

4-Nitro-6-[(8-quinolylamino)methylidene]cyclohexa-2,4-dien-1-one

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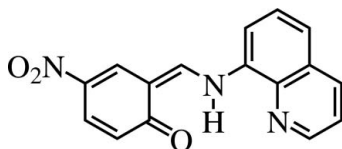
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Key indicators: single-crystal X-ray study; $T = 93$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.130; data-to-parameter ratio = 14.7.

The molecule of the title compound, $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O}_3$, exists in the keto form and the $\text{C}=\text{O}$ and $\text{N}-\text{H}$ bonds are mutually *cis* in the crystal structure. There are two crystallographically independent molecules per asymmetric unit with broadly similar structural data. The only noticeable difference between the two is the dihedral angles between the benzene and the quinoline rings: 1.04 (4) and 3.07 (4)°. In the structure, intramolecular $\text{N}-\text{H}\cdots\text{O}$ (carbonyl) and $\text{N}-\text{H}\cdots\text{N}$ (pyridine) hydrogen bonds exist but there is no evidence of formal intermolecular hydrogen-bonding associations.

Related literature

For a related structure, see: Shibahara *et al.* (2010).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{11}\text{N}_3\text{O}_3$
 $M_r = 293.28$
 Triclinic, $P\bar{1}$
 $a = 7.1583$ (6) Å

$b = 8.2978$ (7) Å
 $c = 22.040$ (2) Å
 $\alpha = 87.432$ (9)°
 $\beta = 86.258$ (12)°

$\gamma = 83.518$ (11)°
 $V = 1297.1$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.11$ mm⁻¹
 $T = 93$ K
 $0.25 \times 0.23 \times 0.18$ mm

Data collection

Rigaku Mercury70 CCD diffractometer
 Absorption correction: multi-scan (REQAB; Jacobson, 1998)
 $T_{\min} = 0.881$, $T_{\max} = 0.981$

16456 measured reflections
 5854 independent reflections
 4472 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.130$
 $S = 1.06$
 5854 reflections

397 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.32$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---------------------------------------|--------------|--------------------|-------------|----------------------|
| $\text{N2}-\text{H2N}\cdots\text{O1}$ | 0.88 | 2.01 | 2.6849 (15) | 132 |
| $\text{N2}-\text{H2N}\cdots\text{N3}$ | 0.88 | 2.31 | 2.6942 (16) | 107 |
| $\text{N5}-\text{H5N}\cdots\text{O6}$ | 0.88 | 1.88 | 2.5915 (14) | 137 |
| $\text{N5}-\text{H5N}\cdots\text{N6}$ | 0.88 | 2.25 | 2.6645 (15) | 109 |

Data collection: *CrystalClear-SM Expert* (Rigaku, 1999); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2007); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2173).

References

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supplementary materials

Acta Cryst. (2010). E66, o1892 [doi:10.1107/S1600536810025250]

4-Nitro-6-[(8-quinolylamino)methylidene]cyclohexa-2,4-dien-1-one

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Comment

In the present work, the title compound, (I), was prepared and the structure determined to explore the substituent effects of Schiff base ligands on the fluorescence of metal complexes (Shibahara *et al.*, 2010). The molecule of (I) (Fig. 1) exists in the keto form and the C=O and N–H bonds are mutually *cis*. In the structure of (I), N–H···O carbonyl and N–H···N pyridine intramolecular hydrogen bonds exist (Table 1) but there is no evidence of formal intermolecular hydrogen-bonding associations (Fig. 2).

Experimental

8-Aminoquinoline (290.4 mg, 2.0 mmol) in toluene (14.5 ml) and 5-nitrosalicylaldehyde (333.6 mg, 1.0 mmol) in toluene (50.5 ml) were dissolved, respectively, and kept at 60 °C for one hour. The two solutions were mixed and kept at 60 °C overnight. Red brown plate-like crystals deposited: yield 438.7 mg (71%). Anal. Found (calcd for C₁₆H₁₁N₃O₃): C, 65.58(65.53); H, 3.76(3.78); N, 14.29(14.33)%.

Refinement

The unit cell contains two crystallographically independent molecules. Trying of higher space groups, *e.g.* P2₁/c, was not successful.

Figures

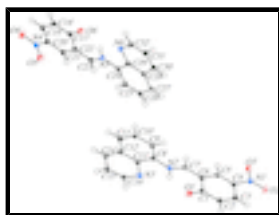


Fig. 1. Molecular configuration and atom-numbering scheme for (I) with displacement ellipsoids drawn at the 50% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

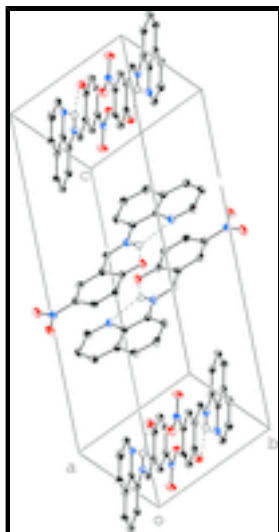


Fig. 2. Molecular packing of (I) in the unit cell.

4-Nitro-6-[(8-quinolylamino)methylidene]cyclohexa-2,4-dien-1-one

Crystal data

$C_{16}H_{11}N_3O_3$

$M_r = 293.28$

Triclinic, *PT*

Hall symbol: -P 1

$a = 7.1583$ (6) Å

$b = 8.2978$ (7) Å

$c = 22.040$ (2) Å

$\alpha = 87.432$ (9)°

$\beta = 86.258$ (12)°

$\gamma = 83.518$ (11)°

$V = 1297.1$ (2) Å³

$Z = 4$

$F(000) = 608.00$

$D_x = 1.502$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 3025 reflections

$\theta = 3.0$ – 27.5 °

$\mu = 0.11$ mm⁻¹

$T = 93$ K

Block, orange

$0.25 \times 0.23 \times 0.18$ mm

Data collection

Rigaku Mercury70 CCD
diffractometer

Detector resolution: 7.314 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(REQAB; Jacobson, 1998)

$T_{\min} = 0.881$, $T_{\max} = 0.981$

16456 measured reflections

5854 independent reflections

4472 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.040$

$\theta_{\text{max}} = 27.5$ °

$h = -9 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -28 \rightarrow 28$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

| | |
|--|--|
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.130$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.0744P)^2 + 0.0495P]$ |
| 5854 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 397 parameters | $(\Delta/\sigma)_{\max} < 0.001$ |
| 0 restraints | $\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$ |

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-------|---------------|--------------|--------------|----------------------------------|
| O(1) | 0.43832 (13) | 0.62852 (12) | -0.07215 (4) | 0.0217 (2) |
| O(2) | 1.19749 (13) | 0.87041 (12) | -0.17075 (4) | 0.0231 (2) |
| O(3) | 1.17251 (13) | 0.96692 (12) | -0.08065 (4) | 0.0236 (2) |
| O(4) | -0.16904 (14) | 0.93926 (13) | 0.67941 (5) | 0.0267 (2) |
| O(5) | -0.10119 (15) | 1.04935 (12) | 0.59061 (5) | 0.0266 (2) |
| O(6) | 0.25414 (13) | 0.33488 (11) | 0.55531 (4) | 0.0208 (2) |
| N(1) | 1.11180 (15) | 0.89084 (13) | -0.12067 (5) | 0.0169 (2) |
| N(2) | 0.42381 (15) | 0.75275 (13) | 0.03868 (5) | 0.0156 (2) |
| N(3) | 0.09322 (15) | 0.63056 (13) | 0.06404 (5) | 0.0170 (2) |
| N(4) | -0.09901 (15) | 0.93035 (14) | 0.62653 (5) | 0.0195 (3) |
| N(5) | 0.33339 (14) | 0.46786 (13) | 0.44950 (5) | 0.0157 (2) |
| N(6) | 0.48679 (15) | 0.16726 (13) | 0.42680 (5) | 0.0167 (2) |
| C(1) | 0.58855 (18) | 0.69178 (16) | -0.08436 (6) | 0.0167 (3) |
| C(2) | 0.69123 (19) | 0.68063 (16) | -0.14301 (6) | 0.0183 (3) |
| C(3) | 0.85732 (19) | 0.74407 (16) | -0.15485 (6) | 0.0180 (3) |
| C(4) | 0.93538 (18) | 0.82506 (16) | -0.10854 (6) | 0.0152 (3) |
| C(5) | 0.84328 (18) | 0.84505 (16) | -0.05262 (6) | 0.0159 (3) |
| C(6) | 0.67036 (18) | 0.78176 (16) | -0.03944 (6) | 0.0153 (3) |
| C(7) | 0.58246 (18) | 0.80688 (16) | 0.01895 (6) | 0.0160 (3) |
| C(8) | 0.33581 (18) | 0.77655 (16) | 0.09739 (6) | 0.0153 (3) |
| C(9) | 0.40980 (18) | 0.85949 (16) | 0.14119 (6) | 0.0167 (3) |
| C(10) | 0.31248 (18) | 0.88074 (16) | 0.19822 (6) | 0.0178 (3) |
| C(11) | 0.14418 (18) | 0.81891 (16) | 0.21149 (6) | 0.0175 (3) |
| C(12) | 0.06553 (18) | 0.73253 (16) | 0.16752 (6) | 0.0166 (3) |
| C(13) | 0.16067 (18) | 0.71080 (15) | 0.10943 (6) | 0.0152 (3) |
| C(14) | -0.10795 (18) | 0.66561 (17) | 0.17778 (6) | 0.0188 (3) |
| C(15) | -0.17462 (19) | 0.58457 (17) | 0.13279 (6) | 0.0198 (3) |

supplementary materials

| | | | | |
|-------|---------------|---------------|-------------|------------|
| C(16) | -0.06864 (18) | 0.57026 (16) | 0.07644 (6) | 0.0176 (3) |
| C(17) | 0.17001 (18) | 0.47021 (16) | 0.57108 (6) | 0.0166 (3) |
| C(18) | 0.07574 (19) | 0.49201 (17) | 0.63044 (6) | 0.0188 (3) |
| C(19) | -0.01010 (18) | 0.63861 (17) | 0.64786 (6) | 0.0183 (3) |
| C(20) | -0.01113 (18) | 0.77500 (16) | 0.60666 (6) | 0.0174 (3) |
| C(21) | 0.07089 (18) | 0.76247 (16) | 0.54887 (6) | 0.0174 (3) |
| C(22) | 0.16227 (18) | 0.61281 (16) | 0.52996 (6) | 0.0158 (3) |
| C(23) | 0.24603 (18) | 0.60299 (16) | 0.47035 (6) | 0.0168 (3) |
| C(24) | 0.41639 (17) | 0.44225 (16) | 0.39051 (6) | 0.0151 (3) |
| C(25) | 0.41950 (18) | 0.56114 (16) | 0.34503 (6) | 0.0173 (3) |
| C(26) | 0.50404 (18) | 0.52268 (17) | 0.28730 (6) | 0.0185 (3) |
| C(27) | 0.58376 (18) | 0.36854 (16) | 0.27533 (6) | 0.0176 (3) |
| C(28) | 0.58052 (17) | 0.24344 (16) | 0.32126 (6) | 0.0157 (3) |
| C(29) | 0.49608 (17) | 0.27981 (16) | 0.37962 (6) | 0.0149 (3) |
| C(30) | 0.65786 (19) | 0.08012 (17) | 0.31225 (6) | 0.0195 (3) |
| C(31) | 0.64855 (19) | -0.03123 (17) | 0.35941 (6) | 0.0199 (3) |
| C(32) | 0.56198 (19) | 0.01744 (16) | 0.41627 (6) | 0.0186 (3) |
| H(2) | 0.6408 | 0.6271 | -0.1744 | 0.022* |
| H(2N) | 0.3677 | 0.6974 | 0.0135 | 0.019* |
| H(3) | 0.9211 | 0.7344 | -0.1939 | 0.022* |
| H(5) | 0.8961 | 0.9018 | -0.0226 | 0.019* |
| H(5N) | 0.3412 | 0.3835 | 0.4752 | 0.019* |
| H(7) | 0.6427 | 0.8675 | 0.0460 | 0.019* |
| H(9) | 0.5267 | 0.9024 | 0.1329 | 0.020* |
| H(10) | 0.3641 | 0.9389 | 0.2281 | 0.021* |
| H(11) | 0.0804 | 0.8342 | 0.2503 | 0.021* |
| H(14) | -0.1774 | 0.6772 | 0.2158 | 0.023* |
| H(15) | -0.2903 | 0.5385 | 0.1392 | 0.024* |
| H(16) | -0.1171 | 0.5136 | 0.0455 | 0.021* |
| H(18) | 0.0736 | 0.4012 | 0.6582 | 0.023* |
| H(19) | -0.0693 | 0.6497 | 0.6875 | 0.022* |
| H(21) | 0.0659 | 0.8548 | 0.5217 | 0.021* |
| H(23) | 0.2387 | 0.6978 | 0.4445 | 0.020* |
| H(25) | 0.3648 | 0.6686 | 0.3526 | 0.021* |
| H(26) | 0.5059 | 0.6052 | 0.2560 | 0.022* |
| H(27) | 0.6413 | 0.3454 | 0.2362 | 0.021* |
| H(30) | 0.7153 | 0.0490 | 0.2738 | 0.023* |
| H(31) | 0.6998 | -0.1408 | 0.3542 | 0.024* |
| H(32) | 0.5577 | -0.0619 | 0.4486 | 0.022* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|------------|------------|------------|-------------|-------------|-------------|
| O(1) | 0.0191 (5) | 0.0227 (5) | 0.0249 (5) | -0.0076 (4) | -0.0017 (4) | -0.0031 (4) |
| O(2) | 0.0227 (5) | 0.0284 (6) | 0.0169 (5) | -0.0024 (4) | 0.0083 (4) | -0.0029 (4) |
| O(3) | 0.0219 (5) | 0.0276 (6) | 0.0231 (5) | -0.0097 (4) | 0.0037 (4) | -0.0098 (4) |
| O(4) | 0.0310 (6) | 0.0273 (6) | 0.0208 (5) | 0.0010 (5) | 0.0060 (4) | -0.0096 (4) |
| O(5) | 0.0334 (6) | 0.0171 (6) | 0.0271 (6) | 0.0043 (4) | 0.0027 (4) | -0.0015 (4) |

| | | | | | | |
|-------|------------|------------|------------|-------------|-------------|-------------|
| O(6) | 0.0257 (5) | 0.0156 (5) | 0.0196 (5) | 0.0030 (4) | 0.0012 (4) | -0.0005 (4) |
| N(1) | 0.0183 (6) | 0.0156 (6) | 0.0159 (6) | -0.0006 (5) | 0.0031 (4) | -0.0018 (5) |
| N(2) | 0.0145 (5) | 0.0156 (6) | 0.0168 (6) | -0.0026 (4) | 0.0005 (4) | -0.0018 (4) |
| N(3) | 0.0169 (6) | 0.0146 (6) | 0.0190 (6) | -0.0003 (4) | -0.0011 (4) | -0.0005 (5) |
| N(4) | 0.0191 (6) | 0.0200 (6) | 0.0191 (6) | 0.0004 (5) | 0.0005 (5) | -0.0049 (5) |
| N(5) | 0.0173 (6) | 0.0135 (6) | 0.0155 (6) | 0.0008 (4) | 0.0000 (4) | -0.0008 (4) |
| N(6) | 0.0174 (6) | 0.0149 (6) | 0.0170 (6) | 0.0002 (4) | 0.0006 (4) | -0.0003 (4) |
| C(1) | 0.0174 (7) | 0.0128 (7) | 0.0199 (7) | 0.0001 (5) | -0.0034 (5) | -0.0001 (5) |
| C(2) | 0.0201 (7) | 0.0168 (7) | 0.0186 (7) | -0.0019 (5) | -0.0044 (5) | -0.0040 (5) |
| C(3) | 0.0229 (7) | 0.0164 (7) | 0.0138 (6) | 0.0020 (5) | -0.0000 (5) | -0.0027 (5) |
| C(4) | 0.0150 (6) | 0.0130 (7) | 0.0172 (7) | -0.0009 (5) | 0.0003 (5) | -0.0001 (5) |
| C(5) | 0.0174 (7) | 0.0135 (7) | 0.0168 (7) | -0.0008 (5) | -0.0019 (5) | -0.0022 (5) |
| C(6) | 0.0155 (6) | 0.0135 (7) | 0.0165 (7) | -0.0001 (5) | 0.0002 (5) | -0.0005 (5) |
| C(7) | 0.0165 (6) | 0.0130 (7) | 0.0187 (7) | -0.0012 (5) | -0.0020 (5) | -0.0012 (5) |
| C(8) | 0.0161 (6) | 0.0133 (7) | 0.0156 (6) | 0.0012 (5) | 0.0010 (5) | 0.0005 (5) |
| C(9) | 0.0149 (6) | 0.0144 (7) | 0.0204 (7) | -0.0014 (5) | -0.0006 (5) | 0.0008 (5) |
| C(10) | 0.0199 (7) | 0.0147 (7) | 0.0190 (7) | -0.0001 (5) | -0.0032 (5) | -0.0029 (5) |
| C(11) | 0.0190 (7) | 0.0166 (7) | 0.0158 (7) | 0.0010 (5) | 0.0022 (5) | -0.0023 (5) |
| C(12) | 0.0164 (6) | 0.0140 (7) | 0.0183 (7) | 0.0012 (5) | 0.0003 (5) | 0.0003 (5) |
| C(13) | 0.0154 (6) | 0.0118 (7) | 0.0178 (7) | 0.0006 (5) | -0.0012 (5) | 0.0001 (5) |
| C(14) | 0.0178 (7) | 0.0200 (7) | 0.0178 (7) | -0.0007 (5) | 0.0040 (5) | -0.0013 (5) |
| C(15) | 0.0150 (6) | 0.0191 (7) | 0.0251 (7) | -0.0024 (5) | 0.0006 (5) | 0.0008 (6) |
| C(16) | 0.0175 (7) | 0.0157 (7) | 0.0196 (7) | -0.0005 (5) | -0.0025 (5) | -0.0003 (5) |
| C(17) | 0.0164 (6) | 0.0148 (7) | 0.0187 (7) | -0.0003 (5) | -0.0031 (5) | -0.0019 (5) |
| C(18) | 0.0208 (7) | 0.0184 (7) | 0.0169 (7) | -0.0010 (6) | -0.0017 (5) | 0.0016 (5) |
| C(19) | 0.0177 (7) | 0.0228 (8) | 0.0146 (6) | -0.0014 (5) | -0.0002 (5) | -0.0040 (5) |
| C(20) | 0.0168 (6) | 0.0152 (7) | 0.0201 (7) | 0.0009 (5) | -0.0013 (5) | -0.0046 (5) |
| C(21) | 0.0178 (6) | 0.0159 (7) | 0.0185 (7) | -0.0004 (5) | -0.0024 (5) | -0.0007 (5) |
| C(22) | 0.0154 (6) | 0.0161 (7) | 0.0160 (7) | -0.0015 (5) | -0.0006 (5) | -0.0024 (5) |
| C(23) | 0.0164 (6) | 0.0157 (7) | 0.0180 (7) | -0.0001 (5) | -0.0020 (5) | -0.0006 (5) |
| C(24) | 0.0130 (6) | 0.0172 (7) | 0.0152 (6) | -0.0012 (5) | -0.0005 (5) | -0.0020 (5) |
| C(25) | 0.0159 (6) | 0.0139 (7) | 0.0216 (7) | 0.0010 (5) | -0.0005 (5) | -0.0013 (5) |
| C(26) | 0.0184 (7) | 0.0190 (7) | 0.0174 (7) | -0.0012 (5) | -0.0006 (5) | 0.0040 (5) |
| C(27) | 0.0169 (6) | 0.0208 (7) | 0.0146 (6) | -0.0007 (5) | 0.0011 (5) | -0.0006 (5) |
| C(28) | 0.0134 (6) | 0.0173 (7) | 0.0164 (7) | -0.0010 (5) | -0.0010 (5) | -0.0021 (5) |
| C(29) | 0.0130 (6) | 0.0161 (7) | 0.0158 (6) | -0.0021 (5) | -0.0011 (5) | -0.0016 (5) |
| C(30) | 0.0207 (7) | 0.0212 (7) | 0.0158 (7) | 0.0008 (6) | 0.0014 (5) | -0.0039 (5) |
| C(31) | 0.0232 (7) | 0.0151 (7) | 0.0207 (7) | 0.0016 (5) | 0.0007 (5) | -0.0040 (5) |
| C(32) | 0.0212 (7) | 0.0147 (7) | 0.0191 (7) | -0.0004 (5) | 0.0010 (5) | 0.0011 (5) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|-------------|-------------|
| O(1)—C(1) | 1.2576 (17) | C(19)—C(20) | 1.4186 (19) |
| O(2)—N(1) | 1.2362 (14) | C(20)—C(21) | 1.3705 (18) |
| O(3)—N(1) | 1.2358 (15) | C(21)—C(22) | 1.4040 (18) |
| O(4)—N(4) | 1.2402 (15) | C(22)—C(23) | 1.4100 (18) |
| O(5)—N(4) | 1.2370 (15) | C(24)—C(25) | 1.3755 (18) |
| O(6)—C(17) | 1.2647 (16) | C(24)—C(29) | 1.4274 (18) |
| N(1)—C(4) | 1.4362 (17) | C(25)—C(26) | 1.4069 (18) |

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| N(2)—C(7) | 1.3091 (17) | C(26)—C(27) | 1.3700 (19) |
| N(2)—C(8) | 1.4137 (17) | C(27)—C(28) | 1.4181 (18) |
| N(3)—C(13) | 1.3684 (18) | C(28)—C(29) | 1.4153 (18) |
| N(3)—C(16) | 1.3209 (17) | C(28)—C(30) | 1.4223 (19) |
| N(4)—C(20) | 1.4425 (17) | C(30)—C(31) | 1.3628 (19) |
| N(5)—C(23) | 1.3076 (16) | C(31)—C(32) | 1.4160 (18) |
| N(5)—C(24) | 1.4085 (17) | N(2)—H(2N) | 0.880 |
| N(6)—C(29) | 1.3696 (17) | N(5)—H(5N) | 0.880 |
| N(6)—C(32) | 1.3219 (17) | C(2)—H(2) | 0.950 |
| C(1)—C(2) | 1.4461 (18) | C(3)—H(3) | 0.950 |
| C(1)—C(6) | 1.4564 (20) | C(5)—H(5) | 0.950 |
| C(2)—C(3) | 1.3591 (20) | C(7)—H(7) | 0.950 |
| C(3)—C(4) | 1.4235 (20) | C(9)—H(9) | 0.950 |
| C(4)—C(5) | 1.3670 (18) | C(10)—H(10) | 0.950 |
| C(5)—C(6) | 1.4066 (19) | C(11)—H(11) | 0.950 |
| C(6)—C(7) | 1.4086 (18) | C(14)—H(14) | 0.950 |
| C(8)—C(9) | 1.3765 (20) | C(15)—H(15) | 0.950 |
| C(8)—C(13) | 1.4275 (19) | C(16)—H(16) | 0.950 |
| C(9)—C(10) | 1.4050 (18) | C(18)—H(18) | 0.950 |
| C(10)—C(11) | 1.3712 (19) | C(19)—H(19) | 0.950 |
| C(11)—C(12) | 1.4122 (20) | C(21)—H(21) | 0.950 |
| C(12)—C(13) | 1.4194 (18) | C(23)—H(23) | 0.950 |
| C(12)—C(14) | 1.4175 (19) | C(25)—H(25) | 0.950 |
| C(14)—C(15) | 1.363 (2) | C(26)—H(26) | 0.950 |
| C(15)—C(16) | 1.4149 (18) | C(27)—H(27) | 0.950 |
| C(17)—C(18) | 1.4416 (18) | C(30)—H(30) | 0.950 |
| C(17)—C(22) | 1.4561 (18) | C(31)—H(31) | 0.950 |
| C(18)—C(19) | 1.3591 (19) | C(32)—H(32) | 0.950 |
| O(1)···N(2) | 2.6849 (15) | H(30)···H(31) | 2.3218 |
| O(1)···C(7) | 2.8580 (17) | H(31)···H(32) | 2.3434 |
| O(2)···C(3) | 2.7538 (17) | O(1)···H(2N) ⁱⁱ | 3.1599 |
| O(2)···C(5) | 3.5301 (16) | O(1)···H(15) ⁱⁱⁱ | 2.4380 |
| O(3)···C(3) | 3.5887 (18) | O(1)···H(16) ⁱⁱⁱ | 2.7199 |
| O(3)···C(5) | 2.6927 (17) | O(2)···H(2) ^{iv} | 3.5621 |
| O(4)···C(19) | 2.7227 (17) | O(2)···H(9) ^{vii} | 3.0570 |
| O(4)···C(21) | 3.5417 (17) | O(2)···H(11) ^v | 3.4655 |
| O(5)···C(19) | 3.5852 (17) | O(2)···H(15) ⁱⁱ | 3.4319 |
| O(5)···C(21) | 2.7233 (16) | O(2)···H(27) ^{vi} | 2.4828 |
| O(6)···N(5) | 2.5915 (14) | O(2)···H(30) ^{vi} | 2.4025 |
| O(6)···N(6) | 3.4561 (14) | O(3)···H(2N) ^{iv} | 3.2430 |
| O(6)···C(23) | 2.8409 (16) | O(3)···H(5) ^{vii} | 2.5621 |
| N(2)···N(3) | 2.6942 (16) | O(3)···H(7) ^{vii} | 2.2044 |
| N(2)···C(1) | 2.9277 (17) | O(3)···H(9) ^{vii} | 2.6883 |
| N(3)···C(14) | 2.8182 (17) | O(4)···H(3) ^{xii} | 3.2655 |
| N(5)···N(6) | 2.6645 (15) | O(4)···H(10) ^{ix} | 2.5738 |

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| N(5)···C(17) | 2.8529 (17) | O(4)···H(11) ^{ix} | 2.6445 |
| N(6)···C(30) | 2.8207 (17) | O(4)···H(25) ^{ix} | 3.4554 |
| C(1)···C(4) | 2.8400 (19) | O(4)···H(30) ^x | 3.4840 |
| C(2)···C(5) | 2.807 (2) | O(5)···H(21) ^{ix} | 2.5710 |
| C(3)···C(6) | 2.8092 (19) | O(5)···H(23) ^{ix} | 2.3356 |
| C(7)···C(9) | 2.9199 (19) | O(5)···H(25) ^{ix} | 3.0924 |
| C(8)···C(11) | 2.8017 (18) | O(5)···H(31) ^x | 3.3681 |
| C(8)···C(16) | 3.5902 (20) | O(5)···H(32) ^{viii} | 3.4236 |
| C(9)···C(12) | 2.8044 (19) | O(6)···H(21) ^{viii} | 3.4880 |
| C(10)···C(13) | 2.8053 (20) | O(6)···H(23) ^{viii} | 3.5688 |
| C(12)···C(16) | 2.7479 (20) | O(6)···H(25) ^x | 3.5018 |
| C(13)···C(15) | 2.7351 (20) | O(6)···H(31) ^{xi} | 2.5222 |
| C(17)···C(20) | 2.8279 (18) | O(6)···H(32) ^{xi} | 2.5031 |
| C(18)···C(21) | 2.8105 (19) | N(1)···H(7) ^{vii} | 3.3602 |
| C(19)···C(22) | 2.8093 (18) | N(1)···H(9) ^{vii} | 3.2529 |
| C(23)···C(25) | 2.9719 (19) | N(1)···H(27) ^{vi} | 3.5387 |
| C(24)···C(27) | 2.7983 (18) | N(1)···H(30) ^{vi} | 3.5525 |
| C(24)···C(32) | 3.5920 (19) | N(2)···H(5) ^v | 3.4815 |
| C(25)···C(28) | 2.8127 (18) | N(2)···H(7) ^v | 3.5900 |
| C(26)···C(29) | 2.8014 (19) | N(2)···H(15) ^{iv} | 3.4162 |
| C(28)···C(32) | 2.7545 (19) | N(3)···H(5) ⁱ | 3.1548 |
| C(29)···C(31) | 2.7303 (19) | N(3)···H(16) ⁱⁱⁱ | 2.7290 |
| O(1)···O(2) ⁱ | 3.3227 (13) | N(4)···H(11) ^{ix} | 3.4326 |
| O(1)···O(3) ⁱ | 3.2146 (14) | N(4)···H(23) ^{ix} | 3.4701 |
| O(1)···N(1) ⁱ | 3.2115 (14) | N(4)···H(31) ^x | 3.5704 |
| O(1)···N(2) ⁱⁱ | 3.2723 (15) | N(5)···H(5N) ^x | 3.3226 |
| O(1)···C(15) ⁱⁱⁱ | 3.1258 (18) | N(6)···H(21) ^x | 3.4494 |
| O(1)···C(16) ⁱⁱⁱ | 3.2809 (17) | N(6)···H(32) ^{xi} | 2.8528 |
| O(2)···O(1) ^{iv} | 3.3227 (13) | C(1)···H(2N) ⁱⁱ | 3.5140 |
| O(2)···C(11) ^v | 3.4770 (16) | C(1)···H(9) ^v | 3.5112 |
| O(2)···C(27) ^{vi} | 3.3066 (16) | C(1)···H(15) ⁱⁱⁱ | 3.3366 |
| O(2)···C(30) ^{vi} | 3.2444 (16) | C(2)···H(10) ^v | 3.5949 |
| O(3)···O(1) ^{iv} | 3.2146 (14) | C(2)···H(15) ⁱⁱⁱ | 3.5615 |
| O(3)···N(2) ^{iv} | 3.5761 (15) | C(2)···H(27) ⁱⁱ | 3.2746 |
| O(3)···C(1) ^{iv} | 3.5409 (16) | C(3)···H(10) ^v | 3.3240 |
| O(3)···C(5) ^{vii} | 3.3767 (17) | C(3)···H(19) ^{xiii} | 3.5875 |
| O(3)···C(7) ^{vii} | 3.1196 (18) | C(4)···H(16) ⁱⁱ | 3.2525 |
| O(3)···C(12) ^v | 3.4391 (16) | C(5)···H(5) ^{vii} | 3.4991 |
| O(3)···C(13) ^v | 3.4420 (16) | C(5)···H(16) ^{iv} | 3.4195 |
| O(4)···N(6) ^{viii} | 3.5733 (17) | C(5)···H(16) ⁱⁱ | 3.3767 |
| O(4)···C(10) ^{ix} | 3.1957 (17) | C(6)···H(7) ^v | 3.4706 |

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| O(4)···C(11) ^{ix} | 3.2263 (18) | C(6)···H(9) ^v | 3.4871 |
| O(4)···C(28) ^{viii} | 3.4627 (17) | C(6)···H(16) ^{iv} | 3.1633 |
| O(4)···C(29) ^{viii} | 3.4710 (18) | C(7)···H(7) ^v | 3.3041 |
| O(4)···C(30) ^{viii} | 3.5134 (17) | C(7)···H(15) ^{iv} | 3.4837 |
| O(4)···C(31) ^{viii} | 3.5819 (17) | C(7)···H(16) ^{iv} | 3.1220 |
| O(5)···N(6) ^{viii} | 3.5096 (16) | C(8)···H(5) ^v | 3.3999 |
| O(5)···C(21) ^{ix} | 3.3904 (17) | C(8)···H(15) ^{iv} | 3.2983 |
| O(5)···C(23) ^{ix} | 3.2189 (16) | C(9)···H(15) ^{iv} | 3.2270 |
| O(5)···C(31) ^x | 3.4750 (18) | C(9)···H(26) | 3.2792 |
| O(5)···C(32) ^{viii} | 3.4199 (18) | C(10)···H(3) ^v | 3.4339 |
| O(6)···N(5) ^x | 3.5275 (15) | C(10)···H(26) | 2.8325 |
| O(6)···C(21) ^{viii} | 3.5533 (17) | C(11)···H(26) | 3.1547 |
| O(6)···C(24) ^x | 3.4581 (17) | C(12)···H(2) ⁱⁱ | 3.4540 |
| O(6)···C(25) ^x | 3.5102 (17) | C(13)···H(2) ⁱⁱ | 3.3068 |
| O(6)···C(31) ^{xi} | 3.1172 (16) | C(14)···H(3) ⁱⁱ | 3.4476 |
| O(6)···C(32) ^{xi} | 3.1219 (16) | C(14)···H(9) ⁱ | 3.2684 |
| N(1)···O(1) ^{iv} | 3.2115 (14) | C(14)···H(26) ⁱ | 3.2372 |
| N(1)···C(11) ^v | 3.4950 (17) | C(14)···H(27) ⁱ | 3.5220 |
| N(1)···C(12) ^v | 3.3809 (17) | C(15)···H(3) ⁱⁱ | 3.3208 |
| N(2)···O(1) ⁱⁱ | 3.2723 (15) | C(15)···H(7) ⁱ | 3.1802 |
| N(2)···O(3) ⁱ | 3.5761 (15) | C(15)···H(9) ⁱ | 3.2019 |
| N(3)···C(1) ⁱⁱ | 3.3457 (17) | C(15)···H(26) ⁱ | 3.4320 |
| N(3)···C(2) ⁱⁱ | 3.3356 (17) | C(15)···H(27) ⁱ | 3.2646 |
| N(3)···C(5) ⁱ | 3.5286 (17) | C(16)···H(5) ⁱ | 3.4314 |
| N(4)···N(6) ^{viii} | 3.2805 (17) | C(16)···H(7) ⁱ | 3.1122 |
| N(4)···C(29) ^{viii} | 3.5113 (18) | C(16)···H(16) ⁱⁱⁱ | 2.9944 |
| N(4)···C(30) ^x | 3.5049 (18) | C(17)···H(23) ^{viii} | 3.4232 |
| N(4)···C(31) ^x | 3.4579 (18) | C(17)···H(31) ^{xi} | 3.2059 |
| N(4)···C(32) ^{viii} | 3.4796 (18) | C(18)···H(23) ^{viii} | 3.4341 |
| N(5)···O(6) ^x | 3.5275 (15) | C(18)···H(25) ^{viii} | 3.5517 |
| N(5)···N(5) ^x | 3.4664 (15) | C(18)···H(31) ^{xi} | 3.1807 |
| N(5)···C(18) ^{viii} | 3.4918 (18) | C(20)···H(5N) ^{viii} | 3.4693 |
| N(5)···C(19) ^{viii} | 3.4670 (18) | C(21)···H(5N) ^{viii} | 3.3937 |
| N(5)···C(20) ^{viii} | 3.5441 (18) | C(21)···H(21) ^{ix} | 3.5381 |
| N(5)···C(23) ^x | 3.5681 (17) | C(22)···H(5N) ^x | 3.5524 |
| N(6)···O(4) ^{viii} | 3.5733 (17) | C(23)···H(5N) ^x | 3.2762 |
| N(6)···O(5) ^{viii} | 3.5096 (16) | C(24)···H(19) ^{viii} | 3.2891 |
| N(6)···N(4) ^{viii} | 3.2805 (17) | C(25)···H(18) ^{viii} | 3.5130 |
| N(6)···C(20) ^{viii} | 3.5064 (17) | C(25)···H(19) ^{viii} | 3.3464 |
| N(6)···C(21) ^x | 3.3644 (18) | C(25)···H(31) ^{xiv} | 3.3768 |
| N(6)···C(22) ^x | 3.4717 (18) | C(26)···H(2) ⁱⁱ | 3.1170 |

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| C(1)···O(3) ⁱ | 3.5409 (16) | C(26)···H(14) ^{iv} | 3.0551 |
| C(1)···N(3) ⁱⁱ | 3.3457 (17) | C(26)···H(15) ^{iv} | 3.4964 |
| C(2)···N(3) ⁱⁱ | 3.3356 (17) | C(26)···H(18) ^x | 3.4580 |
| C(2)···C(13) ⁱⁱ | 3.3661 (18) | C(26)···H(19) ^{viii} | 3.5704 |
| C(2)···C(16) ⁱⁱ | 3.5720 (19) | C(27)···H(2) ⁱⁱ | 2.8250 |
| C(3)···C(10) ^v | 3.3338 (18) | C(27)···H(14) ^{iv} | 3.4053 |
| C(3)···C(15) ⁱⁱ | 3.3851 (19) | C(27)···H(15) ^{iv} | 3.3712 |
| C(3)···C(16) ⁱⁱ | 3.3353 (18) | C(29)···H(19) ^{viii} | 3.4606 |
| C(4)···C(9) ^v | 3.4753 (18) | C(30)···H(10) ^{xv} | 3.2400 |
| C(4)···C(10) ^v | 3.4730 (18) | C(31)···H(18) ^{xi} | 3.4871 |
| C(4)···C(16) ⁱⁱ | 3.3681 (18) | C(31)···H(25) ^{xv} | 3.4007 |
| C(5)···O(3) ^{vii} | 3.3767 (17) | C(32)···H(21) ^x | 3.3663 |
| C(5)···N(3) ^{iv} | 3.5286 (17) | C(32)···H(32) ^{xi} | 3.0711 |
| C(5)···C(8) ^v | 3.3845 (18) | H(2)···O(2) ⁱ | 3.5621 |
| C(5)···C(9) ^v | 3.4833 (18) | H(2)···C(12) ⁱⁱ | 3.4540 |
| C(6)···C(16) ^{iv} | 3.5460 (19) | H(2)···C(13) ⁱⁱ | 3.3068 |
| C(7)···O(3) ^{vii} | 3.1196 (18) | H(2)···C(26) ⁱⁱ | 3.1170 |
| C(7)···C(7) ^v | 3.3760 (19) | H(2)···C(27) ⁱⁱ | 2.8250 |
| C(7)···C(15) ^{iv} | 3.4860 (19) | H(2)···H(15) ⁱⁱⁱ | 3.0355 |
| C(7)···C(16) ^{iv} | 3.2835 (18) | H(2)···H(19) ^{xiii} | 3.5800 |
| C(8)···C(5) ^v | 3.3845 (18) | H(2)···H(26) ⁱⁱ | 3.0110 |
| C(9)···C(4) ^v | 3.4753 (18) | H(2)···H(27) ⁱⁱ | 2.4923 |
| C(9)···C(5) ^v | 3.4833 (18) | H(2N)···O(1) ⁱⁱ | 3.1599 |
| C(9)···C(15) ^{iv} | 3.5386 (18) | H(2N)···O(3) ⁱ | 3.2430 |
| C(10)···O(4) ^{ix} | 3.1957 (17) | H(2N)···C(1) ⁱⁱ | 3.5140 |
| C(10)···C(3) ^v | 3.3338 (18) | H(2N)···H(16) ⁱⁱⁱ | 3.0316 |
| C(10)···C(4) ^v | 3.4730 (18) | H(3)···O(4) ^{xiii} | 3.2655 |
| C(11)···O(2) ^v | 3.4770 (16) | H(3)···C(10) ^v | 3.4339 |
| C(11)···O(4) ^{ix} | 3.2263 (18) | H(3)···C(14) ⁱⁱ | 3.4476 |
| C(11)···N(1) ^v | 3.4950 (17) | H(3)···C(15) ⁱⁱ | 3.3208 |
| C(12)···O(3) ^v | 3.4391 (16) | H(3)···H(10) ^v | 3.2944 |
| C(12)···N(1) ^v | 3.3809 (17) | H(3)···H(15) ⁱⁱ | 3.5195 |
| C(13)···O(3) ^v | 3.4420 (16) | H(3)···H(19) ^{xiii} | 2.7307 |
| C(13)···C(2) ⁱⁱ | 3.3661 (18) | H(3)···H(27) ^{vi} | 3.2127 |
| C(15)···O(1) ⁱⁱⁱ | 3.1258 (18) | H(5)···O(3) ^{vii} | 2.5621 |
| C(15)···C(3) ⁱⁱ | 3.3851 (19) | H(5)···N(2) ^v | 3.4815 |
| C(15)···C(7) ⁱ | 3.4860 (19) | H(5)···N(3) ^{iv} | 3.1548 |
| C(15)···C(9) ⁱ | 3.5386 (18) | H(5)···C(5) ^{vii} | 3.4991 |
| C(16)···O(1) ⁱⁱⁱ | 3.2809 (17) | H(5)···C(8) ^v | 3.3999 |
| C(16)···C(2) ⁱⁱ | 3.5720 (19) | H(5)···C(16) ^{iv} | 3.4314 |
| C(16)···C(3) ⁱⁱ | 3.3353 (18) | H(5)···H(5) ^{vii} | 2.5980 |

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| C(16)···C(4) ⁱⁱ | 3.3681 (18) | H(5)···H(16) ^{iv} | 3.5008 |
| C(16)···C(6) ⁱ | 3.5460 (19) | H(5N)···N(5) ^x | 3.3226 |
| C(16)···C(7) ⁱ | 3.2835 (18) | H(5N)···C(20) ^{viii} | 3.4693 |
| C(17)···C(22) ^{viii} | 3.5057 (20) | H(5N)···C(21) ^{viii} | 3.3937 |
| C(17)···C(23) ^{viii} | 3.2993 (19) | H(5N)···C(22) ^x | 3.5524 |
| C(17)···C(24) ^x | 3.2981 (19) | H(5N)···C(23) ^x | 3.2762 |
| C(17)···C(25) ^x | 3.5516 (19) | H(5N)···H(5N) ^x | 3.4077 |
| C(17)···C(29) ^x | 3.5856 (20) | H(5N)···H(23) ^x | 3.5725 |
| C(18)···N(5) ^{viii} | 3.4918 (18) | H(5N)···H(32) ^{xi} | 3.1277 |
| C(18)···C(23) ^{viii} | 3.478 (2) | H(7)···O(3) ^{vii} | 2.2044 |
| C(18)···C(24) ^{viii} | 3.5605 (19) | H(7)···N(1) ^{vii} | 3.3602 |
| C(18)···C(26) ^x | 3.5999 (20) | H(7)···N(2) ^v | 3.5900 |
| C(19)···N(5) ^{viii} | 3.4670 (18) | H(7)···C(6) ^v | 3.4706 |
| C(19)···C(24) ^{viii} | 3.2305 (19) | H(7)···C(7) ^v | 3.3041 |
| C(19)···C(25) ^{viii} | 3.5176 (20) | H(7)···C(15) ^{iv} | 3.1802 |
| C(19)···C(27) ^x | 3.5788 (19) | H(7)···C(16) ^{iv} | 3.1122 |
| C(19)···C(28) ^x | 3.4481 (19) | H(7)···H(7) ^v | 3.4988 |
| C(19)···C(29) ^{viii} | 3.5544 (18) | H(7)···H(15) ^{iv} | 3.3512 |
| C(20)···N(5) ^{viii} | 3.5441 (18) | H(7)···H(16) ^{iv} | 3.2314 |
| C(20)···N(6) ^{viii} | 3.5064 (17) | H(9)···O(2) ^{vii} | 3.0570 |
| C(20)···C(24) ^{viii} | 3.5800 (19) | H(9)···O(3) ^{vii} | 2.6883 |
| C(20)···C(28) ^x | 3.5439 (19) | H(9)···N(1) ^{vii} | 3.2529 |
| C(20)···C(29) ^{viii} | 3.5435 (18) | H(9)···C(1) ^v | 3.5112 |
| C(20)···C(30) ^x | 3.536 (2) | H(9)···C(6) ^v | 3.4871 |
| C(21)···O(5) ^{ix} | 3.3904 (17) | H(9)···C(14) ^{iv} | 3.2684 |
| C(21)···O(6) ^{viii} | 3.5533 (17) | H(9)···C(15) ^{iv} | 3.2019 |
| C(21)···N(6) ^x | 3.3644 (18) | H(9)···H(14) ^{iv} | 3.2600 |
| C(21)···C(29) ^x | 3.5438 (19) | H(9)···H(15) ^{iv} | 3.1538 |
| C(21)···C(32) ^x | 3.508 (2) | H(9)···H(26) | 3.5922 |
| C(22)···N(6) ^x | 3.4717 (18) | H(10)···O(4) ^{ix} | 2.5738 |
| C(22)···C(17) ^{viii} | 3.5057 (20) | H(10)···C(2) ^v | 3.5949 |
| C(22)···C(22) ^{viii} | 3.5000 (19) | H(10)···C(3) ^v | 3.3240 |
| C(22)···C(23) ^{viii} | 3.5964 (20) | H(10)···C(30) ^{xiv} | 3.2400 |
| C(22)···C(24) ^x | 3.5616 (19) | H(10)···H(3) ^v | 3.2944 |
| C(22)···C(29) ^x | 3.4690 (20) | H(10)···H(25) | 3.4647 |
| C(23)···O(5) ^{ix} | 3.2189 (16) | H(10)···H(26) | 2.8935 |
| C(23)···N(5) ^x | 3.5681 (17) | H(10)···H(30) ^{xiv} | 3.0175 |
| C(23)···C(17) ^{viii} | 3.2993 (19) | H(11)···O(2) ^v | 3.4655 |
| C(23)···C(18) ^{viii} | 3.478 (2) | H(11)···O(4) ^{ix} | 2.6445 |
| C(23)···C(22) ^{viii} | 3.5964 (20) | H(11)···N(4) ^{ix} | 3.4326 |
| C(24)···O(6) ^x | 3.4581 (17) | H(11)···H(18) ^{viii} | 2.9897 |

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| C(24)···C(17) ^x | 3.2981 (19) | H(11)···H(25) | 3.2864 |
| C(24)···C(18) ^{viii} | 3.5605 (19) | H(11)···H(26) | 3.4097 |
| C(24)···C(19) ^{viii} | 3.2305 (19) | H(11)···H(30) ^{xvi} | 3.0218 |
| C(24)···C(20) ^{viii} | 3.5800 (19) | H(11)···H(31) ^{xvi} | 3.4360 |
| C(24)···C(22) ^x | 3.5616 (19) | H(14)···C(26) ⁱ | 3.0551 |
| C(25)···O(6) ^x | 3.5102 (17) | H(14)···C(27) ⁱ | 3.4053 |
| C(25)···C(17) ^x | 3.5516 (19) | H(14)···H(9) ⁱ | 3.2600 |
| C(25)···C(19) ^{viii} | 3.5176 (20) | H(14)···H(18) ^{viii} | 2.9462 |
| C(26)···C(18) ^x | 3.5999 (20) | H(14)···H(26) ⁱ | 2.5054 |
| C(27)···O(2) ^{vi} | 3.3066 (16) | H(14)···H(27) ⁱ | 3.1754 |
| C(27)···C(19) ^x | 3.5788 (19) | H(14)···H(30) ^{xvi} | 3.3813 |
| C(28)···O(4) ^{viii} | 3.4627 (17) | H(14)···H(31) ^{xvi} | 3.4801 |
| C(28)···C(19) ^x | 3.4481 (19) | H(15)···O(1) ⁱⁱⁱ | 2.4380 |
| C(28)···C(20) ^x | 3.5439 (19) | H(15)···O(2) ⁱⁱ | 3.4319 |
| C(29)···O(4) ^{viii} | 3.4710 (18) | H(15)···N(2) ⁱ | 3.4162 |
| C(29)···N(4) ^{viii} | 3.5113 (18) | H(15)···C(1) ⁱⁱⁱ | 3.3366 |
| C(29)···C(17) ^x | 3.5856 (20) | H(15)···C(2) ⁱⁱⁱ | 3.5615 |
| C(29)···C(19) ^{viii} | 3.5544 (18) | H(15)···C(7) ⁱ | 3.4837 |
| C(29)···C(20) ^{viii} | 3.5435 (18) | H(15)···C(8) ⁱ | 3.2983 |
| C(29)···C(21) ^x | 3.5438 (19) | H(15)···C(9) ⁱ | 3.2270 |
| C(29)···C(22) ^x | 3.4690 (20) | H(15)···C(26) ⁱ | 3.4964 |
| C(30)···O(2) ^{vi} | 3.2444 (16) | H(15)···C(27) ⁱ | 3.3712 |
| C(30)···O(4) ^{viii} | 3.5134 (17) | H(15)···H(2) ⁱⁱⁱ | 3.0355 |
| C(30)···N(4) ^x | 3.5049 (18) | H(15)···H(3) ⁱⁱ | 3.5195 |
| C(30)···C(20) ^x | 3.536 (2) | H(15)···H(7) ⁱ | 3.3512 |
| C(31)···O(4) ^{viii} | 3.5819 (17) | H(15)···H(9) ⁱ | 3.1538 |
| C(31)···O(5) ^x | 3.4750 (18) | H(15)···H(26) ⁱ | 2.9198 |
| C(31)···O(6) ^{xi} | 3.1172 (16) | H(15)···H(27) ⁱ | 2.6667 |
| C(31)···N(4) ^x | 3.4579 (18) | H(16)···O(1) ⁱⁱⁱ | 2.7199 |
| C(32)···O(5) ^{viii} | 3.4199 (18) | H(16)···N(3) ⁱⁱⁱ | 2.7290 |
| C(32)···O(6) ^{xi} | 3.1219 (16) | H(16)···C(4) ⁱⁱ | 3.2525 |
| C(32)···N(4) ^{viii} | 3.4796 (18) | H(16)···C(5) ⁱ | 3.4195 |
| C(32)···C(21) ^x | 3.508 (2) | H(16)···C(5) ⁱⁱ | 3.3767 |
| O(1)···H(2) | 2.5982 | H(16)···C(6) ⁱ | 3.1633 |
| O(1)···H(2N) | 2.0128 | H(16)···C(7) ⁱ | 3.1220 |
| O(2)···H(3) | 2.4770 | H(16)···C(16) ⁱⁱⁱ | 2.9944 |
| O(3)···H(5) | 2.3857 | H(16)···H(2N) ⁱⁱⁱ | 3.0316 |
| O(4)···H(19) | 2.4301 | H(16)···H(5) ⁱ | 3.5008 |
| O(5)···H(21) | 2.4272 | H(16)···H(7) ⁱ | 3.2314 |
| O(6)···H(5N) | 1.8755 | H(16)···H(16) ⁱⁱⁱ | 2.5294 |
| O(6)···H(18) | 2.5855 | H(18)···C(25) ^{viii} | 3.5130 |

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| N(1)···H(3) | 2.6513 | H(18)···C(26) ^x | 3.4580 |
| N(1)···H(5) | 2.5714 | H(18)···C(31) ^{xi} | 3.4871 |
| N(2)···H(9) | 2.6515 | H(18)···H(11) ^{viii} | 2.9897 |
| N(3)···H(2N) | 2.3052 | H(18)···H(14) ^{viii} | 2.9462 |
| N(3)···H(15) | 3.2598 | H(18)···H(23) ^{viii} | 3.4689 |
| N(4)···H(19) | 2.6307 | H(18)···H(25) ^{viii} | 3.2803 |
| N(4)···H(21) | 2.5948 | H(18)···H(31) ^{xi} | 2.5653 |
| N(5)···H(25) | 2.6635 | H(19)···C(3) ^{xii} | 3.5875 |
| N(6)···H(5N) | 2.2464 | H(19)···C(24) ^{viii} | 3.2891 |
| N(6)···H(31) | 3.2539 | H(19)···C(25) ^{viii} | 3.3464 |
| C(1)···H(2N) | 2.5884 | H(19)···C(26) ^{viii} | 3.5704 |
| C(1)···H(3) | 3.3144 | H(19)···C(29) ^{viii} | 3.4606 |
| C(1)···H(5) | 3.3474 | H(19)···H(2) ^{xii} | 3.5800 |
| C(1)···H(7) | 3.3429 | H(19)···H(3) ^{xii} | 2.7307 |
| C(3)···H(5) | 3.2882 | H(19)···H(27) ^x | 3.5945 |
| C(4)···H(2) | 3.2632 | H(21)···O(5) ^{ix} | 2.5710 |
| C(5)···H(3) | 3.2810 | H(21)···O(6) ^{viii} | 3.4880 |
| C(5)···H(7) | 2.5273 | H(21)···N(6) ^x | 3.4494 |
| C(6)···H(2) | 3.3204 | H(21)···C(21) ^{ix} | 3.5381 |
| C(6)···H(2N) | 2.5465 | H(21)···C(32) ^x | 3.3663 |
| C(7)···H(5) | 2.5626 | H(21)···H(21) ^{ix} | 2.6477 |
| C(7)···H(9) | 2.6583 | H(21)···H(32) ^x | 3.4667 |
| C(8)···H(7) | 2.5790 | H(23)···O(5) ^{ix} | 2.3356 |
| C(8)···H(10) | 3.2614 | H(23)···O(6) ^{viii} | 3.5688 |
| C(9)···H(2N) | 3.2193 | H(23)···N(4) ^{ix} | 3.4701 |
| C(9)···H(7) | 2.5968 | H(23)···C(17) ^{viii} | 3.4232 |
| C(9)···H(11) | 3.2734 | H(23)···C(18) ^{viii} | 3.4341 |
| C(11)···H(9) | 3.2686 | H(23)···H(5N) ^x | 3.5725 |
| C(11)···H(14) | 2.6951 | H(23)···H(18) ^{viii} | 3.4689 |
| C(12)···H(10) | 3.2687 | H(23)···H(32) ^{xiv} | 3.2042 |
| C(12)···H(15) | 3.2701 | H(25)···O(4) ^{ix} | 3.4554 |
| C(13)···H(2N) | 2.5009 | H(25)···O(5) ^{ix} | 3.0924 |
| C(13)···H(9) | 3.2942 | H(25)···O(6) ^x | 3.5018 |
| C(13)···H(11) | 3.3076 | H(25)···C(18) ^{viii} | 3.5517 |
| C(13)···H(14) | 3.2847 | H(25)···C(31) ^{xiv} | 3.4007 |
| C(13)···H(16) | 3.1500 | H(25)···H(10) | 3.4647 |
| C(14)···H(11) | 2.6905 | H(25)···H(11) | 3.2864 |
| C(14)···H(16) | 3.2355 | H(25)···H(18) ^{viii} | 3.2803 |
| C(16)···H(2N) | 3.5833 | H(25)···H(31) ^{xiv} | 3.0205 |
| C(16)···H(14) | 3.2574 | H(25)···H(32) ^{xiv} | 3.5902 |
| C(17)···H(5N) | 2.4667 | H(26)···C(9) | 3.2792 |

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| C(17)···H(19) | 3.3064 | H(26)···C(10) | 2.8325 |
| C(17)···H(21) | 3.3438 | H(26)···C(11) | 3.1547 |
| C(17)···H(23) | 3.3402 | H(26)···C(14) ^{iv} | 3.2372 |
| C(19)···H(21) | 3.2897 | H(26)···C(15) ^{iv} | 3.4320 |
| C(20)···H(18) | 3.2600 | H(26)···H(2) ⁱⁱ | 3.0110 |
| C(21)···H(19) | 3.2829 | H(26)···H(9) | 3.5922 |
| C(21)···H(23) | 2.5753 | H(26)···H(10) | 2.8935 |
| C(22)···H(5N) | 2.4845 | H(26)···H(11) | 3.4097 |
| C(22)···H(18) | 3.3238 | H(26)···H(14) ^{iv} | 2.5054 |
| C(23)···H(21) | 2.5925 | H(26)···H(15) ^{iv} | 2.9198 |
| C(23)···H(25) | 2.7294 | H(26)···H(31) ^{xiv} | 3.5373 |
| C(24)···H(23) | 2.6359 | H(27)···O(2) ^{vi} | 2.4828 |
| C(24)···H(26) | 3.2577 | H(27)···N(1) ^{vi} | 3.5387 |
| C(25)···H(5N) | 3.2120 | H(27)···C(2) ⁱⁱ | 3.2746 |
| C(25)···H(23) | 2.6988 | H(27)···C(14) ^{iv} | 3.5220 |
| C(25)···H(27) | 3.2756 | H(27)···C(15) ^{iv} | 3.2646 |
| C(27)···H(25) | 3.2719 | H(27)···H(2) ⁱⁱ | 2.4923 |
| C(27)···H(30) | 2.7123 | H(27)···H(3) ^{vi} | 3.2127 |
| C(28)···H(26) | 3.2731 | H(27)···H(14) ^{iv} | 3.1754 |
| C(28)···H(31) | 3.2677 | H(27)···H(15) ^{iv} | 2.6667 |
| C(29)···H(5N) | 2.4594 | H(27)···H(19) ^x | 3.5945 |
| C(29)···H(25) | 3.2962 | H(30)···O(2) ^{vi} | 2.4025 |
| C(29)···H(27) | 3.3045 | H(30)···O(4) ^x | 3.4840 |
| C(29)···H(30) | 3.2877 | H(30)···N(1) ^{vi} | 3.5525 |
| C(29)···H(32) | 3.1569 | H(30)···H(10) ^{xv} | 3.0175 |
| C(30)···H(27) | 2.7034 | H(30)···H(11) ^{xvii} | 3.0218 |
| C(30)···H(32) | 3.2448 | H(30)···H(14) ^{xvii} | 3.3813 |
| C(32)···H(5N) | 3.5228 | H(31)···O(5) ^x | 3.3681 |
| C(32)···H(30) | 3.2663 | H(31)···O(6) ^{xi} | 2.5222 |
| H(2)···H(3) | 2.2939 | H(31)···N(4) ^x | 3.5704 |
| H(2N)···H(7) | 2.6984 | H(31)···C(17) ^{xi} | 3.2059 |
| H(2N)···H(9) | 3.5131 | H(31)···C(18) ^{xi} | 3.1807 |
| H(5)···H(7) | 2.3191 | H(31)···C(25) ^{xv} | 3.3768 |
| H(5N)···H(23) | 2.6976 | H(31)···H(11) ^{xvii} | 3.4360 |
| H(5N)···H(25) | 3.5203 | H(31)···H(14) ^{xvii} | 3.4801 |
| H(7)···H(9) | 2.0562 | H(31)···H(18) ^{xi} | 2.5653 |
| H(9)···H(10) | 2.3471 | H(31)···H(25) ^{xv} | 3.0205 |
| H(10)···H(11) | 2.3129 | H(31)···H(26) ^{xv} | 3.5373 |
| H(11)···H(14) | 2.5485 | H(32)···O(5) ^{viii} | 3.4236 |
| H(14)···H(15) | 2.3232 | H(32)···O(6) ^{xi} | 2.5031 |
| H(15)···H(16) | 2.3424 | H(32)···N(6) ^{xi} | 2.8528 |

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| H(18)···H(19) | 2.2961 | H(32)···C(32) ^{xi} | 3.0711 |
| H(21)···H(23) | 2.3843 | H(32)···H(5N) ^{xi} | 3.1277 |
| H(23)···H(25) | 2.1751 | H(32)···H(21) ^x | 3.4667 |
| H(25)···H(26) | 2.3504 | H(32)···H(23) ^{xv} | 3.2042 |
| H(26)···H(27) | 2.3097 | H(32)···H(25) ^{xv} | 3.5902 |
| H(27)···H(30) | 2.5687 | H(32)···H(32) ^{xi} | 2.5768 |
| O(2)—N(1)—O(3) | 122.13 (11) | C(25)—C(26)—C(27) | 121.26 (12) |
| O(2)—N(1)—C(4) | 119.13 (11) | C(26)—C(27)—C(28) | 120.16 (12) |
| O(3)—N(1)—C(4) | 118.74 (10) | C(27)—C(28)—C(29) | 119.39 (12) |
| C(7)—N(2)—C(8) | 124.94 (12) | C(27)—C(28)—C(30) | 123.60 (12) |
| C(13)—N(3)—C(16) | 116.79 (11) | C(29)—C(28)—C(30) | 117.01 (12) |
| O(4)—N(4)—O(5) | 122.50 (11) | N(6)—C(29)—C(24) | 117.68 (11) |
| O(4)—N(4)—C(20) | 118.35 (11) | N(6)—C(29)—C(28) | 123.54 (12) |
| O(5)—N(4)—C(20) | 119.16 (11) | C(24)—C(29)—C(28) | 118.78 (12) |
| C(23)—N(5)—C(24) | 127.29 (11) | C(28)—C(30)—C(31) | 119.17 (12) |
| C(29)—N(6)—C(32) | 117.14 (11) | C(30)—C(31)—C(32) | 119.55 (12) |
| O(1)—C(1)—C(2) | 122.95 (13) | N(6)—C(32)—C(31) | 123.59 (12) |
| O(1)—C(1)—C(6) | 121.39 (12) | C(7)—N(2)—H(2N) | 117.526 |
| C(2)—C(1)—C(6) | 115.65 (12) | C(8)—N(2)—H(2N) | 117.532 |
| C(1)—C(2)—C(3) | 122.35 (13) | C(23)—N(5)—H(5N) | 116.360 |
| C(2)—C(3)—C(4) | 119.79 (12) | C(24)—N(5)—H(5N) | 116.349 |
| N(1)—C(4)—C(3) | 119.96 (11) | C(1)—C(2)—H(2) | 118.830 |
| N(1)—C(4)—C(5) | 118.85 (12) | C(3)—C(2)—H(2) | 118.824 |
| C(3)—C(4)—C(5) | 121.17 (12) | C(2)—C(3)—H(3) | 120.110 |
| C(4)—C(5)—C(6) | 120.09 (13) | C(4)—C(3)—H(3) | 120.105 |
| C(1)—C(6)—C(5) | 120.86 (12) | C(4)—C(5)—H(5) | 119.957 |
| C(1)—C(6)—C(7) | 121.86 (12) | C(6)—C(5)—H(5) | 119.955 |
| C(5)—C(6)—C(7) | 117.27 (13) | N(2)—C(7)—H(7) | 117.631 |
| N(2)—C(7)—C(6) | 124.73 (13) | C(6)—C(7)—H(7) | 117.636 |
| N(2)—C(8)—C(9) | 123.28 (12) | C(8)—C(9)—H(9) | 119.987 |
| N(2)—C(8)—C(13) | 116.17 (12) | C(10)—C(9)—H(9) | 119.974 |
| C(9)—C(8)—C(13) | 120.54 (12) | C(9)—C(10)—H(10) | 119.473 |
| C(8)—C(9)—C(10) | 120.04 (12) | C(11)—C(10)—H(10) | 119.465 |
| C(9)—C(10)—C(11) | 121.06 (13) | C(10)—C(11)—H(11) | 119.951 |
| C(10)—C(11)—C(12) | 120.09 (12) | C(12)—C(11)—H(11) | 119.955 |
| C(11)—C(12)—C(13) | 119.79 (12) | C(12)—C(14)—H(14) | 120.147 |
| C(11)—C(12)—C(14) | 123.36 (12) | C(15)—C(14)—H(14) | 120.151 |
| C(13)—C(12)—C(14) | 116.85 (12) | C(14)—C(15)—H(15) | 120.576 |
| N(3)—C(13)—C(8) | 118.00 (11) | C(16)—C(15)—H(15) | 120.575 |
| N(3)—C(13)—C(12) | 123.53 (12) | N(3)—C(16)—H(16) | 117.860 |
| C(8)—C(13)—C(12) | 118.47 (12) | C(15)—C(16)—H(16) | 117.867 |
| C(12)—C(14)—C(15) | 119.70 (12) | C(17)—C(18)—H(18) | 119.021 |
| C(14)—C(15)—C(16) | 118.85 (13) | C(19)—C(18)—H(18) | 119.027 |
| N(3)—C(16)—C(15) | 124.27 (13) | C(18)—C(19)—H(19) | 120.077 |
| O(6)—C(17)—C(18) | 122.08 (12) | C(20)—C(19)—H(19) | 120.083 |
| O(6)—C(17)—C(22) | 121.67 (11) | C(20)—C(21)—H(21) | 120.090 |
| C(18)—C(17)—C(22) | 116.25 (11) | C(22)—C(21)—H(21) | 120.102 |

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| C(17)—C(18)—C(19) | 121.95 (12) | N(5)—C(23)—H(23) | 118.877 |
| C(18)—C(19)—C(20) | 119.84 (12) | C(22)—C(23)—H(23) | 118.848 |
| N(4)—C(20)—C(19) | 118.97 (11) | C(24)—C(25)—H(25) | 120.175 |
| N(4)—C(20)—C(21) | 119.55 (11) | C(26)—C(25)—H(25) | 120.176 |
| C(19)—C(20)—C(21) | 121.48 (12) | C(25)—C(26)—H(26) | 119.375 |
| C(20)—C(21)—C(22) | 119.81 (12) | C(27)—C(26)—H(26) | 119.367 |
| C(17)—C(22)—C(21) | 120.63 (12) | C(26)—C(27)—H(27) | 119.913 |
| C(17)—C(22)—C(23) | 120.58 (11) | C(28)—C(27)—H(27) | 119.923 |
| C(21)—C(22)—C(23) | 118.78 (12) | C(28)—C(30)—H(30) | 120.419 |
| N(5)—C(23)—C(22) | 122.27 (12) | C(31)—C(30)—H(30) | 120.408 |
| N(5)—C(24)—C(25) | 124.01 (11) | C(30)—C(31)—H(31) | 120.222 |
| N(5)—C(24)—C(29) | 115.21 (11) | C(32)—C(31)—H(31) | 120.227 |
| C(25)—C(24)—C(29) | 120.76 (12) | N(6)—C(32)—H(32) | 118.204 |
| C(24)—C(25)—C(26) | 119.65 (12) | C(31)—C(32)—H(32) | 118.209 |
| O(2)—N(1)—C(4)—C(3) | -2.84 (16) | C(11)—C(12)—C(13)—C(8) | 0.56 (17) |
| O(3)—N(1)—C(4)—C(5) | -1.75 (16) | C(13)—C(12)—C(14)—C(15) | 0.26 (17) |
| C(7)—N(2)—C(8)—C(9) | -0.65 (19) | C(14)—C(12)—C(13)—N(3) | 0.26 (18) |
| C(13)—N(3)—C(16)—C(15) | 0.39 (17) | C(12)—C(14)—C(15)—C(16) | -0.43 (18) |
| C(16)—N(3)—C(13)—C(12) | -0.57 (17) | C(14)—C(15)—C(16)—N(3) | 0.10 (19) |
| O(4)—N(4)—C(20)—C(19) | 0.75 (17) | O(6)—C(17)—C(22)—C(23) | 1.31 (20) |
| O(5)—N(4)—C(20)—C(21) | 1.07 (18) | C(18)—C(17)—C(22)—C(21) | 1.45 (18) |
| C(23)—N(5)—C(24)—C(25) | 1.0 (2) | C(22)—C(17)—C(18)—C(19) | -2.17 (19) |
| C(29)—N(6)—C(32)—C(31) | -0.54 (19) | C(17)—C(18)—C(19)—C(20) | 1.1 (2) |
| C(32)—N(6)—C(29)—C(28) | 0.14 (18) | C(18)—C(19)—C(20)—C(21) | 0.84 (20) |
| O(1)—C(1)—C(6)—C(7) | -2.14 (18) | C(19)—C(20)—C(21)—C(22) | -1.53 (20) |
| C(2)—C(1)—C(6)—C(5) | -3.13 (17) | C(20)—C(21)—C(22)—C(17) | 0.32 (19) |
| C(6)—C(1)—C(2)—C(3) | 2.60 (17) | C(17)—C(22)—C(23)—N(5) | -0.1 (2) |
| C(1)—C(2)—C(3)—C(4) | -0.08 (18) | N(5)—C(24)—C(29)—N(6) | -0.88 (17) |
| C(2)—C(3)—C(4)—C(5) | -2.11 (18) | C(25)—C(24)—C(29)—C(28) | 0.72 (18) |
| C(3)—C(4)—C(5)—C(6) | 1.54 (18) | C(29)—C(24)—C(25)—C(26) | -0.71 (19) |
| C(4)—C(5)—C(6)—C(1) | 1.17 (18) | C(24)—C(25)—C(26)—C(27) | 0.00 (20) |
| C(1)—C(6)—C(7)—N(2) | 0.57 (19) | C(25)—C(26)—C(27)—C(28) | 0.69 (20) |
| N(2)—C(8)—C(13)—N(3) | 0.29 (16) | C(26)—C(27)—C(28)—C(29) | -0.67 (19) |
| C(9)—C(8)—C(13)—C(12) | -0.22 (17) | C(27)—C(28)—C(29)—C(24) | -0.02 (18) |
| C(13)—C(8)—C(9)—C(10) | -0.30 (18) | C(29)—C(28)—C(30)—C(31) | -0.49 (18) |
| C(8)—C(9)—C(10)—C(11) | 0.49 (18) | C(30)—C(28)—C(29)—N(6) | 0.37 (19) |
| C(9)—C(10)—C(11)—C(12) | -0.14 (18) | C(28)—C(30)—C(31)—C(32) | 0.15 (20) |
| C(10)—C(11)—C(12)—C(13) | -0.39 (18) | C(30)—C(31)—C(32)—N(6) | 0.4 (2) |

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y+1, -z$; (iv) $x+1, y, z$; (v) $-x+1, -y+2, -z$; (vi) $-x+2, -y+1, -z$; (vii) $-x+2, -y+2, -z$; (viii) $-x, -y+1, -z+1$; (ix) $-x, -y+2, -z+1$; (x) $-x+1, -y+1, -z+1$; (xi) $-x+1, -y, -z+1$; (xii) $x-1, y, z+1$; (xiii) $x+1, y, z-1$; (xiv) $x, y+1, z$; (xv) $x, y-1, z$; (xvi) $x-1, y+1, z$; (xvii) $x+1, y-1, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------|-------|-------------|-------------|---------------|
| N2—H2N \cdots O1 | 0.880 | 2.013 | 2.6849 (15) | 132.26 |
| N2—H2N \cdots N3 | 0.880 | 2.305 | 2.6942 (16) | 106.77 |
| N5—H5N \cdots O6 | 0.880 | 1.875 | 2.5915 (14) | 137.26 |
| N5—H5N \cdots N6 | 0.880 | 2.246 | 2.6645 (15) | 108.87 |

Fig. 1

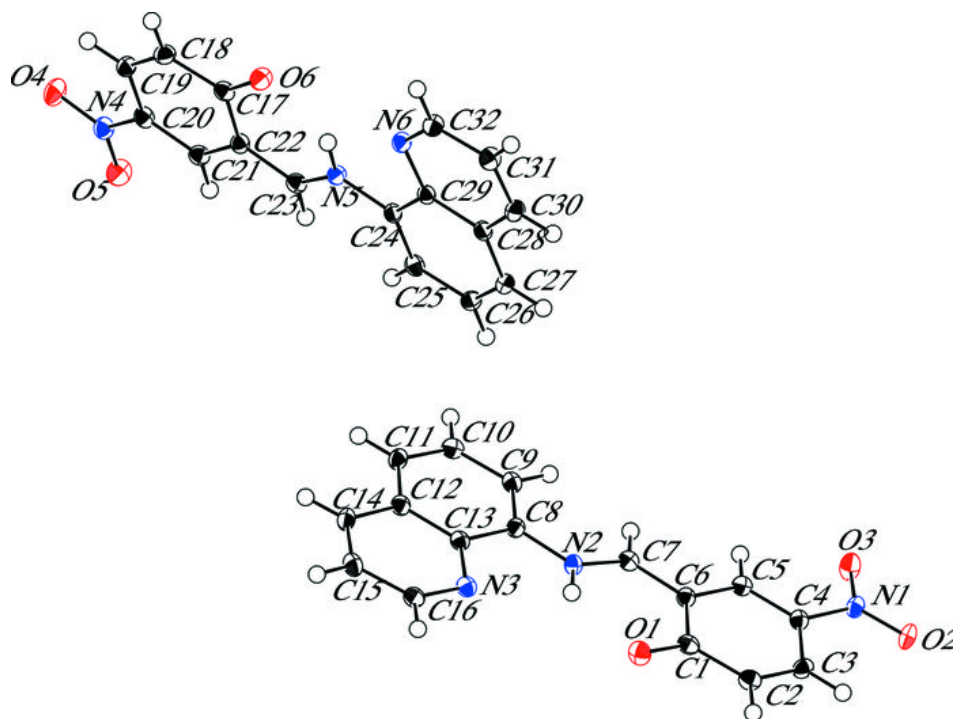


Fig. 2

