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trans-Bis{2-[bis(1*H*-pyrazol-1-yl)methyl]-1-methyl-1*H*-benzimidazole}iron(II) bis(perchlorate) acetonitrile disolvate

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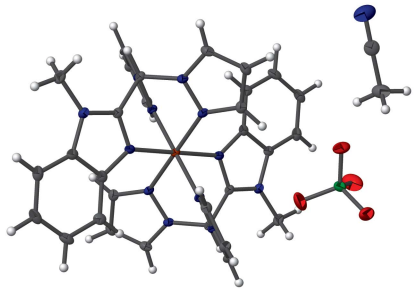
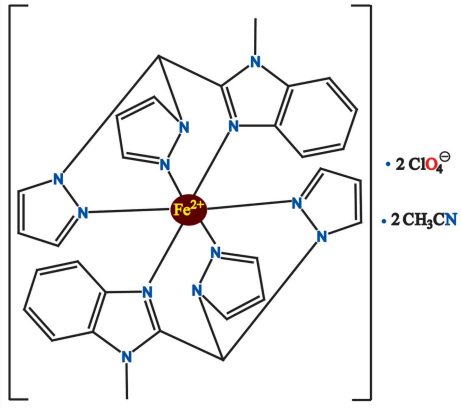
Structural data: full structural data are available from iucrdata.iucr.org

In the structure of the title complex, $[Fe(C_{15}H_{14}N_6)_2](ClO_4)_2\cdot 2C_2H_3N$, the asymmetric unit contains one complete ligand molecule, one perchlorate and one acetonitrile solvent molecule. The iron(II) atom, situated on an inversion centre, is surrounded by six nitrogen atoms from two ligands in an octahedral coordination sphere in which the two benzimidazole units adopt a *trans*-configuration. The crystal structure is stablized by extensive weak C—H···O and C—H···N interactions.

3D view



Chemical scheme



Structure description

Spin-crossover (SCO) complexes are an important class of compounds with respect to new molecular materials and nanoscience research. Moreover, SCO complexes exhibit electronic transitions that involve a change of the spin state at the metal ion in a material, causing changes in a number of its physical properties including its colour, magnetism and conductivity (Guionneau, 2014; Kahn & Martinez, 1998; Matsuda & Tajima, 2007). The present work is part of an ongoing structural study of heterocyclic compounds (Faizi *et al.*, 2016) and their utilization in the synthesis of metal complexes (Faizi & Prisyazhnaya, 2015), excited-state proton-transfer compounds and fluorescent chemosensors (Faizi *et al.*, 2018; Kumar *et al.*, 2018; Mukherjee *et al.*, 2018). Herein we report the synthesis and crystal structure of a new Fe^{II} complex with 2-(di-pyrazol-1-yl-methyl)-1-methyl-1*H*-benzo[*d*]imidazole ligands.

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N7^{i}	0.95	2.57	3.494 (3)	164
C4—H4···O1^{ii}	0.95	2.42	3.308 (3)	155
C5—H5···O3^{iii}	0.95	2.60	3.449 (3)	149
C7—H7···O4^{ii}	1.00	2.32	3.308 (3)	170
C16—H16A···O1^{iv}	0.98	2.40	3.300 (3)	152
C16—H16B···O3	0.98	2.47	3.303 (3)	143

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

The title compound (Fig. 1) crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one complete ligand molecule, one perchlorate and one acetonitrile solvent molecule. As the iron(II) atom is situated on a crystallographic centre of inversion, another ligand, the second perchlorate and another solvent molecule are observed as symmetry equivalents. The iron(II) atom is surrounded by six nitrogen atoms from two ligands in an octahedral coordination sphere in which the two benzimidazole units adopt a *trans*-configuration. The non-coordinating perchlorate counter-ions and solvent molecules connect the complex molecules through weak C—H···O and C—H···N hydrogen-bonding interactions (Table 1, Fig. 2).

Synthesis and crystallization

To a stirred solution of 2-(di-pyrazol-1-yl-methyl)-1-methyl-1*H*-benzo[*d*]imidazole (100 mg, 0.36 mmol) in methanol

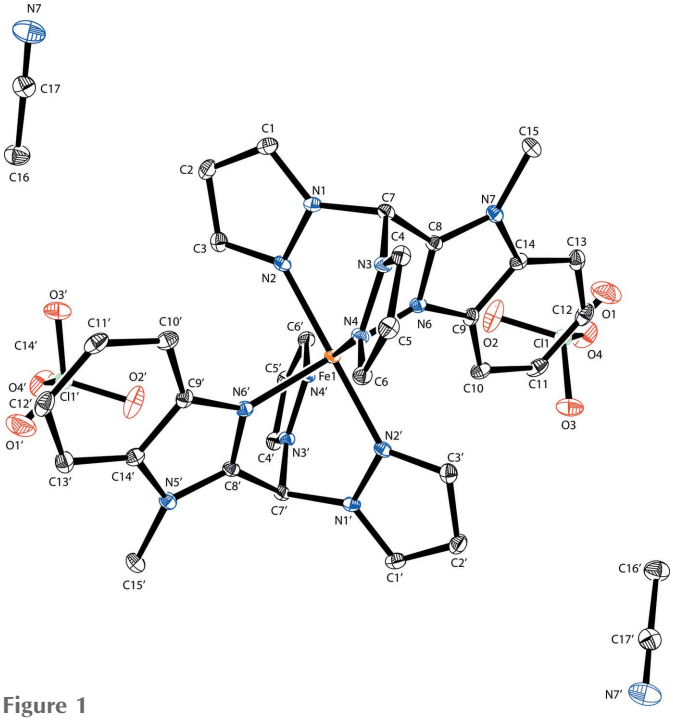


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids at the 40% probability level for non-H atoms. H atoms are omitted for the sake of clarity. [Symmetry code: (′) $-x+1, -y+1, -z+1$.].

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{15}H_{14}N_6)_2](ClO_4)_2\cdot 2C_2H_3N$
M_r	893.50
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	11.3128 (5), 11.7818 (5), 14.1459 (6)
β (°)	99.965 (1)
V (Å^3)	1856.99 (14)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.62
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23607, 3638, 3137
R_{int}	0.042
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.076, 1.06
No. of reflections	3638
No. of parameters	270
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.43

Computer programs: *APEX* and *SMART* (Bruker, 2007), *SAINT-Plus* (Bruker, 2007), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012).

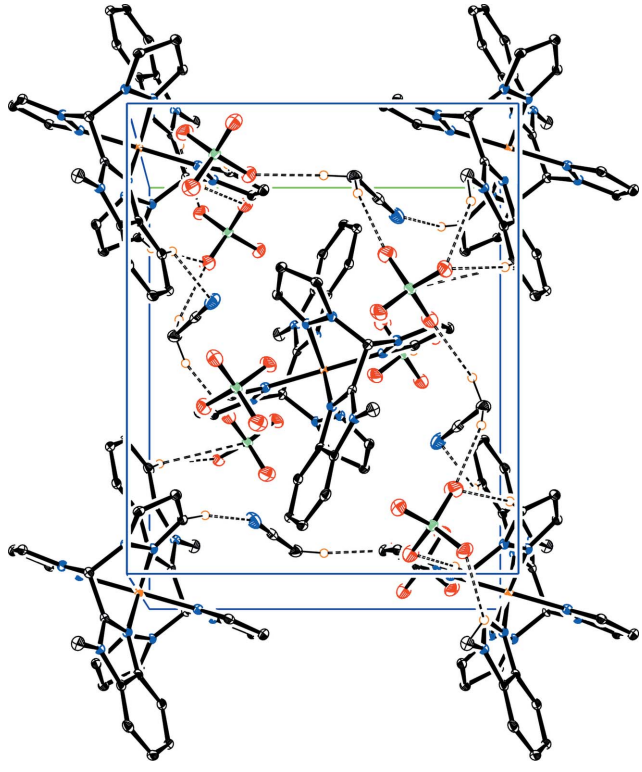


Figure 2
A view along the *a* axis, emphasizing the weak C—H···O and C—H···N interactions which promote the crystal packing in the unit cell of the title compound. Only H atoms involved in these interactions are shown.

(3 ml) solid $[Fe^{II}(H_2O)_6](ClO_4)_2$ (65 mg, 0.18 mmol) was added in small portions under nitrogen. The colour of the solution turned from light yellow to dark yellow without any observed precipitation. After 15 min of stirring, 3 ml of diethyl ether was added, leading to a bright-yellow precipitate that was collected by filtration, washed with 2 ml of methanol/diethyl ether (1:5) and dried *in vacuo* (yield: 110 mg, 78%). The title compound was recrystallized from an acetonitrile/toluene/diethyl ether (4:1:1) mixture (yield: 75 mg, 53%).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190050 [https://doi.org/10.1107/S2414314619000506]

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trans-Bis{2-[bis(1*H*-pyrazol-1-yl)methyl]-1-methyl-1*H*-benzimidazole}iron(II) bis(perchlorate) acetonitrile disolvate

Crystal data

$[Fe(C_{30}H_{28}N_{12})](ClO_4)_2\cdot 2C_2H_3N$
M_r = 893.50
Monoclinic, $P2_1/c$
a = 11.3128 (5) Å
b = 11.7818 (5) Å
c = 14.1459 (6) Å
β = 99.965 (1)°
V = 1856.99 (14) Å^3
Z = 2
$F(000)$ = 920
D_x = 1.598 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 819 reflections
θ = 2.4–20.7°
μ = 0.62 mm^{-1}
T = 100 K
Prism, brown
0.3 × 0.25 × 0.2 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
23607 measured reflections
3638 independent reflections
3137 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.0°, θ_{min} = 2.9°
h = −13→13
k = −14→14
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.076
S = 1.06
3638 reflections
270 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0168P)^2 + 2.7931P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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. All non-hydrogen atoms were refined anisotropically. All H atoms were placed in calculated positions with d(C—H) = 0.95 Å for aromatic, 0.99 for CH and 0.98 Å for CH_3 hydrogen atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.500000	0.500000	0.500000	0.00973 (11)
Cl1	0.05039 (5)	0.27781 (5)	0.40185 (4)	0.01701 (13)
O3	0.12532 (15)	0.19176 (15)	0.37156 (12)	0.0279 (4)
O4	−0.03438 (16)	0.22572 (16)	0.45362 (13)	0.0321 (4)
N1	0.37147 (15)	0.69590 (15)	0.54879 (12)	0.0125 (4)
N5	0.17075 (15)	0.58282 (15)	0.35199 (12)	0.0132 (4)
N3	0.29224 (15)	0.52189 (14)	0.59044 (12)	0.0119 (4)
N2	0.48187 (15)	0.65942 (15)	0.53656 (12)	0.0119 (4)
N6	0.35795 (15)	0.52172 (14)	0.40051 (12)	0.0115 (4)
N4	0.39132 (15)	0.45709 (15)	0.58812 (12)	0.0120 (4)
O2	0.12218 (17)	0.35829 (16)	0.46189 (13)	0.0358 (5)
C2	0.4930 (2)	0.83730 (19)	0.59389 (15)	0.0172 (5)
H2	0.524998	0.908882	0.616231	0.021*
C9	0.32286 (18)	0.49076 (17)	0.30497 (14)	0.0131 (4)
C11	0.3218 (2)	0.41027 (18)	0.15131 (15)	0.0186 (5)
H11	0.360895	0.370447	0.107091	0.022*
C1	0.3762 (2)	0.80282 (18)	0.58468 (15)	0.0160 (4)
H1	0.311041	0.845477	0.600384	0.019*
C12	0.2026 (2)	0.44547 (19)	0.12219 (15)	0.0195 (5)
H12	0.162356	0.427008	0.059441	0.023*
N7	0.3653 (2)	−0.19358 (19)	0.32491 (16)	0.0336 (5)
C10	0.3839 (2)	0.43188 (18)	0.24239 (15)	0.0160 (5)
H10	0.464626	0.407797	0.261703	0.019*
C14	0.20482 (19)	0.52798 (17)	0.27436 (15)	0.0135 (4)
C3	0.55583 (19)	0.74560 (18)	0.56368 (15)	0.0150 (4)
H3	0.639584	0.745042	0.562708	0.018*
C17	0.2894 (2)	−0.1444 (2)	0.34915 (16)	0.0214 (5)
C6	0.38856 (19)	0.37666 (18)	0.65344 (15)	0.0148 (4)
H6	0.447066	0.318586	0.668362	0.018*
C4	0.22846 (18)	0.48295 (18)	0.65559 (14)	0.0138 (4)
H4	0.156295	0.514501	0.669858	0.017*
C8	0.26536 (18)	0.57538 (17)	0.42446 (15)	0.0117 (4)
C5	0.28718 (19)	0.38935 (18)	0.69738 (15)	0.0156 (4)
H5	0.264205	0.342743	0.745928	0.019*
C13	0.1422 (2)	0.50623 (19)	0.18237 (15)	0.0173 (5)
H13	0.062226	0.531874	0.162153	0.021*
C7	0.27116 (18)	0.61768 (18)	0.52547 (14)	0.0124 (4)
H7	0.194396	0.656411	0.532181	0.015*
C15	0.05201 (19)	0.6289 (2)	0.35561 (16)	0.0196 (5)
H15A	0.001099	0.621263	0.292431	0.029*

H15B	0.059185	0.709316	0.373456	0.029*
H15C	0.015932	0.587172	0.403368	0.029*
C16	0.1912 (2)	−0.0816 (2)	0.37885 (17)	0.0266 (6)
H16A	0.118696	−0.090154	0.330248	0.040*
H16B	0.212640	−0.001088	0.385914	0.040*
H16C	0.176149	−0.111334	0.440372	0.040*
O1	−0.01354 (18)	0.33506 (17)	0.31901 (13)	0.0409 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0089 (2)	0.0101 (2)	0.0108 (2)	0.00113 (16)	0.00303 (15)	0.00068 (17)
Cl1	0.0179 (3)	0.0173 (3)	0.0160 (3)	0.0022 (2)	0.0032 (2)	−0.0024 (2)
O3	0.0238 (9)	0.0270 (9)	0.0349 (10)	0.0101 (7)	0.0110 (8)	−0.0015 (8)
O4	0.0296 (10)	0.0327 (10)	0.0387 (11)	−0.0091 (8)	0.0191 (8)	−0.0085 (9)
N1	0.0120 (9)	0.0127 (9)	0.0134 (9)	0.0026 (7)	0.0038 (7)	−0.0003 (7)
N5	0.0110 (9)	0.0147 (9)	0.0140 (9)	0.0001 (7)	0.0026 (7)	0.0017 (7)
N3	0.0108 (8)	0.0124 (9)	0.0132 (8)	0.0011 (7)	0.0040 (7)	−0.0005 (7)
N2	0.0098 (8)	0.0138 (9)	0.0127 (8)	0.0019 (7)	0.0035 (7)	0.0016 (7)
N6	0.0122 (9)	0.0111 (9)	0.0119 (8)	0.0005 (7)	0.0037 (7)	−0.0004 (7)
N4	0.0092 (8)	0.0132 (9)	0.0137 (9)	0.0019 (7)	0.0025 (7)	−0.0001 (7)
O2	0.0447 (11)	0.0334 (11)	0.0293 (10)	−0.0195 (9)	0.0058 (8)	−0.0111 (8)
C2	0.0213 (12)	0.0139 (11)	0.0157 (11)	−0.0021 (9)	0.0011 (9)	−0.0026 (9)
C9	0.0157 (10)	0.0106 (10)	0.0131 (10)	−0.0031 (9)	0.0023 (8)	0.0017 (8)
C11	0.0309 (13)	0.0124 (11)	0.0134 (10)	0.0001 (10)	0.0068 (9)	−0.0006 (9)
C1	0.0214 (11)	0.0134 (10)	0.0133 (10)	0.0040 (9)	0.0033 (9)	0.0000 (9)
C12	0.0298 (13)	0.0156 (11)	0.0120 (10)	−0.0055 (10)	0.0004 (9)	−0.0001 (9)
N7	0.0341 (13)	0.0322 (13)	0.0373 (13)	0.0105 (11)	0.0144 (10)	0.0127 (11)
C10	0.0208 (11)	0.0115 (10)	0.0168 (11)	−0.0002 (9)	0.0060 (9)	0.0019 (9)
C14	0.0159 (11)	0.0106 (10)	0.0150 (10)	−0.0017 (8)	0.0055 (8)	0.0015 (8)
C3	0.0156 (11)	0.0161 (11)	0.0128 (10)	−0.0017 (9)	0.0010 (8)	0.0022 (8)
C17	0.0261 (13)	0.0195 (12)	0.0186 (11)	0.0007 (10)	0.0037 (10)	0.0073 (10)
C6	0.0164 (11)	0.0127 (10)	0.0149 (10)	0.0001 (9)	0.0014 (8)	0.0010 (9)
C4	0.0120 (10)	0.0174 (11)	0.0136 (10)	−0.0020 (8)	0.0062 (8)	−0.0022 (9)
C8	0.0111 (10)	0.0104 (10)	0.0139 (10)	0.0005 (8)	0.0028 (8)	0.0024 (8)
C5	0.0169 (11)	0.0156 (11)	0.0152 (10)	−0.0028 (9)	0.0056 (8)	0.0009 (9)
C13	0.0175 (11)	0.0155 (11)	0.0177 (11)	−0.0042 (9)	−0.0006 (9)	0.0040 (9)
C7	0.0102 (10)	0.0131 (10)	0.0140 (10)	0.0011 (8)	0.0025 (8)	0.0012 (8)
C15	0.0120 (11)	0.0216 (12)	0.0241 (12)	0.0021 (9)	0.0003 (9)	−0.0010 (10)
C16	0.0309 (14)	0.0284 (14)	0.0217 (12)	0.0078 (11)	0.0076 (10)	0.0022 (10)
O1	0.0475 (12)	0.0425 (12)	0.0287 (10)	0.0233 (10)	−0.0045 (9)	0.0034 (9)

Geometric parameters (Å, º)

Fe1—N6^{i}	1.9610 (17)	C9—C14	1.401 (3)
Fe1—N6	1.9610 (17)	C11—C10	1.380 (3)
Fe1—N4^{i}	1.9626 (17)	C11—C12	1.403 (3)
Fe1—N4	1.9626 (17)	C11—H11	0.9500

Fe1—N2	1.9683 (17)	C1—H1	0.9500
Fe1—N2^{i}	1.9683 (17)	C12—C13	1.380 (3)
Cl1—O2	1.4287 (18)	C12—H12	0.9500
Cl1—O3	1.4338 (17)	N7—C17	1.136 (3)
Cl1—O1	1.4346 (18)	C10—H10	0.9500
Cl1—O4	1.4407 (17)	C14—C13	1.393 (3)
N1—C1	1.356 (3)	C3—H3	0.9500
N1—N2	1.360 (2)	C17—C16	1.456 (3)
N1—C7	1.455 (3)	C6—C5	1.404 (3)
N5—C8	1.351 (3)	C6—H6	0.9500
N5—C14	1.385 (3)	C4—C5	1.368 (3)
N5—C15	1.458 (3)	C4—H4	0.9500
N3—C4	1.346 (3)	C8—C7	1.504 (3)
N3—N4	1.361 (2)	C5—H5	0.9500
N3—C7	1.449 (3)	C13—H13	0.9500
N2—C3	1.329 (3)	C7—H7	1.0000
N6—C8	1.317 (3)	C15—H15A	0.9800
N6—C9	1.390 (3)	C15—H15B	0.9800
N4—C6	1.328 (3)	C15—H15C	0.9800
C2—C1	1.367 (3)	C16—H16A	0.9800
C2—C3	1.400 (3)	C16—H16B	0.9800
C2—H2	0.9500	C16—H16C	0.9800
C9—C10	1.398 (3)		

N6^{i}—Fe1—N6	180.0	N1—C1—H1	126.7
N6^{i}—Fe1—N4^{i}	87.92 (7)	C2—C1—H1	126.7
N6—Fe1—N4^{i}	92.08 (7)	C13—C12—C11	121.7 (2)
N6^{i}—Fe1—N4	92.08 (7)	C13—C12—H12	119.2
N6—Fe1—N4	87.93 (7)	C11—C12—H12	119.2
N4^{i}—Fe1—N4	180.0	C11—C10—C9	117.1 (2)
N6^{i}—Fe1—N2	92.62 (7)	C11—C10—H10	121.5
N6—Fe1—N2	87.38 (7)	C9—C10—H10	121.5
N4^{i}—Fe1—N2	91.51 (7)	N5—C14—C13	131.3 (2)
N4—Fe1—N2	88.49 (7)	N5—C14—C9	106.38 (18)
N6^{i}—Fe1—N2^{i}	87.38 (7)	C13—C14—C9	122.3 (2)
N6—Fe1—N2^{i}	92.62 (7)	N2—C3—C2	110.49 (19)
N4^{i}—Fe1—N2^{i}	88.49 (7)	N2—C3—H3	124.8
N4—Fe1—N2^{i}	91.51 (7)	C2—C3—H3	124.8
N2—Fe1—N2^{i}	180.0	N7—C17—C16	179.2 (3)
O2—Cl1—O3	110.02 (12)	N4—C6—C5	110.58 (19)
O2—Cl1—O1	109.14 (12)	N4—C6—H6	124.7
O3—Cl1—O1	109.20 (11)	C5—C6—H6	124.7
O2—Cl1—O4	109.90 (11)	N3—C4—C5	107.04 (18)
O3—Cl1—O4	109.31 (11)	N3—C4—H4	126.5
O1—Cl1—O4	109.24 (12)	C5—C4—H4	126.5
C1—N1—N2	111.32 (17)	N6—C8—N5	113.39 (18)
C1—N1—C7	130.72 (18)	N6—C8—C7	119.84 (18)
N2—N1—C7	117.93 (16)	N5—C8—C7	126.74 (18)

C8—N5—C14	106.19 (17)	C4—C5—C6	105.50 (19)
C8—N5—C15	127.69 (18)	C4—C5—H5	127.2
C14—N5—C15	125.87 (18)	C6—C5—H5	127.2
C4—N3—N4	111.51 (17)	C12—C13—C14	116.5 (2)
C4—N3—C7	130.63 (17)	C12—C13—H13	121.8
N4—N3—C7	117.87 (16)	C14—C13—H13	121.8
C3—N2—N1	105.54 (17)	N3—C7—N1	108.26 (16)
C3—N2—Fe1	135.70 (15)	N3—C7—C8	108.66 (17)
N1—N2—Fe1	118.35 (13)	N1—C7—C8	109.23 (16)
C8—N6—C9	105.67 (17)	N3—C7—H7	110.2
C8—N6—Fe1	117.87 (14)	N1—C7—H7	110.2
C9—N6—Fe1	136.41 (14)	C8—C7—H7	110.2
C6—N4—N3	105.37 (16)	N5—C15—H15A	109.5
C6—N4—Fe1	135.95 (15)	N5—C15—H15B	109.5
N3—N4—Fe1	118.67 (13)	H15A—C15—H15B	109.5
C1—C2—C3	105.95 (19)	N5—C15—H15C	109.5
C1—C2—H2	127.0	H15A—C15—H15C	109.5
C3—C2—H2	127.0	H15B—C15—H15C	109.5
N6—C9—C10	131.1 (2)	C17—C16—H16A	109.5
N6—C9—C14	108.36 (18)	C17—C16—H16B	109.5
C10—C9—C14	120.58 (19)	H16A—C16—H16B	109.5
C10—C11—C12	121.8 (2)	C17—C16—H16C	109.5
C10—C11—H11	119.1	H16A—C16—H16C	109.5
C12—C11—H11	119.1	H16B—C16—H16C	109.5
N1—C1—C2	106.68 (19)		

C1—N1—N2—C3	−1.1 (2)	N3—N4—C6—C5	0.4 (2)
C7—N1—N2—C3	−179.34 (17)	Fe1—N4—C6—C5	178.59 (16)
C1—N1—N2—Fe1	172.72 (13)	N4—N3—C4—C5	−0.1 (2)
C7—N1—N2—Fe1	−5.6 (2)	C7—N3—C4—C5	179.51 (19)
C4—N3—N4—C6	−0.1 (2)	C9—N6—C8—N5	−0.1 (2)
C7—N3—N4—C6	−179.84 (17)	Fe1—N6—C8—N5	−177.98 (13)
C4—N3—N4—Fe1	−178.73 (13)	C9—N6—C8—C7	177.93 (18)
C7—N3—N4—Fe1	1.6 (2)	Fe1—N6—C8—C7	0.0 (2)
C8—N6—C9—C10	−179.7 (2)	C14—N5—C8—N6	0.6 (2)
Fe1—N6—C9—C10	−2.4 (4)	C15—N5—C8—N6	175.19 (19)
C8—N6—C9—C14	−0.5 (2)	C14—N5—C8—C7	−177.20 (19)
Fe1—N6—C9—C14	176.79 (15)	C15—N5—C8—C7	−2.6 (3)
N2—N1—C1—C2	1.4 (2)	N3—C4—C5—C6	0.4 (2)
C7—N1—C1—C2	179.36 (19)	N4—C6—C5—C4	−0.5 (2)
C3—C2—C1—N1	−1.1 (2)	C11—C12—C13—C14	−1.7 (3)
C10—C11—C12—C13	1.8 (3)	N5—C14—C13—C12	−178.1 (2)
C12—C11—C10—C9	0.0 (3)	C9—C14—C13—C12	0.1 (3)
N6—C9—C10—C11	177.5 (2)	C4—N3—C7—N1	118.7 (2)
C14—C9—C10—C11	−1.6 (3)	N4—N3—C7—N1	−61.6 (2)
C8—N5—C14—C13	177.5 (2)	C4—N3—C7—C8	−122.7 (2)
C15—N5—C14—C13	2.8 (4)	N4—N3—C7—C8	56.9 (2)
C8—N5—C14—C9	−0.9 (2)	C1—N1—C7—N3	−113.8 (2)

C15—N5—C14—C9	−175.60 (19)	N2—N1—C7—N3	64.1 (2)
N6—C9—C14—N5	0.9 (2)	C1—N1—C7—C8	128.1 (2)
C10—C9—C14—N5	−179.82 (18)	N2—N1—C7—C8	−54.0 (2)
N6—C9—C14—C13	−177.68 (19)	N6—C8—C7—N3	−59.2 (2)
C10—C9—C14—C13	1.6 (3)	N5—C8—C7—N3	118.5 (2)
N1—N2—C3—C2	0.3 (2)	N6—C8—C7—N1	58.7 (2)
Fe1—N2—C3—C2	−171.80 (15)	N5—C8—C7—N1	−123.6 (2)
C1—C2—C3—N2	0.5 (2)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N7^{ii}	0.95	2.57	3.494 (3)	164
C4—H4···O1^{iii}	0.95	2.42	3.308 (3)	155
C5—H5···O3^{iv}	0.95	2.60	3.449 (3)	149
C7—H7···O4^{iii}	1.00	2.32	3.308 (3)	170
C16—H16*A*···O1^{v}	0.98	2.40	3.300 (3)	152
C16—H16*B*···O3	0.98	2.47	3.303 (3)	143

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