Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Tetrakis(2,4,6-triamino-1,3,5-triazin-1-ium) tris(pyridine-2,6-dicarboxylato)-calcate(II) hexahydrate

**Hossein Aghabozorg,[a]* Shirin Daneshvar[b] and Andya Nemati[a]**

[a]Faculty of Chemistry, Tarbiat Moallem University, Tehran, Iran, and [b]Department of Chemistry, Islamic Azad University, Ardabil Branch, Ardabil, Iran
Correspondence e-mail: haghabozorg@yahoo.com

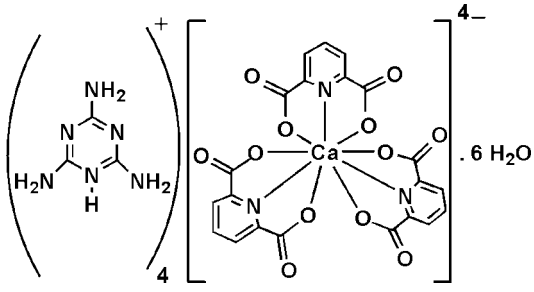
Received 26 June 2008; accepted 21 July 2008

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.052; $wR$ factor = 0.127; data-to-parameter ratio = 17.0.

The title compound, $(C_3H_7N_6)_4[Ca(C_7H_3NO_4)_3]\cdot 6H_2O$ or $(tataH)_4[Ca(pydc)_3]\cdot 6H_2O$ (where tata is 2,4,6-triamino-1,3,5-triazine and $pydcH_2$ is pyridine-2,6-dicarboxylic acid), was obtained by reaction of $Ca(NO_3)_2\cdot 4H_2O$ with the proton-transfer compound $(tataH)_2(pydc)$ in aqueous solution. The $[Ca(pydc)_3]^{4-}$ anion has twofold crystallographic symmetry. It is a nine-coordinate $Ca^{II}$ complex with a distorted tricapped trigonal-prismatic coordination geometry. The structure also contains four $tataH^+$ cations and six uncoordinated water molecules. There are extensive O—H···O, O—H···N, N—H···O, N—H···N and C—H···O hydrogen bonds in the crystal structure.

## Related literature

For related literature, see: Aghabozorg *et al.* (2006); Aghabozorg, Attar Gharamaleki *et al.* (2008); Aghabozorg, Manteghi & Sheshmani (2008); Aghajani *et al.* (2006); Sharif *et al.* (2007).




## Experimental

### Crystal data

$(C_3H_7N_6)_4[Ca(C_7H_3NO_4)_3]\cdot 6H_2O$
$M_r$ = 1152.07
Monoclinic, $C2/c$
$a$ = 17.9605 (15) Å
$b$ = 10.1672 (9) Å
$c$ = 25.922 (2) Å
$\beta$ = 94.467 (2)°
$V$ = 4719.1 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.24 mm$^{-1}$
$T$ = 100 (2) K
0.30 × 0.20 × 0.20 mm

### Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.928, $T_{max}$ = 0.954
16983 measured reflections
6215 independent reflections
4412 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.127
$S$ = 1.09
6215 reflections
365 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.77 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1*W*—H1*WB*···O2$^{i}$ | 0.84 | 1.91 | 2.710 (3) | 160 |
| O1*W*—H1*WA*···O6$^{ii}$ | 0.84 | 1.92 | 2.751 (3) | 170 |
| O2*W*—H2*WB*···N4$^{iii}$ | 0.84 | 2.26 | 3.022 (3) | 151 |
| N3—H3*N*···O2 | 0.88 | 1.79 | 2.667 (2) | 176 |
| O2*W*—H2*WA*···O5 | 0.84 | 2.05 | 2.888 (3) | 175 |
| O3*W*—H3*WB*···O2*W*$^{iv}$ | 0.84 | 2.18 | 2.963 (3) | 154 |
| O3*W*—H3*WA*···N14$^{v}$ | 0.84 | 2.17 | 3.007 (3) | 180 |
| N6—H6*NA*···O1*W*$^{i}$ | 0.88 | 2.45 | 3.294 (3) | 162 |
| N6—H6*NB*···O1*W* | 0.88 | 1.90 | 2.740 (3) | 160 |
| N7—H7*NA*···N11$^{v}$ | 0.88 | 2.22 | 3.103 (3) | 176 |
| N7—H7*NB*···O2*W*$^{ii}$ | 0.88 | 2.44 | 3.205 (3) | 146 |
| N7—H7*NB*···O4$^{ii}$ | 0.88 | 2.53 | 3.111 (2) | 124 |
| N8—H8*NA*···O1 | 0.88 | 2.07 | 2.948 (2) | 172 |
| N12—H11*A*···N10$^{vi}$ | 0.88 | 2.23 | 3.109 (2) | 178 |
| N12—H11*B*···O5 | 0.88 | 2.32 | 3.196 (2) | 175 |
| N8—H8*NB*···O3*W* | 0.88 | 2.15 | 2.832 (4) | 134 |
| N9—H9*NA*···O3 | 0.88 | 1.89 | 2.754 (2) | 165 |
| N13—H13*A*···O4$^{vii}$ | 0.88 | 2.08 | 2.925 (2) | 160 |
| N13—H13*B*···O6$^{vi}$ | 0.88 | 1.96 | 2.790 (2) | 157 |
| N14—H14*A*···O3 | 0.88 | 2.39 | 3.143 (2) | 144 |
| N14—H14*B*···N5$^{viii}$ | 0.88 | 2.10 | 2.978 (3) | 178 |
| C4—H4*A*···O2$^{ix}$ | 0.95 | 2.55 | 3.370 (3) | 145 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2249).

## References


Aghabozorg, H., Aghajani, Z. & Sharif, M. A. (2006). *Acta Cryst.* E**62**, m1930–m1932.

Aghabozorg, H., Attar Gharamaleki, J., Daneshvar, S., Ghadermazi, M. & Khavasi, H. R. (2008). *Acta Cryst.* E**64**, m187–m188.

Aghabozorg, H., Manteghi, F. & Sheshmani, S. (2008). *J. Iran. Chem. Soc.* **5,** 184-227.

Aghajani, Z., Sharif, M. A., Aghabozorg, H. & Naderpour, A. (2006). *Acta Cryst.* E**62**, m830–m832.

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.

Sharif, M. A., Aghabozorg, H. & Moghimi, A. (2007). *Acta Cryst.* E**63**, m1599–m1601.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2008). E**64**, m1063–m1064 [doi:10.1107/S1600536808022873]

# Tetrakis(2,4,6-triamino-1,3,5-triazin-1-ium) tris(pyridine-2,6-dicarboxylato)calcate(II) hexahydrate

**Hossein Aghabozorg, Shirin Daneshvar and Andya Nemati**

## S1. Comment

Hydrogen bonding plays a key role in chemical, catalytic and biochemical processes, as well as in supramolecular chemistry and crystal engineering. Recently we have reported the reaction between the proton-transfer compound, $(tataH)_2(pydc)$ with metal salts $Co(NO_3)_2.6H_2O$, $Bi(NO_3)_3.5H_2O$, $Zn(NO_3)_2.4H_2O$ and $Cd(NO_3)_2.2H_2O$ in a 2:1 molar ratio. These reactions lead to the formation of the $(tataH)_2[Co(H_2O)_6][Co(pydc)_2]_2.4H_2O$ (Aghabozorg, Attar Gharamaleki *et al.*, 2008), $(tataH)_n$ $[Bi(pydc)_2(H_2O)]_n$(Sharif *et al.*, 2007), $(tataH)_2$ $[Zn(pydc)_2].10H_2O$ (Aghajani *et al.*, 2006) and $(tataH)_2$ $[Cd(pydc)_2]$ (Aghabozorg, Aghajani *et al.*, 2006) compounds respectively. For more details and related literature see our recent review article (Aghabozorg, Manteghi *et al.*, 2008).

The structure of the title compound is shown in Fig.1. The anion has crystallographic 2-fold symmetry. The compound contains $[Ca(pydc)_3]^{4-}$ anion, four $(tataH)^+$ cations and six uncoordinated water molecules. In the $[Ca(pydc)_3]^{4-}$ anions, $Ca^{II}$ atom is nine-coordinated by three N atoms (N1, N1a and N2) and six O atoms (O1, O1a, O3, O3a, O5 and O5a) with the range of 2.5031 (14)–2.5472 (15)Å from the carboxylate groups of three $(pydc)^{2-}$ groups that act as tridentate ligands. The coordination geometry around the $Ca^{II}$ atom is distorted tricapped trigonal prism (Fig.2). Three N atoms (N1, N1a and N2) occupying three cap positions and make a flat triangle with N1—Ca1—N1a: 119.78 (8)°, N1—Ca1—N2: 120.11 (4)° and N1a—Ca1—N2: 120.11 (4)° that the sum of these angles is 360.00° and six O atoms (O1, O1a, O3, O3a, O5 and O5a) forming the trigonal prism positions.

There are various hydrogen bonds such as O—H···O, O—H···N, N—H···O and N—H···N [in the range 2.667 (2)–3.294 (3) Å] in this structure (Fig.3) and C—H···O hydrogen bonds [with D···A 3.370 (3) Å] are also present (Table 1). These extensive hydrogen bonds between $[Ca(pydc)_3]^{4-}$ anions, $(tataH)^+$ cations and uncoordinated water molecules play an important role in stabilization of the crystal packing.

## S2. Experimental

The proton-transfer compound, $(tataH)_2(pydc)$, was prepared by the reaction of pyridine-2,6-dicarboxylic acid ($pydcH_2$) with 2,4,6-triamino-1,3,5-triazine (tata). The reaction between $Ca(NO_3)_2.4H_2O$ (118 mg, 0.5 mmol) in water (20 ml) and $(tataH)_2(pydc)$ (420 mg, 1.0 mmol) in water (20 ml), in 1:2 molar ratio gave a colorless compound after slow evaporation of the solvent at the room temperature.

## S3. Refinement

The hydrogen atoms of NH groups and also H atoms of water molecule were found in difference Fourier synthesis. The hydrogen atoms of the H(C) atom positions were calculated. All hydrogen atoms were refined in isotropic approximation in riding model with the $U_{iso}$(H) parameters equal to 1.2 $U_{eq}$(Xi), where U(Xi) the equivalent thermal parameters of the carbon or nitrogen or oxygen atom to which corresponding H atom is bonded. Distances employed in the riding model

are, N-H, 0.88 Å; O-H, 0.84 Å; C-H, 0.95 Å.

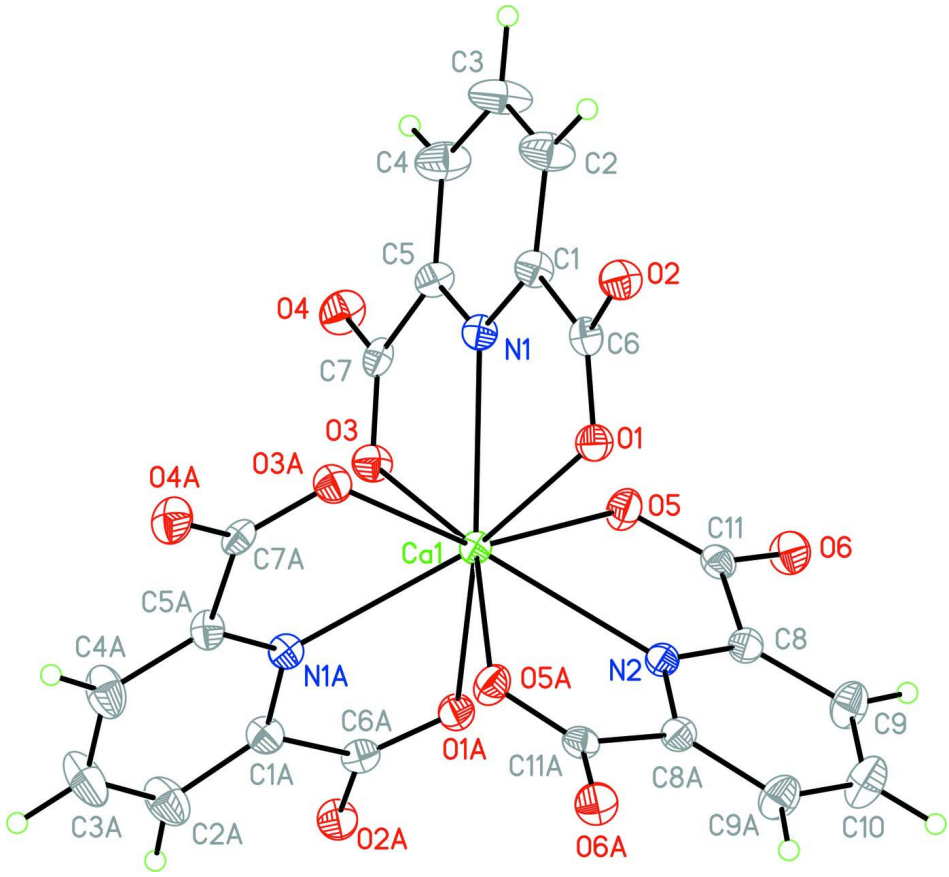



**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. The anion is located on a 2-fold axis and thus, the asymmetric unit contains one half anion, two cations and three water molecules.

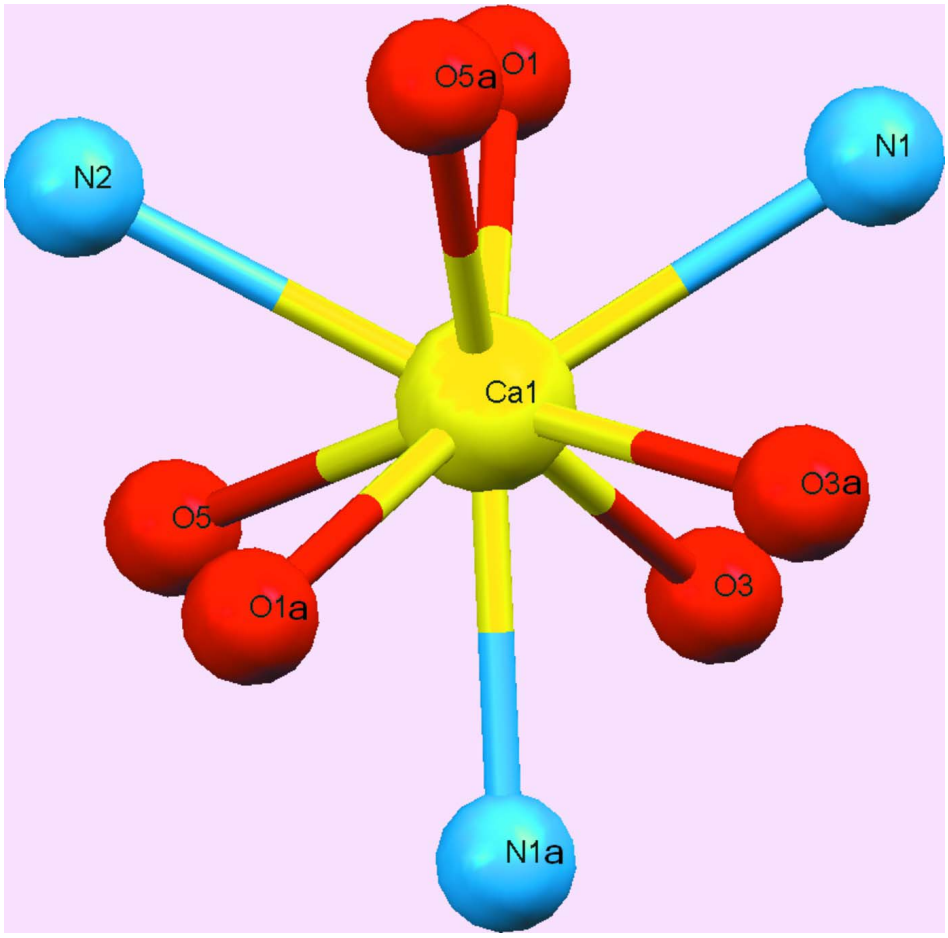



**Figure 2**

A view of the distorted tricapped trigonal prism around the $Ca^{II}$ atom.

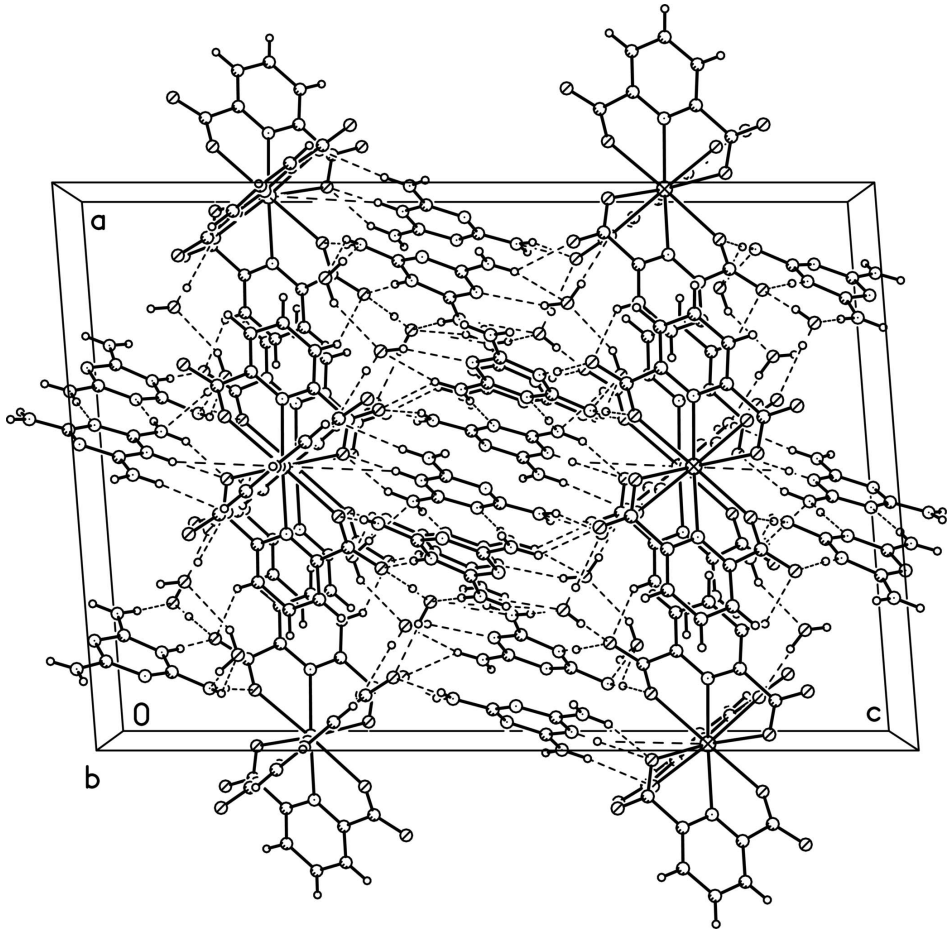



**Figure 3**

Crystal packing with hydrogen bonds shown as dashed lines.

**Tetrakis(2,4,6-triamino-1,3,5-triazin-1-ium) tris(pyridine-2,6-dicarboxylato)calcate(II) hexahydrate**

*Crystal data*

$(C_3H_7N_6)_4[Ca(C_7H_3NO_4)_3]\cdot 6H_2O$
$M_r = 1152.07$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 17.9605\ (15)$ Å
$b = 10.1672\ (9)$ Å
$c = 25.922\ (2)$ Å
$\beta = 94.467\ (2)°$
$V = 4719.1\ (7)$ Å$^3$
$Z = 4$
$F(000) = 2400$
$D_x = 1.622$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 935 reflections
$\theta = 3–29°$
$\mu = 0.24$ mm$^{-1}$
$T = 100$ K
Prism, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.928$, $T_{max} = 0.954$
16983 measured reflections
6215 independent reflections
4412 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.031
$\theta_{max}$ = 29.0°, $\theta_{min}$ = 1.6°
$h$ = −19→24
$k$ = −13→13
$l$ = −35→35

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.127
$S$ = 1.09
6215 reflections
365 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
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 1P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.77 e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ca1 | 0.0000 | 0.32225 (5) | 0.2500 | 0.01468 (13) |
| C1 | 0.17008 (12) | 0.2206 (2) | 0.21823 (8) | 0.0189 (4) |
| N1 | 0.12161 (10) | 0.19798 (16) | 0.25401 (6) | 0.0167 (3) |
| O1 | 0.08882 (8) | 0.38891 (14) | 0.18496 (5) | 0.0198 (3) |
| O1W | 0.25538 (11) | 0.3625 (2) | −0.08194 (7) | 0.0511 (6) |
| H1WB | 0.2800 | 0.3196 | −0.1025 | 0.061* |
| H1WA | 0.2150 | 0.3792 | −0.0992 | 0.061* |
| O2W | 0.20543 (11) | 0.3177 (2) | 0.38198 (7) | 0.0464 (5) |
| H2WB | 0.2093 | 0.3575 | 0.4105 | 0.056* |
| H2WA | 0.1704 | 0.3502 | 0.3627 | 0.056* |
| O2 | 0.18167 (9) | 0.32683 (15) | 0.13789 (6) | 0.0225 (3) |
| N2 | 0.0000 | 0.5723 (2) | 0.2500 | 0.0160 (5) |
| C2 | 0.23993 (13) | 0.1634 (3) | 0.21999 (9) | 0.0291 (5) |
| H2A | 0.2733 | 0.1824 | 0.1943 | 0.035* |
| O3W | 0.16530 (16) | 0.8783 (3) | 0.17830 (10) | 0.0743 (8) |
| H3WB | 0.2094 | 0.8677 | 0.1704 | 0.089* |
| H3WA | 0.1367 | 0.9132 | 0.1550 | 0.089* |
| N3 | 0.16153 (10) | 0.53273 (18) | 0.07458 (7) | 0.0222 (4) |
| H3N | 0.1666 | 0.4663 | 0.0963 | 0.027* |
| O3 | 0.02261 (8) | 0.15716 (14) | 0.32346 (5) | 0.0203 (3) |
| C3 | 0.26030 (14) | 0.0777 (3) | 0.26017 (9) | 0.0345 (6) |
| H3A | 0.3079 | 0.0366 | 0.2624 | 0.041* |

| | | | | |
|---|---|---|---|---|
| O4 | 0.10324 (9) | 0.02965 (15) | 0.37134 (6) | 0.0252 (3) |
| C4 | 0.21035 (14) | 0.0525 (2) | 0.29714 (9) | 0.0292 (5) |
| H4A | 0.2230 | −0.0063 | 0.3249 | 0.035* |
| N4 | 0.18475 (10) | 0.62366 (18) | −0.00573 (7) | 0.0217 (4) |
| O5 | 0.08073 (9) | 0.43271 (14) | 0.32086 (6) | 0.0220 (3) |
| C5 | 0.14127 (12) | 0.1153 (2) | 0.29278 (8) | 0.0183 (4) |
| N5 | 0.12433 (10) | 0.75024 (17) | 0.05810 (7) | 0.0207 (4) |
| N6 | 0.22996 (11) | 0.41835 (19) | 0.01860 (8) | 0.0275 (4) |
| H6NA | 0.2338 | 0.3554 | 0.0419 | 0.033* |
| H6NB | 0.2477 | 0.4118 | −0.0120 | 0.033* |
| O6 | 0.11801 (9) | 0.61386 (15) | 0.36402 (6) | 0.0236 (3) |
| C6 | 0.14421 (12) | 0.3194 (2) | 0.17714 (7) | 0.0174 (4) |
| N7 | 0.13887 (10) | 0.83102 (18) | −0.02277 (7) | 0.0224 (4) |
| H7NA | 0.1188 | 0.9049 | −0.0129 | 0.027* |
| H7NB | 0.1526 | 0.8246 | −0.0545 | 0.027* |
| C7 | 0.08494 (12) | 0.09839 (19) | 0.33279 (8) | 0.0171 (4) |
| N8 | 0.09931 (11) | 0.64715 (19) | 0.13431 (7) | 0.0257 (4) |
| H8NA | 0.0972 | 0.5743 | 0.1525 | 0.031* |
| H8NB | 0.0923 | 0.7219 | 0.1503 | 0.031* |
| C8 | 0.04098 (11) | 0.6393 (2) | 0.28661 (8) | 0.0175 (4) |
| N9 | −0.02526 (10) | 0.21627 (17) | 0.41916 (6) | 0.0189 (4) |
| H9NA | −0.0085 | 0.2124 | 0.3882 | 0.023* |
| C9 | 0.04259 (14) | 0.7762 (2) | 0.28768 (9) | 0.0250 (5) |
| H9A | 0.0724 | 0.8215 | 0.3138 | 0.030* |
| C10 | 0.0000 | 0.8452 (3) | 0.2500 | 0.0301 (8) |
| H10A | 0.0000 | 0.9386 | 0.2500 | 0.036* |
| N10 | −0.03939 (10) | 0.32331 (17) | 0.49808 (6) | 0.0179 (4) |
| C11 | 0.08390 (11) | 0.5555 (2) | 0.32701 (8) | 0.0170 (4) |
| N11 | −0.07504 (10) | 0.09514 (17) | 0.48552 (7) | 0.0187 (4) |
| N12 | 0.01468 (10) | 0.42995 (18) | 0.43181 (7) | 0.0219 (4) |
| H11A | 0.0226 | 0.4986 | 0.4522 | 0.041 (8)* |
| H11B | 0.0304 | 0.4273 | 0.4005 | 0.033 (7)* |
| C12 | 0.15006 (12) | 0.7326 (2) | 0.01068 (8) | 0.0199 (4) |
| N13 | −0.08510 (11) | 0.19908 (18) | 0.56239 (7) | 0.0230 (4) |
| H13A | −0.0983 | 0.1240 | 0.5759 | 0.039 (8)* |
| H13B | −0.0842 | 0.2683 | 0.5828 | 0.029 (7)* |
| C13 | 0.12875 (12) | 0.6464 (2) | 0.08866 (8) | 0.0206 (4) |
| N14 | −0.06375 (11) | 0.00349 (19) | 0.40544 (7) | 0.0273 (4) |
| H14A | −0.0459 | 0.0126 | 0.3750 | 0.033 (7)* |
| H14B | −0.0830 | −0.0706 | 0.4158 | 0.036 (8)* |
| C14 | 0.19208 (12) | 0.5258 (2) | 0.02825 (8) | 0.0217 (4) |
| C15 | −0.01687 (11) | 0.3235 (2) | 0.45053 (8) | 0.0171 (4) |
| C16 | −0.06599 (12) | 0.2060 (2) | 0.51433 (8) | 0.0183 (4) |
| C17 | −0.05485 (11) | 0.1040 (2) | 0.43758 (8) | 0.0188 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ca1 | 0.0160 (3) | 0.0136 (3) | 0.0145 (3) | 0.000 | 0.0015 (2) | 0.000 |
| C1 | 0.0193 (11) | 0.0216 (10) | 0.0160 (9) | 0.0004 (8) | 0.0023 (8) | 0.0019 (8) |
| N1 | 0.0178 (9) | 0.0173 (8) | 0.0150 (8) | −0.0001 (7) | 0.0020 (6) | −0.0004 (6) |
| O1 | 0.0198 (8) | 0.0186 (7) | 0.0215 (7) | 0.0008 (6) | 0.0044 (6) | 0.0036 (6) |
| O1W | 0.0303 (10) | 0.0852 (16) | 0.0357 (10) | 0.0236 (10) | −0.0111 (8) | −0.0261 (10) |
| O2W | 0.0510 (12) | 0.0472 (12) | 0.0378 (10) | 0.0222 (10) | −0.0160 (9) | −0.0154 (9) |
| O2 | 0.0240 (8) | 0.0243 (8) | 0.0200 (7) | 0.0016 (6) | 0.0077 (6) | 0.0054 (6) |
| N2 | 0.0160 (12) | 0.0156 (11) | 0.0168 (11) | 0.000 | 0.0044 (9) | 0.000 |
| C2 | 0.0240 (12) | 0.0416 (14) | 0.0227 (11) | 0.0080 (11) | 0.0074 (9) | 0.0077 (10) |
| O3W | 0.089 (2) | 0.0615 (16) | 0.0691 (17) | 0.0005 (15) | −0.0175 (14) | −0.0047 (13) |
| N3 | 0.0229 (10) | 0.0190 (9) | 0.0250 (9) | 0.0023 (7) | 0.0041 (8) | 0.0065 (7) |
| O3 | 0.0202 (8) | 0.0223 (8) | 0.0187 (7) | 0.0012 (6) | 0.0037 (6) | 0.0027 (6) |
| C3 | 0.0242 (13) | 0.0500 (16) | 0.0300 (13) | 0.0167 (11) | 0.0075 (10) | 0.0120 (11) |
| O4 | 0.0322 (9) | 0.0242 (8) | 0.0197 (7) | 0.0030 (7) | 0.0047 (6) | 0.0077 (6) |
| C4 | 0.0303 (13) | 0.0347 (13) | 0.0227 (11) | 0.0120 (11) | 0.0038 (9) | 0.0097 (10) |
| N4 | 0.0190 (9) | 0.0227 (9) | 0.0230 (9) | 0.0009 (7) | 0.0003 (7) | 0.0035 (7) |
| O5 | 0.0249 (8) | 0.0161 (7) | 0.0238 (8) | −0.0007 (6) | −0.0048 (6) | −0.0004 (6) |
| C5 | 0.0209 (11) | 0.0182 (10) | 0.0160 (9) | 0.0029 (8) | 0.0022 (8) | 0.0008 (7) |
| N5 | 0.0205 (9) | 0.0192 (9) | 0.0220 (9) | −0.0017 (7) | 0.0004 (7) | 0.0015 (7) |
| N6 | 0.0297 (11) | 0.0248 (10) | 0.0290 (10) | 0.0063 (8) | 0.0080 (8) | 0.0063 (8) |
| O6 | 0.0250 (8) | 0.0246 (8) | 0.0205 (7) | −0.0011 (7) | −0.0031 (6) | −0.0052 (6) |
| C6 | 0.0188 (10) | 0.0183 (10) | 0.0149 (9) | −0.0030 (8) | 0.0006 (8) | 0.0002 (7) |
| N7 | 0.0233 (10) | 0.0222 (9) | 0.0217 (9) | 0.0012 (8) | 0.0006 (7) | 0.0037 (7) |
| C7 | 0.0231 (11) | 0.0117 (9) | 0.0167 (9) | −0.0021 (8) | 0.0029 (8) | −0.0013 (7) |
| N8 | 0.0339 (11) | 0.0198 (9) | 0.0241 (9) | 0.0005 (8) | 0.0065 (8) | 0.0028 (7) |
| C8 | 0.0183 (10) | 0.0171 (9) | 0.0178 (9) | −0.0006 (8) | 0.0055 (8) | −0.0011 (7) |
| N9 | 0.0219 (9) | 0.0207 (9) | 0.0147 (8) | 0.0016 (7) | 0.0050 (7) | 0.0009 (7) |
| C9 | 0.0322 (13) | 0.0194 (10) | 0.0228 (11) | −0.0025 (9) | −0.0019 (9) | −0.0030 (8) |
| C10 | 0.044 (2) | 0.0179 (15) | 0.0273 (17) | 0.000 | −0.0032 (15) | 0.000 |
| N10 | 0.0215 (9) | 0.0158 (8) | 0.0167 (8) | 0.0008 (7) | 0.0032 (7) | 0.0012 (6) |
| C11 | 0.0146 (10) | 0.0199 (10) | 0.0168 (9) | −0.0012 (8) | 0.0034 (7) | −0.0010 (7) |
| N11 | 0.0197 (9) | 0.0173 (8) | 0.0193 (8) | −0.0011 (7) | 0.0038 (7) | −0.0011 (7) |
| N12 | 0.0249 (10) | 0.0214 (9) | 0.0200 (9) | −0.0006 (8) | 0.0068 (7) | 0.0025 (7) |
| C12 | 0.0144 (10) | 0.0228 (10) | 0.0217 (10) | −0.0031 (8) | −0.0035 (8) | 0.0027 (8) |
| N13 | 0.0356 (11) | 0.0160 (9) | 0.0182 (8) | −0.0043 (8) | 0.0071 (8) | −0.0012 (7) |
| C13 | 0.0185 (10) | 0.0201 (10) | 0.0227 (10) | −0.0027 (8) | −0.0004 (8) | 0.0012 (8) |
| N14 | 0.0353 (11) | 0.0258 (10) | 0.0221 (9) | −0.0079 (9) | 0.0106 (8) | −0.0068 (8) |
| C14 | 0.0152 (10) | 0.0234 (11) | 0.0265 (11) | −0.0008 (8) | 0.0009 (8) | 0.0033 (8) |
| C15 | 0.0150 (10) | 0.0172 (9) | 0.0189 (9) | 0.0024 (8) | 0.0004 (7) | 0.0021 (8) |
| C16 | 0.0170 (10) | 0.0183 (10) | 0.0197 (10) | 0.0016 (8) | 0.0014 (8) | 0.0009 (8) |
| C17 | 0.0155 (10) | 0.0206 (10) | 0.0204 (10) | 0.0015 (8) | 0.0020 (8) | −0.0013 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ca1—O1 | 2.5031 (14) | O5—C11 | 1.259 (2) |
| Ca1—O1$^{i}$ | 2.5032 (14) | C5—C7 | 1.514 (3) |
| Ca1—O5$^{i}$ | 2.5145 (15) | N5—C13 | 1.319 (3) |
| Ca1—O5 | 2.5145 (15) | N5—C12 | 1.358 (3) |
| Ca1—N1$^{i}$ | 2.5184 (18) | N6—C14 | 1.321 (3) |
| Ca1—N1 | 2.5184 (18) | N6—H6NA | 0.8800 |
| Ca1—N2 | 2.542 (2) | N6—H6NB | 0.8798 |
| Ca1—O3$^{i}$ | 2.5472 (15) | O6—C11 | 1.248 (2) |
| Ca1—O3 | 2.5472 (15) | N7—C12 | 1.329 (3) |
| C1—N1 | 1.340 (3) | N7—H7NA | 0.8800 |
| C1—C2 | 1.380 (3) | N7—H7NB | 0.8800 |
| C1—C6 | 1.511 (3) | N8—C13 | 1.333 (3) |
| N1—C5 | 1.337 (3) | N8—H8NA | 0.8800 |
| O1—C6 | 1.250 (2) | N8—H8NB | 0.8800 |
| O1W—H1WB | 0.8400 | C8—C9 | 1.393 (3) |
| O1W—H1WA | 0.8400 | C8—C11 | 1.514 (3) |
| O2W—H2WB | 0.8400 | N9—C15 | 1.362 (3) |
| O2W—H2WA | 0.8400 | N9—C17 | 1.361 (3) |
| O2—C6 | 1.265 (2) | N9—H9NA | 0.8800 |
| N2—C8$^{i}$ | 1.340 (2) | C9—C10 | 1.384 (3) |
| N2—C8 | 1.340 (2) | C9—H9A | 0.9500 |
| C2—C3 | 1.385 (3) | C10—C9$^{i}$ | 1.384 (3) |
| C2—H2A | 0.9500 | C10—H10A | 0.9500 |
| O3W—H3WB | 0.8400 | N10—C15 | 1.327 (3) |
| O3W—H3WA | 0.8401 | N10—C16 | 1.363 (3) |
| N3—C13 | 1.360 (3) | N11—C17 | 1.324 (3) |
| N3—C14 | 1.360 (3) | N11—C16 | 1.355 (3) |
| N3—H3N | 0.8800 | N12—C15 | 1.330 (3) |
| O3—C7 | 1.275 (3) | N12—H11A | 0.8801 |
| C3—C4 | 1.386 (3) | N12—H11B | 0.8799 |
| C3—H3A | 0.9500 | N13—C16 | 1.319 (3) |
| O4—C7 | 1.243 (2) | N13—H13A | 0.8800 |
| C4—C5 | 1.392 (3) | N13—H13B | 0.8799 |
| C4—H4A | 0.9500 | N14—C17 | 1.320 (3) |
| N4—C14 | 1.329 (3) | N14—H14A | 0.8800 |
| N4—C12 | 1.356 (3) | N14—H14B | 0.8800 |
| | | | |
| O1—Ca1—O1$^{i}$ | 148.58 (7) | N1—C5—C4 | 122.08 (19) |
| O1—Ca1—O5$^{i}$ | 75.43 (5) | N1—C5—C7 | 115.77 (18) |
| O1$^{i}$—Ca1—O5$^{i}$ | 90.55 (5) | C4—C5—C7 | 122.11 (19) |
| O1—Ca1—O5 | 90.55 (5) | C13—N5—C12 | 115.43 (19) |
| O1$^{i}$—Ca1—O5 | 75.43 (5) | C14—N6—H6NA | 119.0 |
| O5$^{i}$—Ca1—O5 | 126.94 (7) | C14—N6—H6NB | 117.5 |
| O1—Ca1—N1$^{i}$ | 134.76 (5) | H6NA—N6—H6NB | 123.4 |
| O1$^{i}$—Ca1—N1$^{i}$ | 64.37 (5) | O1—C6—O2 | 125.19 (19) |
| O5$^{i}$—Ca1—N1$^{i}$ | 75.23 (5) | O1—C6—C1 | 117.84 (17) |

| | | | |
|---|---|---|---|
| O5—Ca1—N1$^{i}$ | 134.68 (5) | O2—C6—C1 | 116.96 (18) |
| O1—Ca1—N1 | 64.37 (5) | C12—N7—H7NA | 119.8 |
| O1$^{i}$—Ca1—N1 | 134.76 (5) | C12—N7—H7NB | 121.1 |
| O5$^{i}$—Ca1—N1 | 134.68 (5) | H7NA—N7—H7NB | 119.1 |
| O5—Ca1—N1 | 75.23 (5) | O4—C7—O3 | 126.11 (19) |
| N1$^{i}$—Ca1—N1 | 119.78 (8) | O4—C7—C5 | 117.75 (19) |
| O1—Ca1—N2 | 74.29 (4) | O3—C7—C5 | 116.14 (17) |
| O1$^{i}$—Ca1—N2 | 74.29 (4) | C13—N8—H8NA | 120.4 |
| O5$^{i}$—Ca1—N2 | 63.47 (4) | C13—N8—H8NB | 120.4 |
| O5—Ca1—N2 | 63.47 (4) | H8NA—N8—H8NB | 117.4 |
| N1$^{i}$—Ca1—N2 | 120.11 (4) | N2—C8—C9 | 122.1 (2) |
| N1—Ca1—N2 | 120.11 (4) | N2—C8—C11 | 115.19 (18) |
| O1—Ca1—O3$^{i}$ | 75.39 (5) | C9—C8—C11 | 122.70 (19) |
| O1$^{i}$—Ca1—O3$^{i}$ | 127.53 (5) | C15—N9—C17 | 119.35 (17) |
| O5$^{i}$—Ca1—O3$^{i}$ | 72.48 (5) | C15—N9—H9NA | 123.4 |
| O5—Ca1—O3$^{i}$ | 152.84 (5) | C17—N9—H9NA | 117.0 |
| N1$^{i}$—Ca1—O3$^{i}$ | 63.34 (5) | C10—C9—C8 | 118.9 (2) |
| N1—Ca1—O3$^{i}$ | 77.73 (5) | C10—C9—H9A | 120.6 |
| N2—Ca1—O3$^{i}$ | 131.22 (3) | C8—C9—H9A | 120.6 |
| O1—Ca1—O3 | 127.53 (5) | C9$^{i}$—C10—C9 | 119.1 (3) |
| O1$^{i}$—Ca1—O3 | 75.39 (5) | C9$^{i}$—C10—H10A | 120.5 |
| O5$^{i}$—Ca1—O3 | 152.84 (5) | C9—C10—H10A | 120.5 |
| O5—Ca1—O3 | 72.48 (5) | C15—N10—C16 | 115.35 (18) |
| N1$^{i}$—Ca1—O3 | 77.73 (5) | O6—C11—O5 | 125.73 (19) |
| N1—Ca1—O3 | 63.34 (5) | O6—C11—C8 | 117.19 (18) |
| N2—Ca1—O3 | 131.22 (3) | O5—C11—C8 | 117.06 (18) |
| O3$^{i}$—Ca1—O3 | 97.56 (7) | C17—N11—C16 | 115.51 (18) |
| N1—C1—C2 | 122.86 (19) | C15—N12—H11A | 118.7 |
| N1—C1—C6 | 114.91 (18) | C15—N12—H11B | 119.2 |
| C2—C1—C6 | 122.16 (19) | H11A—N12—H11B | 121.9 |
| C5—N1—C1 | 118.70 (18) | N7—C12—N4 | 117.41 (19) |
| C5—N1—Ca1 | 121.61 (13) | N7—C12—N5 | 116.5 (2) |
| C1—N1—Ca1 | 119.56 (13) | N4—C12—N5 | 126.05 (19) |
| C6—O1—Ca1 | 120.86 (12) | C16—N13—H13A | 121.4 |
| H1WB—O1W—H1WA | 104.1 | C16—N13—H13B | 122.1 |
| H2WB—O2W—H2WA | 109.9 | H13A—N13—H13B | 116.5 |
| C8$^{i}$—N2—C8 | 118.9 (2) | N5—C13—N8 | 121.3 (2) |
| C8$^{i}$—N2—Ca1 | 120.53 (12) | N5—C13—N3 | 121.8 (2) |
| C8—N2—Ca1 | 120.53 (12) | N8—C13—N3 | 116.96 (19) |
| C3—C2—C1 | 118.4 (2) | C17—N14—H14A | 116.7 |
| C3—C2—H2A | 120.8 | C17—N14—H14B | 120.1 |
| C1—C2—H2A | 120.8 | H14A—N14—H14B | 123.0 |
| H3WB—O3W—H3WA | 114.4 | N6—C14—N4 | 121.3 (2) |
| C13—N3—C14 | 119.60 (18) | N6—C14—N3 | 117.3 (2) |
| C13—N3—H3N | 120.4 | N4—C14—N3 | 121.4 (2) |
| C14—N3—H3N | 119.8 | N10—C15—N12 | 120.64 (19) |
| C7—O3—Ca1 | 122.48 (12) | N10—C15—N9 | 121.73 (18) |
| C2—C3—C4 | 119.2 (2) | N12—C15—N9 | 117.63 (18) |

| | | | |
|---|---|---|---|
| C2—C3—H3A | 120.4 | N13—C16—N11 | 116.54 (19) |
| C4—C3—H3A | 120.4 | N13—C16—N10 | 117.51 (19) |
| C3—C4—C5 | 118.7 (2) | N11—C16—N10 | 125.96 (18) |
| C3—C4—H4A | 120.7 | N14—C17—N11 | 120.7 (2) |
| C5—C4—H4A | 120.7 | N14—C17—N9 | 117.33 (19) |
| C14—N4—C12 | 115.36 (18) | N11—C17—N9 | 121.95 (19) |
| C11—O5—Ca1 | 123.58 (13) | | |

| | | | |
|---|---|---|---|
| C2—C1—N1—C5 | −0.8 (3) | N1—Ca1—O5—C11 | 138.44 (17) |
| C6—C1—N1—C5 | −177.72 (18) | N2—Ca1—O5—C11 | 3.08 (14) |
| C2—C1—N1—Ca1 | 175.25 (18) | O3$^{i}$—Ca1—O5—C11 | 132.90 (16) |
| C6—C1—N1—Ca1 | −1.6 (2) | O3—Ca1—O5—C11 | −155.35 (17) |
| O1—Ca1—N1—C5 | 171.11 (17) | C1—N1—C5—C4 | 0.2 (3) |
| O1$^{i}$—Ca1—N1—C5 | 22.09 (19) | Ca1—N1—C5—C4 | −175.81 (17) |
| O5$^{i}$—Ca1—N1—C5 | −158.97 (14) | C1—N1—C5—C7 | 177.82 (18) |
| O5—Ca1—N1—C5 | 73.20 (15) | Ca1—N1—C5—C7 | 1.8 (2) |
| N1$^{i}$—Ca1—N1—C5 | −60.19 (14) | C3—C4—C5—N1 | 0.4 (4) |
| N2—Ca1—N1—C5 | 119.81 (14) | C3—C4—C5—C7 | −177.1 (2) |
| O3$^{i}$—Ca1—N1—C5 | −109.38 (16) | Ca1—O1—C6—O2 | 162.52 (16) |
| O3—Ca1—N1—C5 | −4.32 (14) | Ca1—O1—C6—C1 | −19.1 (2) |
| O1—Ca1—N1—C1 | −4.88 (14) | N1—C1—C6—O1 | 13.5 (3) |
| O1$^{i}$—Ca1—N1—C1 | −153.89 (14) | C2—C1—C6—O1 | −163.4 (2) |
| O5$^{i}$—Ca1—N1—C1 | 25.05 (18) | N1—C1—C6—O2 | −167.97 (18) |
| O5—Ca1—N1—C1 | −102.78 (15) | C2—C1—C6—O2 | 15.1 (3) |
| N1$^{i}$—Ca1—N1—C1 | 123.83 (16) | Ca1—O3—C7—O4 | 170.52 (16) |
| N2—Ca1—N1—C1 | −56.17 (16) | Ca1—O3—C7—C5 | −9.4 (2) |
| O3$^{i}$—Ca1—N1—C1 | 74.64 (15) | N1—C5—C7—O4 | −175.02 (18) |
| O3—Ca1—N1—C1 | 179.70 (17) | C4—C5—C7—O4 | 2.6 (3) |
| O1$^{i}$—Ca1—O1—C6 | 148.51 (15) | N1—C5—C7—O3 | 4.9 (3) |
| O5$^{i}$—Ca1—O1—C6 | −145.46 (15) | C4—C5—C7—O3 | −177.5 (2) |
| O5—Ca1—O1—C6 | 86.33 (15) | C8$^{i}$—N2—C8—C9 | −0.29 (15) |
| N1$^{i}$—Ca1—O1—C6 | −94.42 (16) | Ca1—N2—C8—C9 | 179.71 (15) |
| N1—Ca1—O1—C6 | 13.04 (14) | C8$^{i}$—N2—C8—C11 | 178.57 (19) |
| N2—Ca1—O1—C6 | 148.51 (15) | Ca1—N2—C8—C11 | −1.43 (19) |
| O3$^{i}$—Ca1—O1—C6 | −70.16 (15) | N2—C8—C9—C10 | 0.6 (3) |
| O3—Ca1—O1—C6 | 18.19 (17) | C11—C8—C9—C10 | −178.21 (17) |
| O1—Ca1—N2—C8$^{i}$ | 80.76 (10) | C8—C9—C10—C9$^{i}$ | −0.27 (14) |
| O1$^{i}$—Ca1—N2—C8$^{i}$ | −99.24 (10) | Ca1—O5—C11—O6 | 173.48 (15) |
| O5$^{i}$—Ca1—N2—C8$^{i}$ | −0.53 (11) | Ca1—O5—C11—C8 | −5.0 (2) |
| O5—Ca1—N2—C8$^{i}$ | 179.47 (11) | N2—C8—C11—O6 | −174.49 (16) |
| N1$^{i}$—Ca1—N2—C8$^{i}$ | −52.29 (11) | C9—C8—C11—O6 | 4.4 (3) |
| N1—Ca1—N2—C8$^{i}$ | 127.71 (11) | N2—C8—C11—O5 | 4.1 (3) |
| O3$^{i}$—Ca1—N2—C8$^{i}$ | 27.26 (11) | C9—C8—C11—O5 | −177.1 (2) |
| O3—Ca1—N2—C8$^{i}$ | −152.74 (11) | C14—N4—C12—N7 | −177.40 (19) |
| O1—Ca1—N2—C8 | −99.24 (10) | C14—N4—C12—N5 | 1.4 (3) |
| O1$^{i}$—Ca1—N2—C8 | 80.76 (10) | C13—N5—C12—N7 | 172.95 (19) |
| O5$^{i}$—Ca1—N2—C8 | 179.47 (11) | C13—N5—C12—N4 | −5.9 (3) |
| O5—Ca1—N2—C8 | −0.53 (11) | C12—N5—C13—N8 | −173.9 (2) |

| | | | |
|---|---|---|---|
| N1$^{i}$—Ca1—N2—C8 | 127.71 (11) | C12—N5—C13—N3 | 4.3 (3) |
| N1—Ca1—N2—C8 | −52.29 (11) | C14—N3—C13—N5 | 1.3 (3) |
| O3$^{i}$—Ca1—N2—C8 | −152.74 (11) | C14—N3—C13—N8 | 179.6 (2) |
| O3—Ca1—N2—C8 | 27.26 (11) | C12—N4—C14—N6 | −174.6 (2) |
| N1—C1—C2—C3 | 0.8 (4) | C12—N4—C14—N3 | 4.7 (3) |
| C6—C1—C2—C3 | 177.5 (2) | C13—N3—C14—N6 | 173.2 (2) |
| O1—Ca1—O3—C7 | 2.23 (17) | C13—N3—C14—N4 | −6.2 (3) |
| O1$^{i}$—Ca1—O3—C7 | −153.52 (15) | C16—N10—C15—N12 | −175.54 (19) |
| O5$^{i}$—Ca1—O3—C7 | 145.59 (14) | C16—N10—C15—N9 | 4.7 (3) |
| O5—Ca1—O3—C7 | −74.48 (15) | C17—N9—C15—N10 | −2.6 (3) |
| N1$^{i}$—Ca1—O3—C7 | 140.11 (15) | C17—N9—C15—N12 | 177.67 (18) |
| N1—Ca1—O3—C7 | 7.43 (14) | C17—N11—C16—N13 | −179.39 (19) |
| N2—Ca1—O3—C7 | −100.42 (14) | C17—N11—C16—N10 | 0.9 (3) |
| O3$^{i}$—Ca1—O3—C7 | 79.58 (14) | C15—N10—C16—N13 | 176.27 (19) |
| C1—C2—C3—C4 | −0.2 (4) | C15—N10—C16—N11 | −4.0 (3) |
| C2—C3—C4—C5 | −0.4 (4) | C16—N11—C17—N14 | −177.5 (2) |
| O1—Ca1—O5—C11 | 75.17 (16) | C16—N11—C17—N9 | 1.6 (3) |
| O1$^{i}$—Ca1—O5—C11 | −76.38 (16) | C15—N9—C17—N14 | 178.31 (19) |
| O5$^{i}$—Ca1—O5—C11 | 3.08 (14) | C15—N9—C17—N11 | −0.8 (3) |
| N1$^{i}$—Ca1—O5—C11 | −104.08 (16) | | |

Symmetry code: (i) $-x, y, -z+1/2$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*WB*···O2$^{ii}$ | 0.84 | 1.91 | 2.710 (3) | 160 |
| O1*W*—H1*WA*···O6$^{iii}$ | 0.84 | 1.92 | 2.751 (3) | 170 |
| O2*W*—H2*WB*···N4$^{iv}$ | 0.84 | 2.26 | 3.022 (3) | 151 |
| N3—H3*N*···O2 | 0.88 | 1.79 | 2.667 (2) | 176 |
| O2*W*—H2*WA*···O5 | 0.84 | 2.05 | 2.888 (3) | 175 |
| O3*W*—H3*WB*···O2*W*$^{v}$ | 0.84 | 2.18 | 2.963 (3) | 154 |
| O3*W*—H3*WA*···N14$^{vi}$ | 0.84 | 2.17 | 3.007 (3) | 180 |
| N6—H6*NA*···O1*W*$^{ii}$ | 0.88 | 2.45 | 3.294 (3) | 162 |
| N6—H6*NB*···O1*W* | 0.88 | 1.90 | 2.740 (3) | 160 |
| N7—H7*NA*···N11$^{vi}$ | 0.88 | 2.22 | 3.103 (3) | 176 |
| N7—H7*NB*···O2*W*$^{iii}$ | 0.88 | 2.44 | 3.205 (3) | 146 |
| N7—H7*NB*···O4$^{iii}$ | 0.88 | 2.53 | 3.111 (2) | 124 |
| N8—H8*NA*···O1 | 0.88 | 2.07 | 2.948 (2) | 172 |
| N12—H11*A*···N10$^{vii}$ | 0.88 | 2.23 | 3.109 (2) | 178 |
| N12—H11*B*···O5 | 0.88 | 2.32 | 3.196 (2) | 175 |
| N8—H8*NB*···O3*W* | 0.88 | 2.15 | 2.832 (4) | 134 |
| N9—H9*NA*···O3 | 0.88 | 1.89 | 2.754 (2) | 165 |
| N13—H13*A*···O4$^{viii}$ | 0.88 | 2.08 | 2.925 (2) | 160 |
| N13—H13*B*···O6$^{vii}$ | 0.88 | 1.96 | 2.790 (2) | 157 |
| N14—H14*A*···O3 | 0.88 | 2.39 | 3.143 (2) | 144 |

| | | | | |
|---|---|---|---|---|
| N14—H14*B*···N5$^{ix}$ | 0.88 | 2.10 | 2.978 (3) | 178 |
| C4—H4*A*···O2$^{x}$ | 0.95 | 2.55 | 3.370 (3) | 145 |

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