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# 2,2′-{[(1*E*,1′*E*)-(Cyclohexane-1,4-diyl)-bis(azanylylidene)]bis(ethan-1-yl-1-yl-idene)}diphenol

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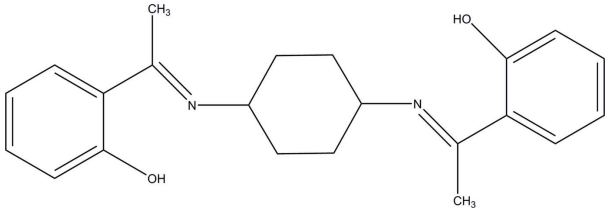
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.060; $wR$ factor = 0.239; data-to-parameter ratio = 13.4.

The title compound, $C_{22}H_{26}N_2O_2$, crystallizes with three independent molecules, two of which are situated on inversion centers, so the asymmetric unit contains two independent half-molecules and one molecule in a general position. The two hydroxy groups in each molecule are involved in intramolecular O—H···N hydrogen bonds, which generate $S$(6) rings. In the crystal, weak intermolecular C—H···$\pi$ interactions link the molecules into two crystallographically independent columns propagating along [001]; one column consists of molecules in general positions, while the other column is built from alternating independent centrosymmetric molecules.

## Related literature

For applications of Schiff base ligands in coordination chemistry, see: Gao & Zheng (2002); Hamil *et al.* (2012); Chu *et al.* (2008); More *et al.* (2001); Vigato & Tamburini (2004). For details of the synthesis, see: Huang *et al.* (2008).




## Experimental

### Crystal data

$C_{22}H_{26}N_2O_2$
$M_r$ = 350.45
Triclinic, $P\overline{1}$
$a$ = 9.0299 (6) Å
$b$ = 11.4718 (8) Å
$c$ = 17.9652 (13) Å
$\alpha$ = 92.946 (3)°
$\beta$ = 95.521 (4)°
$\gamma$ = 91.204 (3)°
$V$ = 1849.3 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 298 K
0.25 × 0.20 × 0.10 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.980, $T_{max}$ = 0.992
20050 measured reflections
6387 independent reflections
2646 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.239
$S$ = 1.02
6387 reflections
477 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C17–C22, C1–C6, C34–C39 and C23–C28 benzene rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O6—H6···N4 | 0.82 | 1.79 | 2.526 (5) | 147 |
| O5—H5···N3 | 0.82 | 1.80 | 2.523 (5) | 147 |
| O2—H2*A*···N2 | 0.82 | 1.80 | 2.516 (5) | 145 |
| O1—H1*A*···N1 | 0.82 | 1.79 | 2.520 (5) | 147 |
| C11—H11*A*···*Cg*1$^{i}$ | 0.97 | 2.64 | 3.552 (3) | 155 |
| C14—H14*A*···*Cg*2$^{ii}$ | 0.97 | 2.63 | 3.540 (1) | 156 |
| C33—H33*B*···*Cg*3$^{iii}$ | 0.97 | 2.62 | 3.510 (4) | 151 |
| C44—H44*A*···*Cg*4$^{iv}$ | 0.97 | 2.61 | 3.504 (4) | 152 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

The authors acknowledge the Department of Chemistry, IIT Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5426).

## References

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# supporting information

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## 2,2′-{[(1*E*,1′*E*)-(Cyclohexane-1,4-diyl)bis(azanylylidene)]bis(ethan-1-yl-1-yl-idene)}diphenol

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### S1. Comment

The research field dealing with Schiff base coordination chemistry has expanded enormously (Chu *et al.*, 2008; Gao *et al.*, 2002; Hamil *et al.*, 2012); the presence of a lone pair of electrons in an $sp^2$ hybridized orbital of nitrogen atom of the azomethine group is of considerable chemical and biological importance (More *et al.*, 2001). Because of the relative easiness of preparation, synthetic flexibility, and the special property of C=N group, Schiff bases are generally excellent chelating agents (Vigato *et al.*, 2004). In azomethine derivatives, the C=N linkage is essential for biological activity, several azomethines were reported to possess remarkable antibacterial, antifungal, anticancer and diuretic activities. Herewith we present the crystal structure of the title compound.

The title compound crystallizes with two half-molecules situated on inversion centers and one molecule in general position (Fig. 1). Two hydroxy groups in each molecule are involved in intramolecular O—H···N hydrogen bonds (Table 1), which generate S(6) rings. In the crystal, weak intermolecular C—H···$\pi$ interactions (Table 1) link the molecules into two crystallographically independent columns propagated in [001] - one column consists from the molecules in general positions, while another column is built from the alternating independent centrosymmetric molecules.

### S2. Experimental

The title compound was prepared by treating trans1, 4-diamino cyclohexane with 2-hydroxy acetophenone in the stoichiometric ratio in the ethanolic solution and refluxed for 5 h. The reaction mixture was then cooled slowly to room temperature; a yellow crystalline product was obtained and further washed with cold ethanol respectively (Huang *et al.*, 2008). It was then recrystallized from chloroform. The yellow like single-crystal of the title compound used in X-ray diffraction studies were grown in a chloroform solution by slow evaporation of the solvent at room temperature.

### S3. Refinement

All hydrogen atoms were fixed geometrically (C—H 0.93–0.98 Å) and refined as riding, with $U_{iso}$(H) = 1.2–1.5 $U_{eq}$(C).

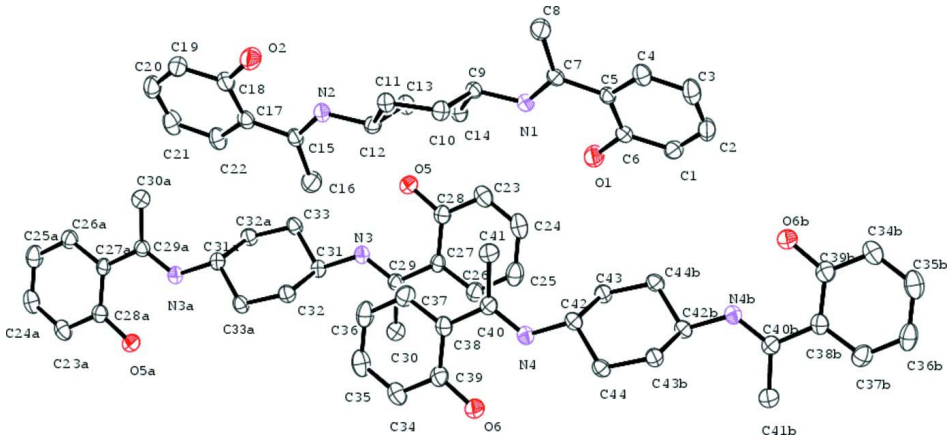


**Figure 1**

Three crystallographically independent molecules showing the atomic numbering and 30% probability displacement ellipsoids [symmetry codes: (*a*) -*x*, 1 - *y*, -*z*; (*b*) 2 - *x*, 1 - *y*, 1 - *z*]. H atoms omitted for clarity.

**2,2′-{[(1*E*,1′*E*)-(Cyclohexane-1,4-diyl)bis(azanylylidene)]bis(ethan-1-yl-1-ylidene)}diphenol**

*Crystal data*

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.0299$ (6) Å
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$\alpha = 92.946$ (3)°
$\beta = 95.521$ (4)°
$\gamma = 91.204$ (3)°
$V = 1849.3$ (2) Å$^3$
$Z = 4$
$F(000) = 752$
$D_x = 1.259$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5628 reflections
$\theta = 0.0$–$0.0°$
$\mu = 0.08$ mm$^{-1}$
$T = 298$ K
Block, yellow
0.25 × 0.20 × 0.10 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.980$, $T_{max} = 0.992$
20050 measured reflections
6387 independent reflections
2646 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.1°$
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.239$
$S = 1.02$
6387 reflections
477 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
$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2 + 2.2422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.8319 (7) | 1.1440 (5) | 0.6061 (3) | 0.0575 (17) |
| H1 | 0.8150 | 1.2200 | 0.6233 | 0.069* |
| C2 | 0.9279 (7) | 1.0768 (6) | 0.6478 (3) | 0.0603 (18) |
| H2 | 0.9765 | 1.1078 | 0.6927 | 0.072* |
| C3 | 0.9532 (6) | 0.9640 (6) | 0.6240 (3) | 0.0594 (17) |
| H3 | 1.0188 | 0.9187 | 0.6525 | 0.071* |
| C4 | 0.8809 (6) | 0.9185 (5) | 0.5577 (3) | 0.0464 (14) |
| H4 | 0.8989 | 0.8422 | 0.5416 | 0.056* |
| C5 | 0.7805 (6) | 0.9842 (4) | 0.5136 (3) | 0.0362 (13) |
| C6 | 0.7589 (6) | 1.1000 (4) | 0.5381 (3) | 0.0439 (14) |
| C7 | 0.7032 (6) | 0.9339 (4) | 0.4427 (3) | 0.0365 (12) |
| C8 | 0.7086 (7) | 0.8049 (4) | 0.4243 (3) | 0.0579 (17) |
| H8A | 0.6480 | 0.7854 | 0.3783 | 0.087* |
| H8B | 0.6718 | 0.7631 | 0.4640 | 0.087* |
| H8C | 0.8095 | 0.7838 | 0.4189 | 0.087* |
| C9 | 0.5504 (6) | 0.9694 (4) | 0.3276 (3) | 0.0353 (13) |
| H9 | 0.5033 | 0.8923 | 0.3307 | 0.042* |
| C10 | 0.6546 (6) | 0.9646 (4) | 0.2661 (3) | 0.0408 (13) |
| H10A | 0.7259 | 0.9037 | 0.2754 | 0.049* |
| H10B | 0.7095 | 1.0383 | 0.2669 | 0.049* |
| C11 | 0.5697 (6) | 0.9406 (4) | 0.1895 (3) | 0.0398 (13) |
| H11A | 0.6391 | 0.9416 | 0.1516 | 0.048* |
| H11B | 0.5234 | 0.8632 | 0.1873 | 0.048* |
| C12 | 0.4503 (6) | 1.0297 (4) | 0.1724 (3) | 0.0389 (13) |
| H12 | 0.4978 | 1.1067 | 0.1694 | 0.047* |
| C13 | 0.3456 (6) | 1.0352 (4) | 0.2340 (3) | 0.0418 (13) |
| H13A | 0.2750 | 1.0966 | 0.2247 | 0.050* |
| H13B | 0.2899 | 0.9618 | 0.2332 | 0.050* |
| C14 | 0.4303 (6) | 1.0587 (4) | 0.3110 (3) | 0.0396 (13) |
| H14A | 0.3608 | 1.0570 | 0.3488 | 0.048* |
| H14B | 0.4763 | 1.1362 | 0.3136 | 0.048* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.2981 (6) | 1.0670 (4) | 0.0578 (3) | 0.0405 (13) |
| C16 | 0.2927 (7) | 1.1947 (4) | 0.0751 (3) | 0.0628 (18) |
| H16A | 0.3690 | 1.2176 | 0.1144 | 0.094* |
| H16B | 0.1971 | 1.2134 | 0.0909 | 0.094* |
| H16C | 0.3085 | 1.2356 | 0.0311 | 0.094* |
| C17 | 0.2196 (6) | 1.0170 (5) | −0.0128 (3) | 0.0425 (14) |
| C18 | 0.2409 (7) | 0.9003 (5) | −0.0371 (3) | 0.0507 (15) |
| C19 | 0.1686 (7) | 0.8566 (5) | −0.1058 (3) | 0.0591 (17) |
| H19 | 0.1866 | 0.7810 | −0.1233 | 0.071* |
| C20 | 0.0720 (7) | 0.9235 (6) | −0.1473 (3) | 0.0608 (18) |
| H20 | 0.0233 | 0.8924 | −0.1921 | 0.073* |
| C21 | 0.0462 (7) | 1.0362 (6) | −0.1235 (3) | 0.0608 (18) |
| H21 | −0.0203 | 1.0811 | −0.1517 | 0.073* |
| C22 | 0.1200 (6) | 1.0821 (5) | −0.0574 (3) | 0.0509 (15) |
| H22 | 0.1029 | 1.1588 | −0.0419 | 0.061* |
| C23 | 0.3019 (7) | 0.3440 (5) | 0.3478 (3) | 0.0517 (15) |
| H23 | 0.2733 | 0.2697 | 0.3603 | 0.062* |
| C24 | 0.4097 (6) | 0.4066 (5) | 0.3931 (3) | 0.0570 (17) |
| H24 | 0.4552 | 0.3738 | 0.4354 | 0.068* |
| C25 | 0.4508 (6) | 0.5175 (5) | 0.3762 (3) | 0.0584 (17) |
| H25 | 0.5239 | 0.5595 | 0.4071 | 0.070* |
| C26 | 0.3841 (6) | 0.5662 (5) | 0.3139 (3) | 0.0487 (15) |
| H26 | 0.4127 | 0.6415 | 0.3034 | 0.058* |
| C27 | 0.2739 (6) | 0.5058 (4) | 0.2651 (3) | 0.0378 (12) |
| C28 | 0.2345 (6) | 0.3910 (4) | 0.2828 (3) | 0.0418 (14) |
| C29 | 0.2037 (6) | 0.5571 (4) | 0.1977 (3) | 0.0398 (13) |
| C30 | 0.2285 (6) | 0.6845 (4) | 0.1877 (3) | 0.0567 (16) |
| H30A | 0.1619 | 0.7084 | 0.1467 | 0.085* |
| H30B | 0.3294 | 0.6986 | 0.1773 | 0.085* |
| H30C | 0.2100 | 0.7284 | 0.2327 | 0.085* |
| C31 | 0.0496 (6) | 0.5264 (4) | 0.0803 (3) | 0.0379 (13) |
| H31 | 0.0089 | 0.6039 | 0.0888 | 0.045* |
| C32 | 0.1573 (6) | 0.5315 (4) | 0.0199 (3) | 0.0424 (13) |
| H32A | 0.2344 | 0.5905 | 0.0350 | 0.051* |
| H32B | 0.2046 | 0.4568 | 0.0146 | 0.051* |
| C33 | −0.0771 (6) | 0.4398 (4) | 0.0546 (3) | 0.0420 (13) |
| H33A | −0.0377 | 0.3619 | 0.0502 | 0.050* |
| H33B | −0.1476 | 0.4398 | 0.0921 | 0.050* |
| C34 | 0.6985 (7) | 0.6551 (5) | 0.1526 (3) | 0.0535 (16) |
| H34 | 0.7273 | 0.7295 | 0.1404 | 0.064* |
| C35 | 0.5913 (7) | 0.5937 (6) | 0.1067 (3) | 0.0614 (18) |
| H35 | 0.5471 | 0.6267 | 0.0641 | 0.074* |
| C36 | 0.5488 (6) | 0.4827 (6) | 0.1238 (3) | 0.0605 (18) |
| H36 | 0.4750 | 0.4411 | 0.0932 | 0.073* |
| C37 | 0.6156 (6) | 0.4339 (5) | 0.1860 (3) | 0.0521 (15) |
| H37 | 0.5873 | 0.3585 | 0.1964 | 0.063* |
| C38 | 0.7259 (6) | 0.4945 (4) | 0.2347 (3) | 0.0403 (13) |
| C39 | 0.7655 (6) | 0.6083 (4) | 0.2172 (3) | 0.0450 (14) |

| | | | | |
|---|---|---|---|---|
| C40 | 0.7956 (6) | 0.4409 (4) | 0.3026 (3) | 0.0382 (13) |
| C41 | 0.7717 (7) | 0.3141 (4) | 0.3121 (3) | 0.0582 (18) |
| H41A | 0.8326 | 0.2915 | 0.3555 | 0.087* |
| H41B | 0.7982 | 0.2703 | 0.2686 | 0.087* |
| H41C | 0.6689 | 0.2987 | 0.3184 | 0.087* |
| C42 | 0.9513 (5) | 0.4732 (4) | 0.4197 (3) | 0.0382 (13) |
| H42 | 0.9922 | 0.3957 | 0.4113 | 0.046* |
| C43 | 0.8430 (5) | 0.4678 (4) | 0.4798 (3) | 0.0398 (13) |
| H43A | 0.7947 | 0.5422 | 0.4846 | 0.048* |
| H43B | 0.7666 | 0.4083 | 0.4647 | 0.048* |
| C44 | 1.0776 (6) | 0.5597 (4) | 0.4452 (3) | 0.0391 (13) |
| H44A | 1.1486 | 0.5588 | 0.4079 | 0.047* |
| H44B | 1.0383 | 0.6376 | 0.4489 | 0.047* |
| N1 | 0.6309 (5) | 1.0050 (3) | 0.3999 (2) | 0.0394 (11) |
| N2 | 0.3692 (5) | 0.9952 (3) | 0.1003 (2) | 0.0408 (11) |
| N3 | 0.1238 (5) | 0.4889 (3) | 0.1507 (2) | 0.0397 (11) |
| N4 | 0.8768 (5) | 0.5101 (3) | 0.3495 (2) | 0.0406 (11) |
| O1 | 0.6695 (6) | 1.1708 (3) | 0.4976 (2) | 0.0688 (13) |
| H1A | 0.6349 | 1.1355 | 0.4588 | 0.103* |
| O2 | 0.3297 (6) | 0.8290 (3) | 0.0025 (2) | 0.0714 (13) |
| H2A | 0.3707 | 0.8653 | 0.0397 | 0.107* |
| O5 | 0.1332 (5) | 0.3254 (3) | 0.2392 (2) | 0.0574 (11) |
| H5 | 0.1070 | 0.3598 | 0.2014 | 0.086* |
| O6 | 0.8666 (5) | 0.6742 (3) | 0.2608 (2) | 0.0581 (11) |
| H6 | 0.8922 | 0.6402 | 0.2987 | 0.087* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.079 (5) | 0.054 (3) | 0.039 (3) | −0.023 (3) | 0.012 (3) | −0.002 (3) |
| C2 | 0.056 (4) | 0.088 (5) | 0.035 (3) | −0.022 (3) | −0.002 (3) | 0.007 (3) |
| C3 | 0.044 (4) | 0.093 (5) | 0.041 (4) | −0.001 (3) | −0.002 (3) | 0.012 (3) |
| C4 | 0.040 (4) | 0.060 (3) | 0.041 (3) | 0.004 (3) | 0.007 (3) | 0.007 (3) |
| C5 | 0.036 (3) | 0.042 (3) | 0.031 (3) | −0.005 (2) | 0.004 (3) | 0.006 (2) |
| C6 | 0.057 (4) | 0.041 (3) | 0.035 (3) | −0.007 (3) | 0.008 (3) | 0.006 (2) |
| C7 | 0.035 (3) | 0.040 (3) | 0.036 (3) | 0.002 (2) | 0.010 (3) | 0.007 (2) |
| C8 | 0.077 (5) | 0.044 (3) | 0.051 (4) | 0.012 (3) | −0.007 (3) | 0.004 (3) |
| C9 | 0.036 (3) | 0.038 (3) | 0.032 (3) | −0.002 (2) | 0.004 (3) | 0.004 (2) |
| C10 | 0.031 (3) | 0.049 (3) | 0.042 (3) | 0.003 (2) | 0.001 (3) | 0.001 (2) |
| C11 | 0.035 (3) | 0.048 (3) | 0.037 (3) | 0.003 (2) | 0.004 (3) | 0.002 (2) |
| C12 | 0.039 (3) | 0.039 (3) | 0.039 (3) | 0.001 (2) | 0.001 (3) | 0.001 (2) |
| C13 | 0.036 (3) | 0.051 (3) | 0.039 (3) | 0.004 (2) | 0.006 (3) | 0.003 (2) |
| C14 | 0.038 (4) | 0.047 (3) | 0.035 (3) | 0.004 (2) | 0.009 (3) | 0.001 (2) |
| C15 | 0.040 (3) | 0.049 (3) | 0.032 (3) | −0.001 (2) | 0.005 (3) | 0.006 (3) |
| C16 | 0.077 (5) | 0.051 (3) | 0.058 (4) | 0.006 (3) | −0.009 (4) | 0.003 (3) |
| C17 | 0.039 (4) | 0.055 (3) | 0.036 (3) | −0.004 (3) | 0.011 (3) | 0.007 (3) |
| C18 | 0.055 (4) | 0.056 (4) | 0.040 (3) | −0.008 (3) | −0.002 (3) | 0.009 (3) |
| C19 | 0.070 (5) | 0.061 (4) | 0.045 (4) | −0.017 (3) | 0.007 (4) | −0.002 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20 | 0.053 (5) | 0.087 (5) | 0.040 (4) | −0.021 (3) | 0.000 (3) | −0.001 (3) |
| C21 | 0.037 (4) | 0.097 (5) | 0.048 (4) | 0.001 (3) | −0.005 (3) | 0.014 (3) |
| C22 | 0.042 (4) | 0.069 (4) | 0.042 (3) | 0.006 (3) | 0.002 (3) | 0.009 (3) |
| C23 | 0.061 (4) | 0.053 (3) | 0.044 (3) | 0.018 (3) | 0.015 (3) | 0.006 (3) |
| C24 | 0.051 (4) | 0.083 (4) | 0.038 (3) | 0.019 (3) | 0.004 (3) | 0.007 (3) |
| C25 | 0.040 (4) | 0.087 (4) | 0.046 (4) | 0.000 (3) | 0.000 (3) | −0.005 (3) |
| C26 | 0.043 (4) | 0.062 (4) | 0.041 (3) | −0.007 (3) | 0.008 (3) | −0.002 (3) |
| C27 | 0.038 (3) | 0.045 (3) | 0.030 (3) | 0.003 (2) | 0.008 (3) | −0.005 (2) |
| C28 | 0.040 (4) | 0.047 (3) | 0.039 (3) | 0.005 (3) | 0.010 (3) | −0.002 (3) |
| C29 | 0.041 (3) | 0.043 (3) | 0.037 (3) | 0.001 (2) | 0.007 (3) | 0.002 (2) |
| C30 | 0.069 (4) | 0.051 (3) | 0.049 (3) | −0.006 (3) | 0.004 (3) | 0.001 (3) |
| C31 | 0.038 (4) | 0.042 (3) | 0.033 (3) | 0.005 (2) | 0.002 (3) | 0.001 (2) |
| C32 | 0.034 (3) | 0.052 (3) | 0.042 (3) | −0.001 (2) | 0.005 (3) | 0.005 (2) |
| C33 | 0.039 (3) | 0.053 (3) | 0.035 (3) | 0.000 (2) | 0.007 (3) | 0.008 (2) |
| C34 | 0.059 (4) | 0.058 (3) | 0.045 (3) | 0.016 (3) | 0.009 (3) | 0.009 (3) |
| C35 | 0.050 (4) | 0.089 (5) | 0.046 (4) | 0.023 (4) | 0.002 (3) | 0.005 (3) |
| C36 | 0.040 (4) | 0.092 (5) | 0.047 (4) | 0.007 (3) | −0.008 (3) | −0.006 (3) |
| C37 | 0.039 (4) | 0.064 (4) | 0.053 (4) | −0.005 (3) | 0.007 (3) | −0.004 (3) |
| C38 | 0.035 (4) | 0.052 (3) | 0.035 (3) | 0.006 (3) | 0.011 (3) | −0.001 (2) |
| C39 | 0.052 (4) | 0.043 (3) | 0.041 (3) | 0.009 (3) | 0.009 (3) | −0.005 (3) |
| C40 | 0.035 (4) | 0.045 (3) | 0.036 (3) | 0.001 (2) | 0.014 (3) | −0.006 (2) |
| C41 | 0.074 (5) | 0.046 (3) | 0.052 (4) | −0.007 (3) | −0.004 (4) | 0.004 (3) |
| C42 | 0.039 (3) | 0.039 (3) | 0.038 (3) | 0.005 (2) | 0.006 (3) | 0.006 (2) |
| C43 | 0.032 (3) | 0.049 (3) | 0.039 (3) | 0.000 (2) | 0.003 (3) | 0.005 (2) |
| C44 | 0.035 (3) | 0.045 (3) | 0.039 (3) | 0.001 (2) | 0.011 (3) | 0.007 (2) |
| N1 | 0.041 (3) | 0.040 (2) | 0.037 (2) | −0.0011 (19) | 0.002 (2) | 0.0043 (19) |
| N2 | 0.041 (3) | 0.048 (3) | 0.034 (3) | 0.001 (2) | 0.002 (2) | 0.003 (2) |
| N3 | 0.040 (3) | 0.046 (2) | 0.034 (2) | 0.002 (2) | 0.004 (2) | 0.0005 (19) |
| N4 | 0.044 (3) | 0.044 (2) | 0.035 (2) | 0.002 (2) | 0.005 (2) | 0.0022 (19) |
| O1 | 0.111 (4) | 0.040 (2) | 0.052 (3) | 0.008 (2) | −0.008 (3) | −0.0017 (19) |
| O2 | 0.104 (4) | 0.046 (2) | 0.059 (3) | 0.008 (2) | −0.015 (3) | 0.000 (2) |
| O5 | 0.077 (3) | 0.044 (2) | 0.048 (2) | −0.008 (2) | −0.005 (2) | 0.0011 (18) |
| O6 | 0.079 (3) | 0.043 (2) | 0.050 (3) | −0.006 (2) | −0.004 (2) | 0.0034 (18) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| C1—C2 | 1.367 (8) | C24—C25 | 1.374 (7) |
| C1—C6 | 1.397 (7) | C24—H24 | 0.9300 |
| C1—H1 | 0.9300 | C25—C26 | 1.370 (7) |
| C2—C3 | 1.373 (8) | C25—H25 | 0.9300 |
| C2—H2 | 0.9300 | C26—C27 | 1.407 (6) |
| C3—C4 | 1.375 (7) | C26—H26 | 0.9300 |
| C3—H3 | 0.9300 | C27—C28 | 1.417 (7) |
| C4—C5 | 1.403 (6) | C27—C29 | 1.468 (7) |
| C4—H4 | 0.9300 | C28—O5 | 1.338 (5) |
| C5—C6 | 1.402 (6) | C29—N3 | 1.279 (6) |
| C5—C7 | 1.476 (6) | C29—C30 | 1.497 (6) |
| C6—O1 | 1.346 (6) | C30—H30A | 0.9600 |

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|---|---|---|---|
| C7—N1 | 1.293 (6) | C30—H30B | 0.9600 |
| C7—C8 | 1.502 (6) | C30—H30C | 0.9600 |
| C8—H8A | 0.9600 | C31—N3 | 1.462 (6) |
| C8—H8B | 0.9600 | C31—C33 | 1.522 (6) |
| C8—H8C | 0.9600 | C31—C32 | 1.528 (7) |
| C9—N1 | 1.460 (5) | C31—H31 | 0.9800 |
| C9—C10 | 1.519 (7) | C32—C33$^{i}$ | 1.514 (6) |
| C9—C14 | 1.526 (6) | C32—H32A | 0.9700 |
| C9—H9 | 0.9800 | C32—H32B | 0.9700 |
| C10—C11 | 1.519 (6) | C33—C32$^{i}$ | 1.514 (6) |
| C10—H10A | 0.9700 | C33—H33A | 0.9700 |
| C10—H10B | 0.9700 | C33—H33B | 0.9700 |
| C11—C12 | 1.522 (6) | C34—C35 | 1.367 (7) |
| C11—H11A | 0.9700 | C34—C39 | 1.394 (7) |
| C11—H11B | 0.9700 | C34—H34 | 0.9300 |
| C12—N2 | 1.457 (6) | C35—C36 | 1.381 (8) |
| C12—C13 | 1.524 (7) | C35—H35 | 0.9300 |
| C12—H12 | 0.9800 | C36—C37 | 1.368 (7) |
| C13—C14 | 1.523 (6) | C36—H36 | 0.9300 |
| C13—H13A | 0.9700 | C37—C38 | 1.407 (7) |
| C13—H13B | 0.9700 | C37—H37 | 0.9300 |
| C14—H14A | 0.9700 | C38—C39 | 1.406 (7) |
| C14—H14B | 0.9700 | C38—C40 | 1.485 (7) |
| C15—N2 | 1.291 (6) | C39—O6 | 1.338 (6) |
| C15—C17 | 1.474 (7) | C40—N4 | 1.290 (6) |
| C15—C16 | 1.484 (7) | C40—C41 | 1.487 (6) |
| C16—H16A | 0.9600 | C41—H41A | 0.9600 |
| C16—H16B | 0.9600 | C41—H41B | 0.9600 |
| C16—H16C | 0.9600 | C41—H41C | 0.9600 |
| C17—C22 | 1.400 (7) | C42—N4 | 1.459 (6) |
| C17—C18 | 1.409 (7) | C42—C44 | 1.517 (6) |
| C18—O2 | 1.341 (6) | C42—C43 | 1.528 (6) |
| C18—C19 | 1.403 (7) | C42—H42 | 0.9800 |
| C19—C20 | 1.367 (8) | C43—C44$^{ii}$ | 1.516 (6) |
| C19—H19 | 0.9300 | C43—H43A | 0.9700 |
| C20—C21 | 1.372 (8) | C43—H43B | 0.9700 |
| C20—H20 | 0.9300 | C44—C43$^{ii}$ | 1.516 (6) |
| C21—C22 | 1.379 (7) | C44—H44A | 0.9700 |
| C21—H21 | 0.9300 | C44—H44B | 0.9700 |
| C22—H22 | 0.9300 | O1—H1A | 0.8200 |
| C23—C24 | 1.373 (7) | O2—H2A | 0.8200 |
| C23—C28 | 1.402 (7) | O5—H5 | 0.8201 |
| C23—H23 | 0.9300 | O6—H6 | 0.8201 |
| | | | |
| C2—C1—C6 | 120.8 (6) | C23—C24—H24 | 119.6 |
| C2—C1—H1 | 119.4 | C25—C24—H24 | 120.0 |
| C6—C1—H1 | 119.8 | C26—C25—C24 | 120.0 (5) |
| C3—C2—C1 | 120.6 (5) | C26—C25—H25 | 120.0 |

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|---|---|---|---|
| C3—C2—H2 | 119.7 | C24—C25—H25 | 120.0 |
| C1—C2—H2 | 119.7 | C25—C26—C27 | 122.1 (5) |
| C2—C3—C4 | 119.5 (5) | C25—C26—H26 | 119.0 |
| C2—C3—H3 | 120.4 | C27—C26—H26 | 118.9 |
| C4—C3—H3 | 120.1 | C26—C27—C28 | 117.1 (5) |
| C3—C4—C5 | 121.7 (5) | C26—C27—C29 | 122.2 (5) |
| C3—C4—H4 | 119.2 | C28—C27—C29 | 120.6 (4) |
| C5—C4—H4 | 119.1 | O5—C28—C23 | 118.5 (5) |
| C4—C5—C6 | 117.9 (4) | O5—C28—C27 | 121.8 (5) |
| C4—C5—C7 | 121.1 (4) | C23—C28—C27 | 119.8 (5) |
| C6—C5—C7 | 121.0 (4) | N3—C29—C27 | 117.3 (4) |
| O1—C6—C1 | 118.7 (5) | N3—C29—C30 | 123.8 (5) |
| O1—C6—C5 | 121.8 (4) | C27—C29—C30 | 118.9 (4) |
| C1—C6—C5 | 119.5 (5) | C29—C30—H30A | 109.5 |
| N1—C7—C5 | 117.1 (4) | C29—C30—H30B | 109.7 |
| N1—C7—C8 | 123.3 (4) | H30A—C30—H30B | 109.5 |
| C5—C7—C8 | 119.6 (4) | C29—C30—H30C | 109.2 |
| C7—C8—H8A | 109.6 | H30A—C30—H30C | 109.5 |
| C7—C8—H8B | 109.5 | H30B—C30—H30C | 109.5 |
| H8A—C8—H8B | 109.5 | N3—C31—C33 | 108.2 (4) |
| C7—C8—H8C | 109.4 | N3—C31—C32 | 111.4 (4) |
| H8A—C8—H8C | 109.5 | C33—C31—C32 | 109.6 (4) |
| H8B—C8—H8C | 109.5 | N3—C31—H31 | 109.3 |
| N1—C9—C10 | 110.9 (4) | C33—C31—H31 | 109.1 |
| N1—C9—C14 | 107.6 (4) | C32—C31—H31 | 109.2 |
| C10—C9—C14 | 110.1 (4) | C33$^{i}$—C32—C31 | 111.1 (4) |
| N1—C9—H9 | 109.4 | C33$^{i}$—C32—H32A | 109.4 |
| C10—C9—H9 | 109.4 | C31—C32—H32A | 109.3 |
| C14—C9—H9 | 109.3 | C33$^{i}$—C32—H32B | 109.6 |
| C9—C10—C11 | 111.4 (4) | C31—C32—H32B | 109.4 |
| C9—C10—H10A | 109.2 | H32A—C32—H32B | 108.0 |
| C11—C10—H10A | 109.4 | C32$^{i}$—C33—C31 | 112.3 (4) |
| C9—C10—H10B | 109.6 | C32$^{i}$—C33—H33A | 109.3 |
| C11—C10—H10B | 109.3 | C31—C33—H33A | 109.0 |
| H10A—C10—H10B | 107.9 | C32$^{i}$—C33—H33B | 109.1 |
| C12—C11—C10 | 112.4 (4) | C31—C33—H33B | 109.2 |
| C12—C11—H11A | 109.1 | H33A—C33—H33B | 107.9 |
| C10—C11—H11A | 109.1 | C35—C34—C39 | 121.3 (5) |
| C12—C11—H11B | 109.1 | C35—C34—H34 | 119.3 |
| C10—C11—H11B | 109.2 | C39—C34—H34 | 119.4 |
| H11A—C11—H11B | 107.9 | C34—C35—C36 | 119.8 (5) |
| N2—C12—C11 | 108.3 (4) | C34—C35—H35 | 120.3 |
| N2—C12—C13 | 110.7 (4) | C36—C35—H35 | 119.9 |
| C11—C12—C13 | 110.0 (4) | C37—C36—C35 | 119.9 (5) |
| N2—C12—H12 | 109.2 | C37—C36—H36 | 120.0 |
| C11—C12—H12 | 109.3 | C35—C36—H36 | 120.1 |
| C13—C12—H12 | 109.2 | C36—C37—C38 | 122.0 (5) |
| C14—C13—C12 | 111.6 (4) | C36—C37—H37 | 119.0 |

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| C14—C13—H13A | 109.3 | C38—C37—H37 | 119.1 |
| C12—C13—H13A | 109.5 | C39—C38—C37 | 117.3 (5) |
| C14—C13—H13B | 109.3 | C39—C38—C40 | 121.4 (4) |
| C12—C13—H13B | 109.1 | C37—C38—C40 | 121.3 (5) |
| H13A—C13—H13B | 108.0 | O6—C39—C34 | 118.3 (5) |
| C13—C14—C9 | 112.3 (4) | O6—C39—C38 | 122.0 (5) |
| C13—C14—H14A | 109.2 | C34—C39—C38 | 119.7 (5) |
| C9—C14—H14A | 109.2 | N4—C40—C38 | 116.0 (4) |
| C13—C14—H14B | 109.0 | N4—C40—C41 | 124.3 (5) |
| C9—C14—H14B | 109.2 | C38—C40—C41 | 119.7 (4) |
| H14A—C14—H14B | 107.8 | C40—C41—H41A | 109.4 |
| N2—C15—C17 | 116.7 (4) | C40—C41—H41B | 109.8 |
| N2—C15—C16 | 124.4 (5) | H41A—C41—H41B | 109.5 |
| C17—C15—C16 | 118.9 (4) | C40—C41—H41C | 109.2 |
| C15—C16—H16A | 109.4 | H41A—C41—H41C | 109.5 |
| C15—C16—H16B | 109.5 | H41B—C41—H41C | 109.5 |
| H16A—C16—H16B | 109.5 | N4—C42—C44 | 108.4 (4) |
| C15—C16—H16C | 109.5 | N4—C42—C43 | 111.0 (4) |
| H16A—C16—H16C | 109.5 | C44—C42—C43 | 109.9 (4) |
| H16B—C16—H16C | 109.5 | N4—C42—H42 | 109.1 |
| C22—C17—C18 | 117.5 (5) | C44—C42—H42 | 109.2 |
| C22—C17—C15 | 121.7 (5) | C43—C42—H42 | 109.2 |
| C18—C17—C15 | 120.7 (5) | C44$^{ii}$—C43—C42 | 111.3 (4) |
| O2—C18—C19 | 118.2 (5) | C44$^{ii}$—C43—H43A | 109.2 |
| O2—C18—C17 | 122.5 (5) | C42—C43—H43A | 109.4 |
| C19—C18—C17 | 119.3 (5) | C44$^{ii}$—C43—H43B | 109.4 |
| C20—C19—C18 | 120.9 (6) | C42—C43—H43B | 109.4 |
| C20—C19—H19 | 119.8 | H43A—C43—H43B | 108.0 |
| C18—C19—H19 | 119.4 | C43$^{ii}$—C44—C42 | 112.3 (4) |
| C19—C20—C21 | 120.7 (5) | C43$^{ii}$—C44—H44A | 109.2 |
| C19—C20—H20 | 119.7 | C42—C44—H44A | 109.1 |
| C21—C20—H20 | 119.6 | C43$^{ii}$—C44—H44B | 109.0 |
| C20—C21—C22 | 119.3 (6) | C42—C44—H44B | 109.3 |
| C20—C21—H21 | 120.2 | H44A—C44—H44B | 107.9 |
| C22—C21—H21 | 120.5 | C7—N1—C9 | 123.8 (4) |
| C21—C22—C17 | 122.2 (6) | C15—N2—C12 | 123.8 (4) |
| C21—C22—H22 | 118.8 | C29—N3—C31 | 123.6 (4) |
| C17—C22—H22 | 119.0 | C40—N4—C42 | 123.5 (4) |
| C24—C23—C28 | 120.6 (5) | C6—O1—H1A | 109.4 |
| C24—C23—H23 | 119.8 | C18—O2—H2A | 109.6 |
| C28—C23—H23 | 119.6 | C28—O5—H5 | 109.4 |
| C23—C24—C25 | 120.4 (5) | C39—O6—H6 | 109.5 |

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| C6—C1—C2—C3 | −0.8 (9) | C26—C27—C28—O5 | −178.5 (5) |
| C1—C2—C3—C4 | −0.1 (9) | C29—C27—C28—O5 | 0.1 (8) |
| C2—C3—C4—C5 | −0.4 (9) | C26—C27—C28—C23 | 1.9 (8) |
| C3—C4—C5—C6 | 1.9 (8) | C29—C27—C28—C23 | −179.5 (5) |
| C3—C4—C5—C7 | −179.7 (5) | C26—C27—C29—N3 | 168.5 (5) |

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| C2—C1—C6—O1 | −177.6 (6) | C28—C27—C29—N3 | −10.1 (8) |
| C2—C1—C6—C5 | 2.2 (9) | C26—C27—C29—C30 | −11.7 (8) |
| C4—C5—C6—O1 | 177.1 (5) | C28—C27—C29—C30 | 169.7 (5) |
| C7—C5—C6—O1 | −1.3 (8) | N3—C31—C32—C33$^{i}$ | 175.1 (4) |
| C4—C5—C6—C1 | −2.7 (8) | C33—C31—C32—C33$^{i}$ | 55.4 (6) |
| C7—C5—C6—C1 | 178.9 (5) | N3—C31—C33—C32$^{i}$ | −177.7 (4) |
| C4—C5—C7—N1 | −169.6 (5) | C32—C31—C33—C32$^{i}$ | −56.0 (6) |
| C6—C5—C7—N1 | 8.8 (7) | C39—C34—C35—C36 | −0.7 (9) |
| C4—C5—C7—C8 | 11.7 (8) | C34—C35—C36—C37 | −0.9 (9) |
| C6—C5—C7—C8 | −169.9 (5) | C35—C36—C37—C38 | 1.2 (9) |
| N1—C9—C10—C11 | −173.8 (4) | C36—C37—C38—C39 | 0.1 (8) |
| C14—C9—C10—C11 | −54.9 (5) | C36—C37—C38—C40 | 179.1 (6) |
| C9—C10—C11—C12 | 56.3 (5) | C35—C34—C39—O6 | −178.1 (5) |
| C10—C11—C12—N2 | −176.4 (4) | C35—C34—C39—C38 | 2.0 (8) |
| C10—C11—C12—C13 | −55.2 (5) | C37—C38—C39—O6 | 178.4 (5) |
| N2—C12—C13—C14 | 174.1 (4) | C40—C38—C39—O6 | −0.6 (8) |
| C11—C12—C13—C14 | 54.3 (5) | C37—C38—C39—C34 | −1.6 (8) |
| C12—C13—C14—C9 | −55.5 (5) | C40—C38—C39—C34 | 179.4 (5) |
| N1—C9—C14—C13 | 176.0 (4) | C39—C38—C40—N4 | 9.9 (8) |
| C10—C9—C14—C13 | 55.0 (5) | C37—C38—C40—N4 | −169.1 (5) |
| N2—C15—C17—C22 | 169.6 (5) | C39—C38—C40—C41 | −169.0 (5) |
| C16—C15—C17—C22 | −11.2 (8) | C37—C38—C40—C41 | 12.0 (8) |
| N2—C15—C17—C18 | −9.4 (8) | N4—C42—C43—C44$^{ii}$ | −174.8 (4) |
| C16—C15—C17—C18 | 169.9 (5) | C44—C42—C43—C44$^{ii}$ | −54.9 (6) |
| C22—C17—C18—O2 | −177.6 (5) | N4—C42—C44—C43$^{ii}$ | 176.9 (4) |
| C15—C17—C18—O2 | 1.4 (9) | C43—C42—C44—C43$^{ii}$ | 55.4 (6) |
| C22—C17—C18—C19 | 3.2 (8) | C5—C7—N1—C9 | 179.2 (4) |
| C15—C17—C18—C19 | −177.8 (5) | C8—C7—N1—C9 | −2.2 (8) |
| O2—C18—C19—C20 | 177.3 (6) | C10—C9—N1—C7 | −83.5 (6) |
| C17—C18—C19—C20 | −3.4 (9) | C14—C9—N1—C7 | 156.0 (5) |
| C18—C19—C20—C21 | 1.5 (10) | C17—C15—N2—C12 | −178.9 (5) |
| C19—C20—C21—C22 | 0.6 (9) | C16—C15—N2—C12 | 1.8 (9) |
| C20—C21—C22—C17 | −0.8 (9) | C11—C12—N2—C15 | −155.7 (5) |
| C18—C17—C22—C21 | −1.1 (9) | C13—C12—N2—C15 | 83.6 (6) |
| C15—C17—C22—C21 | 179.9 (5) | C27—C29—N3—C31 | −178.6 (5) |
| C28—C23—C24—C25 | 1.4 (8) | C30—C29—N3—C31 | 1.6 (8) |
| C23—C24—C25—C26 | 0.0 (9) | C33—C31—N3—C29 | −158.9 (5) |
| C24—C25—C26—C27 | −0.5 (9) | C32—C31—N3—C29 | 80.6 (6) |
| C25—C26—C27—C28 | −0.5 (8) | C38—C40—N4—C42 | 178.8 (5) |
| C25—C26—C27—C29 | −179.1 (5) | C41—C40—N4—C42 | −2.4 (8) |
| C24—C23—C28—O5 | 178.0 (5) | C44—C42—N4—C40 | 159.2 (5) |
| C24—C23—C28—C27 | −2.4 (8) | C43—C42—N4—C40 | −80.0 (6) |

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

*Hydrogen-bond geometry (Å, º)*

Cg1, Cg2, Cg3 and Cg4 are the centroiods of the C17–C22, C1–C6, C34–C39 and C23–C28 benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O6—H6···N4 | 0.82 | 1.79 | 2.526 (5) | 147 |
| O5—H5···N3 | 0.82 | 1.80 | 2.523 (5) | 147 |
| O2—H2*A*···N2 | 0.82 | 1.80 | 2.516 (5) | 145 |
| O1—H1*A*···N1 | 0.82 | 1.79 | 2.520 (5) | 147 |
| C11—H11*A*···*Cg*1$^{iii}$ | 0.97 | 2.64 | 3.552 (3) | 155 |
| C14—H14*A*···*Cg*2$^{iv}$ | 0.97 | 2.63 | 3.540 (1) | 156 |
| C33—H33*B*···*Cg*3$^{v}$ | 0.97 | 2.62 | 3.510 (4) | 151 |
| C44—H44*A*···*Cg*4$^{vi}$ | 0.97 | 2.61 | 3.504 (4) | 152 |

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