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Synthesis and crystal structure of a heterobimetallic cadmium–sodium complex of 1,3,5-triazine-2,4,6-trione, $[CdNa_2(C_3H_2N_3O_3)_4(H_2O)_8]$

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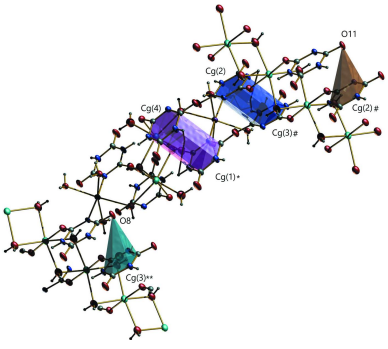
Heterobimetallic crystals of a cadmium–sodium complex of 1,3,5-triazine-2,4,6-trione, namely, μ-aqua-1:2κ^2O:O-heptaaqua-1κ^3O,2κ^2O,3κ^2O-bis(μ-4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazin-2-olato)-1:2κ^2O^2:N^1;2:3κ^2N^1:O^2-bis(4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazin-2-olato)-1κO^2,3κO^2-2-cadmium-1,3-disodium, $[CdNa_2(C_3H_2N_3O_3)_4(H_2O)_8]$, were grown by the single gel diffusion technique. The asymmetric unit of the title compound comprises four 1,3,5-triazine-2,4,6-trione ligands, two sodium atoms and one cadmium atom. Of the four ligands, two are monodentately coordinated to two Na atoms. The third ligand is coordinated bidentately to one Na and the Cd atom and the fourth is also coordinated bidentately to the Cd atom and the other Na atom. All the metal atoms are six-coordinate with a distorted octahedral geometry. The water molecules bridge the Na atoms, constructing coordination polymer chains along the *a* axis and hence are linked by two Cd and one Na coordinations through the cyanuric acid ligands present in the coordination polymer chains, generating a two-dimensional coordination polymer in the (110) plane. The polymer formation is further assisted by means of many intermolecular and intramolecular N—H···O, O—H···O and O–H···N hydrogen bonds between the water molecules and the ligands.

1. Chemical context

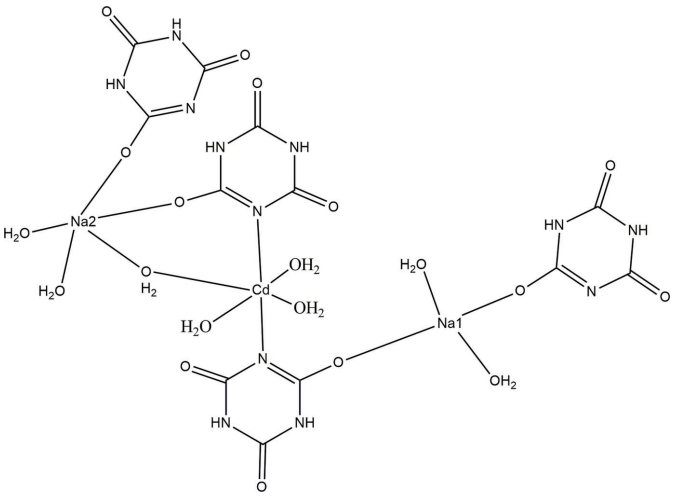
Chelation is considered as the preferred method for the reduction of toxic effects of heavy metals, in which the metals are removed in the form of stable complex chelates. Cadmium, one of the most toxic heavy metals, can accumulate in the human body, leading to renal dysfunction, lung cancer, *etc*. In addition, chelation reactions are utilized in the determination of cadmium toxicity (Flora & Pachauri, 2010) with 1,3,5-triazine-2,4,6-trione, also known as cyanuric acid, being the preferred ligand used for the chelation as it has multiple hydrogen-bond donor centres (Mistri *et al.*, 2014). 1,3,5-Triazine-2,4,6-trione exists in either the keto or enol form but the most stable isomer is the keto form (Reva, 2015). In this work, we report the crystal structure of a heterobimetallic cadmium and sodium complex of 1,3,5-triazine-2,4,6-trione.



2. Structural commentary

The title complex crystallizes in the triclinic space group $P\overline{1}$. Fig. 1 shows the asymmetric unit of the crystal, which consists of four cyanuric acid ligands, two sodium atoms (Na1 and Na2) and one cadmium atom. Of the four ligands, two are

monodentately coordinated to Na1 and Na2 atoms each. The third ligand is coordinated bidentately to Na1 and Cd1 atoms and the fourth one also coordinated bidentately to Na2 and Cd1 atoms. The sodium atom Na2 is coordinated to oxygen atoms of two cyanuric acid ligands [O5—Na2—O14 = 94.52 (6)°]. The Na1 atom is also coordinated to oxygen atoms of two cyanuric acid ligands [O10—Na1—O13 = 173.39 (7)°]. The Cd1 atom is coordinated to nitrogen atoms of two cyanuric acid ligands [N1—Cd1—N4 = 174.58 (6)]°. In addition to the ligand coordination, atoms Na1, Na2 and Cd1 are also coordinated by two, three and four water molecules, respectively.



The title compound forms a two dimensional coordination polymer. In the coordination environment of the polymer, the Na1 atom is six-coordinate with the coordination angle varying from 90° [78.82 (6)–90.60 (6)°], forming a distorted octahedral geometry. Atom Na2 also exhibits a distorted octahedral geometry, with the coordination angles ranging from 77.17 (6) to 91.77 (6)°. The cadmium atom also shows a

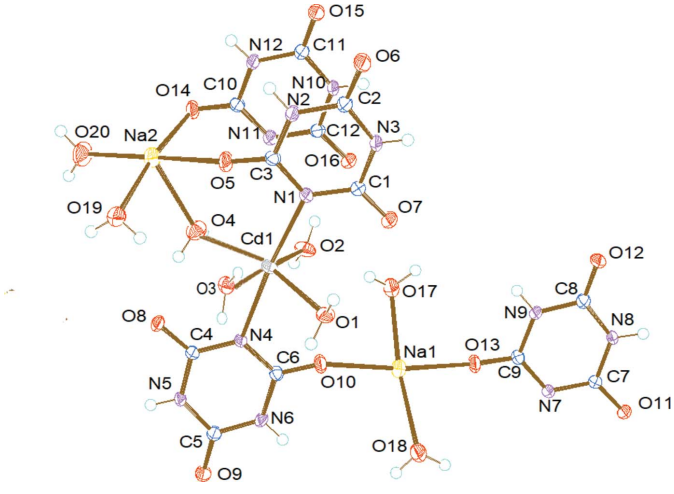


Figure 1
The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N11^{i}	0.98	1.82	2.788 (2)	168
O1—H1B···N7^{ii}	0.98	1.89	2.860 (2)	169
N2—H2···O15^{iii}	0.86	1.96	2.817 (2)	173
O2—H2A···O13^{iv}	0.98	1.77	2.716 (2)	161
O2—H2B···N11	0.98	2.53	3.236 (2)	128
O2—H2B···O16	0.98	1.79	2.753 (2)	167
N3—H3···O11^{v}	0.86	1.92	2.773 (2)	173
O3—H3A···O14^{i}	0.98	1.91	2.871 (2)	166
O3—H3B···O11^{ii}	0.98	1.87	2.842 (2)	169
N5—H5···O16^{vi}	0.86	2.10	2.938 (2)	164
N6—H6···O12^{vi}	0.86	2.13	2.979 (2)	168
N10—H10···O8^{vii}	0.86	1.94	2.792 (2)	172
N8—H8···O7^{v}	0.86	2.02	2.862 (2)	167
N12—H12···O6^{iii}	0.86	2.03	2.882 (2)	173
N9—H9···O9^{vii}	0.86	2.04	2.885 (2)	169
O20—H20B···O6^{viii}	0.98	2.30	2.903 (2)	119
O20—H20A···O14^{ix}	0.98	2.14	3.008 (2)	147
O4—H4A···O8	0.98	1.88	2.725 (2)	143
O17—H17B···O2	0.99	1.87	2.768 (2)	149
O17—H17A···O9^{vii}	0.98	1.81	2.790 (2)	171
O18—H18B···O12^{vi}	0.98	1.91	2.852 (2)	160

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

distorted octahedral geometry with coordination angles in the range 87.94 (5) to 95.46 (6)°. A similar geometry is observed for the Cd atom in the heterobimetallic compound tetraaquabis(malonato)cadmium(II)copper(II) (Dhanya *et al.*, 2014). Na1—O bond distances [2.3471 (16) to 2.4195 (18) Å] show a decrease compared to the value reported for a free Na—O bond (2.421 Å; Brown & Shannon, 1973). The Na2—O bonds, which vary from 2.3067 (17) to 2.4997 (18) Å, are longer than the reported value for a free Na—O bond. This observed range of Na—O bonds also shows close agreement with values reported for sodium 2-aminoterephthalate where the sodium atom adopts a similar six-coordinate geometry (2.326–2.505 Å; Sienkiewicz-Gromiuk *et al.*, 2012). The Cd1—N4 bond distance [2.3210 (15) Å] is comparable to the reported value in a similar coordinated geometry (2.324 Å; Hashemian & Mangeli, 2017). The water molecules are tetrahedrally coordinated to the cadmium atom, forming bond angles ranging from 81.59 (5) to 111.45 (5)°. Three water molecules are coordinated to Na2, with bond angles ranging from 85.43 (6) to 102.25 (7)°. Two water molecules are coordinated to Na1, forming a bond angle of 170.94 (7)°. The two water molecules coordinated to Na1 bridge adjacent Na1 atoms on both sides, forming a coordination polymer chain along the *a* axis. These chains are interconnected by means of two Cd1 and Na2 coordinations through the cyanuric acid ligands present in the Na1 coordination polymer chain on both sides to build a 2D coordination polymer in the (110) plane.

3. Supramolecular features

There are 25 intramolecular and intermolecular hydrogen-bonding interactions involving the ligands and the coordinated

Table 2
Analysis of π–π interactions (Å, °).

α is the dihedral angle between planes *I* and *J*. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1–N3/C1–C3, N4–N6/C4–C6, N7–N9/C7–C9 and N10–N12/C10–C12 rings, respectively.

$Cg(I)\cdots Cg(J)$	$Cg\cdots Cg$	α
$Cg1\cdots Cg4^{i}$	3.5174 (12)	2.42 (10)
$Cg2\cdots Cg3^{ii}$	3.4893 (11)	2.59 (9)

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

water molecules with $D\cdots A$ distances ranging from 2.716 (2) to 3.236 (2) Å (Table 1). Two types of π–π interactions (Table 2) occur between the cyanurate rings of different units, having centroid–centroid distances of 3.5174 (12) and 3.4893 (11) Å, and two types of C—O$\cdots\pi$ interactions (Table 3) with different cyanurate rings with $X\cdots Cg$ distances of 3.6086 (2) and 3.4783 (2) Å are also present in the complex (Fig. 2). A packing diagram is presented in Fig. 3.

4. Synthesis and crystallization

Needle-shaped transparent single crystals were obtained by the single gel diffusion method (Chandran *et al.*, 2017). 1,3,5-Triazine-2,4,6-trione, acetic acid, sodium metasilicate and cadmium chloride hydrate were used for the growth in a single glass test tube of length 20 cm and diameter 2.5 cm. The preparation of silica gel of specific gravity 1.03–1.05 g cm^{-3} involved dissolution of sodium metasilicate (SMS) in double-distilled water to which 1,3,5-triazine-2,4,6-trione (0.01–0.02 *M* concentration) was added. The resulting SMS solution was acidified with drops of glacial acetic acid to adjust the pH to within the range 4–7. The test tubes were filled with 30 ml of the above solution for gel setting. Over the set gel, cadmium chloride solution (0.25–1 *M*) was added carefully along the sides of the test tube to prevent the gel breakage. Finally, the test tube was sealed with a transparent plastic sheet to prevent contamination and kept undisturbed for crystal growth. Crystals formed within the gel after two weeks and growth was completed in a month. A series of trials was undertaken to obtain the optimum conditions to grow well-defined single crystals. 1,3,5-Triazine-2,4,6-trione (0.02 *M*) was used as inner reactant and cadmium chloride (0.25 *M*) as the top solution. Well-defined good-quality single crystals suitable for single-crystal XRD studies were grown in a gel medium of pH 6 and density 1.03 g cm^{-3}.

Table 3
Analysis of $Y-X\cdots Cg$ (π-ring) interactions (Å, °).

$Y-X(I)\cdots Cg(J)$	$X\cdots Cg$	$Y-X\cdots Cg$	$Y\cdots Cg$
C4—O8$\cdots Cg3^{i}$	3.6086 (2)	68.07 (11)	3.349 (2)
C7—O11$\cdots Cg2^{ii}$	3.4783 (2)	68.37 (11)	3.233 (2)

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

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. Some reflections truncated by beamstop were omitted. The nitrogen-bound H atoms were placed in calculated positions (N—H = 0.86 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) set to 1.2U_{eq}(N). H atoms attached to water molecules were located from difference-Fourier maps and

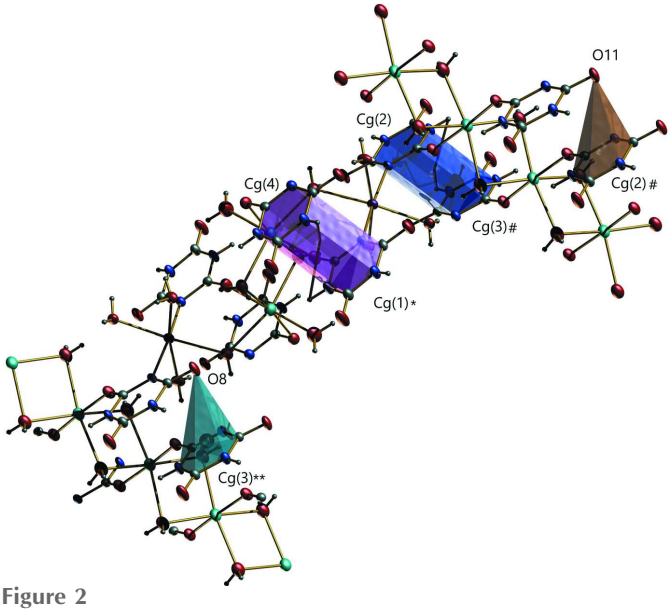


Figure 2
$\pi\cdots\pi$ and C—O$\cdots\pi$ interactions present in the complex. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1–N3/C1–C3, N4–N6/C4–C6, N7–N9/C7–C9 and N10–N12/C10–C12 rings, respectively. Symmetry codes: (*) $x-1, y, z$; (**) $1-x, -y, -z$; (#) $2-x, -y, -z$.

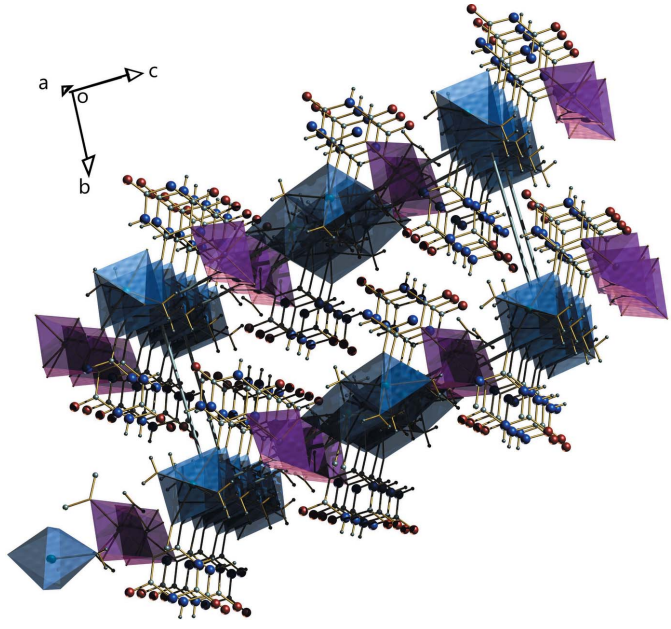


Figure 3
The packing, viewed down the *a* axis, showing the coordination polyhedra.

Table 4
Experimental details.

Crystal data	
Chemical formula	$[CdNa_2(C_3H_2N_3O_3)_4(H_2O)_8]$
M_r	814.81
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	7.0501 (3), 10.0314 (5), 19.5058 (9)
α, β, γ (°)	101.023 (1), 90.468 (1), 97.233 (1)
V (Å^3)	1342.53 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.96
Crystal size (mm)	0.15 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker Kappa *APEX3* CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.870, 0.901
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52745, 5912, 5460
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.643
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.063, 1.20
No. of reflections	5912
No. of parameters	430
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.88, −0.57

Computer programs: *APEX3*, *SAINT* and *XPREP* (Bruker, 2016), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2010).

were refined with isotropic displacement parameters [U_{iso}(H) = 1.5U_{eq}(O)].

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supporting information

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Synthesis and crystal structure of a heterobimetallic cadmium–sodium complex of 1,3,5-triazine-2,4,6-trione, $[CdNa_2(C_3H_2N_3O_3)_4(H_2O)_8]$

R. Divya, B. R. Bijini, V. S. Dhanya, K. Rajendra Babu and M. Sithambaresan

Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *APEX3* and *SAINT* (Bruker, 2016); data reduction: *SAINT* andXPREP (Bruker, 2016); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL2018/3* (Sheldrick, 2015b).

μ-Aqua-1:2κ^2O:*O*-heptaaqua-1κ^3O,2κ^2O,3κ^2O-bis(μ-4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazin-2-olato)-1:2κ^2O^2:N^1;2:3κ^2N^1:O^2-bis(4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazin-2-olato)-1κO^2,3κO^2-2-cadmium-1,3-disodium

Crystal data

$[CdNa_2(C_3H_2N_3O_3)_4(H_2O)_8]$
M_r = 814.81
Triclinic, $P\overline{1}$
a = 7.0501 (3) Å
b = 10.0314 (5) Å
c = 19.5058 (9) Å
α = 101.023 (1)°
β = 90.468 (1)°
γ = 97.233 (1)°
V = 1342.53 (11) Å^3
Z = 2
$F(000)$ = 820
D_x = 2.016 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9962 reflections
θ = 3.1–29.6°
μ = 0.96 mm^{-1}
T = 293 K
Block, colourless
0.15 × 0.10 × 0.10 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.870, T_{max} = 0.901
52745 measured reflections
5912 independent reflections
5460 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.2°, θ_{min} = 3.2°
h = −9→9
k = −12→12
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.20
5912 reflections
430 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.9925P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8025 (3)	0.33005 (19)	0.28213 (10)	0.0172 (4)
C2	0.8168 (3)	0.4798 (2)	0.39643 (11)	0.0216 (4)
C3	0.6821 (3)	0.24087 (19)	0.37866 (10)	0.0172 (4)
C4	0.5623 (3)	−0.32929 (19)	0.20544 (10)	0.0160 (4)
C5	0.6255 (3)	−0.4699 (2)	0.09476 (10)	0.0194 (4)
C6	0.6837 (3)	−0.22094 (19)	0.11527 (10)	0.0157 (4)
C7	0.9520 (3)	0.33435 (19)	−0.20488 (10)	0.0157 (4)
C8	0.8810 (3)	0.4855 (2)	−0.09848 (10)	0.0190 (4)
C9	0.8168 (3)	0.23791 (19)	−0.11439 (10)	0.0158 (4)
C10	0.1780 (3)	0.23787 (19)	0.37549 (10)	0.0166 (4)
C11	0.3200 (3)	0.4760 (2)	0.39865 (11)	0.0213 (4)
C12	0.3021 (3)	0.3339 (2)	0.28316 (10)	0.0170 (4)
N1	0.7207 (2)	0.22287 (16)	0.30988 (8)	0.0169 (3)
N2	0.7326 (3)	0.36898 (17)	0.42028 (9)	0.0226 (4)
H2	0.709160	0.378905	0.464036	0.027*
N3	0.8481 (3)	0.45615 (17)	0.32672 (9)	0.0215 (4)
H3	0.899616	0.523714	0.309038	0.026*
N4	0.6247 (2)	−0.21351 (16)	0.18213 (8)	0.0152 (3)
N5	0.5607 (2)	−0.45516 (16)	0.16086 (8)	0.0187 (3)
H5	0.516292	−0.527734	0.175881	0.022*
N6	0.6887 (3)	−0.35041 (17)	0.07445 (8)	0.0195 (3)
H6	0.734942	−0.354974	0.033533	0.023*
N7	0.8839 (2)	0.22246 (16)	−0.17957 (8)	0.0172 (3)
N8	0.9513 (2)	0.46392 (16)	−0.16400 (9)	0.0187 (3)
H8	0.997548	0.533894	−0.180868	0.022*
N9	0.8147 (3)	0.36876 (17)	−0.07555 (9)	0.0203 (4)
H9	0.768803	0.376704	−0.034471	0.024*
N10	0.3519 (3)	0.45707 (17)	0.32895 (9)	0.0215 (4)
H10	0.406119	0.525452	0.312499	0.026*
N11	0.2119 (2)	0.22607 (17)	0.30703 (9)	0.0188 (3)
N12	0.2315 (3)	0.36306 (17)	0.41995 (9)	0.0219 (4)
H12	0.207301	0.369553	0.463517	0.026*
O1	0.9770 (2)	0.03762 (14)	0.20860 (7)	0.0215 (3)
H1A	1.065349	0.092864	0.245551	0.032*
H1B	1.036161	−0.047201	0.203744	0.032*
O2	0.4449 (2)	0.06725 (15)	0.18140 (8)	0.0256 (3)

H2A	0.363198	−0.014609	0.156501	0.038*
H2B	0.391157	0.153416	0.196860	0.038*
O3	0.8349 (2)	−0.08797 (15)	0.33509 (8)	0.0241 (3)
H3A	0.939632	−0.020504	0.358856	0.036*
H3B	0.901723	−0.163676	0.311768	0.036*
O4	0.3757 (2)	−0.08155 (17)	0.30812 (8)	0.0290 (3)
H4A	0.369042	−0.181741	0.301003	0.044*
H4B	0.265442	−0.057541	0.284123	0.044*
O5	0.6035 (2)	0.14863 (15)	0.40559 (8)	0.0280 (3)
O6	0.8599 (3)	0.59241 (16)	0.43440 (8)	0.0368 (4)
O7	0.8382 (2)	0.32046 (15)	0.21994 (8)	0.0269 (3)
O8	0.5039 (2)	−0.32832 (15)	0.26519 (8)	0.0262 (3)
O9	0.6280 (3)	−0.58152 (15)	0.05625 (8)	0.0312 (4)
O10	0.7346 (2)	−0.11970 (15)	0.09073 (8)	0.0241 (3)
O11	1.0167 (2)	0.32568 (15)	−0.26437 (8)	0.0246 (3)
O12	0.8765 (3)	0.59950 (15)	−0.06270 (8)	0.0308 (4)
O13	0.7540 (2)	0.13948 (15)	−0.08785 (8)	0.0236 (3)
O14	0.1013 (2)	0.14177 (14)	0.40139 (8)	0.0227 (3)
O15	0.3689 (3)	0.58556 (16)	0.43856 (8)	0.0353 (4)
O16	0.3458 (2)	0.32703 (15)	0.22117 (7)	0.0248 (3)
O17	0.5338 (2)	0.13908 (16)	0.05424 (9)	0.0313 (4)
H17A	0.559228	0.239151	0.059155	0.047*
H18A	1.002488	−0.103967	−0.120403	0.047*
O18	0.9774 (2)	−0.12084 (16)	−0.07304 (8)	0.0295 (4)
H18B	0.956220	−0.221324	−0.079922	0.044*
H17B	0.545676	0.133976	0.104027	0.044*
O19	0.5872 (2)	−0.13881 (16)	0.44927 (8)	0.0299 (3)
H19A	0.537228	−0.235403	0.447693	0.045*
H19B	0.694698	−0.133273	0.417733	0.045*
O20	0.0908 (3)	−0.14107 (19)	0.46154 (10)	0.0411 (4)
H20A	0.081618	−0.129379	0.512560	0.062*
H20B	0.114905	−0.236594	0.446586	0.062*
Na1	0.75518 (12)	0.00016 (9)	−0.00173 (4)	0.02498 (19)
Na2	0.34777 (12)	0.00440 (9)	0.43414 (5)	0.02616 (19)
Cd1	0.66796 (2)	0.00416 (2)	0.25149 (2)	0.01845 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0207 (9)	0.0147 (9)	0.0163 (9)	0.0027 (7)	0.0031 (7)	0.0031 (7)
C2	0.0283 (11)	0.0171 (10)	0.0170 (10)	−0.0031 (8)	0.0054 (8)	0.0010 (8)
C3	0.0177 (9)	0.0141 (9)	0.0184 (9)	0.0006 (7)	0.0014 (7)	0.0002 (7)
C4	0.0190 (9)	0.0123 (9)	0.0156 (9)	0.0004 (7)	0.0014 (7)	0.0015 (7)
C5	0.0246 (10)	0.0157 (9)	0.0164 (9)	0.0004 (8)	0.0038 (8)	0.0011 (7)
C6	0.0175 (9)	0.0145 (9)	0.0146 (9)	0.0003 (7)	0.0000 (7)	0.0030 (7)
C7	0.0181 (9)	0.0133 (9)	0.0154 (9)	0.0020 (7)	0.0022 (7)	0.0017 (7)
C8	0.0241 (10)	0.0162 (9)	0.0158 (9)	0.0003 (8)	0.0036 (7)	0.0022 (7)
C9	0.0173 (9)	0.0137 (9)	0.0161 (9)	0.0006 (7)	−0.0005 (7)	0.0028 (7)

C10	0.0166 (9)	0.0156 (9)	0.0173 (9)	0.0020 (7)	−0.0002 (7)	0.0023 (7)
C11	0.0276 (11)	0.0175 (10)	0.0168 (9)	−0.0019 (8)	0.0051 (8)	0.0015 (8)
C12	0.0190 (9)	0.0164 (9)	0.0156 (9)	0.0033 (7)	0.0021 (7)	0.0020 (7)
N1	0.0221 (8)	0.0122 (8)	0.0150 (8)	−0.0003 (6)	0.0026 (6)	0.0011 (6)
N2	0.0357 (10)	0.0150 (8)	0.0140 (8)	−0.0052 (7)	0.0074 (7)	0.0000 (6)
N3	0.0335 (10)	0.0126 (8)	0.0170 (8)	−0.0037 (7)	0.0079 (7)	0.0032 (6)
N4	0.0220 (8)	0.0107 (7)	0.0120 (7)	−0.0003 (6)	0.0023 (6)	0.0011 (6)
N5	0.0293 (9)	0.0099 (7)	0.0156 (8)	−0.0018 (6)	0.0069 (7)	0.0021 (6)
N6	0.0301 (9)	0.0149 (8)	0.0121 (8)	−0.0006 (7)	0.0074 (7)	0.0006 (6)
N7	0.0246 (9)	0.0120 (7)	0.0151 (8)	0.0024 (6)	0.0044 (6)	0.0028 (6)
N8	0.0284 (9)	0.0109 (7)	0.0169 (8)	0.0001 (6)	0.0072 (7)	0.0040 (6)
N9	0.0307 (9)	0.0156 (8)	0.0138 (8)	0.0006 (7)	0.0088 (7)	0.0020 (6)
N10	0.0332 (10)	0.0135 (8)	0.0159 (8)	−0.0042 (7)	0.0076 (7)	0.0028 (6)
N11	0.0233 (8)	0.0152 (8)	0.0165 (8)	−0.0011 (6)	0.0017 (6)	0.0019 (6)
N12	0.0335 (10)	0.0159 (8)	0.0138 (8)	−0.0046 (7)	0.0059 (7)	0.0016 (6)
O1	0.0228 (7)	0.0180 (7)	0.0211 (7)	−0.0004 (6)	0.0020 (6)	−0.0010 (6)
O2	0.0313 (8)	0.0192 (7)	0.0241 (8)	0.0063 (6)	−0.0049 (6)	−0.0029 (6)
O3	0.0274 (8)	0.0226 (7)	0.0217 (7)	0.0048 (6)	−0.0015 (6)	0.0021 (6)
O4	0.0302 (8)	0.0309 (9)	0.0235 (8)	−0.0006 (7)	0.0018 (6)	0.0020 (7)
O5	0.0382 (9)	0.0185 (7)	0.0250 (8)	−0.0085 (6)	0.0073 (7)	0.0063 (6)
O6	0.0630 (12)	0.0175 (8)	0.0222 (8)	−0.0136 (8)	0.0136 (8)	−0.0040 (6)
O7	0.0431 (9)	0.0213 (7)	0.0149 (7)	0.0000 (7)	0.0082 (6)	0.0028 (6)
O8	0.0443 (9)	0.0171 (7)	0.0162 (7)	−0.0007 (6)	0.0125 (6)	0.0029 (6)
O9	0.0558 (11)	0.0132 (7)	0.0214 (8)	−0.0006 (7)	0.0148 (7)	−0.0019 (6)
O10	0.0374 (9)	0.0163 (7)	0.0186 (7)	−0.0023 (6)	0.0030 (6)	0.0071 (6)
O11	0.0382 (9)	0.0175 (7)	0.0180 (7)	0.0028 (6)	0.0128 (6)	0.0034 (6)
O12	0.0530 (10)	0.0135 (7)	0.0232 (8)	−0.0003 (7)	0.0145 (7)	−0.0008 (6)
O13	0.0347 (8)	0.0172 (7)	0.0190 (7)	−0.0023 (6)	0.0044 (6)	0.0071 (6)
O14	0.0279 (8)	0.0171 (7)	0.0229 (7)	−0.0046 (6)	0.0026 (6)	0.0079 (6)
O15	0.0595 (11)	0.0178 (8)	0.0212 (8)	−0.0124 (7)	0.0131 (7)	−0.0035 (6)
O16	0.0374 (9)	0.0206 (7)	0.0155 (7)	0.0013 (6)	0.0071 (6)	0.0025 (6)
O17	0.0421 (10)	0.0223 (8)	0.0290 (9)	−0.0001 (7)	0.0074 (7)	0.0066 (7)
O18	0.0414 (9)	0.0196 (8)	0.0263 (8)	−0.0002 (7)	0.0064 (7)	0.0039 (6)
O19	0.0358 (9)	0.0242 (8)	0.0292 (8)	0.0013 (7)	0.0088 (7)	0.0051 (6)
O20	0.0497 (11)	0.0333 (10)	0.0365 (10)	−0.0116 (8)	0.0067 (8)	0.0078 (8)
Na1	0.0304 (5)	0.0240 (4)	0.0226 (4)	0.0034 (4)	0.0040 (4)	0.0096 (3)
Na2	0.0257 (4)	0.0243 (4)	0.0284 (5)	−0.0008 (3)	0.0033 (3)	0.0073 (4)
Cd1	0.02259 (8)	0.01318 (8)	0.01772 (8)	0.00042 (5)	0.00074 (5)	−0.00040 (5)

Geometric parameters (Å, º)

C1—O7	1.229 (2)	N6—H6	0.8600
C1—N1	1.361 (2)	N8—H8	0.8600
C1—N3	1.390 (3)	N9—H9	0.8600
C2—O6	1.227 (3)	N10—H10	0.8600
C2—N2	1.357 (3)	N12—H12	0.8600
C2—N3	1.360 (3)	O1—Cd1	2.3478 (14)
C3—O5	1.225 (2)	O1—H1A	0.9836

C3—N1	1.354 (3)	O1—H1B	0.9829
C3—N2	1.385 (2)	O2—Cd1	2.2996 (15)
C4—O8	1.238 (2)	O2—H2A	0.9828
C4—N4	1.351 (2)	O2—H2B	0.9831
C4—N5	1.388 (2)	O3—Cd1	2.3913 (15)
C5—O9	1.225 (2)	O3—H3A	0.9830
C5—N6	1.357 (3)	O3—H3B	0.9833
C5—N5	1.359 (3)	O4—Na2	2.4627 (18)
C6—O10	1.219 (2)	O4—Cd1	2.4817 (16)
C6—N4	1.363 (2)	O4—H4A	0.9830
C6—N6	1.392 (2)	O4—H4B	0.9828
C7—O11	1.242 (2)	O5—Na2	2.3067 (17)
C7—N7	1.347 (2)	O10—Na1	2.3471 (16)
C7—N8	1.389 (2)	O13—Na1	2.3824 (16)
C8—O12	1.224 (2)	O14—Na2	2.4997 (18)
C8—N9	1.363 (3)	O17—Na1	2.3584 (19)
C8—N8	1.363 (2)	O17—Na1^{i}	2.4195 (19)
C9—O13	1.236 (2)	O17—H17A	0.9832
C9—N7	1.348 (2)	O17—H17B	0.9857
C9—N9	1.386 (2)	O18—Na1	2.3939 (18)
C10—O14	1.240 (2)	O18—Na1^{ii}	2.4192 (19)
C10—N11	1.344 (3)	O18—H18A	0.9841
C10—N12	1.389 (3)	O18—H18B	0.9830
C11—O15	1.227 (3)	O19—Na2	2.4009 (19)
C11—N12	1.361 (3)	O19—Na2^{iii}	2.4197 (18)
C11—N10	1.361 (3)	O19—H19A	0.9830
C12—O16	1.242 (2)	O19—H19B	0.9830
C12—N11	1.347 (3)	O20—Na2	2.3118 (19)
C12—N10	1.383 (3)	O20—H20A	0.9831
N1—Cd1	2.2541 (16)	O20—H20B	0.9833
N2—H2	0.8600	Na1—Na1^{ii}	3.4526 (17)
N3—H3	0.8600	Na1—Na1^{i}	3.5988 (17)
N4—Cd1	2.3210 (15)	Na2—Na2^{iii}	3.3557 (18)
N5—H5	0.8600		

O7—C1—N1	123.25 (18)	C10—O14—Na2	110.29 (13)
O7—C1—N3	118.73 (18)	Na1—O17—Na1^{i}	97.73 (6)
N1—C1—N3	118.01 (17)	Na1—O17—H17A	119.9
O6—C2—N2	122.93 (19)	Na1^{i}—O17—H17A	124.6
O6—C2—N3	122.67 (19)	Na1—O17—H17B	104.9
N2—C2—N3	114.40 (17)	Na1^{i}—O17—H17B	110.2
O5—C3—N1	122.71 (18)	H17A—O17—H17B	98.3
O5—C3—N2	118.59 (18)	Na1—O18—Na1^{ii}	91.67 (6)
N1—C3—N2	118.70 (17)	Na1—O18—H18A	120.5
O8—C4—N4	122.70 (17)	Na1^{ii}—O18—H18A	107.0
O8—C4—N5	117.98 (17)	Na1—O18—H18B	116.6
N4—C4—N5	119.31 (17)	Na1^{ii}—O18—H18B	118.1
O9—C5—N6	122.21 (18)	H18A—O18—H18B	103.3

O9—C5—N5	123.24 (18)	Na2—O19—Na2^{iii}	88.23 (6)
N6—C5—N5	114.55 (17)	Na2—O19—H19A	114.5
O10—C6—N4	122.79 (17)	Na2^{iii}—O19—H19A	114.5
O10—C6—N6	119.38 (17)	Na2—O19—H19B	114.5
N4—C6—N6	117.82 (16)	Na2^{iii}—O19—H19B	114.5
O11—C7—N7	121.84 (17)	H19A—O19—H19B	109.5
O11—C7—N8	118.25 (17)	Na2—O20—H20A	109.9
N7—C7—N8	119.91 (17)	Na2—O20—H20B	109.5
O12—C8—N9	122.17 (18)	H20A—O20—H20B	104.2
O12—C8—N8	123.57 (18)	O10—Na1—O17	88.93 (6)
N9—C8—N8	114.26 (17)	O10—Na1—O13	173.39 (7)
O13—C9—N7	122.52 (18)	O17—Na1—O13	84.51 (6)
O13—C9—N9	118.21 (17)	O10—Na1—O18	100.11 (6)
N7—C9—N9	119.27 (17)	O17—Na1—O18	170.94 (7)
O14—C10—N11	123.13 (18)	O13—Na1—O18	86.45 (6)
O14—C10—N12	117.85 (17)	O10—Na1—O17^{i}	89.31 (6)
N11—C10—N12	119.02 (17)	O17—Na1—O17^{i}	82.27 (6)
O15—C11—N12	123.32 (19)	O13—Na1—O17^{i}	90.60 (6)
O15—C11—N10	122.43 (19)	O18—Na1—O17^{i}	97.21 (6)
N12—C11—N10	114.24 (17)	O10—Na1—O18^{ii}	78.82 (6)
O16—C12—N11	122.52 (18)	O17—Na1—O18^{ii}	93.97 (6)
O16—C12—N10	117.89 (18)	O13—Na1—O18^{ii}	100.80 (6)
N11—C12—N10	119.58 (17)	O18—Na1—O18^{ii}	88.33 (6)
C3—N1—C1	120.31 (16)	O17^{i}—Na1—O18^{ii}	167.64 (7)
C3—N1—Cd1	114.93 (12)	O10—Na1—Na1^{ii}	89.19 (5)
C1—N1—Cd1	124.46 (13)	O17—Na1—Na1^{ii}	137.16 (6)
C2—N2—C3	124.18 (17)	O13—Na1—Na1^{ii}	95.07 (5)
C2—N2—H2	117.9	O18—Na1—Na1^{ii}	44.46 (4)
C3—N2—H2	117.9	O17^{i}—Na1—Na1^{ii}	140.49 (6)
C2—N3—C1	124.38 (17)	O18^{ii}—Na1—Na1^{ii}	43.88 (4)
C2—N3—H3	117.8	O10—Na1—Na1^{i}	88.84 (5)
C1—N3—H3	117.8	O17—Na1—Na1^{i}	41.77 (4)
C4—N4—C6	120.03 (16)	O13—Na1—Na1^{i}	86.81 (5)
C4—N4—Cd1	124.47 (12)	O18—Na1—Na1^{i}	137.02 (6)
C6—N4—Cd1	115.24 (12)	O17^{i}—Na1—Na1^{i}	40.49 (4)
C5—N5—C4	123.55 (16)	O18^{ii}—Na1—Na1^{i}	134.60 (6)
C5—N5—H5	118.2	Na1^{ii}—Na1—Na1^{i}	177.78 (5)
C4—N5—H5	118.2	O5—Na2—O20	179.41 (8)
C5—N6—C6	124.54 (16)	O5—Na2—O19	83.92 (6)
C5—N6—H6	117.7	O20—Na2—O19	96.15 (7)
C6—N6—H6	117.7	O5—Na2—O19^{iii}	83.78 (6)
C7—N7—C9	119.30 (16)	O20—Na2—O19^{iii}	96.81 (7)
C8—N8—C7	123.21 (16)	O19—Na2—O19^{iii}	91.77 (6)
C8—N8—H8	118.4	O5—Na2—O4	77.17 (6)
C7—N8—H8	118.4	O20—Na2—O4	102.25 (7)
C8—N9—C9	124.01 (17)	O19—Na2—O4	85.43 (6)
C8—N9—H9	118.0	O19^{iii}—Na2—O4	160.92 (7)
C9—N9—H9	118.0	O5—Na2—O14	94.52 (6)

C11—N10—C12	123.56 (17)	O20—Na2—O14	85.34 (7)
C11—N10—H10	118.2	O19—Na2—O14	172.40 (7)
C12—N10—H10	118.2	O19^{iii}—Na2—O14	95.47 (6)
C10—N11—C12	119.66 (17)	O4—Na2—O14	86.97 (6)
C11—N12—C10	123.89 (17)	O5—Na2—Na2^{iii}	81.14 (5)
C11—N12—H12	118.1	O20—Na2—Na2^{iii}	99.33 (6)
C10—N12—H12	118.1	O19—Na2—Na2^{iii}	46.11 (4)
Cd1—O1—H1A	110.2	O19^{iii}—Na2—Na2^{iii}	45.65 (5)
Cd1—O1—H1B	110.1	O4—Na2—Na2^{iii}	128.64 (6)
H1A—O1—H1B	97.0	O14—Na2—Na2^{iii}	141.06 (6)
Cd1—O2—H2A	109.8	N1—Cd1—O2	88.83 (6)
Cd1—O2—H2B	119.7	N1—Cd1—N4	174.58 (6)
H2A—O2—H2B	120.2	O2—Cd1—N4	88.80 (5)
Cd1—O3—H3A	111.0	N1—Cd1—O1	87.44 (5)
Cd1—O3—H3B	110.8	O2—Cd1—O1	111.45 (5)
H3A—O3—H3B	103.1	N4—Cd1—O1	88.89 (5)
Na2—O4—Cd1	117.77 (6)	N1—Cd1—O3	95.46 (6)
Na2—O4—H4A	107.4	O2—Cd1—O3	166.49 (5)
Cd1—O4—H4A	107.4	N4—Cd1—O3	87.94 (5)
Na2—O4—H4B	107.3	O1—Cd1—O3	81.59 (5)
Cd1—O4—H4B	107.3	N1—Cd1—O4	100.77 (6)
H4A—O4—H4B	109.5	O2—Cd1—O4	81.82 (6)
C3—O5—Na2	155.60 (16)	N4—Cd1—O4	83.72 (5)
C6—O10—Na1	152.13 (14)	O1—Cd1—O4	164.73 (5)
C9—O13—Na1	153.27 (14)	O3—Cd1—O4	84.79 (5)

O5—C3—N1—C1	177.79 (19)	O11—C7—N7—C9	179.44 (18)
N2—C3—N1—C1	−1.9 (3)	N8—C7—N7—C9	−0.5 (3)
O5—C3—N1—Cd1	−8.2 (3)	O13—C9—N7—C7	−179.33 (19)
N2—C3—N1—Cd1	172.08 (14)	N9—C9—N7—C7	1.7 (3)
O7—C1—N1—C3	−178.84 (19)	O12—C8—N8—C7	−178.5 (2)
N3—C1—N1—C3	1.4 (3)	N9—C8—N8—C7	1.4 (3)
O7—C1—N1—Cd1	7.8 (3)	O11—C7—N8—C8	178.91 (19)
N3—C1—N1—Cd1	−172.02 (13)	N7—C7—N8—C8	−1.2 (3)
O6—C2—N2—C3	179.9 (2)	O12—C8—N9—C9	179.9 (2)
N3—C2—N2—C3	0.4 (3)	N8—C8—N9—C9	0.0 (3)
O5—C3—N2—C2	−178.7 (2)	O13—C9—N9—C8	179.48 (19)
N1—C3—N2—C2	1.0 (3)	N7—C9—N9—C8	−1.5 (3)
O6—C2—N3—C1	179.5 (2)	O15—C11—N10—C12	178.5 (2)
N2—C2—N3—C1	−0.9 (3)	N12—C11—N10—C12	−0.8 (3)
O7—C1—N3—C2	−179.7 (2)	O16—C12—N10—C11	−176.9 (2)
N1—C1—N3—C2	0.1 (3)	N11—C12—N10—C11	1.9 (3)
O8—C4—N4—C6	−178.62 (19)	O14—C10—N11—C12	−177.67 (19)
N5—C4—N4—C6	0.6 (3)	N12—C10—N11—C12	2.1 (3)
O8—C4—N4—Cd1	7.4 (3)	O16—C12—N11—C10	176.32 (19)
N5—C4—N4—Cd1	−173.39 (13)	N10—C12—N11—C10	−2.5 (3)
O10—C6—N4—C4	177.24 (19)	O15—C11—N12—C10	−179.0 (2)
N6—C6—N4—C4	−4.1 (3)	N10—C11—N12—C10	0.3 (3)

O10—C6—N4—Cd1	−8.3 (2)	O14—C10—N12—C11	178.8 (2)
N6—C6—N4—Cd1	170.42 (13)	N11—C10—N12—C11	−1.0 (3)
O9—C5—N5—C4	178.2 (2)	N1—C3—O5—Na2	−79.6 (4)
N6—C5—N5—C4	−1.6 (3)	N2—C3—O5—Na2	100.1 (4)
O8—C4—N5—C5	−178.30 (19)	N4—C6—O10—Na1	−143.5 (2)
N4—C4—N5—C5	2.5 (3)	N6—C6—O10—Na1	37.8 (4)
O9—C5—N6—C6	178.0 (2)	N7—C9—O13—Na1	118.8 (3)
N5—C5—N6—C6	−2.3 (3)	N9—C9—O13—Na1	−62.3 (4)
O10—C6—N6—C5	−176.13 (19)	N11—C10—O14—Na2	87.6 (2)
N4—C6—N6—C5	5.1 (3)	N12—C10—O14—Na2	−92.13 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N11^{iv}	0.98	1.82	2.788 (2)	168
O1—H1*B*···N7^{ii}	0.98	1.89	2.860 (2)	169
N2—H2···O15^{v}	0.86	1.96	2.817 (2)	173
O2—H2*A*···O13^{i}	0.98	1.77	2.716 (2)	161
O2—H2*B*···N11	0.98	2.53	3.236 (2)	128
O2—H2*B*···O16	0.98	1.79	2.753 (2)	167
N3—H3···O11^{vi}	0.86	1.92	2.773 (2)	173
O3—H3*A*···O14^{iv}	0.98	1.91	2.871 (2)	166
O3—H3*B*···O11^{ii}	0.98	1.87	2.842 (2)	169
N5—H5···O16^{vii}	0.86	2.10	2.938 (2)	164
N6—H6···O12^{vii}	0.86	2.13	2.979 (2)	168
N10—H10···O8^{viii}	0.86	1.94	2.792 (2)	172
N8—H8···O7^{vi}	0.86	2.02	2.862 (2)	167
N12—H12···O6^{v}	0.86	2.03	2.882 (2)	173
N9—H9···O9^{viii}	0.86	2.04	2.885 (2)	169
O20—H20*B*···O6^{ix}	0.98	2.30	2.903 (2)	119
O20—H20*A*···O14^{x}	0.98	2.14	3.008 (2)	147
O4—H4*A*···O8	0.98	1.88	2.725 (2)	143
O17—H17*B*···O2	0.99	1.87	2.768 (2)	149
O17—H17*A*···O9^{viii}	0.98	1.81	2.790 (2)	171
O18—H18*B*···O12^{vii}	0.98	1.91	2.852 (2)	160

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*+2, −*y*, −*z*; (iv) *x*+1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*+1; (vi) −*x*+2, −*y*+1, −*z*; (vii) *x*, *y*−1, *z*; (viii) *x*, *y*+1, *z*; (ix) *x*−1, *y*−1, *z*; (x) −*x*, −*y*, −*z*+1.