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# Crystal structure of a 2:1 co-crystal of the anticancer drug lenalidomide with 1,3-resorcinol

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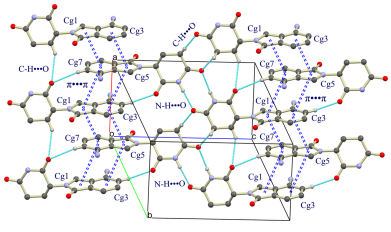
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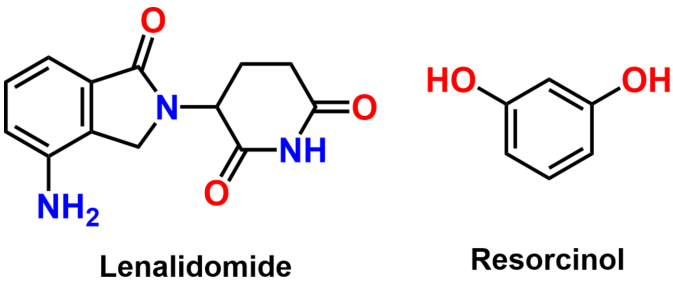
A 2:1 cocrystal of lenalidomide and 1,3-resorcinol [systematic name: 3-(4-amino-1-oxo-1,3-dihydro-2*H*-isoindol-2-yl)piperidine-2,6-dione–benzene-1,3-diol (2/1), $2C_{13}H_{13}N_3O_3{\cdot}C_6H_6O_2$] was synthesized, and its crystal structure was elucidated by single-crystal X-ray diffraction (SCXRD). The cocrystal crystallizes in the triclinic space group $P\overline{1}$. The two symmetry-independent lenalidomide molecules form a hydrogen-bonded dimeric assembly through N—H···O interactions, generating an $R_2^2(8)$ ring motif. In addition, O—H···O hydrogen bonds involving the hydroxyl groups of 1,3-resorcinol and the carbonyl oxygen atoms of the isoindolinone and glutarimide moieties of lenalidomide further contribute to the cohesion and organization of the crystal packing. The crystal structure is further consolidated by several close $\pi$–$\pi$ stacking interactions involving the $\pi$-electrons of the isoindolinone moiety. Hirshfeld surface analysis and the corresponding two-dimensional fingerprint plots were employed to identify and quantify the principal intermolecular contacts contributing to the cohesion of the cocrystal structure.

## 1. Chemical context

Lenalidomide (**LEN**), a synthetic thalidomide analogue, is an immunomodulatory drug used in the treatment of multiple myeloma and myelodysplastic syndromes associated with deletion of chromosome 5q [del(5q)] (Richardson *et al.*, 2002; List *et al.*, 2006). Reported pharmacological effects include immunomodulatory and antiangiogenic activity (Kotla *et al.*, 2009). Also in multiple myeloma, lenalidomide has also been shown to promote cereblon-dependent degradation of IKZF1 and IKZF3 (Krönke *et al.*, 2014). The solid-state landscape of **LEN** includes anhydrous and hydrated forms, polymorphs and solvates (Ravikumar & Sridhar, 2009; Chennuru *et al.*, 2017; Jia *et al.*, 2019). Cocrystals of **LEN** with urea and 3,5-dihydroxybenzoic acid, gallic acid and nicotinamide have been reported, with selected systems showing changes in apparent solubility or dissolution under the conditions studied (Song *et al.*, 2014, Song *et al.*, 2015; Wang *et al.*, 2022). A crystalline form of lenalidomide (**LEN**) with resorcinol (**RES**) was previously disclosed in patent US 12098136 B2, accompanied by DSC, PXRD and NMR data; however, its crystal structure was not reported (Bhat *et al.*, 2024). Here, we report the single-crystal X-ray structure of the **LEN:RES** cocrystal (2:1), providing a crystallographic description of its molecular arrangement and intermolecular interactions.



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## 2. Structural commentary

The crystal structure of the **LEN:RES** (2:1) cocrystal was unambiguously established by single-crystal X-ray diffraction (SCXRD) analysis. The cocrystal crystallizes in the triclinic crystal system with the centrosymmetric space group $P\overline{1}$ (space group No. 2). The asymmetric unit comprises two independent molecules of **LEN** and one molecule of **RES**, corresponding to a 2:1 stoichiometric ratio (Fig. 1*a*). The two crystallographically independent **LEN** molecules are designated *A* and *B*. A structural overlay of molecules *A* and *B* reveals a distinct conformational difference in the glutarimide ring (Fig. 1*b*). The dihedral angle between a plane between the isoindolinone-derived aromatic system and the glutarimide ring is 86.93 (3)° for molecule *A* and 78.96 (3)° for molecule *B*.

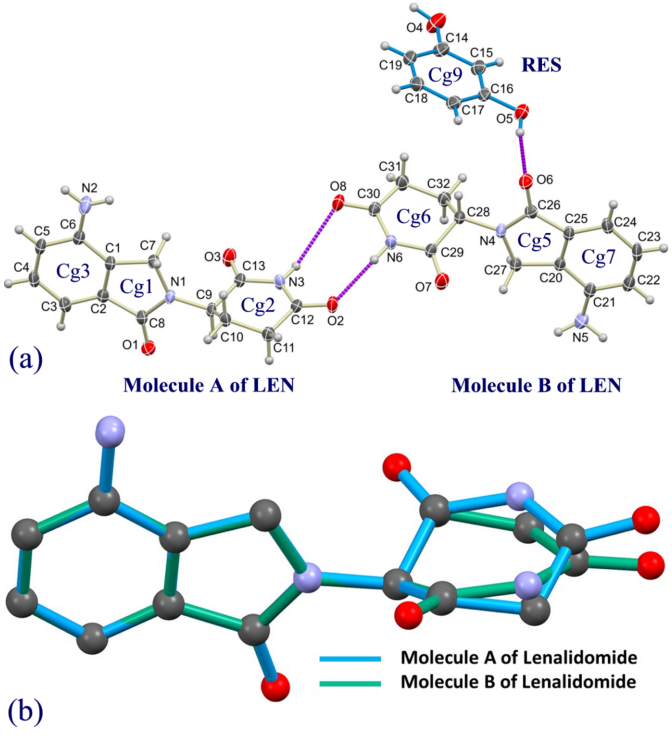



**Figure 1**
(*a*) The **LEN:RES** cocrystal with thermal displacement ellipsoids drawn at the 30% probability level. Atom labelling is provided for identification; hydrogen atoms are depicted as spheres of arbitrary radii for clarity. Hydrogen-bonding interactions are shown as violet dashed lines. (*b*) Overlay of two symmetry-independent molecules of **LEN** within the asymmetric unit of the **LEN:RES** cocrystal.

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

Ring centroids are defined as: *Cg*1 = N1/C7/C1/C2/C8; *Cg*2 = N3/C9–C13; *Cg*3 = C1–C6;*Cg*5 = N4/C20/C25–C27; *Cg*6 = N6/C28–C32; *Cg*7 = C20–C25; and *Cg*9 = C14–C19. *Cg*···*Cg* denotes the centroid—centroid distance associated with $\pi$–$\pi$ interactions.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H1···O8$^{i}$ | 0.93 (3) | 1.92 (3) | 2.816 (3) | 161 (3) |
| O5—H5*A*···O6 | 0.85 (3) | 1.87 (3) | 2.710 (3) | 171 (3) |
| N2—H2*B*···O5$^{ii}$ | 0.78 (3) | 2.56 (3) | 3.310 (3) | 163 (3) |
| N2—H2*A*···O5$^{iii}$ | 0.83 (3) | 2.28 (3) | 3.015 (3) | 148 (3) |
| N3—H3···O1$^{iv}$ | 0.89 (2) | 2.31 (2) | 3.022 (3) | 137 (2) |
| N3—H3···O8 | 0.89 (2) | 2.51 (2) | 3.256 (3) | 141 (2) |
| N5—H1*D*···O2$^{v}$ | 0.92 (3) | 2.23 (3) | 3.144 (3) | 172 (2) |
| N6—H6···O2 | 0.92 (3) | 2.00 (3) | 2.915 (3) | 171 (2) |
| C9—H9···O3$^{iv}$ | 0.98 | 2.65 | 3.409 (3) | 135 |
| C17—H17···O4$^{vi}$ | 0.93 | 2.57 | 3.263 (3) | 131 |
| C27—H27*B*···O7 | 0.97 | 2.58 | 3.106 (3) | 114 |
| C31—H31*B*···O2$^{vii}$ | 0.97 | 2.47 | 3.440 (3) | 178 |
| C10—H10*A*···*Cg*9$^{ii}$ | | 2.65 | 3.581 (3) | 161 |
| *Cg*1···*Cg*7$^{iii}$ | | | 3.7109 (16) | |
| *Cg*1···*Cg*7$^{viii}$ | | | 4.0014 (17) | |
| *Cg*3···*Cg*5$^{iii}$ | | | 3.7997 (17) | |
| *Cg*3···*Cg*5$^{viii}$ | | | 3.9603 (17) | |
| *Cg*3···*Cg*7$^{iii}$ | | | 3.6971 (17) | |
| *Cg*3···*Cg*7$^{viii}$ | | | 3.6644 (17) | |
| *Cg*3···*Cg*8$^{iii}$ | | | 3.5854 (15) | |
| *Cg*3···*Cg*8$^{viii}$ | | | 3.6382 (15) | |
| *Cg*4···*Cg*7$^{iii}$ | | | 3.5410 (15) | |
| *Cg*4···*Cg*7$^{viii}$ | | | 3.6602 (15) | |
| *Cg*4···*Cg*8$^{iii}$ | | | 3.6763 (13) | |
| *Cg*4···*Cg*8$^{viii}$ | | | 3.8723 (13) | |

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

Thus, molecule *A* adopts a more orthogonal, and consequently less twisted, conformation with respect to the defined ring planes than molecule *B*. The molecules present in the asymmetric unit are interconnected through a network of hydrogen-bonding interactions. The two crystallographically independent **LEN** molecules, *A* and *B*, are connected through N—H···O hydrogen bonds, generating a cyclic $R_2^2(8)$ ring motif. In addition, the **RES** molecule participates in O—H···O hydrogen bonding engaging its hydroxyl group with the carbonyl oxygen atom of adjacent **LEN** molecule *B*, thereby further linking the molecular components within the asymmetric unit.

## 3. Supramolecular features

The molecular packing viewed along the *b* axis reveals that the **LEN** molecules are arranged along the *a*-axis direction through short $\pi$–$\pi$ stacking interactions involving the isoindolinone moiety, with centroid-to-centroid distances ranging from 3.5410 (15) to 4.0014 (17) Å (see entries 14-25 of Table 1). These interactions generate a stacked one-dimensional supramolecular assembly extending along the *a*-axis direction. The stacked assemblies are further connected along the *c*-axis direction through dimeric C—H···O and N—H···O hydrogen-bonding interactions (C31—H31*B*···O2$^{vii}$, N3—H3···O8, and N6—H6···O2; Table 1), both forming cyclic $R_2^2(8)$ ring motifs. Consequently, an extended and

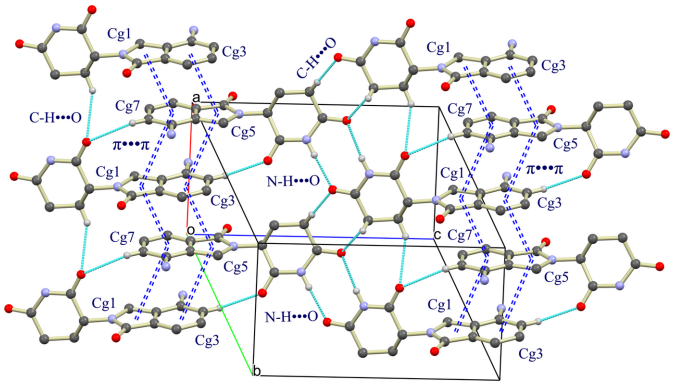



**Figure 2**
View of the molecular packing along the *b* axis in the **LEN:RES** cocrystal, showing the intermolecular C—H···O and N—H···O hydrogen bonds and $\pi$–$\pi$ stacking interactions.

compact supramolecular architecture is generated in the *ac* plane (Fig. 2). The packing arrangement viewed along the *a*-axis shows that the **RES** molecule is positioned between two **LEN** molecules and is involved in N—H···O (N2—H2*B*···O5$^{ii}$ and N3—H3···O1$^{iv}$), O—H···O (O5—H5*A*···O6) and C—H···$\pi$ (C10—H10A···*Cg*9$^{ii}$) interactions. In particular, C—H···$\pi$ interactions occur between the hydrogen atoms associated with the glutarimide moiety of **LEN** and the $\pi$-electron cloud of the aromatic ring of **RES**, contributing to the formation of a one-dimensional supramolecular assembly along the *b*-axis direction. In addition, in the packing along the *c*-axis direction, **RES** interacts with adjacent **LEN** molecules through C—H···O contacts involving hydrogen atoms of **RES** and the carbonyl oxygen atoms of the glutarimide moieties of **LEN** (Fig. 3). These intermolecular interactions collectively consolidate the three-dimensional crystal packing.

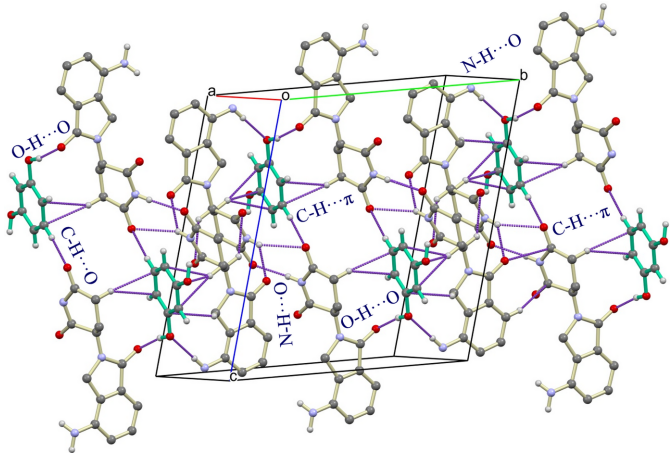
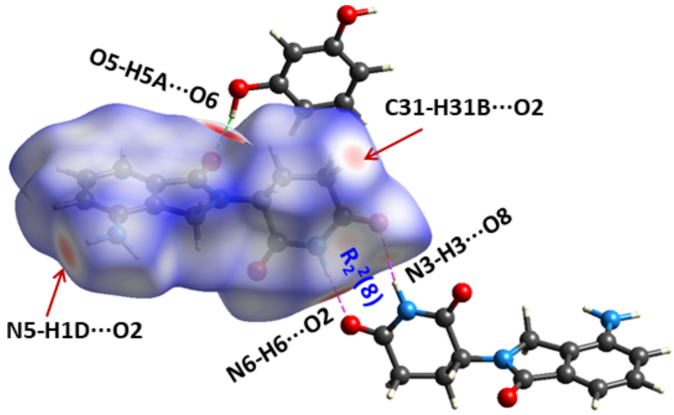



**Figure 3**
View of the molecular packing along the *a* axis in the **LEN:RES** cocrystal, joined using C—H···O, N—H···O, O—H···O and C—H···$\pi$ interactions.



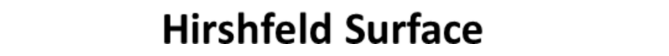




**Figure 4**
Visualization of the Hirshfeld surface of molecule B of **LEN**, within the **LEN:RES** cocrystal.

## 4. Hirshfeld surface analysis

Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) and two-dimensional fingerprint plots (Spackman & McKinnon, 2002) were performed using *CrystalExplorer* (Spackman *et al.*, 2021). The Hirshfeld surface mapped over $d_{norm}$ for molecule *B* of **LEN** in the cocrystal reveals several prominent red spots, indicating close contacts between **LEN** and **RES**. The Hirshfeld surface analysis was performed only for molecule *B* of **LEN** because it participates in O—H···O hydrogen bonding with the **RES** coformer, and N—H···O hydrogen bonding with molecule *A* of **LEN**, forming a dimeric motif. One of the most prominent red spots corresponds to the strong O—H···O hydrogen-bonding interaction between the hydroxyl group of **RES** and the carbonyl oxygen atom of **LEN**. The other prominent red spots are associated with N—H···O

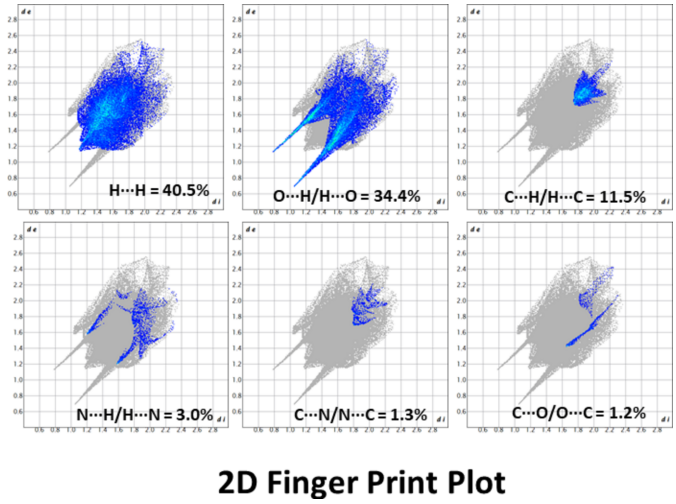






**Figure 5**
Two-dimensional fingerprint plot of molecule *B* of **LEN** in the **LEN:RES** cocrystal, showing the percentage contributions of different intermolecular interactions to the Hirshfeld surface area.

hydrogen-bonding interactions, which generate an $R_2^2(8)$ hydrogen-bonded ring motif (Fig. 4). The two-dimensional fingerprint plots further illustrate the principal intermolecular contacts contributing to the consolidation of the cocrystal structure. In particular, the H···H and O···H/H···O contacts exhibit prominent features at $(d_i + d_e)$ values of approximately 2.4 and 2.0 Å, respectively (Fig. 5). These values are shorter than the corresponding sums of the van der Waals radii, indicating the presence of significant close intermolecular contacts.

## 5. Database survey

A survey of the Cambridge Structural Database (CSD, Version 6.01, Groom *et al.*, 2016) using ConQuest (Bruno *et al.*, 2002) identified 16 crystal structures based on **LEN**. Among these, two structures correspond to polymorphs of **LEN** (AJISES; Ravikumar & Sridhar, 2009, AJISES01; Chennuru *et al.*, 2017), while two are hydrate forms (AJISIW; Ravikumar & Sridhar, 2009, ICOSUR; Chennuru *et al.*, 2017). Solvate structures containing DMF (ICOTEC; Chennuru *et al.*, 2017), acetone (ICOTIG; Chennuru *et al.*, 2017), DMSO (ICOTOM; Chennuru *et al.*, 2017), and acetonitrile (UZULUZ) have also been reported. In addition, **LEN** cocrystals and cocrystal hydrates have been reported with gallic acid (HUVGAI and HUVFUB; Song *et al.*, 2015), 3,5-dihydroxybenzoic acid (XODPIR and XODPEN; Song *et al.*, 2014), urea (XODPOX; Song *et al.*, 2014), melamine (NUNSAU; Screen *et al.*, 2025) and acesulfame (ZIDQUB and ZIDQUB01; Chen *et al.*, 2019). Interestingly, one of the reported crystal structures contains protonated **LEN**, with a chloride ion ($Cl^-$) serving as the counter-ion to maintain charge neutrality (VAGMEZ; Valdivia-Berroeta *et al.*, 2021). However, to the best of our knowledge, no crystal structure of a **LEN:RES** has been reported to date.

## 6. Synthesis and crystallization

The **LEN:RES** cocrystal was prepared by a combination of liquid-assisted grinding and slow-evaporation crystallization. **LEN** (60 mg, 0.231 mmol) and **RES** (25.5 mg, 0.231 mmol) were taken in a 1:1 molar ratio and manually ground together in a mortar and pestle for approximately 10 min in the presence of a few drops of a 1:1 (*v*/*v*) acetone-ethanol solvent mixture. The resulting solid was subsequently dissolved in 1:1:1:1 (*v*/*v*/*v*/*v*) mixture of isopropyl alcohol, methanol, acetonitrile, and water and gently heated to ensure complete dissolution. The resulting solution was filtered to remove any undissolved material and transferred to a crystallization vessel. The solvent was allowed to evaporate slowly at room temperature (298 K). After 4–5 days, yellow, plate-like crystals suitable for single-crystal X-ray diffraction analysis were obtained.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $2C_{13}H_{13}N_3O_3{\cdot}C_6H_6O_2$ |
| $M_r$ | 628.63 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 297 |
| $a, b, c$ (Å) | 7.0508 (3), 14.1141 (6), 16.3951 (9) |
| $\alpha, \beta, \gamma$ (°) | 110.596 (2), 100.956 (2), 101.880 (2) |
| $V$ (Å$^3$) | 1431.91 (12) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.11 |
| Crystal size (mm) | 0.14 × 0.09 × 0.04 |
| | |
| Data collection | |
| Diffractometer | Bruker D8 VENTURE Kappa Duo PHOTON II CPAD |
| Absorption correction | Multi-scan (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.632, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 44385, 7160, 3351 |
| $R_{int}$ | 0.138 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.671 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.061, 0.168, 0.99 |
| No. of reflections | 7160 |
| No. of parameters | 439 |
| No. of restraints | 1 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.30, −0.26 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed in geometrically idealized positions. The H atoms attached to O4 and O5 were located in difference-Fourier maps and refined isotropically. The H atom attached to N3 was placed in a geometrically idealized position and the N3—H3 bond length was restrained to 0.95 Å using a DFIX restraint.

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# supporting information

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## Crystal structure of a 2:1 co-crystal of the anticancer drug lenalidomide with 1,3-resorcinol

**Sejal Kaldoke, Niteen B. Dabke, Nagabhushan Shet and Rajesh G. Gonnade**

### Computing details

**3-(4-Amino-1-oxo-1,3-dihydro-2*H*-isoindol-2-yl)piperidine-2,6-dione–benzene-1,3-diol (2/1)**

*Crystal data*

$2C_{13}H_{13}N_3O_3·C_6H_6O_2$
$M_r = 628.63$
Triclinic, $P\overline{1}$
$a = 7.0508$ (3) Å
$b = 14.1141$ (6) Å
$c = 16.3951$ (9) Å
$\alpha = 110.596$ (2)°
$\beta = 100.956$ (2)°
$\gamma = 101.880$ (2)°
$V = 1431.91$ (12) Å$^3$
$Z = 2$
$F(000) = 660$
$D_x = 1.458$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7164 reflections
$\theta = 2.5$–$28.5°$
$\mu = 0.11$ mm$^{-1}$
$T = 297$ K
Plate, pale yellow
0.14 × 0.09 × 0.04 mm

*Data collection*

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer
Radiation source: micro-focus sealed tube, Incoatech I$\mu$S HB
Multilayer mirrors monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.632$, $T_{max} = 0.746$
44385 measured reflections
7160 independent reflections
3351 reflections with $I > 2\sigma(I)$
$R_{int} = 0.138$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.5°$
$h = -9 \rightarrow 9$
$k = -18 \rightarrow 18$
$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.168$
$S = 0.99$
7160 reflections
439 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.26$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.4392 (3) | 1.21869 (13) | 0.66753 (11) | 0.0466 (5) |
| O2 | 0.1038 (3) | 0.70701 (13) | 0.37776 (11) | 0.0471 (5) |
| O3 | 0.6444 (3) | 0.96443 (14) | 0.58963 (12) | 0.0526 (5) |
| N1 | 0.4203 (3) | 1.06732 (14) | 0.69316 (12) | 0.0335 (5) |
| N2 | 0.6294 (4) | 1.08409 (19) | 0.96980 (16) | 0.0551 (7) |
| N3 | 0.3680 (3) | 0.83778 (15) | 0.48570 (14) | 0.0373 (5) |
| C1 | 0.5573 (4) | 1.14192 (17) | 0.84840 (15) | 0.0322 (6) |
| C2 | 0.5571 (3) | 1.22231 (18) | 0.81917 (16) | 0.0331 (6) |
| C3 | 0.6287 (4) | 1.32822 (18) | 0.87877 (17) | 0.0402 (6) |
| H3A | 0.628058 | 1.382037 | 0.858556 | 0.048* |
| C4 | 0.7014 (4) | 1.34981 (19) | 0.97012 (17) | 0.0442 (7) |
| H4 | 0.750506 | 1.419965 | 1.012339 | 0.053* |
| C5 | 0.7028 (4) | 1.27023 (19) | 0.99993 (16) | 0.0401 (6) |
| H5 | 0.753498 | 1.288036 | 1.061774 | 0.048* |
| C6 | 0.6302 (4) | 1.16338 (19) | 0.93995 (16) | 0.0356 (6) |
| C7 | 0.4697 (4) | 1.03661 (17) | 0.76899 (15) | 0.0340 (6) |
| H7A | 0.567555 | 0.997243 | 0.762260 | 0.041* |
| H7B | 0.349737 | 0.994421 | 0.774725 | 0.041* |
| C8 | 0.4685 (4) | 1.17463 (18) | 0.71944 (16) | 0.0341 (6) |
| C9 | 0.3236 (4) | 0.99346 (18) | 0.60035 (15) | 0.0335 (6) |
| H9 | 0.299217 | 1.035799 | 0.565413 | 0.040* |
| C10 | 0.1187 (4) | 0.91915 (19) | 0.58530 (16) | 0.0385 (6) |
| H10A | 0.134266 | 0.876290 | 0.619736 | 0.046* |
| H10B | 0.029641 | 0.960111 | 0.606562 | 0.046* |
| C11 | 0.0268 (4) | 0.84802 (19) | 0.48517 (17) | 0.0416 (6) |
| H11A | −0.097317 | 0.796450 | 0.477254 | 0.050* |
| H11B | −0.007630 | 0.890553 | 0.452601 | 0.050* |
| C12 | 0.1649 (4) | 0.79088 (19) | 0.44478 (16) | 0.0346 (6) |
| C13 | 0.4619 (4) | 0.93194 (18) | 0.56100 (16) | 0.0345 (6) |
| H3 | 0.443 (4) | 0.8010 (18) | 0.4577 (16) | 0.052* |
| H2A | 0.670 (4) | 1.100 (2) | 1.0250 (19) | 0.052* |
| H2B | 0.592 (4) | 1.026 (2) | 0.9329 (18) | 0.052* |
| O4 | 1.2550 (3) | 0.3382 (2) | 0.38207 (14) | 0.0767 (7) |
| O5 | 0.6176 (3) | 0.16702 (16) | 0.16464 (13) | 0.0563 (6) |
| C14 | 1.0483 (4) | 0.3148 (2) | 0.36367 (19) | 0.0481 (7) |
| C15 | 0.9331 (4) | 0.2529 (2) | 0.27456 (18) | 0.0470 (7) |
| H15 | 0.995148 | 0.228355 | 0.229379 | 0.056* |
| C16 | 0.7265 (4) | 0.22825 (19) | 0.25380 (17) | 0.0400 (6) |
| C17 | 0.6315 (4) | 0.2623 (2) | 0.32043 (18) | 0.0447 (7) |

| | | | | |
|---|---|---|---|---|
| H17 | 0.491186 | 0.243909 | 0.306246 | 0.054* |
| C18 | 0.7511 (5) | 0.3246 (2) | 0.40876 (18) | 0.0484 (7) |
| H18 | 0.689303 | 0.348195 | 0.454229 | 0.058* |
| C19 | 0.9582 (5) | 0.3523 (2) | 0.43099 (17) | 0.0469 (7) |
| H19 | 1.036325 | 0.395666 | 0.490416 | 0.056* |
| H1 | 1.308 (5) | 0.359 (2) | 0.444 (2) | 0.070* |
| H5A | 0.494 (5) | 0.166 (2) | 0.152 (2) | 0.070* |
| O6 | 0.2332 (3) | 0.17291 (13) | 0.11279 (11) | 0.0478 (5) |
| O7 | 0.0550 (3) | 0.46102 (15) | 0.18180 (13) | 0.0553 (5) |
| O8 | 0.5573 (3) | 0.63971 (15) | 0.44179 (12) | 0.0543 (5) |
| N4 | 0.2641 (3) | 0.32938 (14) | 0.09561 (13) | 0.0360 (5) |
| N5 | 0.1058 (4) | 0.3344 (2) | −0.17610 (17) | 0.0524 (7) |
| N6 | 0.3138 (3) | 0.55180 (16) | 0.30871 (14) | 0.0415 (6) |
| C20 | 0.1513 (4) | 0.26472 (18) | −0.06018 (16) | 0.0337 (6) |
| C21 | 0.0881 (4) | 0.24901 (19) | −0.15121 (16) | 0.0375 (6) |
| C22 | 0.0140 (4) | 0.1445 (2) | −0.21483 (17) | 0.0454 (7) |
| H22 | −0.029956 | 0.130577 | −0.276211 | 0.054* |
| C23 | 0.0040 (4) | 0.0602 (2) | −0.18903 (18) | 0.0482 (7) |
| H23 | −0.047229 | −0.008665 | −0.233698 | 0.058* |
| C24 | 0.0678 (4) | 0.07543 (19) | −0.09901 (17) | 0.0434 (7) |
| H24 | 0.062888 | 0.019145 | −0.081646 | 0.052* |
| C25 | 0.1398 (4) | 0.18046 (18) | −0.03610 (16) | 0.0345 (6) |
| C26 | 0.2149 (4) | 0.22211 (18) | 0.06352 (17) | 0.0351 (6) |
| C27 | 0.2335 (4) | 0.36639 (18) | 0.02291 (15) | 0.0369 (6) |
| H27A | 0.359950 | 0.409290 | 0.022747 | 0.044* |
| H27B | 0.137622 | 0.407037 | 0.028206 | 0.044* |
| C28 | 0.3475 (4) | 0.39755 (18) | 0.19125 (16) | 0.0352 (6) |
| H28 | 0.340619 | 0.351277 | 0.223981 | 0.042* |
| C29 | 0.2221 (4) | 0.47085 (19) | 0.22422 (16) | 0.0358 (6) |
| C30 | 0.5058 (4) | 0.57531 (18) | 0.36249 (17) | 0.0389 (6) |
| C31 | 0.6447 (4) | 0.5217 (2) | 0.32072 (17) | 0.0452 (7) |
| H31A | 0.670477 | 0.472816 | 0.347679 | 0.054* |
| H31B | 0.772645 | 0.574642 | 0.335705 | 0.054* |
| C32 | 0.5682 (4) | 0.46140 (19) | 0.21851 (17) | 0.0419 (6) |
| H32A | 0.648126 | 0.414196 | 0.198385 | 0.050* |
| H32B | 0.581853 | 0.510698 | 0.189556 | 0.050* |
| H1C | 0.079 (5) | 0.388 (2) | −0.1394 (19) | 0.063* |
| H1D | 0.046 (4) | 0.315 (2) | −0.2365 (19) | 0.063* |
| H6 | 0.241 (4) | 0.596 (2) | 0.3330 (19) | 0.063* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0613 (13) | 0.0413 (10) | 0.0367 (11) | 0.0153 (9) | 0.0107 (10) | 0.0169 (9) |
| O2 | 0.0483 (12) | 0.0406 (10) | 0.0319 (10) | 0.0099 (9) | 0.0041 (9) | −0.0029 (9) |
| O3 | 0.0350 (12) | 0.0613 (12) | 0.0403 (11) | 0.0071 (10) | 0.0090 (10) | 0.0015 (10) |
| N1 | 0.0424 (13) | 0.0300 (10) | 0.0210 (11) | 0.0069 (9) | 0.0071 (10) | 0.0054 (9) |
| N2 | 0.083 (2) | 0.0437 (14) | 0.0260 (14) | 0.0064 (14) | 0.0098 (15) | 0.0093 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0346 (13) | 0.0359 (11) | 0.0312 (12) | 0.0108 (10) | 0.0107 (10) | 0.0009 (10) |
| C1 | 0.0339 (14) | 0.0323 (13) | 0.0257 (13) | 0.0064 (11) | 0.0114 (11) | 0.0070 (11) |
| C2 | 0.0279 (14) | 0.0361 (13) | 0.0307 (14) | 0.0080 (11) | 0.0096 (11) | 0.0086 (12) |
| C3 | 0.0431 (16) | 0.0291 (13) | 0.0390 (16) | 0.0075 (12) | 0.0106 (13) | 0.0055 (13) |
| C4 | 0.0427 (17) | 0.0335 (14) | 0.0363 (16) | 0.0059 (12) | 0.0076 (13) | −0.0035 (13) |
| C5 | 0.0383 (16) | 0.0432 (15) | 0.0241 (14) | 0.0057 (12) | 0.0069 (12) | 0.0014 (12) |
| C6 | 0.0322 (15) | 0.0402 (14) | 0.0281 (14) | 0.0067 (11) | 0.0090 (12) | 0.0086 (12) |
| C7 | 0.0400 (15) | 0.0316 (12) | 0.0281 (13) | 0.0086 (11) | 0.0109 (12) | 0.0099 (11) |
| C8 | 0.0353 (15) | 0.0329 (13) | 0.0312 (14) | 0.0086 (11) | 0.0127 (12) | 0.0090 (12) |
| C9 | 0.0388 (15) | 0.0338 (12) | 0.0196 (12) | 0.0091 (11) | 0.0065 (11) | 0.0035 (11) |
| C10 | 0.0381 (16) | 0.0380 (13) | 0.0330 (15) | 0.0132 (12) | 0.0124 (12) | 0.0049 (12) |
| C11 | 0.0368 (16) | 0.0415 (14) | 0.0351 (15) | 0.0111 (12) | 0.0047 (13) | 0.0057 (13) |
| C12 | 0.0388 (16) | 0.0370 (13) | 0.0238 (13) | 0.0114 (12) | 0.0057 (12) | 0.0090 (12) |
| C13 | 0.0366 (16) | 0.0369 (13) | 0.0257 (14) | 0.0083 (12) | 0.0099 (12) | 0.0088 (12) |
| O4 | 0.0509 (15) | 0.124 (2) | 0.0492 (14) | 0.0202 (14) | 0.0114 (12) | 0.0327 (16) |
| O5 | 0.0605 (14) | 0.0674 (13) | 0.0331 (11) | 0.0222 (12) | 0.0059 (11) | 0.0138 (10) |
| C14 | 0.0446 (19) | 0.0634 (18) | 0.0416 (17) | 0.0173 (15) | 0.0120 (14) | 0.0270 (15) |
| C15 | 0.0532 (19) | 0.0627 (18) | 0.0337 (16) | 0.0231 (15) | 0.0189 (14) | 0.0227 (15) |
| C16 | 0.0535 (19) | 0.0380 (14) | 0.0285 (15) | 0.0154 (13) | 0.0083 (13) | 0.0143 (13) |
| C17 | 0.0451 (17) | 0.0528 (16) | 0.0412 (17) | 0.0194 (14) | 0.0127 (14) | 0.0219 (15) |
| C18 | 0.060 (2) | 0.0560 (17) | 0.0375 (17) | 0.0286 (16) | 0.0190 (15) | 0.0192 (15) |
| C19 | 0.058 (2) | 0.0485 (16) | 0.0310 (15) | 0.0176 (15) | 0.0085 (14) | 0.0141 (14) |
| O6 | 0.0598 (13) | 0.0374 (10) | 0.0392 (11) | 0.0099 (9) | 0.0066 (10) | 0.0142 (9) |
| O7 | 0.0385 (12) | 0.0613 (12) | 0.0441 (12) | 0.0148 (10) | 0.0013 (10) | 0.0015 (10) |
| O8 | 0.0590 (13) | 0.0559 (12) | 0.0278 (10) | 0.0140 (10) | 0.0012 (10) | 0.0016 (10) |
| N4 | 0.0430 (13) | 0.0301 (11) | 0.0250 (11) | 0.0077 (10) | 0.0048 (10) | 0.0043 (10) |
| N5 | 0.0626 (18) | 0.0578 (16) | 0.0342 (14) | 0.0182 (14) | 0.0108 (13) | 0.0170 (14) |
| N6 | 0.0377 (14) | 0.0402 (12) | 0.0324 (13) | 0.0130 (10) | 0.0031 (11) | 0.0013 (11) |
| C20 | 0.0294 (14) | 0.0374 (13) | 0.0269 (14) | 0.0094 (11) | 0.0063 (11) | 0.0058 (12) |
| C21 | 0.0313 (15) | 0.0440 (15) | 0.0297 (14) | 0.0094 (12) | 0.0084 (12) | 0.0075 (13) |
| C22 | 0.0388 (16) | 0.0566 (17) | 0.0276 (15) | 0.0112 (14) | 0.0074 (13) | 0.0048 (14) |
| C23 | 0.0423 (17) | 0.0411 (15) | 0.0350 (16) | 0.0042 (13) | 0.0086 (14) | −0.0084 (13) |
| C24 | 0.0436 (17) | 0.0355 (14) | 0.0389 (16) | 0.0108 (12) | 0.0096 (14) | 0.0029 (13) |
| C25 | 0.0329 (15) | 0.0357 (13) | 0.0278 (14) | 0.0091 (11) | 0.0086 (12) | 0.0053 (12) |
| C26 | 0.0343 (15) | 0.0317 (13) | 0.0362 (15) | 0.0082 (11) | 0.0099 (12) | 0.0114 (13) |
| C27 | 0.0375 (15) | 0.0351 (13) | 0.0325 (14) | 0.0088 (12) | 0.0086 (12) | 0.0091 (12) |
| C28 | 0.0416 (16) | 0.0311 (12) | 0.0255 (13) | 0.0098 (12) | 0.0052 (12) | 0.0058 (11) |
| C29 | 0.0325 (16) | 0.0374 (14) | 0.0280 (14) | 0.0058 (12) | 0.0043 (12) | 0.0072 (12) |
| C30 | 0.0448 (17) | 0.0328 (13) | 0.0305 (15) | 0.0068 (12) | 0.0051 (13) | 0.0087 (13) |
| C31 | 0.0360 (16) | 0.0429 (15) | 0.0395 (16) | 0.0068 (12) | 0.0040 (13) | 0.0034 (13) |
| C32 | 0.0346 (15) | 0.0412 (14) | 0.0381 (16) | 0.0100 (12) | 0.0051 (13) | 0.0061 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.230 (3) | C15—C16 | 1.371 (4) |
| O2—C12 | 1.220 (3) | C16—C17 | 1.384 (3) |
| O3—C13 | 1.209 (3) | C17—C18 | 1.384 (4) |
| N1—C8 | 1.367 (3) | C18—C19 | 1.371 (4) |

| | | | |
|---|---|---|---|
| N1—C9 | 1.437 (3) | O6—C26 | 1.242 (3) |
| N1—C7 | 1.460 (3) | O7—C29 | 1.202 (3) |
| N2—C6 | 1.370 (3) | O8—C30 | 1.225 (3) |
| N3—C12 | 1.368 (3) | N4—C26 | 1.358 (3) |
| N3—C13 | 1.379 (3) | N4—C28 | 1.444 (3) |
| C1—C2 | 1.378 (3) | N4—C27 | 1.458 (3) |
| C1—C6 | 1.390 (3) | N5—C21 | 1.392 (3) |
| C1—C7 | 1.497 (3) | N6—C30 | 1.370 (3) |
| C2—C3 | 1.385 (3) | N6—C29 | 1.373 (3) |
| C2—C8 | 1.477 (3) | C20—C25 | 1.371 (3) |
| C3—C4 | 1.386 (3) | C20—C21 | 1.396 (3) |
| C4—C5 | 1.375 (3) | C20—C27 | 1.494 (3) |
| C5—C6 | 1.397 (3) | C21—C22 | 1.389 (3) |
| C9—C10 | 1.519 (3) | C22—C23 | 1.390 (4) |
| C9—C13 | 1.522 (3) | C23—C24 | 1.382 (4) |
| C10—C11 | 1.514 (3) | C24—C25 | 1.391 (3) |
| C11—C12 | 1.493 (3) | C25—C26 | 1.470 (3) |
| O4—C14 | 1.375 (3) | C28—C29 | 1.519 (3) |
| O5—C16 | 1.373 (3) | C28—C32 | 1.519 (3) |
| C14—C19 | 1.377 (4) | C30—C31 | 1.482 (3) |
| C14—C15 | 1.384 (4) | C31—C32 | 1.513 (3) |

| | | | |
|---|---|---|---|
| C8—N1—C9 | 122.6 (2) | C15—C16—C17 | 121.2 (3) |
| C8—N1—C7 | 113.20 (19) | O5—C16—C17 | 121.4 (3) |
| C9—N1—C7 | 124.16 (18) | C16—C17—C18 | 118.2 (3) |
| C12—N3—C13 | 127.7 (2) | C19—C18—C17 | 121.7 (3) |
| C2—C1—C6 | 121.4 (2) | C18—C19—C14 | 118.7 (3) |
| C2—C1—C7 | 109.99 (19) | C26—N4—C28 | 122.7 (2) |
| C6—C1—C7 | 128.6 (2) | C26—N4—C27 | 112.5 (2) |
| C1—C2—C3 | 122.2 (2) | C28—N4—C27 | 124.77 (18) |
| C1—C2—C8 | 108.6 (2) | C30—N6—C29 | 127.0 (2) |
| C3—C2—C8 | 129.2 (2) | C25—C20—C21 | 121.0 (2) |
| C2—C3—C4 | 116.5 (2) | C25—C20—C27 | 110.0 (2) |
| C5—C4—C3 | 121.7 (2) | C21—C20—C27 | 129.0 (2) |
| C4—C5—C6 | 121.8 (2) | C22—C21—N5 | 122.4 (2) |
| N2—C6—C1 | 121.8 (2) | C22—C21—C20 | 116.5 (2) |
| N2—C6—C5 | 121.8 (2) | N5—C21—C20 | 121.1 (2) |
| C1—C6—C5 | 116.3 (2) | C21—C22—C23 | 121.6 (2) |
| N1—C7—C1 | 102.00 (18) | C24—C23—C22 | 122.0 (2) |
| O1—C8—N1 | 124.7 (2) | C23—C24—C25 | 115.6 (3) |
| O1—C8—C2 | 129.1 (2) | C20—C25—C24 | 123.2 (2) |
| N1—C8—C2 | 106.2 (2) | C20—C25—C26 | 108.2 (2) |
| N1—C9—C10 | 114.20 (18) | C24—C25—C26 | 128.6 (2) |
| N1—C9—C13 | 111.7 (2) | O6—C26—N4 | 123.9 (2) |
| C10—C9—C13 | 111.10 (19) | O6—C26—C25 | 129.0 (2) |
| C11—C10—C9 | 109.87 (19) | N4—C26—C25 | 107.1 (2) |
| C12—C11—C10 | 113.0 (2) | N4—C27—C20 | 102.16 (18) |
| O2—C12—N3 | 120.2 (2) | N4—C28—C29 | 112.0 (2) |

| | | | |
|---|---|---|---|
| O2—C12—C11 | 123.0 (2) | N4—C28—C32 | 114.32 (19) |
| N3—C12—C11 | 116.8 (2) | C29—C28—C32 | 109.95 (19) |
| O3—C13—N3 | 120.5 (2) | O7—C29—N6 | 120.8 (2) |
| O3—C13—C9 | 123.3 (2) | O7—C29—C28 | 124.4 (2) |
| N3—C13—C9 | 116.1 (2) | N6—C29—C28 | 114.8 (2) |
| O4—C14—C19 | 121.5 (3) | O8—C30—N6 | 119.8 (2) |
| O4—C14—C15 | 117.6 (2) | O8—C30—C31 | 122.6 (2) |
| C19—C14—C15 | 120.9 (3) | N6—C30—C31 | 117.6 (2) |
| C16—C15—C14 | 119.1 (2) | C30—C31—C32 | 114.8 (2) |
| C15—C16—O5 | 117.4 (2) | C31—C32—C28 | 109.7 (2) |
| | | | |
| C6—C1—C2—C3 | 0.0 (4) | O5—C16—C17—C18 | −179.5 (2) |
| C7—C1—C2—C3 | 179.5 (2) | C16—C17—C18—C19 | −0.2 (4) |
| C6—C1—C2—C8 | −179.2 (2) | C17—C18—C19—C14 | −1.6 (4) |
| C7—C1—C2—C8 | 0.4 (3) | O4—C14—C19—C18 | −178.7 (2) |
| C1—C2—C3—C4 | 0.0 (4) | C15—C14—C19—C18 | 2.0 (4) |
| C8—C2—C3—C4 | 179.0 (2) | C25—C20—C21—C22 | 0.0 (3) |
| C2—C3—C4—C5 | 0.2 (4) | C27—C20—C21—C22 | −178.8 (2) |
| C3—C4—C5—C6 | −0.3 (4) | C25—C20—C21—N5 | −177.9 (2) |
| C2—C1—C6—N2 | 179.4 (2) | C27—C20—C21—N5 | 3.3 (4) |
| C7—C1—C6—N2 | −0.1 (4) | N5—C21—C22—C23 | 177.7 (2) |
| C2—C1—C6—C5 | −0.1 (3) | C20—C21—C22—C23 | −0.2 (4) |
| C7—C1—C6—C5 | −179.6 (2) | C21—C22—C23—C24 | −0.3 (4) |
| C4—C5—C6—N2 | −179.2 (2) | C22—C23—C24—C25 | 0.9 (4) |
| C4—C5—C6—C1 | 0.3 (4) | C21—C20—C25—C24 | 0.6 (4) |
| C8—N1—C7—C1 | 0.1 (2) | C27—C20—C25—C24 | 179.7 (2) |
| C9—N1—C7—C1 | −177.6 (2) | C21—C20—C25—C26 | −179.5 (2) |
| C2—C1—C7—N1 | −0.3 (2) | C27—C20—C25—C26 | −0.4 (3) |
| C6—C1—C7—N1 | 179.2 (2) | C23—C24—C25—C20 | −1.0 (4) |
| C9—N1—C8—O1 | −1.6 (4) | C23—C24—C25—C26 | 179.1 (2) |
| C7—N1—C8—O1 | −179.4 (2) | C28—N4—C26—O6 | 1.3 (4) |
| C9—N1—C8—C2 | 177.9 (2) | C27—N4—C26—O6 | 178.2 (2) |
| C7—N1—C8—C2 | 0.1 (3) | C28—N4—C26—C25 | −178.7 (2) |
| C1—C2—C8—O1 | 179.2 (2) | C27—N4—C26—C25 | −1.9 (3) |
| C3—C2—C8—O1 | 0.1 (4) | C20—C25—C26—O6 | −178.7 (2) |
| C1—C2—C8—N1 | −0.3 (3) | C24—C25—C26—O6 | 1.2 (4) |
| C3—C2—C8—N1 | −179.4 (2) | C20—C25—C26—N4 | 1.4 (3) |
| C8—N1—C9—C10 | −119.2 (2) | C24—C25—C26—N4 | −178.7 (2) |
| C7—N1—C9—C10 | 58.3 (3) | C26—N4—C27—C20 | 1.6 (3) |
| C8—N1—C9—C13 | 113.7 (2) | C28—N4—C27—C20 | 178.4 (2) |
| C7—N1—C9—C13 | −68.8 (3) | C25—C20—C27—N4 | −0.7 (3) |
| N1—C9—C10—C11 | 177.73 (19) | C21—C20—C27—N4 | 178.3 (2) |
| C13—C9—C10—C11 | −54.9 (3) | C26—N4—C28—C29 | −124.1 (2) |
| C9—C10—C11—C12 | 53.1 (3) | C27—N4—C28—C29 | 59.5 (3) |
| C13—N3—C12—O2 | 179.7 (2) | C26—N4—C28—C32 | 110.0 (3) |
| C13—N3—C12—C11 | 0.6 (4) | C27—N4—C28—C32 | −66.5 (3) |
| C10—C11—C12—O2 | 154.8 (2) | C30—N6—C29—O7 | −176.8 (2) |
| C10—C11—C12—N3 | −26.2 (3) | C30—N6—C29—C28 | 3.6 (3) |

| | | | |
|---|---|---|---|
| C12—N3—C13—O3 | −179.5 (2) | N4—C28—C29—O7 | 13.1 (3) |
| C12—N3—C13—C9 | −3.2 (3) | C32—C28—C29—O7 | 141.4 (2) |
| N1—C9—C13—O3 | −24.3 (3) | N4—C28—C29—N6 | −167.24 (19) |
| C10—C9—C13—O3 | −153.0 (2) | C32—C28—C29—N6 | −39.0 (3) |
| N1—C9—C13—N3 | 159.58 (19) | C29—N6—C30—O8 | −169.0 (2) |
| C10—C9—C13—N3 | 30.8 (3) | C29—N6—C30—C31 | 11.9 (4) |
| O4—C14—C15—C16 | −179.9 (2) | O8—C30—C31—C32 | −168.9 (2) |
| C19—C14—C15—C16 | −0.6 (4) | N6—C30—C31—C32 | 10.2 (3) |
| C14—C15—C16—O5 | 179.8 (2) | C30—C31—C32—C28 | −44.5 (3) |
| C14—C15—C16—C17 | −1.3 (4) | N4—C28—C32—C31 | −174.74 (19) |
| C15—C16—C17—C18 | 1.6 (4) | C29—C28—C32—C31 | 58.3 (3) |

*Hydrogen-bond geometry (Å, º)*

Ring centroids are defined as: *Cg*1 = N1/C7/C1/C2/C8; *Cg*2 = N3/C9–C13; *Cg*3 = C1–C6;*Cg*5 = N4/C20/C25–C27; *Cg*6 = N6/C28–C32; *Cg*7 = C20–C25; and *Cg*9 = C14–C19. *Cg*···*Cg* denotes the centroid—centroid distance associated with $\pi$–$\pi$ interactions.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H1···O8$^{i}$ | 0.93 (3) | 1.92 (3) | 2.816 (3) | 161 (3) |
| O5—H5*A*···O6 | 0.85 (3) | 1.87 (3) | 2.710 (3) | 171 (3) |
| N2—H2*B*···O5$^{ii}$ | 0.78 (3) | 2.56 (3) | 3.310 (3) | 163 (3) |
| N2—H2*A*···O5$^{iii}$ | 0.83 (3) | 2.28 (3) | 3.015 (3) | 148 (3) |
| N3—H3···O1$^{iv}$ | 0.89 (2) | 2.31 (2) | 3.022 (3) | 137 (2) |
| N3—H3···O8 | 0.89 (2) | 2.51 (2) | 3.256 (3) | 141 (2) |
| N5—H1*D*···O2$^{v}$ | 0.92 (3) | 2.23 (3) | 3.144 (3) | 172 (2) |
| N6—H6···O2 | 0.92 (3) | 2.00 (3) | 2.915 (3) | 171 (2) |
| C9—H9···O3$^{iv}$ | 0.98 | 2.65 | 3.409 (3) | 135 |
| C17—H17···O4$^{vi}$ | 0.93 | 2.57 | 3.263 (3) | 131 |
| C27—H27*B*···O7 | 0.97 | 2.58 | 3.106 (3) | 114 |
| C31—H31*B*···O2$^{vii}$ | 0.97 | 2.47 | 3.440 (3) | 178 |
| C10—H10*A*···Cg9$^{ii}$ | | 2.65 | 3.581 (3) | 161 |
| Cg1···Cg7$^{iii}$ | | | 3.7109 (16) | |
| Cg1···Cg7$^{viii}$ | | | 4.0014 (17) | |
| Cg3···Cg5$^{iii}$ | | | 3.7997 (17) | |
| Cg3···Cg5$^{viii}$ | | | 3.9603 (17) | |
| Cg3···Cg7$^{iii}$ | | | 3.6971 (17) | |
| Cg3···Cg7$^{viii}$ | | | 3.6644 (17) | |
| Cg3···Cg8$^{iii}$ | | | 3.5854 (15) | |
| Cg3···Cg8$^{viii}$ | | | 3.6382 (15) | |
| Cg4···Cg7$^{iii}$ | | | 3.5410 (15) | |
| Cg4···Cg7$^{viii}$ | | | 3.6602 (15) | |
| Cg4···Cg8$^{iii}$ | | | 3.6763 (13) | |
| Cg4···Cg8$^{viii}$ | | | 3.8723 (13) | |

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