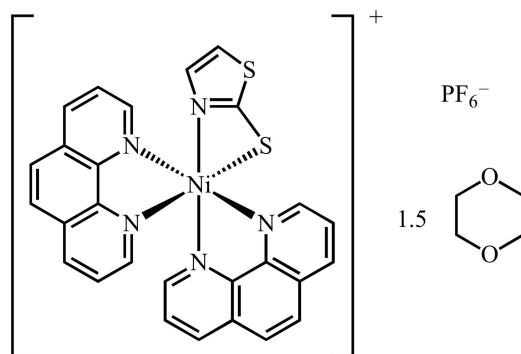
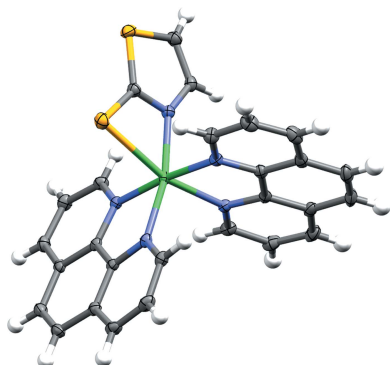
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**Keywords:** crystal structure; 2-mercaptothiazolate;  $\pi$ - $\pi$  stacking; hydrogen bonding; nickel(II) complex.**CCDC reference:** 1539577**Supporting information:** this article has supporting information at [journals.iucr.org/e](http://journals.iucr.org/e)

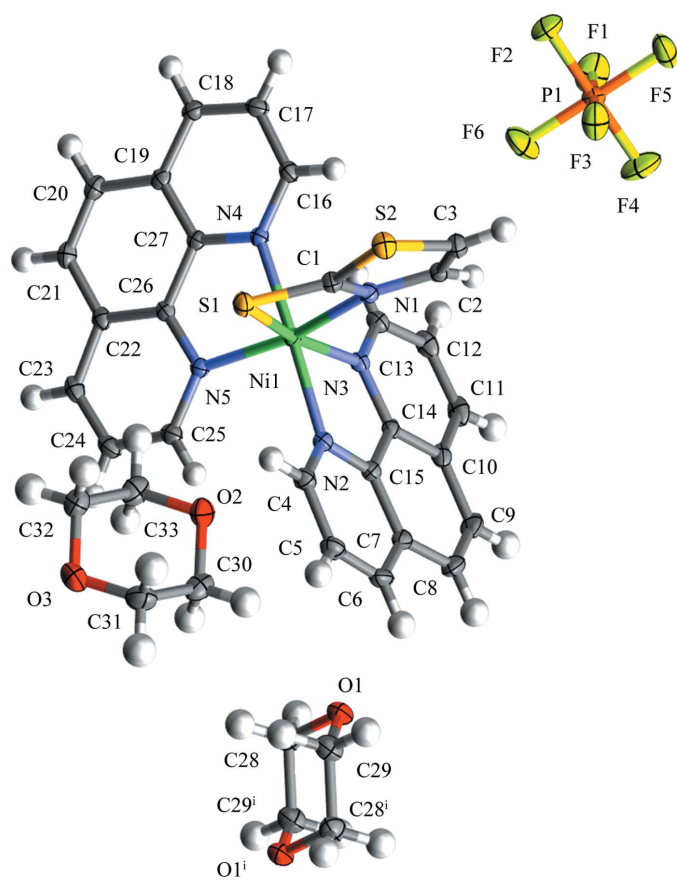
The title salt,  $[\text{Ni}(\text{C}_3\text{H}_2\text{NS}_2)(\text{C}_{12}\text{H}_8\text{N}_2)_2]\text{PF}_6 \cdot 1.5\text{C}_4\text{H}_8\text{O}_2$ , was the unexpected product on making an attempt to prepare an  $[\text{Ni}(\text{2-mercaptothiazolate})-(1,10\text{-phenanthroline})]^+$  complex by reaction of  $[\text{NiCl}_2(1,10\text{-phenanthroline})]$  with 2-mercaptothiazolate. In the resulting complex, the 2-mercaptothiazolate anion acts as a chelating ligand, which coordinates to the  $\text{Ni}^{\text{II}}$  ion with the thiazolyl N and thiolate S atoms. In the crystal,  $\pi$ - $\pi$  stacking interactions between the coordinating 1,10-phenanthroline molecules of adjacent complexes result in a zigzag chain running parallel to the  $c$  axis. Weak  $\text{C}-\text{H} \cdots \text{X}$  ( $\text{X} = \text{O}, \text{F}$ ) hydrogen-bonding interactions between the chains and 1,4-dioxane solvent molecules and  $\text{PF}_6^-$  counter-anions lead to the formation of sheets parallel to the  $ac$  plane.

## 1. Chemical context

2-Mercaptothiazolate (tzS) has three types of atoms available for coordination, namely the thiazolyl N, the thiazolyl S, and the thiolate S atom. Hence the tzS ligand is able to show different coordination modes. The anionic tzS ligand and its protonated neutral form are generally used as bridging ligands [ $\mu_2$ -tzS- $\kappa(N, \text{thiolate } S)$ ] or as monodentate ligands [ $\kappa(\text{thiolate } S)$ ] (Raper *et al.*, 1989, 1990a) whereas transition metal complexes with tzS in a bidentate coordination mode are rare (Raper *et al.*, 1989), although a number of transition metal complexes with 2-mercaptobenzothiazolate as a bidentate ligand exist (Raper *et al.*, 1990b; Ballester *et al.*, 1994; Khan *et al.*, 2010).



In a project intended to prepare the square-planar  $[\text{Ni}(\text{tzS})-(\text{phen})]^+$  cation involving tzS as a bidentate ligand by reaction of  $[\text{NiCl}_2(\text{phen})]$  (phen is 1,10-phenanthroline) with 2-mercaptothiazolate, we obtained the unexpected title dioxane solvate compound  $[\text{Ni}(\text{tzS})(\text{phen})_2](\text{PF}_6) \cdot 1.5(1,4\text{-dioxane})$  in which the tzS ligand acts after all as a bidentate ligand.



**Figure 1**  
The structures of the molecular entities in the title salt, shown with 50% probability displacement ellipsoids. [Symmetry code: (i)  $1 - x, -y, 1 - z$ .]

## 2. Structural commentary

The title salt consists of a complex cation  $[\text{Ni}(\text{tzS})(\text{phen})_2]^+$ , one  $\text{PF}_6^-$  counter-anion, and 1.5 1,4-dioxane solvent mol-

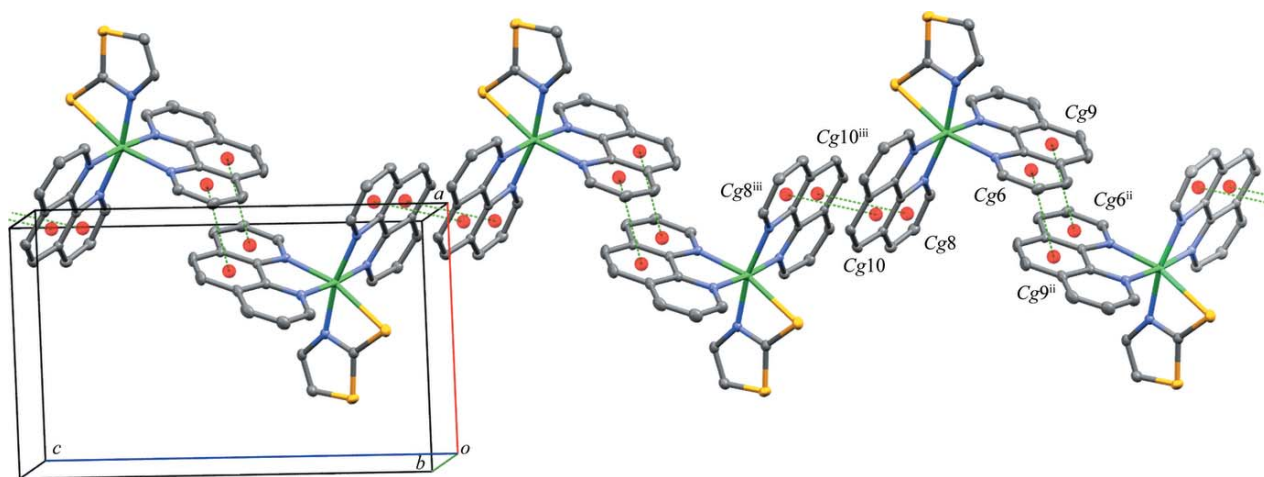
**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ni1–N1	2.0524 (16)	Ni1–N2	2.0780 (15)
Ni1–N5	2.0668 (15)	Ni1–N3	2.0890 (15)
Ni1–N4	2.0735 (15)	Ni1–S1	2.5871 (5)
N5–Ni1–N4	80.54 (6)	N1–Ni1–S1	67.71 (4)
N2–Ni1–N3	79.90 (6)		

ecules of crystallization (one located about a centre of inversion), as shown in Fig. 1. The nickel(II) atom exhibits a considerably distorted octahedral  $\text{N}_5\text{S}$  coordination environment, which is constructed from one bidentate tzS and two bidentate phen ligands whereby the tzS ligand chelates to the  $\text{Ni}^{\text{II}}$  atom through the thiazolyl N and thiolate S atoms. Selected bond lengths and angles are gathered in Table 1. These values are very similar to that of related Ni complexes with bidentate 2-mercaptobenzothiazolate ligands (Raper *et al.*, 1990b; Ballester *et al.*, 1994; Khan *et al.*, 2010). The narrow bite angle involving the tzS ligand (Table 1) is due to formation of a four-membered chelate ring. The averaged Ni–N(phen) distances and bite angles are 2.08  $\text{\AA}$  and  $80.2^\circ$ , which are typical values for Ni–phen complexes (Bouzaid *et al.*, 2012).

## 3. Supramolecular features

In the crystal,  $\pi$ – $\pi$  stacking interactions between phen ligands of adjacent  $[\text{Ni}(\text{tzS})(\text{phen})_2]^+$  exist (Fig. 2). The interactions result in zigzag chains parallel to the  $c$  axis. The distances between the centroids of the rings are 3.8528 (11) for  $\text{Cg}6 \cdots \text{Cg}9^{\text{ii}}$  and  $\text{Cg}9 \cdots \text{Cg}6^{\text{ii}}$ , and 3.6126 (10)  $\text{\AA}$  for  $\text{Cg}8 \cdots \text{Cg}10^{\text{iii}}$  and  $\text{Cg}10 \cdots \text{Cg}8^{\text{iii}}$ , respectively [ $\text{Cg}6$ ,  $\text{Cg}9$ ,  $\text{Cg}8$ , and  $\text{Cg}10$  are the centroids of the N3/C14/C10–C13, C7–C10/C14/C15, N5/C26/C22–C25 and C19–C22/C26/C27 rings, respectively; symmetry codes: (ii)  $2 - x, 1 - y, 1 - z$ ; (iii)  $2 - x, 1 - y, -z$ ]. Such chains in turn are linked by weak C–H $\cdots$ X



**Figure 2**  
The arrangement of the complex cations in the crystal structure, forming zigzag  $\pi$ – $\pi$  stacked chains extending parallel to the  $c$  axis. Green dashed lines represent  $\pi$ – $\pi$  stacking interactions, red spheres represent centroids of the phenyl/pyridyl rings.  $\text{Cg}6$ ,  $\text{Cg}9$ ,  $\text{Cg}8$  and  $\text{Cg}10$  are the centroids of the N3/C14/C10–13, C7–C10/C14/C15, N5/C26/C22–C25 and C19–C22/C26/C27 rings, respectively. [Symmetry codes: (ii)  $2 - x, 1 - y, 1 - z$ ; (iii)  $2 - x, 1 - y, -z$ .]

**Table 2**  
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H1 $\cdots$ O1 <sup>i</sup>	0.95	2.42	3.330 (2)	160
C3—H2 $\cdots$ F6	0.95	2.47	3.074 (2)	122
C4—H3 $\cdots$ O2	0.95	2.51	3.226 (2)	132
C5—H4 $\cdots$ O1	0.95	2.63	3.269 (2)	125
C12—H9 $\cdots$ F4 <sup>ii</sup>	0.95	2.63	3.249 (3)	124
C13—H10 $\cdots$ F6 <sup>ii</sup>	0.95	2.56	3.412 (2)	150
C24—H17 $\cdots$ F1 <sup>iii</sup>	0.95	2.58	3.386 (3)	143
C28—H20 $\cdots$ F3 <sup>iii</sup>	0.99	2.50	3.336 (3)	142
C30—H23 $\cdots$ F1 <sup>iv</sup>	0.99	2.44	3.225 (3)	136

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

( $X = O, F$ ) hydrogen-bonding interactions involving the  $PF_6^-$  counter-anion and 1,4-dioxane solvent molecules, which results in the formation of a sheet structure parallel to the  $ac$  plane (Fig. 3, Table 2).

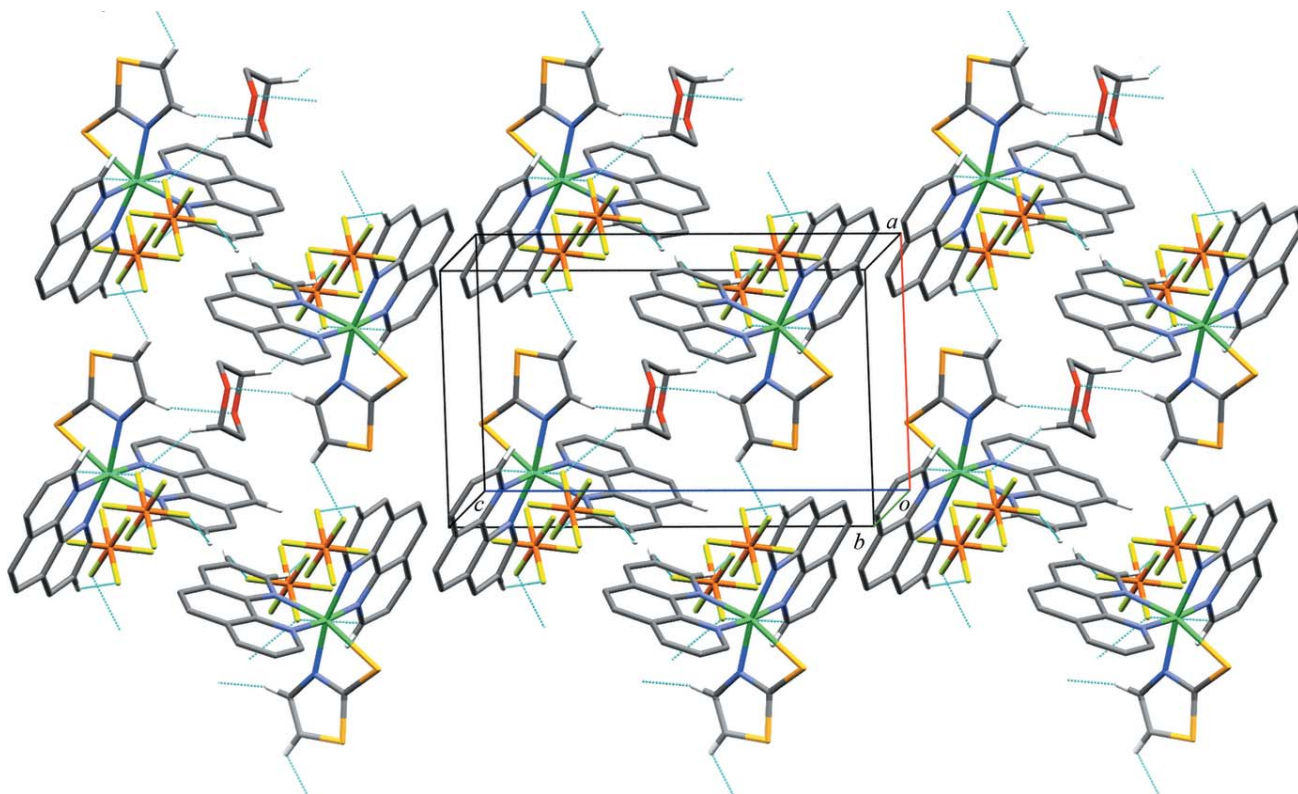
#### 4. Database survey

A search in the Cambridge Structural Database (Groom *et al.*, 2016) reveals four reports of Ni complexes with bidentate 2-mercaptobenzothiazolate ligands. One is a square-planar complex (Banerji *et al.*, 1982), the others being octahedral complexes. Two of them consist of two 2-mercaptobenzothiazolate ligands and another bidentate ligand (Ballester *et al.*, 1994; Khan *et al.*, 2010) whereas the third is a tris-2-

**Table 3**  
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_3H_2NS_2)(C_{12}H_8N_2)_2]PF_6 \cdot 1.5C_4H_8O_2$
$M_r$	812.42
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	110
$a, b, c$ (Å)	9.1800 (2), 12.1460 (2), 14.9005 (3)
$\alpha, \beta, \gamma$ (°)	88.490 (2), 89.166 (2), 83.278 (2)
$V$ (Å <sup>3</sup> )	1649.31 (6)
$Z$	2
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	0.84
Crystal size (mm)	0.27 × 0.24 × 0.16
Data collection	
Diffractometer	Rigaku Saturn 724+ CCD area-detector diffractometer
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku Oxford Diffraction, 2015)
$T_{min}, T_{max}$	0.942, 1.000
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	30580, 9593, 8109
$R_{int}$	0.037
$(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )	0.728
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.041, 0.094, 1.02
No. of reflections	9593
No. of parameters	460
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å <sup>-3</sup> )	1.07, -0.55

Computer programs: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001), *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2016* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2006), *Yadokari-XG* (Kabuto *et al.*, 2009; Wakita, 2001), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).



**Figure 3**  
The sheet structure constructed from chains by  $C-H\cdots X$  ( $X = F, O$ ) hydrogen-bonding interactions (blue dashed lines).

mercaptobenzothiazolate complex (Raper *et al.*, 1990b). In the case of a tzS-Ni complex, one  $\mu_2$ -tzS- $\kappa(N$ , thiolate  $S$ )-Ni<sub>2</sub> complex is reported (Raper *et al.*, 1989).

## 5. Synthesis and crystallization

The title compound was synthesized using [NiCl<sub>2</sub>(phen)], prepared by a literature protocol (Yakhvarov *et al.*, 2007). A mixture of 2-mercaptothiazole ( $8.07 \times 10^{-4}$  mol) and one equivalent of Et<sub>3</sub>N in methanol (10 ml) was added slowly to a solution of [NiCl<sub>2</sub>(phen)] ( $8.07 \times 10^{-4}$  mol) in methanol (20 ml). After stirring overnight, the colour of the solution turned from blue to brown–yellow. 10 equivalents of NH<sub>4</sub>PF<sub>6</sub> were added to the solution, resulting in a pale-brown–yellow precipitate. The precipitate was filtered off and dried *in vacuo*. The crude product containing excess NH<sub>4</sub>PF<sub>6</sub> was purified by recrystallization using 1,4-dioxane vapor diffusion into an acetonitrile solution of the crude product. The title complex was isolated as brown block-like crystals [yield 365 mg, 40.6% (based on Ni)].

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed in calculated positions and refined as riding, with phenyl C–H = 0.95 Å and methylene C–H = 0.99 Å, both with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

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## supporting information

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## Crystal structure of bis(1,10-phenanthroline- $\kappa^2N,N'$ )(1,3-thiazole-2-thiolato- $\kappa^2S^2,N$ )nickel(II) hexafluoridophosphate 1,4-dioxane sesquisolvate

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### Computing details

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); data reduction: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2006) and *Yadokari-XG* (Kabuto *et al.*, 2009; Wakita, 2001); software used to prepare material for publication: *Yadokari-XG* (Kabuto *et al.*, 2009; Wakita, 2001), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

### Bis(1,10-phenanthroline- $\kappa^2N,N'$ )(1,3-thiazole-2-thiolato- $\kappa^2S^2,N$ )nickel(II) hexafluoridophosphate 1,4-dioxane sesquisolvate

#### Crystal data

[Ni(C<sub>3</sub>H<sub>2</sub>NS<sub>2</sub>)(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]PF<sub>6</sub>·1.5C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>

$M_r = 812.42$

Triclinic,  $P\bar{1}$

$a = 9.1800$  (2) Å

$b = 12.1460$  (2) Å

$c = 14.9005$  (3) Å

$\alpha = 88.490$  (2)°

$\beta = 89.166$  (2)°

$\gamma = 83.278$  (2)°

$V = 1649.31$  (6) Å<sup>3</sup>

$Z = 2$

$F(000) = 832$

$D_x = 1.636$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 17089 reflections

$\theta = 2.7\text{--}31.3^\circ$

$\mu = 0.84$  mm<sup>-1</sup>

$T = 110$  K

Block, pale brown

$0.27 \times 0.24 \times 0.16$  mm

#### Data collection

Rigaku Saturn 724+ CCD area-detector diffractometer

$\omega$  scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)

$T_{\min} = 0.942$ ,  $T_{\max} = 1.000$

30580 measured reflections

9593 independent reflections

8109 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 31.1^\circ$ ,  $\theta_{\min} = 2.6^\circ$

$h = -13 \rightarrow 12$

$k = -17 \rightarrow 17$

$l = -21 \rightarrow 21$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.094$

$S = 1.02$

9593 reflections

460 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 1.5145P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.07 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.55 \text{ e } \text{\AA}^{-3}$

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.73044 (2)	0.61812 (2)	0.24062 (2)	0.01241 (6)
S1	0.53398 (5)	0.58427 (4)	0.12496 (3)	0.02027 (10)
S2	0.27542 (5)	0.74630 (4)	0.20072 (3)	0.02077 (10)
N1	0.53418 (17)	0.71330 (13)	0.26332 (10)	0.0156 (3)
N2	0.67416 (17)	0.49693 (12)	0.33146 (10)	0.0149 (3)
N3	0.83585 (16)	0.66322 (12)	0.35503 (10)	0.0141 (3)
N4	0.80703 (16)	0.73517 (12)	0.15381 (10)	0.0135 (3)
N5	0.91276 (17)	0.52383 (12)	0.18870 (10)	0.0145 (3)
C1	0.4540 (2)	0.68055 (15)	0.19814 (12)	0.0168 (3)
C2	0.4575 (2)	0.79119 (15)	0.31651 (12)	0.0163 (3)
H1	0.500491	0.823032	0.365735	0.020*
C3	0.3158 (2)	0.81894 (16)	0.29321 (13)	0.0200 (4)
H2	0.248221	0.870981	0.323482	0.024*
C4	0.5919 (2)	0.41613 (15)	0.31850 (13)	0.0193 (4)
H3	0.556632	0.407017	0.259865	0.023*
C5	0.5550 (2)	0.34380 (16)	0.38736 (14)	0.0233 (4)
H4	0.496199	0.286649	0.375371	0.028*
C6	0.6045 (2)	0.35620 (16)	0.47238 (14)	0.0235 (4)
H5	0.579898	0.307848	0.519931	0.028*
C7	0.6921 (2)	0.44098 (16)	0.48883 (12)	0.0191 (4)
C8	0.7474 (2)	0.46125 (17)	0.57547 (13)	0.0249 (4)
H6	0.726221	0.415078	0.625286	0.030*
C9	0.8292 (2)	0.54520 (18)	0.58738 (13)	0.0254 (4)
H7	0.864927	0.556815	0.645483	0.030*
C10	0.8632 (2)	0.61703 (16)	0.51402 (12)	0.0191 (4)
C11	0.9467 (2)	0.70618 (17)	0.52245 (14)	0.0239 (4)
H8	0.984806	0.721607	0.579105	0.029*
C12	0.9726 (2)	0.77056 (16)	0.44835 (14)	0.0222 (4)
H9	1.029589	0.830557	0.453062	0.027*
C13	0.9142 (2)	0.74704 (15)	0.36545 (13)	0.0178 (4)
H10	0.931415	0.792980	0.314734	0.021*
C14	0.8106 (2)	0.59880 (15)	0.42826 (12)	0.0151 (3)
C15	0.7239 (2)	0.50946 (15)	0.41569 (12)	0.0156 (3)

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C16	0.7508 (2)	0.83886 (15)	0.13609 (12)	0.0169 (3)
H11	0.667891	0.869149	0.169923	0.020*
C17	0.8085 (2)	0.90583 (15)	0.06957 (13)	0.0194 (4)
H12	0.764610	0.979628	0.058505	0.023*
C18	0.9287 (2)	0.86359 (15)	0.02080 (12)	0.0179 (4)
H13	0.968495	0.907501	-0.024998	0.021*
C19	0.9929 (2)	0.75454 (15)	0.03913 (12)	0.0152 (3)
C20	1.1203 (2)	0.70379 (16)	-0.00691 (12)	0.0190 (4)
H14	1.163820	0.744055	-0.053612	0.023*
C21	1.1801 (2)	0.59931 (16)	0.01492 (12)	0.0193 (4)
H15	1.266761	0.568516	-0.015128	0.023*
C22	1.1142 (2)	0.53469 (15)	0.08271 (12)	0.0161 (3)
C23	1.1700 (2)	0.42569 (16)	0.10745 (13)	0.0202 (4)
H16	1.258641	0.392175	0.081252	0.024*
C24	1.0956 (2)	0.36811 (16)	0.16959 (13)	0.0210 (4)
H17	1.131644	0.294102	0.186555	0.025*
C25	0.9656 (2)	0.41942 (15)	0.20793 (12)	0.0178 (4)
H18	0.913046	0.377820	0.249434	0.021*
C26	0.98624 (19)	0.58098 (14)	0.12670 (11)	0.0140 (3)
C27	0.92727 (19)	0.69317 (14)	0.10620 (11)	0.0134 (3)
P1	-0.06216 (5)	1.07671 (4)	0.28379 (3)	0.01764 (10)
F1	0.08571 (15)	1.13260 (13)	0.29517 (10)	0.0407 (4)
F2	-0.07497 (16)	1.12468 (12)	0.18336 (8)	0.0367 (3)
F3	-0.20929 (14)	1.02145 (11)	0.27239 (9)	0.0330 (3)
F4	-0.04921 (18)	1.02975 (13)	0.38455 (9)	0.0462 (4)
F5	-0.15412 (16)	1.18707 (11)	0.31890 (10)	0.0372 (3)
F6	0.02958 (15)	0.96652 (11)	0.24816 (11)	0.0407 (4)
O1	0.46687 (16)	0.11530 (11)	0.48337 (10)	0.0246 (3)
C28	0.6101 (2)	0.05903 (18)	0.46710 (15)	0.0275 (4)
H19	0.684348	0.110335	0.476684	0.033*
H20	0.618213	0.035696	0.403887	0.033*
C29	0.3598 (2)	0.04078 (17)	0.47172 (15)	0.0267 (4)
H21	0.361853	0.017159	0.408583	0.032*
H22	0.260907	0.079038	0.484938	0.032*
O2	0.43879 (16)	0.25330 (12)	0.19127 (10)	0.0258 (3)
C30	0.4199 (2)	0.14818 (19)	0.23091 (14)	0.0279 (5)
H23	0.345190	0.157520	0.279569	0.034*
H24	0.513406	0.114588	0.257485	0.034*
C31	0.3720 (3)	0.07302 (19)	0.16157 (16)	0.0343 (5)
H25	0.358712	0.000165	0.189903	0.041*
H26	0.276598	0.105373	0.136657	0.041*
O3	0.4778 (2)	0.05827 (13)	0.09123 (12)	0.0406 (4)
C32	0.5003 (3)	0.16329 (19)	0.05165 (15)	0.0298 (5)
H27	0.408580	0.197032	0.023020	0.036*
H28	0.577340	0.152711	0.004431	0.036*
C33	0.5455 (2)	0.23982 (19)	0.12063 (15)	0.0275 (4)
H29	0.641539	0.209207	0.145690	0.033*
H30	0.556615	0.312911	0.092026	0.033*

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Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.01357 (11)	0.01267 (11)	0.01108 (11)	-0.00176 (8)	-0.00075 (8)	-0.00039 (8)
S1	0.0239 (2)	0.0193 (2)	0.0174 (2)	-0.00050 (18)	-0.00023 (18)	-0.00451 (17)
S2	0.0155 (2)	0.0246 (2)	0.0219 (2)	-0.00020 (18)	-0.00392 (17)	-0.00288 (18)
N1	0.0160 (7)	0.0166 (7)	0.0140 (7)	-0.0014 (6)	-0.0003 (6)	0.0004 (6)
N2	0.0158 (7)	0.0137 (7)	0.0152 (7)	-0.0014 (6)	0.0007 (6)	-0.0004 (5)
N3	0.0132 (7)	0.0137 (7)	0.0153 (7)	-0.0006 (5)	-0.0018 (5)	-0.0015 (5)
N4	0.0142 (7)	0.0141 (7)	0.0124 (7)	-0.0018 (5)	-0.0019 (5)	-0.0006 (5)
N5	0.0165 (7)	0.0136 (7)	0.0133 (7)	-0.0016 (6)	-0.0016 (6)	-0.0008 (5)
C1	0.0178 (9)	0.0165 (8)	0.0159 (8)	-0.0009 (7)	-0.0001 (7)	-0.0001 (7)
C2	0.0208 (9)	0.0152 (8)	0.0134 (8)	-0.0041 (7)	0.0001 (7)	0.0006 (6)
C3	0.0205 (9)	0.0201 (9)	0.0189 (9)	0.0001 (7)	0.0019 (7)	-0.0026 (7)
C4	0.0216 (9)	0.0160 (9)	0.0209 (9)	-0.0044 (7)	-0.0007 (7)	-0.0009 (7)
C5	0.0263 (10)	0.0153 (9)	0.0288 (10)	-0.0055 (8)	0.0045 (8)	0.0001 (7)
C6	0.0289 (11)	0.0147 (9)	0.0257 (10)	-0.0004 (8)	0.0080 (8)	0.0060 (7)
C7	0.0217 (9)	0.0177 (9)	0.0163 (8)	0.0039 (7)	0.0030 (7)	0.0028 (7)
C8	0.0312 (11)	0.0260 (10)	0.0155 (9)	0.0032 (8)	0.0018 (8)	0.0054 (7)
C9	0.0310 (11)	0.0309 (11)	0.0126 (8)	0.0042 (9)	-0.0036 (8)	-0.0005 (8)
C10	0.0192 (9)	0.0211 (9)	0.0155 (8)	0.0050 (7)	-0.0034 (7)	-0.0032 (7)
C11	0.0233 (10)	0.0272 (10)	0.0206 (9)	0.0021 (8)	-0.0081 (8)	-0.0086 (8)
C12	0.0196 (9)	0.0196 (9)	0.0278 (10)	-0.0021 (7)	-0.0057 (8)	-0.0074 (8)
C13	0.0174 (9)	0.0151 (8)	0.0209 (9)	-0.0014 (7)	-0.0016 (7)	-0.0021 (7)
C14	0.0158 (8)	0.0149 (8)	0.0136 (8)	0.0032 (6)	-0.0009 (6)	-0.0022 (6)
C15	0.0171 (9)	0.0137 (8)	0.0153 (8)	0.0005 (7)	0.0008 (7)	-0.0003 (6)
C16	0.0172 (9)	0.0146 (8)	0.0184 (8)	0.0005 (7)	-0.0003 (7)	-0.0016 (7)
C17	0.0234 (10)	0.0142 (8)	0.0203 (9)	-0.0009 (7)	-0.0023 (7)	0.0020 (7)
C18	0.0219 (9)	0.0174 (9)	0.0151 (8)	-0.0052 (7)	-0.0009 (7)	0.0022 (7)
C19	0.0161 (8)	0.0177 (8)	0.0125 (8)	-0.0039 (7)	-0.0023 (6)	-0.0008 (6)
C20	0.0180 (9)	0.0244 (9)	0.0152 (8)	-0.0046 (7)	0.0023 (7)	-0.0005 (7)
C21	0.0164 (9)	0.0240 (9)	0.0173 (9)	-0.0013 (7)	0.0023 (7)	-0.0043 (7)
C22	0.0162 (8)	0.0175 (8)	0.0148 (8)	-0.0011 (7)	-0.0020 (7)	-0.0031 (6)
C23	0.0173 (9)	0.0194 (9)	0.0229 (9)	0.0036 (7)	-0.0021 (7)	-0.0061 (7)
C24	0.0235 (10)	0.0151 (8)	0.0233 (9)	0.0030 (7)	-0.0049 (8)	-0.0014 (7)
C25	0.0213 (9)	0.0154 (8)	0.0168 (8)	-0.0019 (7)	-0.0039 (7)	-0.0005 (7)
C26	0.0138 (8)	0.0142 (8)	0.0138 (8)	-0.0005 (6)	-0.0032 (6)	-0.0017 (6)
C27	0.0143 (8)	0.0142 (8)	0.0119 (7)	-0.0019 (6)	-0.0032 (6)	-0.0010 (6)
P1	0.0179 (2)	0.0176 (2)	0.0175 (2)	-0.00266 (18)	-0.00070 (18)	0.00178 (17)
F1	0.0282 (7)	0.0550 (9)	0.0433 (8)	-0.0218 (7)	0.0021 (6)	-0.0075 (7)
F2	0.0479 (9)	0.0412 (8)	0.0197 (6)	-0.0024 (7)	-0.0003 (6)	0.0089 (6)
F3	0.0254 (7)	0.0397 (8)	0.0370 (7)	-0.0140 (6)	0.0059 (5)	-0.0143 (6)
F4	0.0601 (10)	0.0546 (10)	0.0254 (7)	-0.0157 (8)	-0.0099 (7)	0.0166 (7)
F5	0.0406 (8)	0.0258 (7)	0.0450 (8)	-0.0014 (6)	0.0112 (6)	-0.0130 (6)
F6	0.0302 (7)	0.0273 (7)	0.0615 (10)	0.0095 (6)	0.0039 (7)	-0.0039 (7)
O1	0.0298 (8)	0.0153 (7)	0.0285 (8)	-0.0022 (6)	0.0013 (6)	-0.0007 (6)
C28	0.0279 (11)	0.0232 (10)	0.0314 (11)	-0.0048 (8)	0.0076 (9)	0.0008 (8)
C29	0.0253 (11)	0.0221 (10)	0.0325 (11)	-0.0013 (8)	-0.0005 (9)	-0.0006 (8)



O2	0.0232 (7)	0.0280 (8)	0.0265 (7)	-0.0036 (6)	0.0015 (6)	-0.0043 (6)
C30	0.0207 (10)	0.0383 (12)	0.0241 (10)	-0.0018 (9)	-0.0007 (8)	0.0059 (9)
C31	0.0444 (14)	0.0247 (11)	0.0345 (12)	-0.0083 (10)	0.0017 (10)	0.0040 (9)
O3	0.0588 (12)	0.0220 (8)	0.0392 (10)	0.0015 (8)	0.0122 (8)	-0.0051 (7)
C32	0.0342 (12)	0.0316 (12)	0.0231 (10)	-0.0022 (9)	0.0043 (9)	-0.0001 (9)
C33	0.0198 (10)	0.0352 (12)	0.0279 (11)	-0.0059 (9)	0.0011 (8)	0.0020 (9)

*Geometric parameters (Å, °)*

Ni1—N1	2.0524 (16)	C17—H12	0.9500
Ni1—N5	2.0668 (15)	C18—C19	1.407 (3)
Ni1—N4	2.0735 (15)	C18—H13	0.9500
Ni1—N2	2.0780 (15)	C19—C27	1.402 (2)
Ni1—N3	2.0890 (15)	C19—C20	1.432 (3)
Ni1—S1	2.5871 (5)	C20—C21	1.355 (3)
S1—C1	1.7143 (19)	C20—H14	0.9500
S2—C3	1.724 (2)	C21—C22	1.433 (3)
S2—C1	1.7377 (19)	C21—H15	0.9500
N1—C1	1.324 (2)	C22—C26	1.403 (2)
N1—C2	1.373 (2)	C22—C23	1.404 (3)
N2—C4	1.326 (2)	C23—C24	1.368 (3)
N2—C15	1.360 (2)	C23—H16	0.9500
N3—C13	1.327 (2)	C24—C25	1.401 (3)
N3—C14	1.359 (2)	C24—H17	0.9500
N4—C16	1.325 (2)	C25—H18	0.9500
N4—C27	1.359 (2)	C26—C27	1.433 (2)
N5—C25	1.329 (2)	P1—F3	1.5901 (13)
N5—C26	1.359 (2)	P1—F2	1.5925 (13)
C2—C3	1.353 (3)	P1—F4	1.5929 (14)
C2—H1	0.9500	P1—F5	1.5944 (14)
C3—H2	0.9500	P1—F6	1.5946 (14)
C4—C5	1.397 (3)	P1—F1	1.6002 (14)
C4—H3	0.9500	O1—C29	1.427 (2)
C5—C6	1.370 (3)	O1—C28	1.430 (3)
C5—H4	0.9500	C28—C29 <sup>i</sup>	1.499 (3)
C6—C7	1.407 (3)	C28—H19	0.9900
C6—H5	0.9500	C28—H20	0.9900
C7—C15	1.402 (2)	C29—H21	0.9900
C7—C8	1.431 (3)	C29—H22	0.9900
C8—C9	1.352 (3)	O2—C30	1.421 (3)
C8—H6	0.9500	O2—C33	1.427 (3)
C9—C10	1.434 (3)	C30—C31	1.500 (3)
C9—H7	0.9500	C30—H23	0.9900
C10—C14	1.405 (2)	C30—H24	0.9900
C10—C11	1.407 (3)	C31—O3	1.419 (3)
C11—C12	1.370 (3)	C31—H25	0.9900
C11—H8	0.9500	C31—H26	0.9900
C12—C13	1.403 (3)	O3—C32	1.427 (3)

C12—H9	0.9500	C32—C33	1.498 (3)
C13—H10	0.9500	C32—H27	0.9900
C14—C15	1.436 (2)	C32—H28	0.9900
C16—C17	1.403 (3)	C33—H29	0.9900
C16—H11	0.9500	C33—H30	0.9900
C17—C18	1.369 (3)		
N1—Ni1—N5	167.32 (6)	C17—C18—H13	120.3
N1—Ni1—N4	93.43 (6)	C19—C18—H13	120.3
N5—Ni1—N4	80.54 (6)	C27—C19—C18	117.60 (17)
N1—Ni1—N2	91.11 (6)	C27—C19—C20	118.87 (17)
N5—Ni1—N2	95.58 (6)	C18—C19—C20	123.53 (17)
N4—Ni1—N2	174.56 (6)	C21—C20—C19	121.19 (17)
N1—Ni1—N3	96.71 (6)	C21—C20—H14	119.4
N5—Ni1—N3	95.07 (6)	C19—C20—H14	119.4
N4—Ni1—N3	96.57 (6)	C20—C21—C22	120.89 (17)
N2—Ni1—N3	79.90 (6)	C20—C21—H15	119.6
N1—Ni1—S1	67.71 (4)	C22—C21—H15	119.6
N5—Ni1—S1	100.94 (4)	C26—C22—C23	117.41 (17)
N4—Ni1—S1	89.91 (4)	C26—C22—C21	119.09 (17)
N2—Ni1—S1	94.59 (4)	C23—C22—C21	123.49 (17)
N3—Ni1—S1	163.53 (4)	C24—C23—C22	119.49 (18)
C1—S1—Ni1	72.66 (6)	C24—C23—H16	120.3
C3—S2—C1	90.25 (9)	C22—C23—H16	120.3
C1—N1—C2	112.89 (16)	C23—C24—C25	119.32 (18)
C1—N1—Ni1	100.84 (12)	C23—C24—H17	120.3
C2—N1—Ni1	146.25 (13)	C25—C24—H17	120.3
C4—N2—C15	118.14 (16)	N5—C25—C24	122.78 (18)
C4—N2—Ni1	128.68 (13)	N5—C25—H18	118.6
C15—N2—Ni1	113.07 (12)	C24—C25—H18	118.6
C13—N3—C14	118.13 (16)	N5—C26—C22	122.98 (16)
C13—N3—Ni1	129.09 (13)	N5—C26—C27	117.26 (16)
C14—N3—Ni1	112.67 (11)	C22—C26—C27	119.76 (16)
C16—N4—C27	118.16 (15)	N4—C27—C19	122.76 (16)
C16—N4—Ni1	129.33 (13)	N4—C27—C26	117.15 (15)
C27—N4—Ni1	112.38 (11)	C19—C27—C26	120.09 (16)
C25—N5—C26	117.93 (16)	F3—P1—F2	90.17 (8)
C25—N5—Ni1	129.51 (13)	F3—P1—F4	90.13 (8)
C26—N5—Ni1	112.56 (11)	F2—P1—F4	179.51 (9)
N1—C1—S1	118.78 (14)	F3—P1—F5	90.39 (8)
N1—C1—S2	111.99 (14)	F2—P1—F5	90.13 (8)
S1—C1—S2	129.24 (11)	F4—P1—F5	89.48 (9)
C3—C2—N1	114.64 (17)	F3—P1—F6	89.55 (8)
C3—C2—H1	122.7	F2—P1—F6	89.58 (8)
N1—C2—H1	122.7	F4—P1—F6	90.81 (9)
C2—C3—S2	110.23 (14)	F5—P1—F6	179.70 (9)
C2—C3—H2	124.9	F3—P1—F1	179.86 (10)
S2—C3—H2	124.9	F2—P1—F1	89.74 (8)

N2—C4—C5	122.83 (18)	F4—P1—F1	89.96 (8)
N2—C4—H3	118.6	F5—P1—F1	89.50 (8)
C5—C4—H3	118.6	F6—P1—F1	90.56 (8)
C6—C5—C4	119.28 (18)	C29—O1—C28	109.56 (15)
C6—C5—H4	120.4	O1—C28—C29 <sup>i</sup>	111.04 (17)
C4—C5—H4	120.4	O1—C28—H19	109.4
C5—C6—C7	119.59 (18)	C29 <sup>i</sup> —C28—H19	109.4
C5—C6—H5	120.2	O1—C28—H20	109.4
C7—C6—H5	120.2	C29 <sup>i</sup> —C28—H20	109.4
C15—C7—C6	117.20 (18)	H19—C28—H20	108.0
C15—C7—C8	119.17 (18)	O1—C29—C28 <sup>i</sup>	110.46 (18)
C6—C7—C8	123.63 (18)	O1—C29—H21	109.6
C9—C8—C7	120.92 (18)	C28 <sup>i</sup> —C29—H21	109.6
C9—C8—H6	119.5	O1—C29—H22	109.6
C7—C8—H6	119.5	C28 <sup>i</sup> —C29—H22	109.6
C8—C9—C10	121.29 (18)	H21—C29—H22	108.1
C8—C9—H7	119.4	C30—O2—C33	109.66 (16)
C10—C9—H7	119.4	O2—C30—C31	110.18 (17)
C14—C10—C11	117.21 (18)	O2—C30—H23	109.6
C14—C10—C9	118.94 (18)	C31—C30—H23	109.6
C11—C10—C9	123.85 (18)	O2—C30—H24	109.6
C12—C11—C10	119.52 (18)	C31—C30—H24	109.6
C12—C11—H8	120.2	H23—C30—H24	108.1
C10—C11—H8	120.2	O3—C31—C30	110.5 (2)
C11—C12—C13	119.36 (18)	O3—C31—H25	109.5
C11—C12—H9	120.3	C30—C31—H25	109.5
C13—C12—H9	120.3	O3—C31—H26	109.5
N3—C13—C12	122.67 (18)	C30—C31—H26	109.5
N3—C13—H10	118.7	H25—C31—H26	108.1
C12—C13—H10	118.7	C31—O3—C32	109.84 (17)
N3—C14—C10	123.10 (17)	O3—C32—C33	111.09 (18)
N3—C14—C15	117.20 (15)	O3—C32—H27	109.4
C10—C14—C15	119.70 (17)	C33—C32—H27	109.4
N2—C15—C7	122.97 (17)	O3—C32—H28	109.4
N2—C15—C14	117.04 (16)	C33—C32—H28	109.4
C7—C15—C14	119.99 (17)	H27—C32—H28	108.0
N4—C16—C17	122.88 (17)	O2—C33—C32	110.56 (17)
N4—C16—H11	118.6	O2—C33—H29	109.5
C17—C16—H11	118.6	C32—C33—H29	109.5
C18—C17—C16	119.20 (17)	O2—C33—H30	109.5
C18—C17—H12	120.4	C32—C33—H30	109.5
C16—C17—H12	120.4	H29—C33—H30	108.1
C17—C18—C19	119.37 (17)		
C2—N1—C1—S1	179.41 (13)	N3—C14—C15—C7	-179.09 (16)
Ni1—N1—C1—S1	-1.39 (16)	C10—C14—C15—C7	0.0 (3)
C2—N1—C1—S2	-0.3 (2)	C27—N4—C16—C17	1.2 (3)
Ni1—N1—C1—S2	178.89 (9)	Ni1—N4—C16—C17	-174.37 (14)

Ni1—S1—C1—N1	1.14 (13)	N4—C16—C17—C18	-0.5 (3)
Ni1—S1—C1—S2	-179.20 (15)	C16—C17—C18—C19	-0.8 (3)
C3—S2—C1—N1	0.03 (15)	C17—C18—C19—C27	1.3 (3)
C3—S2—C1—S1	-179.65 (14)	C17—C18—C19—C20	-178.73 (18)
C1—N1—C2—C3	0.5 (2)	C27—C19—C20—C21	-1.8 (3)
Ni1—N1—C2—C3	-178.06 (17)	C18—C19—C20—C21	178.29 (18)
N1—C2—C3—S2	-0.5 (2)	C19—C20—C21—C22	2.3 (3)
C1—S2—C3—C2	0.25 (15)	C20—C21—C22—C26	0.0 (3)
C15—N2—C4—C5	-0.1 (3)	C20—C21—C22—C23	179.21 (18)
Ni1—N2—C4—C5	-175.92 (14)	C26—C22—C23—C24	2.7 (3)
N2—C4—C5—C6	0.3 (3)	C21—C22—C23—C24	-176.58 (18)
C4—C5—C6—C7	-0.3 (3)	C22—C23—C24—C25	-0.5 (3)
C5—C6—C7—C15	0.2 (3)	C26—N5—C25—C24	2.4 (3)
C5—C6—C7—C8	179.18 (19)	Ni1—N5—C25—C24	-176.95 (13)
C15—C7—C8—C9	0.0 (3)	C23—C24—C25—N5	-2.2 (3)
C6—C7—C8—C9	-179.0 (2)	C25—N5—C26—C22	0.0 (3)
C7—C8—C9—C10	0.2 (3)	Ni1—N5—C26—C22	179.44 (13)
C8—C9—C10—C14	-0.4 (3)	C25—N5—C26—C27	179.54 (15)
C8—C9—C10—C11	179.5 (2)	Ni1—N5—C26—C27	-1.01 (19)
C14—C10—C11—C12	0.2 (3)	C23—C22—C26—N5	-2.5 (3)
C9—C10—C11—C12	-179.65 (19)	C21—C22—C26—N5	176.79 (16)
C10—C11—C12—C13	0.6 (3)	C23—C22—C26—C27	177.96 (16)
C14—N3—C13—C12	0.7 (3)	C21—C22—C26—C27	-2.8 (3)
Ni1—N3—C13—C12	176.59 (14)	C16—N4—C27—C19	-0.5 (2)
C11—C12—C13—N3	-1.1 (3)	Ni1—N4—C27—C19	175.75 (13)
C13—N3—C14—C10	0.1 (3)	C16—N4—C27—C26	179.86 (15)
Ni1—N3—C14—C10	-176.42 (14)	Ni1—N4—C27—C26	-3.88 (19)
C13—N3—C14—C15	179.19 (16)	C18—C19—C27—N4	-0.7 (3)
Ni1—N3—C14—C15	2.7 (2)	C20—C19—C27—N4	179.34 (16)
C11—C10—C14—N3	-0.5 (3)	C18—C19—C27—C26	178.90 (16)
C9—C10—C14—N3	179.28 (17)	C20—C19—C27—C26	-1.0 (2)
C11—C10—C14—C15	-179.60 (17)	N5—C26—C27—N4	3.4 (2)
C9—C10—C14—C15	0.2 (3)	C22—C26—C27—N4	-177.08 (15)
C4—N2—C15—C7	0.0 (3)	N5—C26—C27—C19	-176.28 (15)
Ni1—N2—C15—C7	176.42 (14)	C22—C26—C27—C19	3.3 (2)
C4—N2—C15—C14	-178.94 (16)	C29—O1—C28—C29 <sup>i</sup>	-57.7 (2)
Ni1—N2—C15—C14	-2.5 (2)	C28—O1—C29—C28 <sup>i</sup>	57.4 (2)
C6—C7—C15—N2	0.0 (3)	C33—O2—C30—C31	-58.8 (2)
C8—C7—C15—N2	-179.08 (17)	O2—C30—C31—O3	59.4 (2)
C6—C7—C15—C14	178.90 (17)	C30—C31—O3—C32	-57.7 (3)
C8—C7—C15—C14	-0.2 (3)	C31—O3—C32—C33	56.7 (3)
N3—C14—C15—N2	-0.1 (2)	C30—O2—C33—C32	57.7 (2)
C10—C14—C15—N2	179.01 (16)	O3—C32—C33—O2	-57.0 (2)

Symmetry code: (i)  $-x+1, -y, -z+1$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H1...O1 <sup>ii</sup>	0.95	2.42	3.330 (2)	160
C3—H2...F6	0.95	2.47	3.074 (2)	122
C4—H3...O2	0.95	2.51	3.226 (2)	132
C5—H4...O1	0.95	2.63	3.269 (2)	125
C12—H9...F4 <sup>iii</sup>	0.95	2.63	3.249 (3)	124
C13—H10...F6 <sup>iii</sup>	0.95	2.56	3.412 (2)	150
C24—H17...F1 <sup>iv</sup>	0.95	2.58	3.386 (3)	143
C28—H20...F3 <sup>iv</sup>	0.99	2.50	3.336 (3)	142
C30—H23...F1 <sup>v</sup>	0.99	2.44	3.225 (3)	136

Symmetry codes: (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $x+1, y, z$ ; (iv)  $x+1, y-1, z$ ; (v)  $x, y-1, z$ .