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Bis{2,6-bis[(*E*)-(4-fluorobenzylimino)methyl]-pyridine}nickel(II) dinitrate dihydrate

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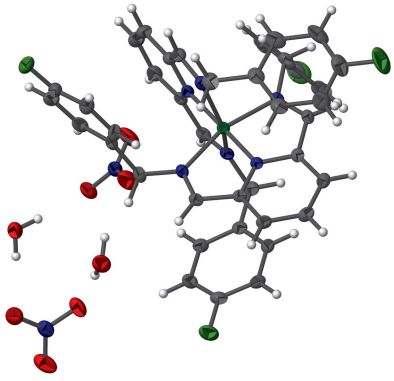
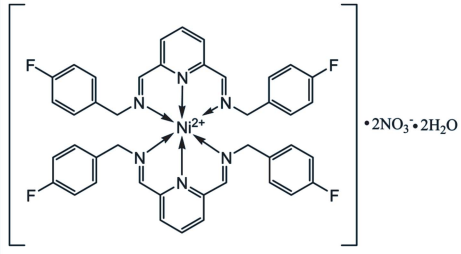
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydrated salt, $[Ni(C_{21}H_{17}F_2N_3)_2](NO_3)_2\cdot 2H_2O$, the central Ni^{II} ion is coordinated by six N atoms from two tridentate chelating 2,6-bis[(*E*)-(4-fluorobenzylimino)methyl]pyridine ligands. While the central Ni^{II} ion is six-coordinate, its environment is distorted from an octahedral structure because of the unequal Ni—N distances. The Ni—N bond lengths vary from 1.8642 (14) to 2.2131 (15) Å, while the N—Ni—N angles range from 79.98 (6) to 104.44 (6)°. Three coordinating sites of each chelating agent are almost coplanar with respect to the pyridine ring, and two pyridine moieties are perpendicular to each other. Two non-coordinating nitrate anions within the asymmetric unit balance the charges of the central metal ion, and are linked with two crystal water molecules, forming a water–nitrate cyclic tetrameric unit [O···O = 2.813 (2) to 3.062 (2) Å]. In an isolated molecule, the fluorophenyl rings of one ligand are stacked with the central ring of the other ligand *via* π–π interactions, with the closest centroid-to-plane distances being 3.359 (6), 3.408 (5), 3.757 (6) and 3.659 (5) Å.

3D view



Chemical scheme



Structure description

Schiff bases containing molecular clefts with multiple donor atoms are attractive chelating ligands in the area of coordination chemistry. The incorporation of transition-metal ions within the Schiff base-derived molecular frameworks can make them potentially useful in a number of biomedical allocations (Chaudhary & Guragain, 2019). Because of the excellent chelating properties of Schiff bases derived from multidentate ligands, they are widely used to coordinate transition-metal ions (Guerriero *et al.*, 1992; Vigato & Tamburini, 2004; Gupta & Sutar, 2008; da Silva *et al.*, 2011). Such complexes

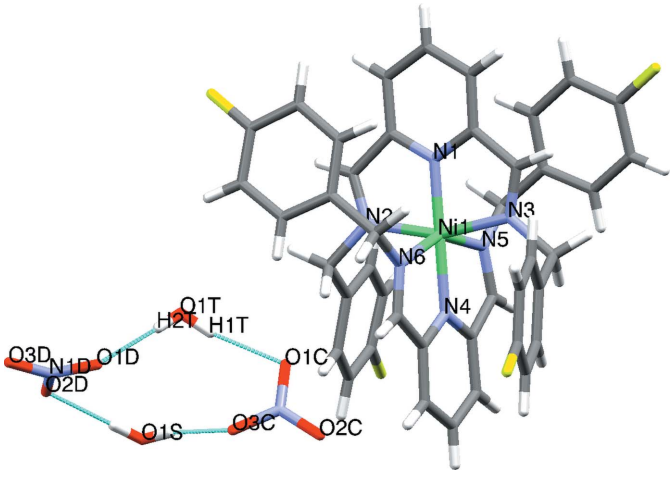


Figure 1
Asymmetric unit of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level; O—H···O hydrogen bonds are shown as light-blue lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1S—H1S···O3C	0.83 (2)	2.00 (2)	2.814 (2)	167 (3)
O1S—H2S···O2D	0.86 (2)	1.96 (2)	2.813 (2)	174 (3)
O1T—H1T···O1C	0.87 (2)	2.03 (2)	2.876 (2)	166 (3)
O1T—H2T···O1D	0.85 (2)	2.21 (2)	3.062 (2)	178 (3)
C2—H2···O3C^{i}	0.95	2.41	3.303 (2)	157
C4—H4···O1S^{ii}	0.95	2.40	3.185 (2)	140
C13—H13···F1^{iii}	0.95	2.39	3.240 (3)	149
C14—H14···O1S^{i}	0.95	2.33	3.227 (2)	158
C15—H15B···O1D^{iv}	0.99	2.55	3.487 (2)	158
C18—H18···F3^{v}	0.95	2.48	3.373 (3)	156
C23—H23···O2C	0.95	2.45	3.239 (3)	140
C27—H27···O3C^{iv}	0.95	2.41	3.343 (2)	166
C28—H28A···O2D^{ii}	0.99	2.56	3.540 (3)	171
C33—H33···F4^{vi}	0.95	2.47	3.320 (3)	150
C35—H35···F3^{vii}	0.95	2.52	3.302 (2)	140

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

have been extensively used in many chemical, biochemical and analytical and antimicrobial applications. Consequently, understanding the structural aspects of Schiff base-derived metal complexes could provide useful information to predict their applications (Skyrianou *et al.*, 2010). Herein we report the crystal structure of an Ni^{II} complex with a Schiff base, bis{2,6-bis[(*E*)-(4-fluorobenzylimino)methyl]pyridine}-nickel(II) dinitrate dihydrate.

The asymmetric unit of the title compound contains one Ni^{II} ion, two 2,6-bis[(*E*)-(4-fluorobenzylimino)methyl]pyridine ligands, two nitrate anions and two water molecules. While the central Ni ion is six-coordinate (Fig. 1), the environment is considerably distorted from an octahedral structure because of the unequal Ni—N bond lengths. The Ni—N bond lengths involving the pyridine rings range from 1.8647 (17) to 2.2131 (18) Å. The coordination sphere of Ni in this N-containing environment is, in comparison with other structures (Matthews *et al.*, 2017; Basaran *et al.*, 2015), in fact unusual. Such a distortion is rather characteristic for Cu^{II} or Mn^{III} complexes (Salaudeen *et al.*, 2008; Halcrow, 2013). However, chemical analysis unambiguously confirmed the presence of Ni^{II} in the title salt. The N—Ni—N angles range from 80.00 (7) to 104.44 (7)°. Three coordinating nitrogen atoms and the pyridine ring (r.m.s. deviation = 0.004 Å) of each chelating group are nearly co-planar, with a dihedral angle of 3.14 (2)°. Two pyridine rings (r.m.s. deviation = 0.004 Å) are almost perpendicular to each other, with a dihedral angle of 89.53 (4)°, and coordinate to the metal ion through nitrogen atoms, as seen in a closely related nickel(II) complex (Basaran *et al.*, 2015).

Two nitrate anions within the asymmetric unit, that are located outside the coordination sphere to balance the charges of the central metal ion, are hydrogen-bonded with two crystal water molecules *via* four hydrogen bonds [O···O = 2.811 (3)–3.061 (3) Å; Table 1], forming an isolated anion–water unit with an $R_4^4(12)$ graph-set motif. In an isolated cationic complex molecule, two fluorophenyl rings of one ligand sandwich the pyridine ring of the other ligand *via* π–π interactions, with the closest centroid-to-plane distances being 3.359 (6), 3.408 (5), 3.757 (6) and 3.659 (5) Å. Charge-assisted C—H···O interactions between the cationic complexes and the nitrate anions as well as C—H···F interactions between adjacent cationic complexes lead to the formation of a three-dimensional network structure. Fig. 2 shows a packing plot, displaying the hydrogen-bonded anionic units together with the packing of the molecules in the unit cell.

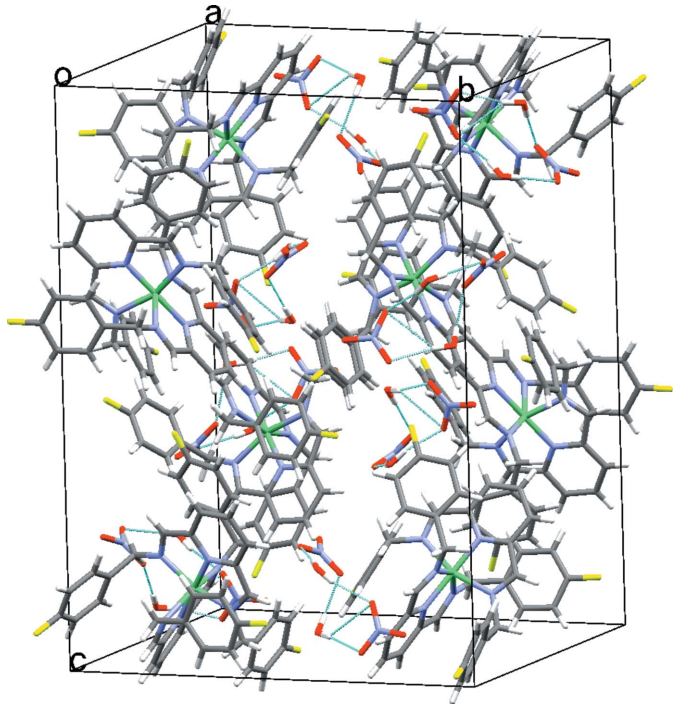


Figure 2
Crystal packing of the title compound showing hydrogen-bonded anionic units (light-blue lines) together with the packing of the molecules in the unit cell, as viewed approximately along the *a* axis. For clarity, C—H···O and C—H···F hydrogen bonds are not shown.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{21}H_{17}F_2N_3)_2](NO_3)_2·2H_2O$
M_r	917.51
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	100
a, *b*, *c* (Å)	17.0353 (13), 18.7759 (14), 25.4659 (18)
V (Å^3)	8145.3 (10)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.56
Crystal size (mm)	0.52 × 0.40 × 0.24
Data collection	
Diffractometer	Bruker *APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.685, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	161343, 8675, 7462
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.109, 1.01
No. of reflections	8675
No. of parameters	580
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.69

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

Synthesis and crystallization

The synthesis of the Schiff base was performed following the method reported previously (Basaran *et al.*, 2015). In a typical reaction, 2,6-diformylpyridine (1.85 mmol) and 4-fluorobenzylamine (3.70 mmol) were mixed in 20 ml of methanol, and the mixture was left overnight with constant stirring at room temperature. The solvent was evaporated to provide a colourless powder. Yield: 90%. ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.51 (*s*, 2H, imine proton), 8.09 (*d*, 2H, *J* = 10 Hz, py—H), 7.81 (*t*, 1H, *J* = 10 Hz, py—H), 7.32 (*m*, *J* = 5 Hz, 4H, Bn—H), 7.04 (*t*, *J* = 5 Hz, 4H, Bn—H), 4.85 (*s*, 4H, NCH_2). ^{13}C NMR (125 MHz, $CDCl_3$,): δ 163.04 (Bn—*C*), 162.45 (two py-*C*), 161.09 (Bn—*C*), 154.13 (two imine-*C*), 137.21 (py—*C*H), 134.26 (Bn—*C*) 134.24 (Bn—*C*), 129.76 (two Bn—*C*H), 129.70 (two Bn—*C*H), 122.65 (two py—*C*H), 115.49 (two Bn—*C*H), 115.32 (two Bn—*C*H), 64.14 (two *C*H_2). ESI-MS: *m*/*z* (+) 350.21 $[M + H]^+$. Analysis calculated for $C_{21}H_{17}F_2N_3$: C, 72.19; H, 4.90; N, 12.03. Found: C, 72.25; H, 4.92; N, 12.05.

The nickel complex was synthesized from the reaction of the ligand with 0.5 equiv. of nickel(II) nitrate in water. Single crystals suitable for X-ray analysis were obtained from the slow evaporation of the complex dissolved in water after two weeks. Analysis calculated for $C_{42}H_{34}F_4N_6Ni(NO_3)_2(H_2O)_2$; C, 54.98; H, 4.17; N, 12.21; Ni, 6.40. Found: C, 54.82; H, 4.21; N, 12.27; Ni, 6.34. Elemental analysis of C, H and N was carried out using an ECS 4010 Analytical Platform (Costech Instrument). The Ni^{II} ion was quantitatively determined from gravimetric analysis of the complex using dimethylglyoxime, confirming the presence of nickel(II) in the complex (Minster, 1946).

Refinement

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

Funding information

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References

Basaran, I., Rhaman, M. M., Powell, D. R. & Hossain, M. A. (2015). *Acta Cryst.* E**71**, m226–m227.
Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Chaudhary, N. K. & Guragain, B. (2019). *Asian J. Chem.* **31**, 951–959.
Guerriero, P., Vigato, P. A., Fenton, D. E. & Hellier, P. C. (1992). *Acta Chem. Scand.* **46**, 1025–1046.
Gupta, K. C. & Sutar, A. K. (2008). *Coord. Chem. Rev.* **252**, 1420–1450.
Halcrow, M. A. (2013). *Chem. Soc. Rev.* **42**, 1784–1795.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, https://doi.org/10.1107/S1600576719014092
Matthews, M., Sendzik, M., Bruggeman, A., Kearns, C., Oliver, A. G. & Babbini, D. C. (2017). *Acta Cryst.* E**73**, 1167–1171.
Minster, J. T. (1946). *Analyst*, **71**, 424–428.
Salaudeen, A. A., Kilner, C. A. & Halcrow, M. A. (2008). *Chem. Commun.* pp. 5200–5202.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Silva, C. M. da, da Silva, D. L., Modolo, L. V., Alves, R. B., de Resende, M. A., Martins, C. V. B. & de Fátima, A. (2011). *J. Adv. Res.* **2**, 1–8.
Skyrianou, K. C., Perdih, F., Turel, I., Kessissoglou, D. P. & Psomas, G. (2010). *J. Inorg. Biochem.* **104**, 161–170.
Vigato, P. A. & Tamburini, S. (2004). *Coord. Chem. Rev.* **248**, 1717–2128.

full crystallographic data

IUCrData (2019). **4**, x191688 [https://doi.org/10.1107/S2414314619016882]

Bis{2,6-bis[(*E*)-(4-fluorobenzylimino)methyl]pyridine}nickel(II) dinitrate dihydrate

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Bis{2,6-bis[(*E*)-(4-fluorobenzylimino)methyl]pyridine}nickel(II) dinitrate dihydrate

Crystal data

$[Ni(C_{21}H_{17}F_2N_3)_2](NO_3)_2·2H_2O$
M_r = 917.51
Orthorhombic, *Pbca*
a = 17.0353 (13) Å
b = 18.7759 (14) Å
c = 25.4659 (18) Å
V = 8145.3 (10) Å^3
Z = 8
F(000) = 3792
D_x = 1.496 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9364 reflections
θ = 2.3–26.7°
μ = 0.56 mm^{-1}
T = 100 K
Block, bluish_black
0.52 × 0.40 × 0.24 mm

Data collection

Bruker APEX CCD diffractometer
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.685, T_{max} = 0.745
161343 measured reflections
8675 independent reflections
7462 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.8°, θ_{min} = 1.6°
h = −21→21
k = −23→23
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.109
S = 1.01
8675 reflections
580 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 7.1P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 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. The H atoms of the water molecules were located from a difference Fourier map and were refined with distance restraints (O—H = 0.85 (2) Å) and with U_{iso}(H) = 1.2U_{eq}(O).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.56405 (2)	0.28869 (2)	0.64363 (2)	0.01841 (8)
F1	0.63434 (12)	0.22324 (10)	0.89733 (6)	0.0683 (5)
F2	0.36925 (9)	−0.03240 (7)	0.57727 (6)	0.0470 (4)
F3	0.89670 (8)	0.41647 (8)	0.50480 (5)	0.0438 (3)
F4	0.31167 (8)	0.55522 (6)	0.61596 (5)	0.0392 (3)
N1	0.52019 (8)	0.34183 (7)	0.69806 (5)	0.0170 (3)
N2	0.55829 (8)	0.38380 (8)	0.60935 (6)	0.0187 (3)
N3	0.55104 (9)	0.21275 (7)	0.69753 (6)	0.0184 (3)
N4	0.61183 (9)	0.23418 (8)	0.58681 (6)	0.0190 (3)
N5	0.69087 (9)	0.29623 (8)	0.66063 (6)	0.0212 (3)
N6	0.46197 (9)	0.25163 (8)	0.59733 (6)	0.0201 (3)
C1	0.49857 (10)	0.30917 (9)	0.74283 (7)	0.0194 (3)
C2	0.46540 (11)	0.34686 (10)	0.78416 (7)	0.0232 (4)
H2	0.449286	0.323263	0.815346	0.028*
C3	0.45641 (11)	0.42011 (10)	0.77864 (8)	0.0254 (4)
H3	0.434032	0.447191	0.806363	0.030*
C4	0.48008 (11)	0.45384 (10)	0.73265 (7)	0.0231 (4)
H4	0.475052	0.503976	0.728884	0.028*
C5	0.51122 (10)	0.41274 (9)	0.69232 (7)	0.0191 (3)
C6	0.53341 (10)	0.43430 (9)	0.63923 (7)	0.0206 (3)
H6	0.529733	0.482243	0.627570	0.025*
C7	0.57583 (11)	0.40007 (10)	0.55444 (7)	0.0234 (4)
H7A	0.554387	0.447612	0.545665	0.028*
H7AB	0.549607	0.364625	0.531617	0.028*
C8	0.66288 (11)	0.39936 (9)	0.54347 (7)	0.0227 (4)
C9	0.71632 (12)	0.42861 (10)	0.57875 (7)	0.0260 (4)
H9	0.698114	0.446061	0.611577	0.031*
C10	0.79573 (12)	0.43276 (11)	0.56685 (8)	0.0302 (4)
H10	0.832377	0.451112	0.591503	0.036*
C11	0.81964 (13)	0.40936 (11)	0.51810 (8)	0.0321 (4)
C12	0.76922 (13)	0.38008 (11)	0.48242 (8)	0.0338 (5)
H12	0.787768	0.364129	0.449264	0.041*
C13	0.69037 (13)	0.37403 (10)	0.49549 (7)	0.0288 (4)
H13	0.654907	0.352446	0.471504	0.035*
C14	0.51882 (10)	0.23369 (9)	0.74059 (7)	0.0203 (3)
H14	0.508897	0.202136	0.768985	0.024*
C15	0.57673 (11)	0.13819 (9)	0.69424 (7)	0.0218 (4)
H15A	0.580371	0.117940	0.730054	0.026*
H15B	0.629590	0.136110	0.678154	0.026*
C16	0.52024 (11)	0.09422 (9)	0.66190 (7)	0.0213 (4)
C17	0.54625 (12)	0.05882 (10)	0.61703 (7)	0.0254 (4)
H17	0.599182	0.064108	0.605950	0.030*

C18	0.49532 (14)	0.01572 (11)	0.58828 (8)	0.0326 (5)
H18	0.512802	−0.008752	0.557796	0.039*
C19	0.41938 (14)	0.00969 (11)	0.60527 (8)	0.0330 (5)
C20	0.39085 (13)	0.04347 (11)	0.64916 (8)	0.0318 (4)
H20	0.337693	0.037982	0.659681	0.038*
C21	0.44252 (11)	0.08608 (10)	0.67776 (8)	0.0253 (4)
H21	0.424493	0.109822	0.708410	0.030*
C22	0.56689 (11)	0.20617 (9)	0.54884 (7)	0.0206 (4)
C23	0.59935 (13)	0.16824 (10)	0.50687 (7)	0.0278 (4)
H23	0.566872	0.149833	0.479749	0.033*
C24	0.67990 (13)	0.15809 (11)	0.50567 (8)	0.0327 (4)
H24	0.703320	0.131766	0.477934	0.039*
C25	0.72610 (12)	0.18666 (11)	0.54530 (8)	0.0297 (4)
H25	0.781380	0.180018	0.545100	0.036*
C26	0.69029 (11)	0.22510 (10)	0.58523 (7)	0.0229 (4)
C27	0.73211 (11)	0.26043 (10)	0.62806 (7)	0.0245 (4)
H27	0.787498	0.256930	0.631529	0.029*
C28	0.73112 (11)	0.33406 (11)	0.70322 (8)	0.0283 (4)
H28A	0.718569	0.385485	0.701435	0.034*
H28B	0.788617	0.328482	0.699332	0.034*
C29	0.70543 (11)	0.30453 (11)	0.75535 (7)	0.0264 (4)
C30	0.66522 (11)	0.34672 (11)	0.79102 (8)	0.0285 (4)
H30	0.654053	0.394904	0.782425	0.034*
C31	0.64102 (13)	0.31965 (13)	0.83910 (8)	0.0368 (5)
H31	0.613410	0.348573	0.863511	0.044*
C32	0.65816 (16)	0.24988 (15)	0.85031 (8)	0.0434 (6)
C33	0.69808 (16)	0.20601 (12)	0.81624 (9)	0.0423 (6)
H33	0.708871	0.157882	0.825219	0.051*
C34	0.72215 (13)	0.23395 (11)	0.76841 (8)	0.0339 (5)
H34	0.750222	0.204811	0.744382	0.041*
C35	0.48277 (11)	0.21748 (9)	0.55641 (7)	0.0218 (4)
H35	0.445293	0.200148	0.531924	0.026*
C36	0.37800 (11)	0.26274 (10)	0.60653 (8)	0.0272 (4)
H36A	0.362563	0.239761	0.639955	0.033*
H36B	0.347472	0.240427	0.577827	0.033*
C37	0.35948 (10)	0.34148 (10)	0.60900 (7)	0.0217 (4)
C38	0.36431 (11)	0.38280 (10)	0.56371 (7)	0.0238 (4)
H38	0.378772	0.361272	0.531371	0.029*
C39	0.34813 (12)	0.45525 (11)	0.56546 (8)	0.0278 (4)
H39	0.351257	0.483902	0.534786	0.033*
C40	0.32736 (11)	0.48422 (10)	0.61331 (8)	0.0265 (4)
C41	0.32144 (11)	0.44549 (11)	0.65888 (7)	0.0257 (4)
H41	0.306529	0.467281	0.691036	0.031*
C42	0.33817 (10)	0.37303 (10)	0.65607 (7)	0.0242 (4)
H42	0.334916	0.344751	0.686930	0.029*
N1C	0.44870 (10)	0.25225 (9)	0.41568 (6)	0.0270 (3)
O1C	0.45857 (12)	0.29359 (9)	0.45374 (6)	0.0453 (4)
O2C	0.46221 (11)	0.18737 (8)	0.41992 (7)	0.0447 (4)

O3C	0.42413 (9)	0.27623 (8)	0.37264 (6)	0.0321 (3)
N1D	0.26557 (10)	0.46087 (9)	0.30779 (7)	0.0300 (4)
O1D	0.26571 (9)	0.41323 (8)	0.34230 (6)	0.0378 (4)
O2D	0.33011 (10)	0.48588 (9)	0.29188 (8)	0.0479 (4)
O3D	0.20287 (10)	0.48652 (9)	0.29197 (8)	0.0516 (5)
O1S	0.45995 (11)	0.39752 (8)	0.31231 (6)	0.0382 (4)
H1S	0.4519 (16)	0.3656 (12)	0.3342 (10)	0.046*
H2S	0.4180 (12)	0.4219 (14)	0.3062 (11)	0.046*
O1T	0.38587 (10)	0.42834 (8)	0.43101 (6)	0.0362 (3)
H1T	0.4134 (15)	0.3897 (11)	0.4336 (11)	0.043*
H2T	0.3526 (14)	0.4229 (15)	0.4063 (9)	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01987 (13)	0.01626 (13)	0.01908 (13)	−0.00008 (8)	−0.00018 (8)	−0.00037 (8)
F1	0.0980 (14)	0.0766 (12)	0.0303 (8)	0.0026 (10)	−0.0023 (8)	0.0246 (7)
F2	0.0559 (9)	0.0391 (7)	0.0459 (8)	−0.0122 (6)	−0.0231 (7)	−0.0091 (6)
F3	0.0330 (7)	0.0560 (8)	0.0424 (7)	0.0115 (6)	0.0156 (6)	0.0121 (6)
F4	0.0540 (8)	0.0238 (6)	0.0398 (7)	0.0121 (6)	0.0005 (6)	−0.0013 (5)
N1	0.0158 (7)	0.0162 (7)	0.0192 (7)	−0.0009 (5)	−0.0010 (5)	−0.0005 (5)
N2	0.0188 (7)	0.0176 (7)	0.0198 (7)	−0.0030 (5)	−0.0022 (5)	0.0023 (6)
N3	0.0191 (7)	0.0154 (7)	0.0208 (7)	−0.0018 (5)	−0.0031 (6)	0.0006 (5)
N4	0.0214 (7)	0.0168 (7)	0.0188 (7)	0.0015 (6)	0.0001 (6)	0.0017 (5)
N5	0.0210 (7)	0.0206 (7)	0.0221 (7)	−0.0027 (6)	−0.0023 (6)	0.0023 (6)
N6	0.0208 (7)	0.0149 (7)	0.0245 (7)	−0.0001 (5)	−0.0021 (6)	0.0017 (6)
C1	0.0174 (8)	0.0209 (8)	0.0197 (8)	−0.0033 (6)	−0.0016 (6)	−0.0002 (6)
C2	0.0212 (9)	0.0267 (9)	0.0216 (8)	−0.0028 (7)	0.0011 (7)	−0.0017 (7)
C3	0.0236 (9)	0.0262 (9)	0.0264 (9)	0.0005 (7)	0.0022 (7)	−0.0083 (7)
C4	0.0224 (9)	0.0175 (8)	0.0295 (9)	0.0001 (7)	0.0006 (7)	−0.0037 (7)
C5	0.0174 (8)	0.0159 (8)	0.0241 (8)	−0.0011 (6)	−0.0015 (6)	−0.0017 (6)
C6	0.0199 (8)	0.0163 (8)	0.0256 (9)	−0.0015 (6)	−0.0031 (7)	0.0015 (6)
C7	0.0296 (9)	0.0220 (9)	0.0185 (8)	−0.0037 (7)	−0.0023 (7)	0.0025 (7)
C8	0.0307 (10)	0.0177 (8)	0.0197 (8)	−0.0009 (7)	0.0020 (7)	0.0034 (6)
C9	0.0314 (10)	0.0268 (9)	0.0200 (8)	−0.0045 (8)	0.0051 (7)	−0.0020 (7)
C10	0.0301 (10)	0.0312 (10)	0.0293 (10)	−0.0035 (8)	0.0029 (8)	0.0008 (8)
C11	0.0322 (10)	0.0316 (10)	0.0325 (10)	0.0078 (8)	0.0103 (8)	0.0100 (8)
C12	0.0449 (12)	0.0317 (10)	0.0249 (9)	0.0152 (9)	0.0068 (9)	0.0010 (8)
C13	0.0428 (11)	0.0220 (9)	0.0215 (9)	0.0071 (8)	−0.0025 (8)	−0.0014 (7)
C14	0.0209 (8)	0.0202 (8)	0.0199 (8)	−0.0031 (7)	−0.0015 (7)	0.0029 (6)
C15	0.0240 (9)	0.0159 (8)	0.0256 (9)	0.0006 (7)	−0.0048 (7)	0.0014 (7)
C16	0.0274 (9)	0.0139 (8)	0.0225 (8)	0.0019 (7)	−0.0052 (7)	0.0033 (6)
C17	0.0339 (10)	0.0184 (8)	0.0238 (9)	0.0022 (7)	−0.0019 (8)	0.0018 (7)
C18	0.0483 (13)	0.0261 (10)	0.0235 (9)	0.0021 (9)	−0.0068 (9)	−0.0030 (8)
C19	0.0446 (12)	0.0232 (9)	0.0311 (10)	−0.0057 (9)	−0.0172 (9)	−0.0006 (8)
C20	0.0286 (10)	0.0280 (10)	0.0386 (11)	−0.0048 (8)	−0.0073 (8)	0.0019 (8)
C21	0.0287 (10)	0.0217 (9)	0.0255 (9)	0.0001 (7)	−0.0026 (7)	−0.0009 (7)
C22	0.0271 (9)	0.0160 (8)	0.0187 (8)	0.0015 (6)	−0.0014 (7)	0.0018 (6)

C23	0.0390 (11)	0.0251 (9)	0.0193 (8)	0.0039 (8)	−0.0010 (8)	−0.0027 (7)
C24	0.0405 (11)	0.0324 (10)	0.0252 (9)	0.0093 (9)	0.0063 (8)	−0.0041 (8)
C25	0.0279 (10)	0.0318 (10)	0.0295 (10)	0.0097 (8)	0.0056 (8)	0.0018 (8)
C26	0.0236 (9)	0.0221 (9)	0.0230 (9)	0.0038 (7)	0.0017 (7)	0.0034 (7)
C27	0.0186 (8)	0.0268 (9)	0.0282 (9)	−0.0003 (7)	−0.0002 (7)	0.0037 (8)
C28	0.0251 (9)	0.0291 (10)	0.0305 (10)	−0.0076 (8)	−0.0063 (8)	−0.0007 (8)
C29	0.0240 (9)	0.0286 (9)	0.0266 (9)	−0.0048 (8)	−0.0109 (7)	0.0004 (7)
C30	0.0259 (9)	0.0308 (10)	0.0288 (9)	−0.0017 (8)	−0.0106 (8)	−0.0005 (8)
C31	0.0357 (11)	0.0479 (13)	0.0267 (10)	0.0013 (10)	−0.0089 (9)	0.0008 (9)
C32	0.0529 (14)	0.0521 (14)	0.0251 (10)	−0.0053 (12)	−0.0098 (10)	0.0112 (10)
C33	0.0570 (15)	0.0335 (11)	0.0364 (12)	0.0013 (10)	−0.0194 (11)	0.0101 (9)
C34	0.0395 (12)	0.0301 (11)	0.0320 (10)	0.0000 (9)	−0.0144 (9)	−0.0023 (8)
C35	0.0266 (9)	0.0171 (8)	0.0218 (8)	−0.0007 (7)	−0.0055 (7)	0.0007 (6)
C36	0.0203 (9)	0.0218 (9)	0.0396 (11)	−0.0035 (7)	0.0007 (8)	−0.0007 (8)
C37	0.0135 (8)	0.0225 (9)	0.0292 (9)	−0.0017 (6)	−0.0029 (7)	−0.0005 (7)
C38	0.0230 (9)	0.0253 (9)	0.0232 (8)	0.0023 (7)	−0.0039 (7)	−0.0031 (7)
C39	0.0313 (10)	0.0284 (10)	0.0238 (9)	0.0047 (8)	−0.0032 (8)	0.0039 (7)
C40	0.0252 (9)	0.0221 (9)	0.0322 (10)	0.0053 (7)	−0.0030 (8)	−0.0024 (7)
C41	0.0209 (9)	0.0313 (10)	0.0249 (9)	0.0057 (7)	0.0002 (7)	−0.0028 (7)
C42	0.0176 (8)	0.0291 (9)	0.0259 (9)	0.0006 (7)	0.0022 (7)	0.0045 (7)
N1C	0.0274 (8)	0.0300 (9)	0.0235 (8)	0.0027 (7)	−0.0005 (6)	0.0046 (6)
O1C	0.0702 (12)	0.0405 (9)	0.0253 (8)	0.0120 (8)	−0.0079 (8)	−0.0044 (6)
O2C	0.0649 (11)	0.0270 (8)	0.0423 (9)	0.0016 (8)	−0.0131 (8)	0.0090 (7)
O3C	0.0400 (8)	0.0296 (7)	0.0268 (7)	0.0021 (6)	−0.0073 (6)	0.0058 (6)
N1D	0.0323 (9)	0.0223 (8)	0.0354 (9)	−0.0052 (7)	−0.0031 (7)	0.0030 (7)
O1D	0.0388 (9)	0.0341 (8)	0.0406 (8)	−0.0086 (7)	−0.0068 (7)	0.0143 (7)
O2D	0.0354 (9)	0.0420 (9)	0.0664 (12)	0.0028 (7)	0.0134 (8)	0.0209 (8)
O3D	0.0333 (9)	0.0421 (9)	0.0795 (13)	−0.0073 (7)	−0.0176 (9)	0.0244 (9)
O1S	0.0492 (10)	0.0299 (8)	0.0353 (8)	0.0083 (7)	0.0144 (7)	0.0072 (6)
O1T	0.0434 (9)	0.0305 (8)	0.0346 (8)	0.0024 (7)	−0.0015 (7)	−0.0018 (6)

Geometric parameters (Å, º)

Ni1—N1	1.8642 (14)	C18—C19	1.369 (3)
Ni1—N4	1.9503 (15)	C18—H18	0.9500
Ni1—N2	1.9901 (15)	C19—C20	1.374 (3)
Ni1—N3	1.9916 (15)	C20—C21	1.395 (3)
Ni1—N5	2.2079 (16)	C20—H20	0.9500
Ni1—N6	2.2131 (15)	C21—H21	0.9500
F1—C32	1.360 (3)	C22—C23	1.398 (3)
F2—C19	1.365 (2)	C22—C35	1.461 (3)
F3—C11	1.362 (2)	C23—C24	1.386 (3)
F4—C40	1.361 (2)	C23—H23	0.9500
N1—C1	1.346 (2)	C24—C25	1.388 (3)
N1—C5	1.348 (2)	C24—H24	0.9500
N2—C6	1.287 (2)	C25—C26	1.388 (3)
N2—C7	1.462 (2)	C25—H25	0.9500
N3—C14	1.288 (2)	C26—C27	1.462 (3)

N3—C15	1.469 (2)	C27—H27	0.9500
N4—C22	1.341 (2)	C28—C29	1.504 (3)
N4—C26	1.348 (2)	C28—H28A	0.9900
N5—C27	1.278 (3)	C28—H28B	0.9900
N5—C28	1.467 (2)	C29—C30	1.386 (3)
N6—C35	1.274 (2)	C29—C34	1.396 (3)
N6—C36	1.464 (2)	C30—C31	1.388 (3)
C1—C2	1.388 (2)	C30—H30	0.9500
C1—C14	1.460 (2)	C31—C32	1.372 (4)
C2—C3	1.391 (3)	C31—H31	0.9500
C2—H2	0.9500	C32—C33	1.376 (4)
C3—C4	1.391 (3)	C33—C34	1.388 (3)
C3—H3	0.9500	C33—H33	0.9500
C4—C5	1.390 (2)	C34—H34	0.9500
C4—H4	0.9500	C35—H35	0.9500
C5—C6	1.461 (2)	C36—C37	1.513 (3)
C6—H6	0.9500	C36—H36A	0.9900
C7—C8	1.509 (3)	C36—H36B	0.9900
C7—H7A	0.9900	C37—C42	1.386 (3)
C7—H7AB	0.9900	C37—C38	1.392 (3)
C8—C9	1.392 (3)	C38—C39	1.389 (3)
C8—C13	1.392 (3)	C38—H38	0.9500
C9—C10	1.388 (3)	C39—C40	1.380 (3)
C9—H9	0.9500	C39—H39	0.9500
C10—C11	1.379 (3)	C40—C41	1.373 (3)
C10—H10	0.9500	C41—C42	1.392 (3)
C11—C12	1.366 (3)	C41—H41	0.9500
C12—C13	1.388 (3)	C42—H42	0.9500
C12—H12	0.9500	N1C—O2C	1.244 (2)
C13—H13	0.9500	N1C—O1C	1.253 (2)
C14—H14	0.9500	N1C—O3C	1.257 (2)
C15—C16	1.512 (2)	N1D—O3D	1.239 (2)
C15—H15A	0.9900	N1D—O1D	1.254 (2)
C15—H15B	0.9900	N1D—O2D	1.262 (2)
C16—C21	1.392 (3)	O1S—H1S	0.830 (17)
C16—C17	1.394 (3)	O1S—H2S	0.862 (17)
C17—C18	1.394 (3)	O1T—H1T	0.867 (17)
C17—H17	0.9500	O1T—H2T	0.853 (17)

N1—Ni1—N4	178.87 (6)	C19—C18—C17	118.05 (19)
N1—Ni1—N2	79.98 (6)	C19—C18—H18	121.0
N4—Ni1—N2	99.56 (6)	C17—C18—H18	121.0
N1—Ni1—N3	79.99 (6)	F2—C19—C18	118.3 (2)
N4—Ni1—N3	100.49 (6)	F2—C19—C20	118.1 (2)
N2—Ni1—N3	159.92 (6)	C18—C19—C20	123.59 (19)
N1—Ni1—N5	102.24 (6)	C19—C20—C21	117.8 (2)
N4—Ni1—N5	76.75 (6)	C19—C20—H20	121.1
N2—Ni1—N5	94.40 (6)	C21—C20—H20	121.1

N3—Ni1—N5	91.12 (6)	C16—C21—C20	120.77 (19)
N1—Ni1—N6	104.44 (6)	C16—C21—H21	119.6
N4—Ni1—N6	76.57 (6)	C20—C21—H21	119.6
N2—Ni1—N6	90.56 (6)	N4—C22—C23	121.68 (17)
N3—Ni1—N6	93.13 (6)	N4—C22—C35	114.07 (16)
N5—Ni1—N6	153.31 (6)	C23—C22—C35	124.23 (17)
C1—N1—C5	120.71 (15)	C24—C23—C22	118.58 (18)
C1—N1—Ni1	119.71 (12)	C24—C23—H23	120.7
C5—N1—Ni1	119.58 (12)	C22—C23—H23	120.7
C6—N2—C7	118.60 (15)	C23—C24—C25	119.51 (18)
C6—N2—Ni1	114.70 (12)	C23—C24—H24	120.2
C7—N2—Ni1	126.64 (12)	C25—C24—H24	120.2
C14—N3—C15	117.80 (15)	C24—C25—C26	118.98 (19)
C14—N3—Ni1	114.56 (12)	C24—C25—H25	120.5
C15—N3—Ni1	127.58 (12)	C26—C25—H25	120.5
C22—N4—C26	119.67 (15)	N4—C26—C25	121.55 (18)
C22—N4—Ni1	120.17 (12)	N4—C26—C27	113.79 (16)
C26—N4—Ni1	120.16 (12)	C25—C26—C27	124.64 (18)
C27—N5—C28	118.53 (16)	N5—C27—C26	117.07 (17)
C27—N5—Ni1	112.14 (12)	N5—C27—H27	121.5
C28—N5—Ni1	129.31 (12)	C26—C27—H27	121.5
C35—N6—C36	118.31 (16)	N5—C28—C29	109.76 (15)
C35—N6—Ni1	112.05 (12)	N5—C28—H28A	109.7
C36—N6—Ni1	129.61 (12)	C29—C28—H28A	109.7
N1—C1—C2	121.42 (16)	N5—C28—H28B	109.7
N1—C1—C14	110.15 (15)	C29—C28—H28B	109.7
C2—C1—C14	128.36 (16)	H28A—C28—H28B	108.2
C1—C2—C3	118.17 (17)	C30—C29—C34	119.16 (19)
C1—C2—H2	120.9	C30—C29—C28	120.77 (18)
C3—C2—H2	120.9	C34—C29—C28	120.07 (19)
C2—C3—C4	120.22 (17)	C29—C30—C31	121.0 (2)
C2—C3—H3	119.9	C29—C30—H30	119.5
C4—C3—H3	119.9	C31—C30—H30	119.5
C5—C4—C3	118.67 (17)	C32—C31—C30	118.0 (2)
C5—C4—H4	120.7	C32—C31—H31	121.0
C3—C4—H4	120.7	C30—C31—H31	121.0
N1—C5—C4	120.77 (16)	F1—C32—C31	118.1 (2)
N1—C5—C6	110.15 (15)	F1—C32—C33	118.8 (2)
C4—C5—C6	128.96 (16)	C31—C32—C33	123.1 (2)
N2—C6—C5	115.35 (15)	C32—C33—C34	118.2 (2)
N2—C6—H6	122.3	C32—C33—H33	120.9
C5—C6—H6	122.3	C34—C33—H33	120.9
N2—C7—C8	112.08 (15)	C33—C34—C29	120.5 (2)
N2—C7—H7A	109.2	C33—C34—H34	119.7
C8—C7—H7A	109.2	C29—C34—H34	119.7
N2—C7—H7AB	109.2	N6—C35—C22	116.99 (16)
C8—C7—H7AB	109.2	N6—C35—H35	121.5
H7A—C7—H7AB	107.9	C22—C35—H35	121.5

C9—C8—C13	118.76 (18)	N6—C36—C37	110.46 (14)
C9—C8—C7	121.31 (16)	N6—C36—H36A	109.6
C13—C8—C7	119.74 (17)	C37—C36—H36A	109.6
C10—C9—C8	121.23 (18)	N6—C36—H36B	109.6
C10—C9—H9	119.4	C37—C36—H36B	109.6
C8—C9—H9	119.4	H36A—C36—H36B	108.1
C11—C10—C9	117.80 (19)	C42—C37—C38	119.60 (17)
C11—C10—H10	121.1	C42—C37—C36	120.55 (17)
C9—C10—H10	121.1	C38—C37—C36	119.85 (17)
F3—C11—C12	118.69 (19)	C39—C38—C37	120.50 (17)
F3—C11—C10	118.5 (2)	C39—C38—H38	119.8
C12—C11—C10	122.8 (2)	C37—C38—H38	119.8
C11—C12—C13	118.80 (18)	C40—C39—C38	117.72 (18)
C11—C12—H12	120.6	C40—C39—H39	121.1
C13—C12—H12	120.6	C38—C39—H39	121.1
C12—C13—C8	120.53 (19)	F4—C40—C41	117.54 (17)
C12—C13—H13	119.7	F4—C40—C39	118.68 (17)
C8—C13—H13	119.7	C41—C40—C39	123.78 (18)
N3—C14—C1	115.50 (15)	C40—C41—C42	117.34 (17)
N3—C14—H14	122.3	C40—C41—H41	121.3
C1—C14—H14	122.3	C42—C41—H41	121.3
N3—C15—C16	111.20 (14)	C37—C42—C41	121.06 (17)
N3—C15—H15A	109.4	C37—C42—H42	119.5
C16—C15—H15A	109.4	C41—C42—H42	119.5
N3—C15—H15B	109.4	O2C—N1C—O1C	120.96 (16)
C16—C15—H15B	109.4	O2C—N1C—O3C	119.22 (17)
H15A—C15—H15B	108.0	O1C—N1C—O3C	119.82 (17)
C21—C16—C17	119.18 (17)	O3D—N1D—O1D	120.45 (18)
C21—C16—C15	120.47 (17)	O3D—N1D—O2D	120.13 (17)
C17—C16—C15	120.29 (17)	O1D—N1D—O2D	119.25 (17)
C16—C17—C18	120.61 (19)	H1S—O1S—H2S	112 (3)
C16—C17—H17	119.7	H1T—O1T—H2T	108 (3)
C18—C17—H17	119.7		

N2—Ni1—N1—C1	175.88 (14)	C18—C19—C20—C21	−0.1 (3)
N3—Ni1—N1—C1	−2.77 (13)	C17—C16—C21—C20	−0.4 (3)
N5—Ni1—N1—C1	−91.74 (13)	C15—C16—C21—C20	−177.62 (17)
N6—Ni1—N1—C1	87.91 (13)	C19—C20—C21—C16	0.4 (3)
N2—Ni1—N1—C5	−4.79 (13)	C26—N4—C22—C23	−0.9 (3)
N3—Ni1—N1—C5	176.56 (14)	Ni1—N4—C22—C23	178.46 (13)
N5—Ni1—N1—C5	87.59 (13)	C26—N4—C22—C35	177.66 (15)
N6—Ni1—N1—C5	−92.76 (13)	Ni1—N4—C22—C35	−3.0 (2)
C5—N1—C1—C2	1.0 (3)	N4—C22—C23—C24	1.7 (3)
Ni1—N1—C1—C2	−179.72 (13)	C35—C22—C23—C24	−176.63 (18)
C5—N1—C1—C14	−176.35 (15)	C22—C23—C24—C25	−1.2 (3)
Ni1—N1—C1—C14	2.98 (19)	C23—C24—C25—C26	−0.2 (3)
N1—C1—C2—C3	−1.3 (3)	C22—N4—C26—C25	−0.6 (3)
C14—C1—C2—C3	175.45 (17)	Ni1—N4—C26—C25	−179.93 (14)

C1—C2—C3—C4	0.2 (3)	C22—N4—C26—C27	178.07 (15)
C2—C3—C4—C5	1.2 (3)	Ni1—N4—C26—C27	−1.3 (2)
C1—N1—C5—C4	0.6 (2)	C24—C25—C26—N4	1.2 (3)
Ni1—N1—C5—C4	−178.77 (13)	C24—C25—C26—C27	−177.37 (18)
C1—N1—C5—C6	−175.78 (15)	C28—N5—C27—C26	−178.27 (16)
Ni1—N1—C5—C6	4.90 (19)	Ni1—N5—C27—C26	3.0 (2)
C3—C4—C5—N1	−1.6 (3)	N4—C26—C27—N5	−1.4 (2)
C3—C4—C5—C6	173.93 (18)	C25—C26—C27—N5	177.20 (18)
C7—N2—C6—C5	175.30 (15)	C27—N5—C28—C29	−117.17 (19)
Ni1—N2—C6—C5	−2.03 (19)	Ni1—N5—C28—C29	61.3 (2)
N1—C5—C6—N2	−1.6 (2)	N5—C28—C29—C30	−116.22 (19)
C4—C5—C6—N2	−177.54 (17)	N5—C28—C29—C34	64.0 (2)
C6—N2—C7—C8	108.60 (18)	C34—C29—C30—C31	−0.5 (3)
Ni1—N2—C7—C8	−74.43 (18)	C28—C29—C30—C31	179.69 (18)
N2—C7—C8—C9	−41.1 (2)	C29—C30—C31—C32	0.1 (3)
N2—C7—C8—C13	143.91 (17)	C30—C31—C32—F1	−179.8 (2)
C13—C8—C9—C10	0.0 (3)	C30—C31—C32—C33	0.1 (4)
C7—C8—C9—C10	−175.08 (18)	F1—C32—C33—C34	−179.9 (2)
C8—C9—C10—C11	2.4 (3)	C31—C32—C33—C34	0.2 (4)
C9—C10—C11—F3	176.66 (18)	C32—C33—C34—C29	−0.6 (3)
C9—C10—C11—C12	−2.6 (3)	C30—C29—C34—C33	0.7 (3)
F3—C11—C12—C13	−178.77 (18)	C28—C29—C34—C33	−179.43 (19)
C10—C11—C12—C13	0.5 (3)	C36—N6—C35—C22	−178.93 (15)
C11—C12—C13—C8	1.9 (3)	Ni1—N6—C35—C22	2.81 (19)
C9—C8—C13—C12	−2.2 (3)	N4—C22—C35—N6	−0.2 (2)
C7—C8—C13—C12	172.98 (17)	C23—C22—C35—N6	178.24 (17)
C15—N3—C14—C1	176.60 (14)	C35—N6—C36—C37	−120.46 (18)
Ni1—N3—C14—C1	−0.9 (2)	Ni1—N6—C36—C37	57.4 (2)
N1—C1—C14—N3	−1.2 (2)	N6—C36—C37—C42	−110.12 (19)
C2—C1—C14—N3	−178.26 (17)	N6—C36—C37—C38	69.5 (2)
C14—N3—C15—C16	103.36 (19)	C42—C37—C38—C39	0.2 (3)
Ni1—N3—C15—C16	−79.53 (18)	C36—C37—C38—C39	−179.45 (17)
N3—C15—C16—C21	−61.9 (2)	C37—C38—C39—C40	0.0 (3)
N3—C15—C16—C17	120.90 (18)	C38—C39—C40—F4	179.65 (17)
C21—C16—C17—C18	0.0 (3)	C38—C39—C40—C41	−0.4 (3)
C15—C16—C17—C18	177.22 (17)	F4—C40—C41—C42	−179.48 (17)
C16—C17—C18—C19	0.4 (3)	C39—C40—C41—C42	0.5 (3)
C17—C18—C19—F2	179.97 (17)	C38—C37—C42—C41	0.0 (3)
C17—C18—C19—C20	−0.3 (3)	C36—C37—C42—C41	179.63 (17)
F2—C19—C20—C21	179.65 (18)	C40—C41—C42—C37	−0.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*S*—H1*S*···O3*C*	0.83 (2)	2.00 (2)	2.814 (2)	167 (3)
O1*S*—H2*S*···O2*D*	0.86 (2)	1.96 (2)	2.813 (2)	174 (3)
O1*T*—H1*T*···O1*C*	0.87 (2)	2.03 (2)	2.876 (2)	166 (3)
O1*T*—H2*T*···O1*D*	0.85 (2)	2.21 (2)	3.062 (2)	178 (3)

C2—H2···O3*C*^{i}	0.95	2.41	3.303 (2)	157
C4—H4···O1*S*^{ii}	0.95	2.40	3.185 (2)	140
C13—H13···F1^{iii}	0.95	2.39	3.240 (3)	149
C14—H14···O1*S*^{i}	0.95	2.33	3.227 (2)	158
C15—H15*B*···O1*D*^{iv}	0.99	2.55	3.487 (2)	158
C18—H18···F3^{v}	0.95	2.48	3.373 (3)	156
C23—H23···O2*C*	0.95	2.45	3.239 (3)	140
C27—H27···O3*C*^{iv}	0.95	2.41	3.343 (2)	166
C28—H28*A*···O2*D*^{ii}	0.99	2.56	3.540 (3)	171
C33—H33···F4^{vi}	0.95	2.47	3.320 (3)	150
C35—H35···F3^{vii}	0.95	2.52	3.302 (2)	140

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) $-x+1$, $-y+1$, $-z+1$; (iii) x, $-y+1/2$, $z-1/2$; (iv) $x+1/2$, $-y+1/2$, $-z+1$; (v) $-x+3/2$, $y-1/2$, z; (vi) $-x+1$, $y-1/2$, $-z+3/2$; (vii) $x-1/2$, $-y+1/2$, $-z+1$.