Supporting Information

Article Title: Synthesis and Structure of Macrocyclic Bis(hydroxynaphthoic Amide)s Connected by an Achiral or Chiral Diamine

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Experimental Section

General. The starting materials and reagents, purchased from commercial suppliers, were used after standard purification. All of the solvents were dried over sodium wire or molecular sieves, and were distilled before use. Reaction flasks were flame-dried under a stream of Ar. All moisture- and oxygen-sensitive reactions were conducted under an Ar atmosphere. Flash chromatography was carried out using silica-gel 60 (70-230 mesh). Preparative TLC (PTLC) was carried out with Wakogel B-5F. "Usual workup" represents the sequence of drying the combined extracts over Na_2SO_4 , filtering off Na_2SO_4 , and concentrating the filtrate under reduced pressure. The melting points are uncorrected. ^1H -NMR (300 or 500 MHz) spectra were measured with Me_4Si as an internal standard when CDCl_3 was used as a solvent, otherwise residual protiated solvent was used as an internal standard; the δ and J values are given in ppm and Hz, respectively. The unit for the values of IR spectra is cm^{-1} .

Compound characterization data of 5b-g

(*R,R*)-5b. mp 208-210 °C; IR (KBr) 3370, 1640; ^1H -NMR (300 MHz, CDCl_3) δ 4.90 (2H, d, $J=13.2$), 5.04 (2H, d, $J=13.5$), 5.71 (2H, d, $J=1.5$), 5.73 (2H, s), 7.20-7.42 (12H, m), 7.39 (2H, t, $J=7.5$), 7.52 (2H, t, $J=7.5$), 7.71 (2H, d, $J=7.8$), 7.84 (2H, d, $J=7.8$), 8.70 (2H, s), 8.96 (2H, d, $J=6.6$). Anal. Calcd for $\text{C}_{40}\text{H}_{32}\text{N}_2\text{O}_4$: C, 79.45; H, 5.33; N, 4.63. Found: C, 79.20; H, 5.38; N, 4.54.

(*S,S*)-5b. mp 208-210 °C; IR (KBr) 3370, 1650; ^1H -NMR (300 MHz, CDCl_3) δ 4.90 (2H, d, $J=13.5$), 5.05 (2H, d, $J=13.5$), 5.72 (2H, d, $J=5.9$), 5.74 (2H, s), 7.20-7.35 (12H, m), 7.40 (2H, t, $J=7.5$), 7.53 (2H, t, $J=7.5$), 7.71 (2H, d, $J=8.1$), 7.85 (2H, d, $J=7.5$), 8.71 (2H, s), 8.96 (2H, d, $J=5.7$). Anal. Calcd for $\text{C}_{40}\text{H}_{32}\text{N}_2\text{O}_4 \cdot 0.5\text{H}_2\text{O}$: C, 78.28; H, 5.42; N, 4.56. Found: C, 78.49; H, 5.38; N, 4.50.

(*R,R*)-5c. mp 215-218 °C; IR (KBr) 3330, 1640; ^1H -NMR (300 MHz, CDCl_3) δ 1.31-1.39 (2H, m), 1.49-1.55 (2H, m), 1.81-1.85 (2H, m), 2.60 (2H, d, $J=12.3$), 4.02-4.07 (2H, m), 4.63 (2H, d, $J=14.1$), 4.91 (2H, d, $J=13.8$), 5.51 (2H, s), 7.18 (2H, s), 7.40 (2H, t, $J=7.7$), 7.50 (2H, t, $J=8.0$), 7.68 (2H, d, $J=8.1$), 7.74-7.76 (2H, m), 7.88 (2H, d, $J=8.4$), 8.58 (2H, s). Anal. Calcd for $\text{C}_{32}\text{H}_{30}\text{N}_2\text{O}_4$: C, 75.87; H, 5.97; N, 5.53. Found: C, 75.48; H, 6.05; N, 5.24.

(S,S)-5c. mp 216-218 °C; IR (KBr) 3330, 1640; ¹H-NMR (300 MHz, CDCl₃) **d** 1.32-1.39 (2H, m), 1.49-1.57 (2H, m), 1.81-1.84 (2H, m), 2.60 (2H, d, *J*=12.9), 4.03-4.07 (2H, m), 4.63 (2H, d, *J*=14.1), 4.91 (2H, d, *J*=14.1), 5.51 (2H, s), 7.18 (2H, s), 7.40 (2H, t, *J*=7.6), 7.50 (2H, t, *J*=7.6), 7.68 (2H, d, *J*=8.1), 7.76 (2H, d, *J*=5.1), 7.88 (2H, d, *J*=8.1), 8.58 (2H, s). Anal. Calcd for C₃₂H₃₀N₂O₄: C, 75.87; H, 5.97; N, 5.53. Found: C, 75.69; H, 5.97; N, 5.40.

5d. mp 207-209 °C; IR (KBr) 3380, 1650; ¹H-NMR (300 MHz, CDCl₃) **d** 1.55 (4H, s), 1.81-1.93 (4H, m), 4.53-4.58 (2H, m), 4.85 (4H, s), 5.76 (2H, s), 7.23 (2H, s), 7.40 (2H, t, *J*=7.5), 7.52 (2H, t, *J*=8.1), 7.71 (2H, d, *J*=8.4), 7.90 (2H, d, *J*=7.8), 8.14-8.16 (2H, m), 8.71 (2H, s). Anal. Calcd for C₃₂H₃₀N₂O₄: C, 75.87; H, 5.97; N, 5.53. Found: C, 75.71; H, 6.21; N, 5.34.

(S,S)-5e. mp 130.9-132.5 °C; IR (KBr) 3400, 1650; ¹H-NMR (300 MHz, CDCl₃) **d** 1.38 (6H, s), 3.82-3.86 (4H, m), 4.09 (2H, s), 4.88 (4H, s), 5.75 (2H, s), 7.27 (2H, s), 7.41 (2H, t, *J*=8.1), 7.51 (2H, t, *J*=7.7), 7.71 (2H, d, *J*=8.1), 7.71-7.75 (2H, m), 7.87 (2H, d, *J*=8.1), 8.51 (2H, s). Anal. Calcd for C₃₃H₃₂N₂O₆: C, 71.72; H, 5.84; N, 5.07. Found: C, 71.57; H, 5.81; N, 5.04.

5f. mp 122.3-124.1 °C; IR (KBr) 3400, 1650; ¹H-NMR (300 MHz, CDCl₃) **d** 1.15 (6H, s), 3.53 (4H, d, *J*=6.0), 4.87 (4H, s), 5.67 (2H, s), 7.24 (2H, s), 7.40 (2H, t, *J*=7.5), 7.50 (2H, t, *J*=7.6), 7.68 (2H, d, *J*=8.1), 7.87 (2H, d, *J*=8.1), 7.97 (2H, t, *J*=6.0), 8.67 (2H, s). Anal. Calcd for C₃₁H₃₀N₂O₄·0.5H₂O: C, 73.94; H, 6.20; N, 5.56. Found: C, 74.16; H, 6.20; N, 5.52.

(R,R)-5g. mp 165.7-166.9 °C; IR (KBr) 3380, 1640; ¹H-NMR (300 MHz, CDCl₃) **d** 1.55 (6H, d, *J*=6.9), 4.52 (4H, s), 5.36 (2H, dt, *J*=14.4, 7.2), 5.47 (2H, s), 7.02 (2H, s), 7.23-7.43 (12H, m), 7.52 (2H, t, *J*=7.5), 7.67 (2H, d, *J*=7.8), 7.88 (2H, d, *J*=8.1), 8.06 (2H, d, *J*=7.8), 8.73 (2H, s). Anal. Calcd for C₄₂H₃₈N₂O₄·H₂O: C, 77.28; H, 6.18; N, 4.29. Found: C, 77.44; H, 6.11; N, 4.24.

Compound characterization data of 6b-g

(R,R)-6b. mp 274-276 °C; IR (KBr) 3430, 1650; ¹H-NMR (300 MHz, CDCl₃) **d** 3.48 (2H, d, *J*=16.5), 3.92 (2H, d, *J*=16.5), 5.47 (2H, m), 5.75 (2H, dd, *J*=3.0, 7.4), 6.80 (2H, dd, *J*=2.4, 7.5), 7.29-7.38 (12H, m), 7.51 (2H, t, *J*=8.1), 7.72 (2H, d, *J*=8.1), 7.78 (2H, s), 8.20 (2H, d, *J*=8.4), 9.99 (2H, s). Anal. Calcd for C₄₀H₃₂N₂O₄·0.5H₂O: C, 78.28; H, 5.42; N, 4.56. Found: C, 78.31; H, 5.72; N, 4.65.

(S,S)-6b. mp 275-277 °C; IR (KBr) 3410, 1650; ¹H-NMR (300 MHz, CDCl₃) **d** 3.49 (2H, d,

$J=16.5$), 3.92 (2H, d, $J=16.5$), 5.48 (2H, m), 5.76 (2H, dd, $J=3.0$, 7.4), 6.81 (2H, dd, $J=3.0$, 7.1), 7.30-7.40 (12H, m), 7.52 (2H, t, $J=7.7$), 7.73 (2H, d, $J=7.8$), 7.79 (2H, s), 8.20 (2H, d, $J=8.7$), 9.98 (2H, s). Anal. Calcd for $C_{40}H_{32}N_2O_4$: C, 79.45; H, 5.33; N, 4.63. Found: C, 79.49; H, 5.48; N, 4.56.

(*R,R*)-6c. mp 270-272 °C; IR (KBr) 3420, 1650; $^1\text{H-NMR}$ (300 MHz, CDCl_3) **d** 1.42-1.64 (4H, m), 1.94 (2H, d, $J=8.1$), 2.12 (2H, d, $J=12.9$), 3.46 (2H, d, $J=16.5$), 3.93 (2H, d, $J=17.1$), 4.18 (2H, dt, $J=8.1$, 12.3), 5.44 (2H, t, $J=2.4$), 6.31 (2H, d, $J=10.2$), 7.31 (2H, t, $J=7.8$), 7.50 (2H, t, $J=8.1$), 7.72 (2H, d, $J=7.5$), 7.78 (2H, s), 8.16 (2H, d, $J=8.4$), 10.38 (2H, s). Anal. Calcd for $C_{32}H_{30}N_2O_4$: C, 75.87; H, 5.97; N, 5.53. Found: C, 76.03; H, 6.01; N, 5.41.

(*S,S*)-6c. mp 271-274 °C; IR (KBr) 3380, 1640; $^1\text{H-NMR}$ (300 MHz, CDCl_3) **d** 1.45-1.66 (4H, m), 1.97 (2H, d, $J=7.5$), 2.15 (2H, d, $J=12.3$), 3.46 (2H, d, $J=16.8$), 3.93 (2H, d, $J=17.1$), 4.20 (2H, dt, $J=3.6$, 12.3), 5.44 (2H, t, $J=2.4$), 6.25 (2H, d, $J=9.6$), 7.32 (2H, t, $J=7.4$), 7.51 (2H, t, $J=7.7$), 7.73 (2H, d, $J=8.1$), 7.78 (2H, s), 8.16 (2H, d, $J=8.4$), 10.36 (2H, s). Anal. Calcd for $C_{32}H_{30}N_2O_4$: C, 75.87; H, 5.97; N, 5.53. Found: C, 75.86; H, 6.18; N, 5.49.

6d. mp 282-284 °C; IR (KBr) 3380, 1660; $^1\text{H-NMR}$ (300 MHz, CDCl_3) **d** 1.61-1.98 (8H, m), 2.44 (1H, br s), 3.70 (4H, s), 4.32 (1H, br s), 5.45 (2H, s), 6.72 (2H, br s), 7.32 (2H, t, $J=8.1$), 7.51 (2H, t, $J=8.1$), 7.74 (2H, d, $J=8.4$), 7.83 (2H, s), 8.15 (2H, d, $J=6.9$), 10.25 (2H, s). Anal. Calcd for $C_{32}H_{30}N_2O_4 \cdot H_2O$: C, 73.26; H, 6.15; N, 5.34. Found: C, 73.43; H, 5.96; N, 5.28.

(*S,S*)-6e. mp 190.0-191.5 °C; IR (KBr) 3350, 2980, 1650; $^1\text{H-NMR}$ (300 MHz, $\text{DMSO-}d_6$) **d** 1.45 (6H, s), 3.14 (2H, br s), 3.46 (2H, d, $J=15.0$), 3.58 (2H, br s), 3.68 (2H, d, $J=15.6$), 4.67 (2H, s), 5.46 (2H, s), 7.26 (2H, t, $J=7.5$), 7.42 (2H, t, $J=7.5$), 7.71 (2H, d, $J=7.8$), 8.04 (2H, d, $J=8.4$), 8.20 (2H, s), 9.34 (2H, s), 11.60 (2H, s). Anal. Calcd for $C_{33}H_{32}N_2O_6$: C, 71.72; H, 5.84; N, 5.07. Found: C, 71.58; H, 5.87; N, 4.87.

6f. mp 262-264 °C; IR (KBr) 3450, 3380, 1650; $^1\text{H-NMR}$ (300 MHz, CD_2Cl_2) **d** 1.26 (6H, s), 3.45 (4H, d, $J=6.3$), 3.70 (4H, s), 5.49 (2H, s), 6.94 (2H, t, $J=6.0$), 7.25 (2H, t, $J=7.4$), 7.40 (2H, t, $J=7.7$), 7.67 (2H, d, $J=8.1$), 7.72 (2H, s), 8.08 (2H, d, $J=8.4$), 10.08 (2H, s). Anal. Calcd for $C_{31}H_{30}N_2O_4$: C, 75.28; H, 6.11; N, 5.66. Found: C, 75.19; H, 6.37; N, 5.43.

(*R,R*)-6g. mp 122.2-122.8 °C; IR (KBr) 3350, 1640; $^1\text{H-NMR}$ (300 MHz, CDCl_3) **d** 1.67 (6H, d, $J=6.9$), 3.99 (4H, s), 4.42 (2H, s), 5.38 (2H, dt, $J=14.4$, 7.2), 6.71 (2H, d, $J=7.5$), 7.24-7.45 (14H, m),

7.71 (2H, d, $J=8.1$), 7.76 (2H, d, $J=8.4$), 7.85 (2H, s), 11.92 (2H, s). Anal. Calcd for $C_{42}H_{38}N_2O_4$: C, 79.47; H, 6.03; N, 4.11. Found: C, 79.28; H, 6.07; N, 4.37.

FIGURE S1. NMR spectrum of **3** in CDCl₃

FIGURE S3. NMR spectrum of **5a** in CDCl₃

FIGURE S4. NMR spectrum of (*R,R*)-**5b** in CDCl₃

FIGURE S5. NMR spectrum of (S,S)-5b in CDCl_3

FIGURE S6. NMR spectrum of (R,R)-5c in CDCl₃

FIGURE S7. NMR spectrum of (S,S)-5c in CDCl_3

FIGURE S8. NMR spectrum of 5d in CDCl₃

FIGURE S9. NMR spectrum of (S,S)-5e in CDCl₃

FIGURE S10. NMR spectrum of **5f** in CDCl₃

FIGURE S11. NMR spectrum of (R,R)-5g in CDCl₃

FIGURE S12. NMR spectrum of **6a** in DMSO-d₆

FIGURE S13. NMR spectrum of (R,R)-6b in CDCl₃

FIGURE S14. NMR spectrum of (S,S)-6b in CDCl_3

FIGURE S15. NMR spectrum of (R,R)-6c in CDCl₃

FIGURE S16. NMR spectrum of (S,S)-6c in CDCl_3

FIGURE S17. NMR spectrum of **6d** in CDCl₃

FIGURE S18. NMR spectrum of (S,S)-6e in DMSO-d₆

FIGURE S19. NMR spectrum of **6f** in CD₂Cl₂

FIGURE S20. NMR spectrum of **(R,R)-6g** in CDCl_3

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CD spectra, X-ray crystallographic analyses, and variable temperature NMR
measurements of the homochiral bis(hydroxynaphthoic amide)s revealed that two
naphthalene rings in the macrocycles took a twisted conformation in a solution
and in the crystalline state because of the steric hindrance between the two
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Single Crystal Structure Analysis Software. Version 1.00.
MSC, 9009 New Trails Drive, The Woodlands, TX, USA 77381-5209.
Rigaku, 3-9-12 Akishima, Tokyo 196-8666, Japan.

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CRYSTALS Issue 10, Chemical Crystallography Laboratory, Oxford, UK.

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_refine_ls_shift/su_max        0.0466
_refine_diff_density_max       0.35
_refine_diff_density_min      -0.43
_refine_ls_extinction_method    none
_refine_ls_extinction_coef      ?
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'C' 'C' 0.003 0.002
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
'H' 'H' 0.000 0.000
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(1992, Vol. C, Table 6.1.1.2)
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;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)

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  'O' 'O' 0.011 0.006
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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_atom_site_fract_z
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_atom_site_adp_type
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_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
O(1) O 1.1173(5) 0.3640(3) 0.6012(1) 0.046(1) Uani 1.00 d . . .
O(2) O 0.8350(5) 0.2914(3) 0.7145(1) 0.041(1) Uani 1.00 d . . .
O(3) O 1.1446(7) 0.1976(3) 0.5691(1) 0.056(1) Uani 1.00 d . . .
O(4) O 0.7115(5) 0.1435(3) 0.6770(1) 0.044(1) Uani 1.00 d . . .
O(5) O 0.3274(8) 0.2611(5) 0.4891(2) 0.086(2) Uani 1.00 d . . .
N(1) N 1.0664(6) 0.0962(3) 0.6251(1) 0.040(1) Uani 1.00 d . . .
N(2) N 0.7108(6) 0.1418(3) 0.5980(1) 0.039(1) Uani 1.00 d . . .
C(1) C 1.0730(7) 0.6090(4) 0.7242(2) 0.047(2) Uani 1.00 d . . .
C(2) C 1.0429(6) 0.5300(4) 0.7044(2) 0.036(1) Uani 1.00 d . . .
C(3) C 1.1843(7) 0.4909(4) 0.6710(2) 0.040(1) Uani 1.00 d . . .
C(4) C 0.8717(7) 0.4766(4) 0.7155(2) 0.039(1) Uani 1.00 d . . .
C(5) C 1.2271(6) 0.3921(4) 0.6774(2) 0.034(1) Uani 1.00 d . . .
C(6) C 1.3099(6) 0.3596(4) 0.7185(2) 0.036(1) Uani 1.00 d . . .
C(7) C 1.3732(7) 0.4180(4) 0.7550(2) 0.046(2) Uani 1.00 d . . .
C(8) C 1.4601(8) 0.3833(6) 0.7938(2) 0.058(2) Uani 1.00 d . . .
C(9) C 1.4818(7) 0.2910(6) 0.8000(2) 0.056(2) Uani 1.00 d . . .
C(10) C 1.4239(7) 0.2324(5) 0.7663(2) 0.047(2) Uani 1.00 d . . .
C(11) C 1.3377(6) 0.2654(4) 0.7247(2) 0.039(1) Uani 1.00 d . . .
C(12) C 1.2822(6) 0.2047(4) 0.6892(2) 0.036(1) Uani 1.00 d . . .
C(13) C 1.2056(6) 0.2372(4) 0.6485(2) 0.034(1) Uani 1.00 d . . .
C(14) C 1.1852(6) 0.3313(4) 0.6422(2) 0.032(1) Uani 1.00 d . . .
C(15) C 1.1400(7) 0.1748(4) 0.6111(2) 0.038(1) Uani 1.00 d . . .
C(16) C 0.9735(7) 0.0340(4) 0.5936(2) 0.037(1) Uani 1.00 d . . .
C(17) C 1.0281(7) -0.0610(4) 0.6053(2) 0.038(1) Uani 1.00 d . . .
C(18) C 0.9921(8) -0.0959(5) 0.6495(2) 0.049(2) Uani 1.00 d . . .
C(19) C 1.0267(10) -0.1853(5) 0.6593(2) 0.059(2) Uani 1.00 d . . .
C(20) C 1.1098(9) -0.1150(5) 0.5722(2) 0.053(2) Uani 1.00 d . . .
C(21) C 1.102(1) -0.2406(5) 0.6256(3) 0.067(2) Uani 1.00 d . . .
C(22) C 1.145(1) -0.2053(6) 0.5821(2) 0.065(2) Uani 1.00 d . . .
C(23) C 0.7557(7) 0.0465(4) 0.5969(2) 0.036(1) Uani 1.00 d . . .
C(24) C 0.6605(7) -0.0044(4) 0.5581(2) 0.037(1) Uani 1.00 d . . .
C(25) C 0.6370(9) -0.0969(5) 0.5613(2) 0.052(2) Uani 1.00 d . . .
C(26) C 0.5572(10) -0.1460(5) 0.5257(2) 0.060(2) Uani 1.00 d . . .
C(27) C 0.4954(8) -0.1019(5) 0.4861(2) 0.054(2) Uani 1.00 d . . .
C(28) C 0.5104(9) -0.0123(6) 0.4826(2) 0.059(2) Uani 1.00 d . . .
C(29) C 0.5948(9) 0.0377(5) 0.5177(2) 0.051(2) Uani 1.00 d . . .
C(30) C 0.7023(6) 0.1864(4) 0.6395(2) 0.034(1) Uani 1.00 d . . .
C(31) C 0.6890(6) 0.2855(4) 0.6386(2) 0.032(1) Uani 1.00 d . . .
C(32) C 0.6114(7) 0.3320(4) 0.6021(2) 0.035(1) Uani 1.00 d . . .
C(33) C 0.6078(6) 0.4264(4) 0.6013(1) 0.035(1) Uani 1.00 d . . .
C(34) C 0.5147(7) 0.4736(4) 0.5652(2) 0.043(2) Uani 1.00 d . . .

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C(35)	C	0.5099(8)	0.5647(5)	0.5646(2)	0.051(2)	Uani	1.00	d	.	.	.
C(36)	C	0.6014(9)	0.6136(4)	0.5999(2)	0.050(2)	Uani	1.00	d	.	.	.
C(37)	C	0.6938(7)	0.5698(4)	0.6352(2)	0.042(2)	Uani	1.00	d	.	.	.
C(38)	C	0.6972(6)	0.4754(4)	0.6376(2)	0.035(1)	Uani	1.00	d	.	.	.
C(39)	C	0.7786(6)	0.4282(4)	0.6754(2)	0.032(1)	Uani	1.00	d	.	.	.
C(40)	C	0.7669(6)	0.3363(4)	0.6769(1)	0.030(1)	Uani	1.00	d	.	.	.
H(1)	H	1.0836	0.3239	0.5769	0.0560	Uiso	1.00	calc	.	.	.
H(2)	H	0.8234	0.2265	0.7112	0.0380	Uiso	1.00	calc	.	.	.
H(3)	H	1.0753	0.0807	0.6572	0.0478	Uiso	1.00	calc	.	.	.
H(4)	H	0.6870	0.1731	0.5697	0.0470	Uiso	1.00	calc	.	.	.
H(5)	H	1.1811	0.6422	0.7157	0.0380	Uiso	1.00	calc	.	.	.
H(6)	H	0.9716	0.6337	0.7422	0.0380	Uiso	1.00	calc	.	.	.
H(7)	H	1.3008	0.5212	0.6670	0.0380	Uiso	1.00	calc	.	.	.
H(8)	H	1.1590	0.4899	0.6374	0.0380	Uiso	1.00	calc	.	.	.
H(9)	H	0.9061	0.4326	0.7394	0.0380	Uiso	1.00	calc	.	.	.
H(10)	H	0.7827	0.5138	0.7307	0.0380	Uiso	1.00	calc	.	.	.
H(11)	H	1.3436	0.4826	0.7507	0.0380	Uiso	1.00	calc	.	.	.
H(12)	H	1.4784	0.4302	0.8170	0.0380	Uiso	1.00	calc	.	.	.
H(13)	H	1.5421	0.2675	0.8279	0.0380	Uiso	1.00	calc	.	.	.
H(14)	H	1.4485	0.1667	0.7701	0.0380	Uiso	1.00	calc	.	.	.
H(15)	H	1.2945	0.1395	0.6906	0.0380	Uiso	1.00	calc	.	.	.
H(16)	H	1.0066	0.0471	0.5619	0.0380	Uiso	1.00	calc	.	.	.
H(17)	H	0.9023	-0.0700	0.6710	0.0380	Uiso	1.00	calc	.	.	.
H(18)	H	0.9992	-0.2088	0.6892	0.0708	Uiso	1.00	calc	.	.	.
H(19)	H	1.1231	-0.3025	0.6318	0.0796	Uiso	1.00	calc	.	.	.
H(20)	H	1.2076	-0.2401	0.5579	0.0380	Uiso	1.00	calc	.	.	.
H(21)	H	1.1424	-0.0912	0.5427	0.0642	Uiso	1.00	calc	.	.	.
H(22)	H	0.7164	0.0211	0.6258	0.0435	Uiso	1.00	calc	.	.	.
H(23)	H	0.6941	-0.1244	0.5881	0.0380	Uiso	1.00	calc	.	.	.
H(24)	H	0.5451	-0.2099	0.5284	0.0717	Uiso	1.00	calc	.	.	.
H(25)	H	0.4288	-0.1391	0.4619	0.0380	Uiso	1.00	calc	.	.	.
H(26)	H	0.4655	0.0238	0.4575	0.0380	Uiso	1.00	calc	.	.	.
H(27)	H	0.6224	0.1017	0.5138	0.0380	Uiso	1.00	calc	.	.	.
H(28)	H	0.5515	0.2991	0.5765	0.0380	Uiso	1.00	calc	.	.	.
H(29)	H	0.4332	0.4474	0.5416	0.0380	Uiso	1.00	calc	.	.	.
H(30)	H	0.4331	0.5991	0.5434	0.0380	Uiso	1.00	calc	.	.	.
H(31)	H	0.5945	0.6802	0.6011	0.0380	Uiso	1.00	calc	.	.	.
H(32)	H	0.7445	0.6067	0.6605	0.0380	Uiso	1.00	calc	.	.	.
H(33)	H	0.3951	0.3125	0.5013	0.1039	Uiso	1.00	calc	.	.	.
H(34)	H	0.3652	0.1942	0.5008	0.0715	Uiso	1.00	calc	.	.	.

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

O(1)	0.058(2)	0.048(3)	0.033(2)	0.001(2)	-0.004(2)	0.005(2)
O(2)	0.049(2)	0.038(3)	0.035(2)	0.003(2)	-0.003(2)	0.009(2)
O(3)	0.078(3)	0.051(3)	0.039(2)	-0.016(2)	0.006(2)	0.003(2)
O(4)	0.055(2)	0.038(3)	0.039(2)	0.004(2)	0.004(2)	0.005(2)
O(5)	0.087(4)	0.105(6)	0.068(3)	0.003(4)	0.001(3)	0.020(3)
N(1)	0.042(2)	0.039(3)	0.039(2)	-0.007(2)	0.004(2)	-0.001(2)
N(2)	0.052(2)	0.030(3)	0.035(2)	0.002(2)	-0.004(2)	0.000(2)
C(1)	0.046(3)	0.042(4)	0.052(3)	-0.003(3)	0.003(2)	-0.009(3)
C(2)	0.036(2)	0.037(4)	0.036(2)	-0.002(2)	0.000(2)	0.001(2)
C(3)	0.044(2)	0.032(3)	0.042(3)	-0.002(2)	0.011(2)	0.003(2)
C(4)	0.044(2)	0.039(4)	0.035(2)	-0.004(3)	0.006(2)	-0.004(2)
C(5)	0.028(2)	0.036(4)	0.038(2)	-0.003(2)	0.006(2)	0.001(2)

C(6)	0.031(2)	0.040(4)	0.036(2)	-0.004(2)	0.005(2)	0.000(2)
C(7)	0.037(2)	0.053(4)	0.047(3)	0.000(3)	-0.003(2)	-0.002(2)
C(8)	0.047(3)	0.085(6)	0.042(3)	-0.008(3)	-0.004(2)	-0.003(3)
C(9)	0.041(3)	0.086(6)	0.041(3)	0.001(3)	-0.007(2)	0.008(3)
C(10)	0.036(2)	0.056(5)	0.049(3)	0.003(3)	-0.004(2)	0.014(3)
C(11)	0.032(2)	0.049(4)	0.037(2)	-0.001(2)	0.001(2)	0.009(2)
C(12)	0.031(2)	0.033(3)	0.045(3)	-0.004(2)	0.001(2)	0.006(2)
C(13)	0.034(2)	0.031(3)	0.037(2)	-0.003(2)	0.007(2)	0.003(2)
C(14)	0.027(2)	0.033(3)	0.035(2)	-0.003(2)	0.001(2)	0.004(2)
C(15)	0.037(2)	0.041(4)	0.037(2)	-0.005(2)	0.005(2)	-0.001(2)
C(16)	0.043(2)	0.033(4)	0.036(2)	-0.002(2)	0.004(2)	-0.002(2)
C(17)	0.042(2)	0.031(3)	0.042(3)	-0.002(2)	0.001(2)	-0.002(2)
C(18)	0.053(3)	0.050(5)	0.043(3)	0.011(3)	-0.002(2)	0.003(2)
C(19)	0.067(4)	0.043(5)	0.067(4)	0.010(3)	-0.008(3)	0.008(3)
C(20)	0.062(3)	0.049(5)	0.049(3)	0.003(3)	0.005(3)	-0.007(3)
C(21)	0.072(4)	0.046(5)	0.082(5)	0.004(4)	-0.016(4)	0.006(3)
C(22)	0.073(4)	0.051(5)	0.070(4)	0.011(4)	-0.003(4)	-0.013(3)
C(23)	0.045(3)	0.026(3)	0.037(2)	-0.002(2)	0.000(2)	0.003(2)
C(24)	0.045(3)	0.027(3)	0.040(2)	0.001(2)	0.000(2)	-0.002(2)
C(25)	0.061(3)	0.041(4)	0.053(3)	-0.007(3)	-0.011(3)	-0.001(3)
C(26)	0.067(4)	0.043(5)	0.070(4)	0.000(3)	-0.013(3)	-0.013(3)
C(27)	0.055(3)	0.057(5)	0.050(3)	-0.006(3)	-0.005(3)	-0.012(3)
C(28)	0.064(4)	0.066(6)	0.047(3)	-0.007(4)	-0.014(3)	0.001(3)
C(29)	0.062(3)	0.043(4)	0.048(3)	-0.012(3)	-0.007(3)	0.002(3)
C(30)	0.034(2)	0.030(3)	0.038(2)	0.006(2)	0.002(2)	0.003(2)
C(31)	0.030(2)	0.028(3)	0.038(2)	0.004(2)	0.003(2)	0.000(2)
C(32)	0.035(2)	0.036(4)	0.034(2)	0.006(2)	-0.003(2)	0.002(2)
C(33)	0.033(2)	0.038(4)	0.033(2)	0.005(2)	-0.002(2)	0.004(2)
C(34)	0.043(3)	0.045(4)	0.041(3)	0.005(3)	-0.006(2)	0.009(2)
C(35)	0.056(3)	0.045(4)	0.052(3)	0.008(3)	-0.004(3)	0.011(3)
C(36)	0.062(3)	0.031(4)	0.056(3)	0.004(3)	0.002(3)	0.007(3)
C(37)	0.046(3)	0.033(4)	0.047(3)	0.003(2)	0.002(2)	0.002(2)
C(38)	0.034(2)	0.037(3)	0.033(2)	0.003(2)	0.007(2)	0.002(2)
C(39)	0.029(2)	0.031(3)	0.035(2)	0.000(2)	0.002(2)	0.001(2)
C(40)	0.026(2)	0.038(4)	0.027(2)	0.002(2)	0.002(2)	0.000(2)

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_computing_structure_refinement 'teXsan Ver. 1.10'
_computing_publication_material 'teXsan Ver. 1.11'
_computing_molecular_graphics   ?
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  _geom_bond_atom_site_label_2
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O(1)      C(14)      1.365(6)    . . yes
O(2)      C(40)      1.360(6)    . . yes
O(3)      C(15)      1.250(6)    . . yes
O(4)      C(30)      1.250(6)    . . yes
N(1)      C(15)      1.345(7)    . . yes
N(1)      C(16)      1.456(7)    . . yes
N(2)      C(23)      1.455(7)    . . yes
N(2)      C(30)      1.362(6)    . . yes
C(1)      C(2)      1.323(8)    . . yes

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C(2)	C(3)	1.517(7)	. . yes
C(2)	C(4)	1.506(7)	. . yes
C(3)	C(5)	1.513(8)	. . yes
C(4)	C(39)	1.513(7)	. . yes
C(5)	C(6)	1.408(6)	. . yes
C(5)	C(14)	1.387(7)	. . yes
C(6)	C(7)	1.433(7)	. . yes
C(6)	C(11)	1.426(8)	. . yes
C(7)	C(8)	1.378(8)	. . yes
C(8)	C(9)	1.39(1)	. . yes
C(9)	C(10)	1.366(9)	. . yes
C(10)	C(11)	1.431(7)	. . yes
C(11)	C(12)	1.420(8)	. . yes
C(12)	C(13)	1.378(7)	. . yes
C(13)	C(14)	1.418(7)	. . yes
C(13)	C(15)	1.495(7)	. . yes
C(16)	C(17)	1.506(8)	. . yes
C(16)	C(23)	1.589(7)	. . yes
C(17)	C(18)	1.392(7)	. . yes
C(17)	C(20)	1.376(8)	. . yes
C(18)	C(19)	1.381(9)	. . yes
C(19)	C(21)	1.379(10)	. . yes
C(20)	C(22)	1.40(1)	. . yes
C(21)	C(22)	1.389(10)	. . yes
C(23)	C(24)	1.511(7)	. . yes
C(24)	C(25)	1.388(8)	. . yes
C(24)	C(29)	1.399(8)	. . yes
C(25)	C(26)	1.380(8)	. . yes
C(26)	C(27)	1.385(9)	. . yes
C(27)	C(28)	1.342(10)	. . yes
C(28)	C(29)	1.391(8)	. . yes
C(30)	C(31)	1.478(7)	. . yes
C(31)	C(32)	1.373(7)	. . yes
C(31)	C(40)	1.446(7)	. . yes
C(32)	C(33)	1.406(8)	. . yes
C(33)	C(34)	1.419(7)	. . yes
C(33)	C(38)	1.425(7)	. . yes
C(34)	C(35)	1.357(9)	. . yes
C(35)	C(36)	1.410(9)	. . yes
C(36)	C(37)	1.376(8)	. . yes
C(37)	C(38)	1.405(8)	. . yes
C(38)	C(39)	1.420(7)	. . yes
C(39)	C(40)	1.372(7)	. . yes

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  _geom_angle_atom_site_label_3
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  _geom_angle_site_symmetry_3
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  C(15)      N(1)      C(16)      123.5(4)    . . . yes
  C(23)      N(2)      C(30)      120.2(4)    . . . yes
  C(1)       C(2)      C(3)       120.0(5)    . . . yes
  C(1)       C(2)      C(4)       120.9(5)    . . . yes
  C(3)       C(2)      C(4)       119.0(5)    . . . yes
  C(2)       C(3)      C(5)       115.8(4)    . . . yes
  C(2)       C(4)      C(39)      117.2(4)    . . . yes
  C(3)       C(5)      C(6)       121.4(5)    . . . yes
```

C(3)	C(5)	C(14)	120.1(4)	. . . yes
C(6)	C(5)	C(14)	118.5(6)	. . . yes
C(5)	C(6)	C(7)	122.5(6)	. . . yes
C(5)	C(6)	C(11)	120.1(5)	. . . yes
C(7)	C(6)	C(11)	117.4(5)	. . . yes
C(6)	C(7)	C(8)	120.4(6)	. . . yes
C(7)	C(8)	C(9)	121.5(6)	. . . yes
C(8)	C(9)	C(10)	120.3(5)	. . . yes
C(9)	C(10)	C(11)	120.1(6)	. . . yes
C(6)	C(11)	C(10)	120.2(5)	. . . yes
C(6)	C(11)	C(12)	119.7(4)	. . . yes
C(10)	C(11)	C(12)	120.1(6)	. . . yes
C(11)	C(12)	C(13)	119.8(5)	. . . yes
C(12)	C(13)	C(14)	119.7(5)	. . . yes
C(12)	C(13)	C(15)	121.0(5)	. . . yes
C(14)	C(13)	C(15)	119.3(4)	. . . yes
O(1)	C(14)	C(5)	118.2(5)	. . . yes
O(1)	C(14)	C(13)	119.9(4)	. . . yes
C(5)	C(14)	C(13)	121.9(4)	. . . yes
O(3)	C(15)	N(1)	122.2(5)	. . . yes
O(3)	C(15)	C(13)	120.8(5)	. . . yes
N(1)	C(15)	C(13)	116.9(4)	. . . yes
N(1)	C(16)	C(17)	109.8(4)	. . . yes
N(1)	C(16)	C(23)	110.3(4)	. . . yes
C(17)	C(16)	C(23)	110.9(5)	. . . yes
C(16)	C(17)	C(18)	120.2(5)	. . . yes
C(16)	C(17)	C(20)	120.5(5)	. . . yes
C(18)	C(17)	C(20)	119.3(6)	. . . yes
C(17)	C(18)	C(19)	120.6(6)	. . . yes
C(18)	C(19)	C(21)	120.2(6)	. . . yes
C(17)	C(20)	C(22)	120.1(6)	. . . yes
C(19)	C(21)	C(22)	119.5(7)	. . . yes
C(20)	C(22)	C(21)	120.2(6)	. . . yes
N(2)	C(23)	C(16)	109.6(5)	. . . yes
N(2)	C(23)	C(24)	113.7(4)	. . . yes
C(16)	C(23)	C(24)	110.5(4)	. . . yes
C(23)	C(24)	C(25)	120.2(5)	. . . yes
C(23)	C(24)	C(29)	122.6(5)	. . . yes
C(25)	C(24)	C(29)	117.2(5)	. . . yes
C(24)	C(25)	C(26)	121.8(6)	. . . yes
C(25)	C(26)	C(27)	119.3(7)	. . . yes
C(26)	C(27)	C(28)	120.4(6)	. . . yes
C(27)	C(28)	C(29)	120.8(6)	. . . yes
C(24)	C(29)	C(28)	120.5(6)	. . . yes
O(4)	C(30)	N(2)	119.9(5)	. . . yes
O(4)	C(30)	C(31)	121.8(5)	. . . yes
N(2)	C(30)	C(31)	118.2(4)	. . . yes
C(30)	C(31)	C(32)	122.9(5)	. . . yes
C(30)	C(31)	C(40)	118.8(4)	. . . yes
C(32)	C(31)	C(40)	118.3(5)	. . . yes
C(31)	C(32)	C(33)	121.6(5)	. . . yes
C(32)	C(33)	C(34)	121.0(5)	. . . yes
C(32)	C(33)	C(38)	119.4(4)	. . . yes
C(34)	C(33)	C(38)	119.6(5)	. . . yes
C(33)	C(34)	C(35)	121.0(5)	. . . yes
C(34)	C(35)	C(36)	119.6(5)	. . . yes
C(35)	C(36)	C(37)	120.7(6)	. . . yes
C(36)	C(37)	C(38)	121.1(5)	. . . yes
C(33)	C(38)	C(37)	117.9(5)	. . . yes
C(33)	C(38)	C(39)	119.5(5)	. . . yes
C(37)	C(38)	C(39)	122.6(5)	. . . yes

C(4)	C(39)	C(38)	121.9(5)	. . .	yes
C(4)	C(39)	C(40)	118.6(4)	. . .	yes
C(38)	C(39)	C(40)	119.4(4)	. . .	yes
O(2)	C(40)	C(31)	119.1(5)	. . .	yes
O(2)	C(40)	C(39)	119.4(4)	. . .	yes
C(31)	C(40)	C(39)	121.5(4)	. . .	yes

#-----

loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

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_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

O(1)	C(14)	C(5)	C(3)	4.5(6)		yes
O(1)	C(14)	C(5)	C(6)	-175.4(4)		yes
O(1)	C(14)	C(13)	C(12)	177.0(4)		yes
O(1)	C(14)	C(13)	C(15)	-4.2(6)		yes
O(2)	C(40)	C(31)	C(30)	-5.9(6)		yes
O(2)	C(40)	C(31)	C(32)	176.4(4)		yes
O(2)	C(40)	C(39)	C(4)	1.5(6)		yes
O(2)	C(40)	C(39)	C(38)	-176.1(4)		yes
O(3)	C(15)	N(1)	C(16)	-4.8(8)		yes
O(3)	C(15)	C(13)	C(12)	-149.5(5)		yes
O(3)	C(15)	C(13)	C(14)	31.7(7)		yes
O(4)	C(30)	N(2)	C(23)	-8.4(7)		yes
O(4)	C(30)	C(31)	C(32)	-154.8(5)		yes
O(4)	C(30)	C(31)	C(40)	27.6(6)		yes
N(1)	C(15)	C(13)	C(12)	34.4(7)		yes
N(1)	C(15)	C(13)	C(14)	-144.4(5)		yes
N(1)	C(16)	C(17)	C(18)	59.8(6)		yes
N(1)	C(16)	C(17)	C(20)	-121.8(5)		yes
N(1)	C(16)	C(23)	N(2)	42.9(6)		yes
N(1)	C(16)	C(23)	C(24)	169.0(4)		yes
N(2)	C(23)	C(16)	C(17)	164.7(4)		yes
N(2)	C(23)	C(24)	C(25)	-158.0(5)		yes
N(2)	C(23)	C(24)	C(29)	22.7(7)		yes
N(2)	C(30)	C(31)	C(32)	27.3(6)		yes
N(2)	C(30)	C(31)	C(40)	-150.3(4)		yes
C(1)	C(2)	C(3)	C(5)	135.9(5)		yes
C(1)	C(2)	C(4)	C(39)	140.2(6)		yes
C(2)	C(3)	C(5)	C(6)	-64.0(6)		yes
C(2)	C(3)	C(5)	C(14)	116.1(5)		yes
C(2)	C(4)	C(39)	C(38)	-64.7(6)		yes
C(2)	C(4)	C(39)	C(40)	117.8(5)		yes
C(3)	C(2)	C(4)	C(39)	-41.4(7)		yes
C(3)	C(5)	C(6)	C(7)	-5.6(6)		yes
C(3)	C(5)	C(6)	C(11)	175.9(4)		yes
C(3)	C(5)	C(14)	C(13)	-173.5(4)		yes
C(4)	C(2)	C(3)	C(5)	-42.5(6)		yes
C(4)	C(39)	C(38)	C(33)	-178.6(4)		yes
C(4)	C(39)	C(38)	C(37)	-1.4(7)		yes
C(4)	C(39)	C(40)	C(31)	-176.5(4)		yes
C(5)	C(6)	C(7)	C(8)	-177.4(4)		yes
C(5)	C(6)	C(11)	C(10)	179.2(4)		yes
C(5)	C(6)	C(11)	C(12)	0.3(6)		yes
C(5)	C(14)	C(13)	C(12)	-5.0(6)		yes

C(5)	C(14)	C(13)	C(15)	173.8(4)	 yes
C(6)	C(5)	C(14)	C(13)	6.6(6)	 yes
C(6)	C(7)	C(8)	C(9)	-2.9(8)	 yes
C(6)	C(11)	C(10)	C(9)	-0.7(7)	 yes
C(6)	C(11)	C(12)	C(13)	1.4(7)	 yes
C(7)	C(6)	C(5)	C(14)	174.3(4)	 yes
C(7)	C(6)	C(11)	C(10)	0.6(7)	 yes
C(7)	C(6)	C(11)	C(12)	-178.3(4)	 yes
C(7)	C(8)	C(9)	C(10)	2.9(8)	 yes
C(8)	C(7)	C(6)	C(11)	1.1(7)	 yes
C(8)	C(9)	C(10)	C(11)	-1.0(8)	 yes
C(9)	C(10)	C(11)	C(12)	178.2(5)	 yes
C(10)	C(11)	C(12)	C(13)	-177.5(4)	 yes
C(11)	C(6)	C(5)	C(14)	-4.2(6)	 yes
C(11)	C(12)	C(13)	C(14)	0.9(6)	 yes
C(11)	C(12)	C(13)	C(15)	-177.9(4)	 yes
C(13)	C(15)	N(1)	C(16)	171.2(4)	 yes
C(15)	N(1)	C(16)	C(17)	138.9(5)	 yes
C(15)	N(1)	C(16)	C(23)	-98.6(6)	 yes
C(16)	C(17)	C(18)	C(19)	174.2(5)	 yes
C(16)	C(17)	C(20)	C(22)	-174.5(6)	 yes
C(16)	C(23)	N(2)	C(30)	-88.8(5)	 yes
C(16)	C(23)	C(24)	C(25)	78.2(6)	 yes
C(16)	C(23)	C(24)	C(29)	-101.1(6)	 yes
C(17)	C(16)	C(23)	C(24)	-69.1(5)	 yes
C(17)	C(18)	C(19)	C(21)	1.6(10)	 yes
C(17)	C(20)	C(22)	C(21)	-1(1)	 yes
C(18)	C(17)	C(16)	C(23)	-62.3(6)	 yes
C(18)	C(17)	C(20)	C(22)	4.0(9)	 yes
C(18)	C(19)	C(21)	C(22)	1(1)	 yes
C(19)	C(18)	C(17)	C(20)	-4.2(9)	 yes
C(19)	C(21)	C(22)	C(20)	-1(1)	 yes
C(20)	C(17)	C(16)	C(23)	116.1(5)	 yes
C(23)	N(2)	C(30)	C(31)	169.4(4)	 yes
C(23)	C(24)	C(25)	C(26)	-177.5(5)	 yes
C(23)	C(24)	C(29)	C(28)	179.1(5)	 yes
C(24)	C(23)	N(2)	C(30)	146.9(4)	 yes
C(24)	C(25)	C(26)	C(27)	-1(1)	 yes
C(24)	C(29)	C(28)	C(27)	-2.1(10)	 yes
C(25)	C(24)	C(29)	C(28)	-0.2(9)	 yes
C(25)	C(26)	C(27)	C(28)	0(1)	 yes
C(26)	C(25)	C(24)	C(29)	1.8(9)	 yes
C(26)	C(27)	C(28)	C(29)	2(1)	 yes
C(30)	C(31)	C(32)	C(33)	-177.2(4)	 yes
C(30)	C(31)	C(40)	C(39)	172.1(4)	 yes
C(31)	C(32)	C(33)	C(34)	-175.0(4)	 yes
C(31)	C(32)	C(33)	C(38)	4.2(7)	 yes
C(31)	C(40)	C(39)	C(38)	6.0(6)	 yes
C(32)	C(31)	C(40)	C(39)	-5.6(6)	 yes
C(32)	C(33)	C(34)	C(35)	179.5(5)	 yes
C(32)	C(33)	C(38)	C(37)	178.8(4)	 yes
C(32)	C(33)	C(38)	C(39)	-3.9(6)	 yes
C(33)	C(32)	C(31)	C(40)	0.4(7)	 yes
C(33)	C(34)	C(35)	C(36)	1.1(9)	 yes
C(33)	C(38)	C(37)	C(36)	2.3(7)	 yes
C(33)	C(38)	C(39)	C(40)	-1.2(6)	 yes
C(34)	C(33)	C(38)	C(37)	-1.9(6)	 yes
C(34)	C(33)	C(38)	C(39)	175.4(4)	 yes
C(34)	C(35)	C(36)	C(37)	-0.7(9)	 yes
C(35)	C(34)	C(33)	C(38)	0.2(7)	 yes
C(35)	C(36)	C(37)	C(38)	-1.0(8)	 yes

C(36)	C(37)	C(38)	C(39)	-174.9(4)	 yes
C(37)	C(38)	C(39)	C(40)	176.0(4)	 yes
C(37)	C(38)	C(39)	C(40)	176.0(4)	 yes

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loop_

_geom_contact_atom_site_label_1

_geom_contact_atom_site_label_2

_geom_contact_distance

_geom_contact_site_symmetry_1

_geom_contact_site_symmetry_2

_geom_contact_publ_flag

O(1)	C(28)	3.349(8)	. 3_556 ?
O(1)	C(34)	3.461(7)	. 1_655 ?
O(2)	C(1)	3.299(7)	. 4_746 ?
O(2)	C(10)	3.437(6)	. 1_455 ?
O(2)	C(9)	3.539(6)	. 1_455 ?
O(3)	O(5)	2.811(6)	. 1_655 ?
O(3)	O(5)	2.902(7)	. 3_556 ?
O(4)	C(12)	3.255(6)	. 1_455 ?
O(4)	C(1)	3.272(6)	. 4_746 ?
O(4)	C(11)	3.532(7)	. 1_455 ?
O(4)	C(10)	3.553(7)	. 1_455 ?
O(5)	N(2)	3.004(6)	. 3_456 ?
O(5)	C(32)	3.343(8)	. 3_456 ?
O(5)	C(29)	3.439(9)	. 3_456 ?
C(1)	C(19)	3.596(9)	. 1_565 ?
C(5)	C(33)	3.549(6)	. 1_655 ?
C(6)	C(40)	3.532(6)	. 1_655 ?
C(11)	C(40)	3.554(6)	. 1_655 ?
C(11)	C(31)	3.555(6)	. 1_655 ?
C(12)	C(30)	3.367(6)	. 1_655 ?
C(12)	C(31)	3.493(6)	. 1_655 ?
C(13)	C(32)	3.517(7)	. 1_655 ?
C(13)	C(31)	3.581(7)	. 1_655 ?
C(14)	C(32)	3.291(6)	. 1_655 ?
C(14)	C(33)	3.567(6)	. 1_655 ?
C(20)	C(26)	3.530(9)	. 1_655 ?
C(22)	C(26)	3.50(1)	. 1_655 ?

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#===END

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data_6c

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CHEMICAL DATA

_chemical_formula_sum	'C36 H42 N2 O6 S2 '
_chemical_formula_moiety	'C32 H30 N2 O4, 2(C2 H6 O S)'
_chemical_formula_weight	662.86
_chemical_melting_point	'270-272 \%C'

#-----

CRYSTAL DATA

_symmetry_cell_setting	orthorhombic
_symmetry_space_group_name_H-M	'P c a 21 '
_symmetry_Int_Tables_number	29

loop_

_symmetry_equiv_pos_as_xyz

x,y,z

-x,-y,1/2+z

1/2-x,y,1/2+z

1/2+x,-y,z

_cell_length_a	20.526(1)
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_cell_length_b	8.7053(5)
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_cell_length_c	18.706(1)
_cell_angle_alpha	90
_cell_angle_beta	90
_cell_angle_gamma	90
_cell_volume	3342.5(7)
_cell_formula_units_Z	4
_cell_measurement_reflns_used	44615
_cell_measurement_theta_min	1.5
_cell_measurement_theta_max	27.5
_cell_measurement_temperature	193.2
#-----	
_exptl_crystal_description	'prism'
_exptl_crystal_colour	'yellow'
_exptl_crystal_size_max	0.580
_exptl_crystal_size_mid	0.300
_exptl_crystal_size_min	0.175
_exptl_crystal_size_rad	?
_exptl_crystal_density_diffn	1.317
_exptl_crystal_density_meas	?
_exptl_crystal_density_method	'not measured'
_exptl_absorpt_coefficient_mu	0.208
_exptl_absorpt_correction_type	multi-scan
_exptl_absorpt_process_details	'(Higashi, 1995)'
_exptl_absorpt_correction_T_min	0.837
_exptl_absorpt_correction_T_max	0.964
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# EXPERIMENTAL DATA	
_diffn_radiation_type	'Mo K\alpha'
_diffn_radiation_wavelength	0.7107
_diffn_measurement_device_type	'Rigaku RAXIS-RAPID Imaging Plate'
_diffn_measurement_method	\w
_diffn_detector_area_resol_mean	10.00
_diffn_reflns_number	28698
_diffn_reflns_av_R_equivalents	0.045
_diffn_reflns_theta_max	27.48
_diffn_measured_fraction_theta_max	1.0000
_diffn_reflns_theta_full	27.48
_diffn_measured_fraction_theta_full	1.0000
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_diffn_reflns_limit_k_min	0
_diffn_reflns_limit_k_max	11
_diffn_reflns_limit_l_min	0
_diffn_reflns_limit_l_max	24
#-----	
# REFINEMENT DATA	
_refine_special_details	
;	
Refinement using reflections with $F^2 > 0.0 \sigma(F^2)$. 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).	
;	
_reflns_number_total	3953
_reflns_number_gt	2928
_reflns_threshold_expression	$F^2 > 2.0 \sigma(F^2)$
_refine_ls_structure_factor_coef	Fsqd
_refine_ls_R_factor_gt	0.0411
_refine_ls_wR_factor_ref	0.1133
_refine_ls_hydrogen_treatment	noref
_refine_ls_number_reflns	3953

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_refine_ls_number_parameters      417
_refine_ls_goodness_of_fit_ref    0.949
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
  'w = 1/[\s^2^(Fo^2^)+ (0.18800(Max(Fo^2^,0) + 2Fc^2^)/3)^2^]'
_refine_ls_shift/su_max           0.0079
_refine_diff_density_max          1.00
_refine_diff_density_min         -0.27
_refine_ls_extinction_method
  'Zachariasen(1967) type 2 Gaussian isotropic'
_refine_ls_extinction_coef        0.003(1)
_refine_ls_abs_structure_details  ?
_refine_ls_abs_structure_Flack    0.2(2)

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;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
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;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'S' 'S' 0.125 0.123
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_fract_z
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_atom_site_occupancy
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_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
S(1)  S  0.83496(6)  0.3887(1)  0.1886(6)  0.0481(3)  Uani  1.00  d  .  .  .
S(2)  S  0.09256(5)  0.3881(1)  0.1863(6)  0.0359(3)  Uani  1.00  d  .  .  .
O(1)  O  0.5784(1)   -0.3076(4)  0.3707(6)  0.0378(8)  Uani  1.00  d  .  .  .
O(2)  O  0.5227(2)   0.0218(4)  0.4977(6)  0.0379(8)  Uani  1.00  d  .  .  .
O(3)  O  0.5140(2)   -0.5065(4)  0.5604(6)  0.0470(9)  Uani  1.00  d  .  .  .
O(4)  O  0.4245(2)   -0.1512(4)  0.5183(6)  0.0440(8)  Uani  1.00  d  .  .  .
O(5)  O  0.8495(2)   0.2967(5)  0.2529(6)  0.053(1)   Uani  1.00  d  .  .  .

```

O(6)	O	0.1362(2)	0.3349(5)	0.2473(6)	0.053(1)	Uani	1.00	d	.	.	.
N(1)	N	0.4924(2)	-0.4731(4)	0.4434(6)	0.0350(10)	Uani	1.00	d	.	.	.
N(2)	N	0.3832(2)	-0.2845(4)	0.4249(6)	0.0324(9)	Uani	1.00	d	.	.	.
C(1)	C	0.7202(3)	0.1897(7)	0.3506(7)	0.058(2)	Uani	1.00	d	.	.	.
C(2)	C	0.6741(2)	0.0979(5)	0.3748(6)	0.040(1)	Uani	1.00	d	.	.	.
C(3)	C	0.6793(2)	-0.0757(5)	0.3687(6)	0.037(1)	Uani	1.00	d	.	.	.
C(4)	C	0.6121(2)	0.1637(5)	0.4071(6)	0.036(1)	Uani	1.00	d	.	.	.
C(5)	C	0.6614(2)	-0.1660(5)	0.4351(6)	0.0309(9)	Uani	1.00	d	.	.	.
C(6)	C	0.6946(2)	-0.1412(5)	0.5007(6)	0.0319(10)	Uani	1.00	d	.	.	.
C(7)	C	0.7497(2)	-0.0419(5)	0.5070(6)	0.037(1)	Uani	1.00	d	.	.	.
C(8)	C	0.7805(2)	-0.0186(6)	0.5714(6)	0.042(1)	Uani	1.00	d	.	.	.
C(9)	C	0.7584(2)	-0.0948(6)	0.6331(6)	0.044(1)	Uani	1.00	d	.	.	.
C(10)	C	0.7070(2)	-0.1924(6)	0.6298(6)	0.039(1)	Uani	1.00	d	.	.	.
C(11)	C	0.6740(2)	-0.2197(5)	0.5637(6)	0.0320(10)	Uani	1.00	d	.	.	.
C(12)	C	0.6207(2)	-0.3214(5)	0.5587(6)	0.0307(10)	Uani	1.00	d	.	.	.
C(13)	C	0.5887(2)	-0.3499(5)	0.4965(6)	0.0285(9)	Uani	1.00	d	.	.	.
C(14)	C	0.6107(2)	-0.2727(5)	0.4327(6)	0.0297(9)	Uani	1.00	d	.	.	.
C(15)	C	0.5291(2)	-0.4520(5)	0.5028(6)	0.0332(10)	Uani	1.00	d	.	.	.
C(16)	C	0.4275(2)	-0.5428(5)	0.4444(6)	0.0340(10)	Uani	1.00	d	.	.	.
C(17)	C	0.4131(2)	-0.6119(5)	0.3714(6)	0.038(1)	Uani	1.00	d	.	.	.
C(18)	C	0.3451(2)	-0.6838(5)	0.3694(6)	0.042(1)	Uani	1.00	d	.	.	.
C(19)	C	0.2933(2)	-0.5642(5)	0.3877(6)	0.042(1)	Uani	1.00	d	.	.	.
C(20)	C	0.3069(2)	-0.4958(6)	0.4615(6)	0.043(1)	Uani	1.00	d	.	.	.
C(21)	C	0.3753(2)	-0.4267(5)	0.4682(6)	0.034(1)	Uani	1.00	d	.	.	.
C(22)	C	0.4172(2)	-0.1653(5)	0.4527(6)	0.0324(9)	Uani	1.00	d	.	.	.
C(23)	C	0.4503(2)	-0.0599(5)	0.4025(6)	0.0296(9)	Uani	1.00	d	.	.	.
C(24)	C	0.4328(2)	-0.0457(5)	0.3316(6)	0.0308(10)	Uani	1.00	d	.	.	.
C(25)	C	0.4706(2)	0.0394(5)	0.2830(6)	0.0309(9)	Uani	1.00	d	.	.	.
C(26)	C	0.4502(2)	0.0604(6)	0.2110(6)	0.038(1)	Uani	1.00	d	.	.	.
C(27)	C	0.4884(3)	0.1376(5)	0.1640(6)	0.043(1)	Uani	1.00	d	.	.	.
C(28)	C	0.5488(2)	0.2002(5)	0.1852(6)	0.043(1)	Uani	1.00	d	.	.	.
C(29)	C	0.5698(2)	0.1836(5)	0.2548(6)	0.036(1)	Uani	1.00	d	.	.	.
C(30)	C	0.5308(2)	0.1046(5)	0.3065(6)	0.0308(9)	Uani	1.00	d	.	.	.
C(31)	C	0.5486(2)	0.0943(5)	0.3798(6)	0.0296(9)	Uani	1.00	d	.	.	.
C(32)	C	0.5072(2)	0.0211(5)	0.4274(6)	0.0294(9)	Uani	1.00	d	.	.	.
C(33)	C	0.8546(3)	0.2704(7)	0.1135(6)	0.057(2)	Uani	1.00	d	.	.	.
C(34)	C	0.7481(3)	0.3849(8)	0.1787(6)	0.070(2)	Uani	1.00	d	.	.	.
C(35)	C	0.0723(3)	0.2198(6)	0.1371(6)	0.051(1)	Uani	1.00	d	.	.	.
C(36)	C	0.0137(2)	0.4191(6)	0.2252(6)	0.043(1)	Uani	1.00	d	.	.	.
H(1)	H	0.6037	-0.3022	0.3287	0.0570	Uiso	1.00	calc	.	.	.
H(2)	H	0.4848	0.0116	0.5206	0.0570	Uiso	1.00	calc	.	.	.
H(3)	H	0.4997	-0.4009	0.4138	0.0570	Uiso	1.00	calc	.	.	.
H(4)	H	0.3787	-0.2985	0.3722	0.0570	Uiso	1.00	calc	.	.	.
H(5)	H	0.7129	0.2808	0.3490	0.0570	Uiso	1.00	calc	.	.	.
H(6)	H	0.7639	0.1404	0.3330	0.0570	Uiso	1.00	calc	.	.	.
H(7)	H	0.7245	-0.0886	0.3482	0.0570	Uiso	1.00	calc	.	.	.
H(8)	H	0.6526	-0.1206	0.3250	0.0570	Uiso	1.00	calc	.	.	.
H(9)	H	0.6090	0.2822	0.3999	0.0570	Uiso	1.00	calc	.	.	.
H(10)	H	0.6155	0.1523	0.4571	0.0570	Uiso	1.00	calc	.	.	.
H(11)	H	0.7613	0.0204	0.4640	0.0570	Uiso	1.00	calc	.	.	.
H(12)	H	0.8244	0.0499	0.5751	0.0570	Uiso	1.00	calc	.	.	.
H(13)	H	0.7866	-0.0678	0.6821	0.0570	Uiso	1.00	calc	.	.	.
H(14)	H	0.6982	-0.2603	0.6709	0.0570	Uiso	1.00	calc	.	.	.
H(15)	H	0.6082	-0.3820	0.6011	0.0570	Uiso	1.00	calc	.	.	.
H(16)	H	0.4294	-0.6277	0.4809	0.0570	Uiso	1.00	calc	.	.	.
H(17)	H	0.4501	-0.6902	0.3663	0.0570	Uiso	1.00	calc	.	.	.
H(18)	H	0.4112	-0.5256	0.3329	0.0570	Uiso	1.00	calc	.	.	.
H(19)	H	0.3309	-0.7444	0.3238	0.0570	Uiso	1.00	calc	.	.	.
H(20)	H	0.3436	-0.7700	0.4039	0.0570	Uiso	1.00	calc	.	.	.
H(21)	H	0.3000	-0.5741	0.5058	0.0570	Uiso	1.00	calc	.	.	.
H(22)	H	0.2756	-0.4137	0.4821	0.0570	Uiso	1.00	calc	.	.	.

H(23)	H	0.2468	-0.6006	0.3846	0.0570	Uiso	1.00	calc	.	.	.
H(24)	H	0.2974	-0.4779	0.3527	0.0570	Uiso	1.00	calc	.	.	.
H(25)	H	0.3900	-0.3939	0.5257	0.0570	Uiso	1.00	calc	.	.	.
H(26)	H	0.3942	-0.1008	0.3173	0.0570	Uiso	1.00	calc	.	.	.
H(27)	H	0.4063	0.0245	0.1986	0.0570	Uiso	1.00	calc	.	.	.
H(28)	H	0.4743	0.1536	0.1123	0.0570	Uiso	1.00	calc	.	.	.
H(29)	H	0.5775	0.2547	0.1483	0.0570	Uiso	1.00	calc	.	.	.
H(30)	H	0.6070	0.2620	0.2688	0.0570	Uiso	1.00	calc	.	.	.
H(31)	H	0.8400	0.3067	0.0828	0.0570	Uiso	1.00	calc	.	.	.
H(32)	H	0.8298	0.1775	0.1173	0.0570	Uiso	1.00	calc	.	.	.
H(33)	H	0.9095	0.2651	0.1165	0.0570	Uiso	1.00	calc	.	.	.
H(34)	H	0.7380	0.4343	0.1412	0.0570	Uiso	1.00	calc	.	.	.
H(35)	H	0.7350	0.4509	0.2156	0.0570	Uiso	1.00	calc	.	.	.
H(36)	H	0.7316	0.2733	0.1668	0.0570	Uiso	1.00	calc	.	.	.
H(37)	H	0.1105	0.1731	0.1142	0.0570	Uiso	1.00	calc	.	.	.
H(38)	H	0.0301	0.2531	0.1053	0.0570	Uiso	1.00	calc	.	.	.
H(39)	H	0.0493	0.1414	0.1741	0.0570	Uiso	1.00	calc	.	.	.
H(40)	H	0.0029	0.2991	0.2433	0.0570	Uiso	1.00	calc	.	.	.
H(41)	H	-0.0168	0.4498	0.1920	0.0570	Uiso	1.00	calc	.	.	.
H(42)	H	0.0164	0.5140	0.2538	0.0570	Uiso	1.00	calc	.	.	.

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

S(1)	0.0549(7)	0.0472(6)	0.0424(6)	0.0010(6)	0.0023(7)	0.0103(6)
S(2)	0.0319(5)	0.0453(6)	0.0304(5)	-0.0018(5)	0.0034(5)	0.0096(5)
O(1)	0.033(2)	0.057(2)	0.024(1)	-0.010(1)	0.001(1)	0.000(2)
O(2)	0.043(2)	0.047(2)	0.024(1)	-0.008(2)	-0.001(1)	-0.001(1)
O(3)	0.048(2)	0.057(2)	0.036(2)	-0.017(2)	-0.002(2)	0.016(2)
O(4)	0.048(2)	0.051(2)	0.032(1)	-0.011(2)	0.007(1)	-0.005(2)
O(5)	0.050(2)	0.063(2)	0.045(2)	0.009(2)	0.001(2)	0.013(2)
O(6)	0.033(2)	0.095(3)	0.031(2)	0.005(2)	-0.001(1)	0.013(2)
N(1)	0.029(2)	0.041(2)	0.035(2)	-0.004(2)	0.001(1)	0.008(2)
N(2)	0.031(2)	0.034(2)	0.032(2)	0.001(1)	0.003(2)	0.001(1)
C(1)	0.049(3)	0.065(3)	0.060(4)	-0.027(3)	-0.003(3)	0.023(3)
C(2)	0.040(2)	0.048(2)	0.032(2)	-0.011(2)	-0.007(2)	0.005(2)
C(3)	0.036(2)	0.049(2)	0.027(2)	-0.004(2)	0.008(2)	0.003(2)
C(4)	0.044(2)	0.037(2)	0.026(2)	-0.010(2)	-0.007(2)	0.000(2)
C(5)	0.026(2)	0.038(2)	0.029(2)	0.004(2)	0.004(2)	0.002(2)
C(6)	0.025(2)	0.038(2)	0.033(2)	0.007(2)	-0.001(2)	0.002(2)
C(7)	0.029(2)	0.043(2)	0.038(2)	0.000(2)	0.000(2)	0.004(2)
C(8)	0.028(2)	0.054(3)	0.044(2)	-0.001(2)	-0.005(2)	-0.005(2)
C(9)	0.036(2)	0.058(3)	0.037(2)	0.005(2)	-0.011(2)	-0.004(2)
C(10)	0.039(2)	0.047(3)	0.030(2)	0.006(2)	-0.008(2)	0.007(2)
C(11)	0.028(2)	0.038(2)	0.030(2)	0.007(1)	-0.003(2)	0.001(2)
C(12)	0.032(2)	0.032(2)	0.028(2)	0.005(2)	0.000(2)	0.008(2)
C(13)	0.026(2)	0.031(2)	0.029(2)	0.005(1)	0.001(1)	0.004(2)
C(14)	0.027(2)	0.037(2)	0.025(2)	0.004(1)	0.003(1)	-0.001(2)
C(15)	0.032(2)	0.034(2)	0.034(2)	0.001(2)	0.000(2)	0.006(2)
C(16)	0.030(2)	0.033(2)	0.039(2)	-0.004(1)	-0.001(2)	0.010(2)
C(17)	0.033(2)	0.035(2)	0.045(2)	0.002(2)	0.000(2)	-0.002(2)
C(18)	0.038(2)	0.035(2)	0.054(3)	-0.005(2)	-0.002(2)	-0.003(2)
C(19)	0.029(2)	0.042(2)	0.055(3)	-0.005(2)	0.000(2)	0.001(2)
C(20)	0.030(2)	0.048(3)	0.052(2)	-0.007(2)	0.013(2)	0.001(2)
C(21)	0.030(2)	0.042(2)	0.030(2)	-0.005(1)	0.004(2)	0.003(2)
C(22)	0.028(2)	0.034(2)	0.035(2)	0.005(2)	0.002(2)	-0.001(2)

C(23)	0.030(2)	0.027(2)	0.032(2)	0.005(1)	0.001(2)	-0.004(2)
C(24)	0.028(2)	0.031(2)	0.033(2)	0.002(2)	-0.005(2)	-0.006(2)
C(25)	0.038(2)	0.026(2)	0.029(2)	0.007(2)	-0.004(2)	-0.003(2)
C(26)	0.041(2)	0.041(2)	0.031(2)	0.009(2)	-0.011(2)	-0.008(2)
C(27)	0.061(3)	0.041(3)	0.026(2)	0.014(2)	-0.005(2)	0.003(2)
C(28)	0.061(3)	0.038(2)	0.030(2)	0.005(2)	0.002(2)	0.011(2)
C(29)	0.044(2)	0.032(2)	0.032(2)	-0.002(2)	0.000(2)	0.005(2)
C(30)	0.039(2)	0.027(2)	0.027(2)	0.005(2)	-0.004(2)	-0.001(2)
C(31)	0.038(2)	0.026(2)	0.025(2)	0.001(2)	-0.004(1)	0.001(2)
C(32)	0.035(2)	0.028(2)	0.025(1)	0.003(1)	-0.004(1)	-0.001(2)
C(33)	0.063(4)	0.065(3)	0.043(3)	-0.010(3)	0.005(3)	-0.005(2)
C(34)	0.056(2)	0.096(4)	0.057(4)	0.027(4)	-0.010(3)	0.004(4)
C(35)	0.051(3)	0.046(3)	0.057(3)	0.008(2)	-0.002(3)	-0.009(2)
C(36)	0.033(2)	0.054(3)	0.041(3)	0.008(2)	0.004(2)	0.005(2)

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_computing_structure_solution  SIR92
_computing_structure_refinement 'teXsan Ver. 1.10'
_computing_publication_material 'teXsan Ver. 1.11'
_computing_molecular_graphics  ?
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_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
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S(1)      O(5)      1.476(4)    . . yes
S(1)      C(33)     1.788(6)    . . yes
S(1)      C(34)     1.792(6)    . . yes
S(2)      O(6)      1.522(4)    . . yes
S(2)      C(35)     1.780(5)    . . yes
S(2)      C(36)     1.795(5)    . . yes
O(1)      C(14)     1.371(5)    . . yes
O(2)      C(32)     1.352(5)    . . yes
O(3)      C(15)     1.218(5)    . . yes
O(4)      C(22)     1.241(6)    . . yes
N(1)      C(15)     1.354(6)    . . yes
N(1)      C(16)     1.465(6)    . . yes
N(2)      C(21)     1.487(5)    . . yes
N(2)      C(22)     1.355(6)    . . yes
C(1)      C(2)      1.319(6)    . . yes
C(2)      C(3)      1.519(7)    . . yes
C(2)      C(4)      1.521(7)    . . yes
C(3)      C(5)      1.514(6)    . . yes
C(4)      C(31)     1.524(6)    . . yes
C(5)      C(6)      1.421(6)    . . yes
C(5)      C(14)     1.396(6)    . . yes
C(6)      C(7)      1.427(6)    . . yes
C(6)      C(11)     1.426(6)    . . yes
C(7)      C(8)      1.376(7)    . . yes
C(8)      C(9)      1.407(7)    . . yes
C(9)      C(10)     1.355(7)    . . yes
C(10)     C(11)     1.431(6)    . . yes
C(11)     C(12)     1.410(6)    . . yes
C(12)     C(13)     1.360(6)    . . yes
C(13)     C(14)     1.441(6)    . . yes
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C(13)	C(15)	1.517(6)	. . yes
C(16)	C(17)	1.521(7)	. . yes
C(16)	C(21)	1.538(6)	. . yes
C(17)	C(18)	1.530(6)	. . yes
C(18)	C(19)	1.527(6)	. . yes
C(19)	C(20)	1.530(7)	. . yes
C(20)	C(21)	1.533(6)	. . yes
C(22)	C(23)	1.479(6)	. . yes
C(23)	C(24)	1.380(6)	. . yes
C(23)	C(32)	1.442(6)	. . yes
C(24)	C(25)	1.405(6)	. . yes
C(25)	C(26)	1.422(6)	. . yes
C(25)	C(30)	1.429(6)	. . yes
C(26)	C(27)	1.356(7)	. . yes
C(27)	C(28)	1.411(7)	. . yes
C(28)	C(29)	1.379(7)	. . yes
C(29)	C(30)	1.431(6)	. . yes
C(30)	C(31)	1.423(6)	. . yes
C(31)	C(32)	1.387(6)	. . yes

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loop_

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_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O(5)	S(1)	C(33)	106.4(2)	. . . yes
O(5)	S(1)	C(34)	106.0(3)	. . . yes
C(33)	S(1)	C(34)	97.6(3)	. . . yes
O(6)	S(2)	C(35)	106.0(2)	. . . yes
O(6)	S(2)	C(36)	105.8(2)	. . . yes
C(35)	S(2)	C(36)	97.1(2)	. . . yes
C(15)	N(1)	C(16)	123.5(3)	. . . yes
C(21)	N(2)	C(22)	119.0(4)	. . . yes
C(1)	C(2)	C(3)	121.8(5)	. . . yes
C(1)	C(2)	C(4)	120.6(4)	. . . yes
C(3)	C(2)	C(4)	117.6(4)	. . . yes
C(2)	C(3)	C(5)	116.0(4)	. . . yes
C(2)	C(4)	C(31)	115.6(4)	. . . yes
C(3)	C(5)	C(6)	120.9(4)	. . . yes
C(3)	C(5)	C(14)	120.0(4)	. . . yes
C(6)	C(5)	C(14)	119.1(4)	. . . yes
C(5)	C(6)	C(7)	122.9(4)	. . . yes
C(5)	C(6)	C(11)	119.9(4)	. . . yes
C(7)	C(6)	C(11)	117.2(4)	. . . yes
C(6)	C(7)	C(8)	121.8(4)	. . . yes
C(7)	C(8)	C(9)	119.9(4)	. . . yes
C(8)	C(9)	C(10)	120.7(4)	. . . yes
C(9)	C(10)	C(11)	120.7(4)	. . . yes
C(6)	C(11)	C(10)	119.6(4)	. . . yes
C(6)	C(11)	C(12)	118.5(4)	. . . yes
C(10)	C(11)	C(12)	121.9(4)	. . . yes
C(11)	C(12)	C(13)	123.0(4)	. . . yes
C(12)	C(13)	C(14)	118.2(4)	. . . yes
C(12)	C(13)	C(15)	115.5(4)	. . . yes
C(14)	C(13)	C(15)	126.2(4)	. . . yes
O(1)	C(14)	C(5)	122.4(4)	. . . yes
O(1)	C(14)	C(13)	116.4(3)	. . . yes

C(5)	C(14)	C(13)	121.2(4)	. . .	yes
O(3)	C(15)	N(1)	122.1(4)	. . .	yes
O(3)	C(15)	C(13)	120.1(4)	. . .	yes
N(1)	C(15)	C(13)	117.7(4)	. . .	yes
N(1)	C(16)	C(17)	109.2(3)	. . .	yes
N(1)	C(16)	C(21)	111.4(3)	. . .	yes
C(17)	C(16)	C(21)	112.6(3)	. . .	yes
C(16)	C(17)	C(18)	111.2(4)	. . .	yes
C(17)	C(18)	C(19)	110.5(3)	. . .	yes
C(18)	C(19)	C(20)	109.9(4)	. . .	yes
C(19)	C(20)	C(21)	113.2(4)	. . .	yes
N(2)	C(21)	C(16)	108.3(3)	. . .	yes
N(2)	C(21)	C(20)	112.5(4)	. . .	yes
C(16)	C(21)	C(20)	110.8(4)	. . .	yes
O(4)	C(22)	N(2)	121.1(4)	. . .	yes
O(4)	C(22)	C(23)	120.8(4)	. . .	yes
N(2)	C(22)	C(23)	117.9(4)	. . .	yes
C(22)	C(23)	C(24)	123.2(4)	. . .	yes
C(22)	C(23)	C(32)	118.0(4)	. . .	yes
C(24)	C(23)	C(32)	118.6(4)	. . .	yes
C(23)	C(24)	C(25)	121.6(4)	. . .	yes
C(24)	C(25)	C(26)	121.2(4)	. . .	yes
C(24)	C(25)	C(30)	119.3(4)	. . .	yes
C(26)	C(25)	C(30)	119.5(4)	. . .	yes
C(25)	C(26)	C(27)	120.6(4)	. . .	yes
C(26)	C(27)	C(28)	121.0(4)	. . .	yes
C(27)	C(28)	C(29)	120.0(4)	. . .	yes
C(28)	C(29)	C(30)	120.9(4)	. . .	yes
C(25)	C(30)	C(29)	117.9(4)	. . .	yes
C(25)	C(30)	C(31)	119.6(4)	. . .	yes
C(29)	C(30)	C(31)	122.5(4)	. . .	yes
C(4)	C(31)	C(30)	121.3(4)	. . .	yes
C(4)	C(31)	C(32)	119.3(4)	. . .	yes
C(30)	C(31)	C(32)	119.4(4)	. . .	yes
O(2)	C(32)	C(23)	120.5(4)	. . .	yes
O(2)	C(32)	C(31)	118.6(4)	. . .	yes
C(23)	C(32)	C(31)	120.8(4)	. . .	yes

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loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

O(1)	C(14)	C(5)	C(3)	4.4(6)		yes
O(1)	C(14)	C(5)	C(6)	-177.1(4)		yes
O(1)	C(14)	C(13)	C(12)	178.3(4)		yes
O(1)	C(14)	C(13)	C(15)	-7.1(6)		yes
O(2)	C(32)	C(23)	C(22)	-11.5(6)		yes
O(2)	C(32)	C(23)	C(24)	173.9(4)		yes
O(2)	C(32)	C(31)	C(4)	3.9(6)		yes
O(2)	C(32)	C(31)	C(30)	-175.4(4)		yes
O(3)	C(15)	N(1)	C(16)	9.1(7)		yes
O(3)	C(15)	C(13)	C(12)	-2.4(6)		yes
O(3)	C(15)	C(13)	C(14)	-177.2(4)		yes
O(4)	C(22)	N(2)	C(21)	-22.4(6)		yes

O(4)	C(22)	C(23)	C(24)	-164.1(4)	 yes
O(4)	C(22)	C(23)	C(32)	21.5(6)	 yes
N(1)	C(15)	C(13)	C(12)	174.5(4)	 yes
N(1)	C(15)	C(13)	C(14)	-0.3(6)	 yes
N(1)	C(16)	C(17)	C(18)	-179.0(3)	 yes
N(1)	C(16)	C(21)	N(2)	50.3(4)	 yes
N(1)	C(16)	C(21)	C(20)	174.1(4)	 yes
N(2)	C(21)	C(16)	C(17)	-72.8(4)	 yes
N(2)	C(21)	C(20)	C(19)	69.5(5)	 yes
N(2)	C(22)	C(23)	C(24)	21.0(6)	 yes
N(2)	C(22)	C(23)	C(32)	-153.3(4)	 yes
C(1)	C(2)	C(3)	C(5)	134.8(5)	 yes
C(1)	C(2)	C(4)	C(31)	131.9(5)	 yes
C(2)	C(3)	C(5)	C(6)	-58.2(6)	 yes
C(2)	C(3)	C(5)	C(14)	120.3(4)	 yes
C(2)	C(4)	C(31)	C(30)	-61.5(5)	 yes
C(2)	C(4)	C(31)	C(32)	119.2(4)	 yes
C(3)	C(2)	C(4)	C(31)	-45.6(6)	 yes
C(3)	C(5)	C(6)	C(7)	-5.7(6)	 yes
C(3)	C(5)	C(6)	C(11)	175.6(4)	 yes
C(3)	C(5)	C(14)	C(13)	-174.3(4)	 yes
C(4)	C(2)	C(3)	C(5)	-47.7(6)	 yes
C(4)	C(31)	C(30)	C(25)	-179.4(4)	 yes
C(4)	C(31)	C(30)	C(29)	-1.8(6)	 yes
C(4)	C(31)	C(32)	C(23)	-173.3(4)	 yes
C(5)	C(6)	C(7)	C(8)	179.3(4)	 yes
C(5)	C(6)	C(11)	C(10)	-179.0(4)	 yes
C(5)	C(6)	C(11)	C(12)	0.2(6)	 yes
C(5)	C(14)	C(13)	C(12)	-2.9(6)	 yes
C(5)	C(14)	C(13)	C(15)	171.7(4)	 yes
C(6)	C(5)	C(14)	C(13)	4.2(6)	 yes
C(6)	C(7)	C(8)	C(9)	0.7(7)	 yes
C(6)	C(11)	C(10)	C(9)	-1.2(7)	 yes
C(6)	C(11)	C(12)	C(13)	1.1(6)	 yes
C(7)	C(6)	C(5)	C(14)	175.8(4)	 yes
C(7)	C(6)	C(11)	C(10)	2.2(6)	 yes
C(7)	C(6)	C(11)	C(12)	-178.5(4)	 yes
C(7)	C(8)	C(9)	C(10)	0.5(7)	 yes
C(8)	C(7)	C(6)	C(11)	-2.0(6)	 yes
C(8)	C(9)	C(10)	C(11)	-0.2(7)	 yes
C(9)	C(10)	C(11)	C(12)	179.6(4)	 yes
C(10)	C(11)	C(12)	C(13)	-179.7(4)	 yes
C(11)	C(6)	C(5)	C(14)	-2.8(6)	 yes
C(11)	C(12)	C(13)	C(14)	0.2(6)	 yes
C(11)	C(12)	C(13)	C(15)	-175.0(4)	 yes
C(13)	C(15)	N(1)	C(16)	-167.7(4)	 yes
C(15)	N(1)	C(16)	C(17)	-155.4(4)	 yes
C(15)	N(1)	C(16)	C(21)	79.6(5)	 yes
C(16)	C(17)	C(18)	C(19)	58.0(5)	 yes
C(16)	C(21)	N(2)	C(22)	-97.1(4)	 yes
C(16)	C(21)	C(20)	C(19)	-51.9(5)	 yes
C(17)	C(16)	C(21)	C(20)	51.0(5)	 yes
C(17)	C(18)	C(19)	C(20)	-57.9(5)	 yes
C(18)	C(17)	C(16)	C(21)	-54.7(4)	 yes
C(18)	C(19)	C(20)	C(21)	55.8(5)	 yes
C(20)	C(21)	N(2)	C(22)	140.0(4)	 yes
C(21)	N(2)	C(22)	C(23)	152.4(4)	 yes
C(22)	C(23)	C(24)	C(25)	-171.2(4)	 yes
C(22)	C(23)	C(32)	C(31)	165.7(4)	 yes
C(23)	C(24)	C(25)	C(26)	-176.5(4)	 yes
C(23)	C(24)	C(25)	C(30)	4.0(6)	 yes

C(23)	C(32)	C(31)	C(30)	7.4(6)	 yes
C(24)	C(23)	C(32)	C(31)	-8.9(6)	 yes
C(24)	C(25)	C(26)	C(27)	-177.4(4)	 yes
C(24)	C(25)	C(30)	C(29)	176.8(4)	 yes
C(24)	C(25)	C(30)	C(31)	-5.6(6)	 yes
C(25)	C(24)	C(23)	C(32)	3.1(6)	 yes
C(25)	C(26)	C(27)	C(28)	-0.6(7)	 yes
C(25)	C(30)	C(29)	C(28)	2.0(6)	 yes
C(25)	C(30)	C(31)	C(32)	-0.1(6)	 yes
C(26)	C(25)	C(30)	C(29)	-2.7(6)	 yes
C(26)	C(25)	C(30)	C(31)	175.0(4)	 yes
C(26)	C(27)	C(28)	C(29)	-0.1(7)	 yes
C(27)	C(26)	C(25)	C(30)	2.0(6)	 yes
C(27)	C(28)	C(29)	C(30)	-0.6(7)	 yes
C(28)	C(29)	C(30)	C(31)	-175.6(4)	 yes
C(29)	C(30)	C(31)	C(32)	177.4(4)	 yes
C(29)	C(30)	C(31)	C(32)	177.4(4)	 yes

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loop_

_geom_contact_atom_site_label_1

_geom_contact_atom_site_label_2

_geom_contact_distance

_geom_contact_site_symmetry_1

_geom_contact_site_symmetry_2

_geom_contact_publ_flag

S(2)	O(3)	3.343(4)	. 3_564 ?
S(2)	O(1)	3.531(4)	. 4_455 ?
O(1)	O(6)	2.605(4)	. 4_555 ?
O(1)	C(36)	3.180(6)	. 4_555 ?
O(2)	C(27)	3.414(5)	. 2_655 ?
O(3)	C(36)	3.201(6)	. 3_545 ?
O(3)	C(35)	3.297(6)	. 3_545 ?
O(3)	C(33)	3.468(7)	. 3_645 ?
O(4)	C(28)	3.200(6)	. 2_655 ?
O(4)	C(27)	3.262(6)	. 2_655 ?
O(4)	C(8)	3.450(6)	. 4_455 ?
O(5)	C(24)	3.141(5)	. 4_555 ?
O(5)	N(2)	3.293(5)	. 4_555 ?
O(5)	C(1)	3.353(6)	. . ?
O(5)	C(36)	3.573(6)	. 1_655 ?
O(6)	C(3)	3.322(6)	. 4_455 ?
O(6)	C(14)	3.549(5)	. 4_455 ?
O(6)	C(34)	3.589(7)	. 4_465 ?
C(12)	C(27)	3.384(6)	. 2_655 ?
C(27)	C(35)	3.592(7)	. 4_555 ?
C(28)	C(36)	3.472(7)	. 4_565 ?

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#===END

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data_6d

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CHEMICAL DATA

_chemical_formula_sum	'C36 H42 N2 O6 S2 '
_chemical_formula_moiety	'C32 H30 N2 O4, 2(C2 H6 O S)'
_chemical_formula_weight	662.86
_chemical_melting_point	'282-284 \%C'

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CRYSTAL DATA

_symmetry_cell_setting	monoclinic
_symmetry_space_group_name_H-M	'P 1 21 1'
_symmetry_Int_Tables_number	4

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loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,1/2+y,-z
_cell_length_a          10.1149(7)
_cell_length_b          9.3228(4)
_cell_length_c          17.515(1)
_cell_angle_alpha       90
_cell_angle_beta        90.413(2)
_cell_angle_gamma       90
_cell_volume            1651.6(2)
_cell_formula_units_Z   2
_cell_measurement_reflns_used 15103
_cell_measurement_theta_min 2.2
_cell_measurement_theta_max 27.5
_cell_measurement_temperature 193.2
#-----
_exptl_crystal_description 'platelet'
_exptl_crystal_colour      'yellow'
_exptl_crystal_size_max    0.540
_exptl_crystal_size_mid    0.360
_exptl_crystal_size_min    0.050
_exptl_crystal_size_rad    ?
_exptl_crystal_density_diffn 1.333
_exptl_crystal_density_meas ?
_exptl_crystal_density_method 'not measured'
_exptl_absorpt_coefficient_mu 0.210
_exptl_absorpt_correction_type multi-scan
_exptl_absorpt_process_details '(Higashi, 1995)'
_exptl_absorpt_correction_T_min 0.861
_exptl_absorpt_correction_T_max 0.990
#-----
# EXPERIMENTAL DATA
_diffn_radiation_type      'Mo K\alpha'
_diffn_radiation_wavelength 0.7107
_diffn_measurement_device_type 'Rigaku RAXIS-RAPID Imaging Plate'
_diffn_measurement_method  \w
_diffn_detector_area_resol_mean ?
_diffn_reflns_number       15978
_diffn_reflns_av_R_equivalents 0.045
_diffn_reflns_theta_max    27.48
_diffn_measured_fraction_theta_max 0.5294
_diffn_reflns_theta_full    27.48
_diffn_measured_fraction_theta_full 0.5294
_diffn_reflns_limit_h_min    0
_diffn_reflns_limit_h_max    13
_diffn_reflns_limit_k_min    0
_diffn_reflns_limit_k_max    12
_diffn_reflns_limit_l_min    -22
_diffn_reflns_limit_l_max    22
#-----
# REFINEMENT DATA
_refine_special_details
;
Refinement using reflections with  $F^2 > 0.0 \sigma(F^2)$ . 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).
;
_reflns_number_total       1331
_reflns_number_gt          3183

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_reflns_threshold_expression      F^2^>2.0\s(F^2^)
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_R_factor_gt           0.0456
_refine_ls_wR_factor_ref         0.1165
_refine_ls_hydrogen_treatment    noref
_refine_ls_number_reflns         4004
_refine_ls_number_parameters     417
_refine_ls_goodness_of_fit_ref   1.127
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
  'w = 1/[\s^2^(Fo^2^) + (0.06200(Max(Fo^2^,0) + 2Fc^2^)/3)^2^]'
_refine_ls_shift/su_max          0.0038
_refine_diff_density_max         0.99
_refine_diff_density_min        -0.38
_refine_ls_extinction_method
  'Zachariasen(1967) type 2 Gaussian isotropic'
_refine_ls_extinction_coef       0.013(3)
_refine_ls_abs_structure_details ?
_refine_ls_abs_structure_Flack   0.0(2)
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
  'C' 'C' 0.003 0.002
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'H' 'H' 0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
  'N' 'N' 0.006 0.003
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'O' 'O' 0.011 0.006
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'S' 'S' 0.125 0.123
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
#-----
# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
S(1) S -0.53575(9) -0.4130(8) -0.47661(5) 0.0366(2) Uani 1.00 d . . .

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S(2)	S	-0.2787(1)	-0.3586(8)	-0.17520(6)	0.0486(3)	Uani	1.00	d	.	.	.
O(1)	O	-0.2864(2)	-0.5640(8)	-0.8910(1)	0.0319(6)	Uani	1.00	d	.	.	.
O(2)	O	-0.2567(2)	-0.3126(8)	-0.6994(1)	0.0305(6)	Uani	1.00	d	.	.	.
O(3)	O	-0.2044(2)	-0.7776(8)	-0.8159(1)	0.0313(6)	Uani	1.00	d	.	.	.
O(4)	O	-0.1453(2)	-0.5070(8)	-0.6241(1)	0.0349(6)	Uani	1.00	d	.	.	.
O(5)	O	-0.5808(3)	-0.2674(8)	-0.4500(1)	0.0451(7)	Uani	1.00	d	.	.	.
O(6)	O	-0.1809(5)	-0.2768(9)	-0.2179(3)	0.117(2)	Uani	1.00	d	.	.	.
N(1)	N	-0.2554(2)	-0.7994(9)	-0.6911(1)	0.0257(6)	Uani	1.00	d	.	.	.
N(2)	N	-0.0057(3)	-0.6598(8)	-0.6820(1)	0.0278(7)	Uani	1.00	d	.	.	.
C(1)	C	-0.4285(4)	-0.0564(9)	-0.9334(2)	0.0380(10)	Uani	1.00	d	.	.	.
C(2)	C	-0.3857(3)	-0.1644(9)	-0.8918(2)	0.0294(8)	Uani	1.00	d	.	.	.
C(3)	C	-0.4333(3)	-0.3150(9)	-0.9074(2)	0.0284(8)	Uani	1.00	d	.	.	.
C(4)	C	-0.2879(3)	-0.1402(8)	-0.8275(2)	0.0286(8)	Uani	1.00	d	.	.	.
C(5)	C	-0.4507(3)	-0.4152(9)	-0.8395(2)	0.0235(7)	Uani	1.00	d	.	.	.
C(6)	C	-0.5461(3)	-0.3880(8)	-0.7820(2)	0.0248(7)	Uani	1.00	d	.	.	.
C(7)	C	-0.6287(3)	-0.2654(9)	-0.7822(2)	0.0320(8)	Uani	1.00	d	.	.	.
C(8)	C	-0.7207(3)	-0.2454(9)	-0.7268(2)	0.0371(9)	Uani	1.00	d	.	.	.
C(9)	C	-0.7370(3)	-0.3459(9)	-0.6677(2)	0.0357(9)	Uani	1.00	d	.	.	.
C(10)	C	-0.6589(3)	-0.4648(9)	-0.6653(2)	0.0317(8)	Uani	1.00	d	.	.	.
C(11)	C	-0.5603(3)	-0.4884(9)	-0.7209(2)	0.0247(7)	Uani	1.00	d	.	.	.
C(12)	C	-0.4734(3)	-0.6060(8)	-0.7155(2)	0.0247(7)	Uani	1.00	d	.	.	.
C(13)	C	-0.3776(3)	-0.6294(8)	-0.7693(2)	0.0227(7)	Uani	1.00	d	.	.	.
C(14)	C	-0.3724(3)	-0.5359(9)	-0.8340(2)	0.0239(7)	Uani	1.00	d	.	.	.
C(15)	C	-0.2742(3)	-0.7426(8)	-0.7606(2)	0.0237(7)	Uani	1.00	d	.	.	.
C(16)	C	-0.1356(3)	-0.8796(9)	-0.6703(2)	0.0269(8)	Uani	1.00	d	.	.	.
C(17)	C	-0.1663(3)	-1.0066(9)	-0.6189(2)	0.0318(8)	Uani	1.00	d	.	.	.
C(18)	C	-0.0412(4)	-1.0886(9)	-0.5988(2)	0.0395(10)	Uani	1.00	d	.	.	.
C(19)	C	0.0591(4)	-0.9925(9)	-0.5600(2)	0.042(1)	Uani	1.00	d	.	.	.
C(20)	C	0.0889(3)	-0.8610(9)	-0.6093(2)	0.0378(9)	Uani	1.00	d	.	.	.
C(21)	C	-0.0354(3)	-0.7794(9)	-0.6315(2)	0.0276(8)	Uani	1.00	d	.	.	.
C(22)	C	-0.0725(3)	-0.5367(9)	-0.6793(2)	0.0249(7)	Uani	1.00	d	.	.	.
C(23)	C	-0.0648(3)	-0.4375(9)	-0.7459(2)	0.0239(7)	Uani	1.00	d	.	.	.
C(24)	C	0.0297(3)	-0.4494(8)	-0.8009(2)	0.0254(7)	Uani	1.00	d	.	.	.
C(25)	C	0.0274(3)	-0.3627(8)	-0.8669(2)	0.0258(7)	Uani	1.00	d	.	.	.
C(26)	C	0.1267(3)	-0.3753(9)	-0.9227(2)	0.0308(8)	Uani	1.00	d	.	.	.
C(27)	C	0.1205(3)	-0.2953(9)	-0.9884(2)	0.0339(8)	Uani	1.00	d	.	.	.
C(28)	C	0.0179(4)	-0.1969(9)	-0.9990(2)	0.0373(9)	Uani	1.00	d	.	.	.
C(29)	C	-0.0778(3)	-0.1795(9)	-0.9453(2)	0.0311(8)	Uani	1.00	d	.	.	.
C(30)	C	-0.0778(3)	-0.2620(8)	-0.8766(2)	0.0257(7)	Uani	1.00	d	.	.	.
C(31)	C	-0.1745(3)	-0.2462(8)	-0.8201(2)	0.0257(7)	Uani	1.00	d	.	.	.
C(32)	C	-0.1652(3)	-0.3298(9)	-0.7549(2)	0.0253(7)	Uani	1.00	d	.	.	.
C(33)	C	-0.3978(4)	-0.3820(10)	-0.5361(2)	0.051(1)	Uani	1.00	d	.	.	.
C(34)	C	-0.4490(4)	-0.4909(10)	-0.3985(2)	0.055(1)	Uani	1.00	d	.	.	.
C(35)	C	-0.3449(4)	-0.2387(9)	-0.1080(2)	0.047(1)	Uani	1.00	d	.	.	.
C(36)	C	-0.1947(5)	-0.4713(9)	-0.1113(3)	0.073(2)	Uani	1.00	d	.	.	.
H(1)	H	-0.2297	-0.6456	-0.8880	0.0371	Uiso	1.00	calc	.	.	.
H(2)	H	-0.2521	-0.3696	-0.6542	0.0344	Uiso	1.00	calc	.	.	.
H(3)	H	-0.3976	0.0379	-0.9235	0.0456	Uiso	1.00	calc	.	.	.
H(4)	H	-0.4902	-0.0724	-0.9741	0.0456	Uiso	1.00	calc	.	.	.
H(5)	H	-0.5169	-0.3089	-0.9324	0.0333	Uiso	1.00	calc	.	.	.
H(6)	H	-0.3716	-0.3599	-0.9404	0.0333	Uiso	1.00	calc	.	.	.
H(7)	H	-0.3357	-0.1421	-0.7810	0.0336	Uiso	1.00	calc	.	.	.
H(8)	H	-0.2506	-0.0481	-0.8347	0.0336	Uiso	1.00	calc	.	.	.
H(9)	H	-0.6205	-0.1978	-0.8226	0.0373	Uiso	1.00	calc	.	.	.
H(10)	H	-0.7744	-0.1618	-0.7282	0.0437	Uiso	1.00	calc	.	.	.
H(11)	H	-0.8015	-0.3302	-0.6290	0.0421	Uiso	1.00	calc	.	.	.
H(12)	H	-0.6717	-0.5348	-0.6261	0.0365	Uiso	1.00	calc	.	.	.
H(13)	H	-0.4808	-0.6706	-0.6735	0.0294	Uiso	1.00	calc	.	.	.
H(14)	H	-0.3221	-0.7878	-0.6533	0.0300	Uiso	1.00	calc	.	.	.
H(15)	H	-0.0966	-0.9155	-0.7160	0.0314	Uiso	1.00	calc	.	.	.
H(16)	H	-0.2061	-0.9736	-0.5734	0.0366	Uiso	1.00	calc	.	.	.

H(17)	H	-0.2257	-1.0701	-0.6448	0.0366	Uiso	1.00	calc	.	.	.
H(18)	H	-0.0639	-1.1659	-0.5643	0.0460	Uiso	1.00	calc	.	.	.
H(19)	H	-0.0045	-1.1289	-0.6433	0.0460	Uiso	1.00	calc	.	.	.
H(20)	H	0.0244	-0.9613	-0.5123	0.0480	Uiso	1.00	calc	.	.	.
H(21)	H	0.1380	-1.0450	-0.5512	0.0480	Uiso	1.00	calc	.	.	.
H(22)	H	0.1467	-0.7995	-0.5820	0.0441	Uiso	1.00	calc	.	.	.
H(23)	H	0.1311	-0.8927	-0.6548	0.0441	Uiso	1.00	calc	.	.	.
H(24)	H	-0.0746	-0.7429	-0.5854	0.0319	Uiso	1.00	calc	.	.	.
H(25)	H	0.0644	-0.6701	-0.7180	0.0324	Uiso	1.00	calc	.	.	.
H(26)	H	0.0985	-0.5197	-0.7949	0.0295	Uiso	1.00	calc	.	.	.
H(27)	H	0.1988	-0.4402	-0.9147	0.0374	Uiso	1.00	calc	.	.	.
H(28)	H	0.1865	-0.3077	-1.0262	0.0410	Uiso	1.00	calc	.	.	.
H(29)	H	0.0152	-0.1424	-1.0448	0.0437	Uiso	1.00	calc	.	.	.
H(30)	H	-0.1461	-0.1111	-0.9535	0.0358	Uiso	1.00	calc	.	.	.
H(31)	H	-0.3294	-0.3373	-0.5075	0.0602	Uiso	1.00	calc	.	.	.
H(32)	H	-0.3654	-0.4730	-0.5545	0.0602	Uiso	1.00	calc	.	.	.
H(33)	H	-0.4227	-0.3250	-0.5779	0.0602	Uiso	1.00	calc	.	.	.
H(34)	H	-0.4181	-0.5853	-0.4131	0.0647	Uiso	1.00	calc	.	.	.
H(35)	H	-0.3768	-0.4343	-0.3844	0.0647	Uiso	1.00	calc	.	.	.
H(36)	H	-0.5075	-0.5029	-0.3564	0.0647	Uiso	1.00	calc	.	.	.
H(37)	H	-0.3815	-0.1581	-0.1332	0.0534	Uiso	1.00	calc	.	.	.
H(38)	H	-0.4115	-0.2855	-0.0790	0.0534	Uiso	1.00	calc	.	.	.
H(39)	H	-0.2763	-0.2074	-0.0739	0.0534	Uiso	1.00	calc	.	.	.
H(40)	H	-0.2568	-0.5284	-0.0839	0.0837	Uiso	1.00	calc	.	.	.
H(41)	H	-0.1443	-0.4161	-0.0763	0.0837	Uiso	1.00	calc	.	.	.
H(42)	H	-0.1371	-0.5338	-0.1387	0.0837	Uiso	1.00	calc	.	.	.

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

S(1)	0.0278(4)	0.0506(6)	0.0314(4)	-0.0009(4)	0.0071(3)	-0.0093(4)
S(2)	0.0599(6)	0.0426(6)	0.0434(5)	-0.0033(5)	0.0066(4)	-0.0030(5)
O(1)	0.039(1)	0.031(1)	0.026(1)	0.007(1)	0.0105(9)	0.000(1)
O(2)	0.034(1)	0.032(1)	0.026(1)	0.004(1)	0.0107(9)	-0.0024(10)
O(3)	0.041(1)	0.029(1)	0.024(1)	0.008(1)	0.0059(9)	-0.0029(10)
O(4)	0.045(1)	0.035(1)	0.024(1)	0.009(1)	0.0088(9)	0.002(1)
O(5)	0.049(2)	0.051(2)	0.036(1)	0.007(1)	0.014(1)	-0.004(1)
O(6)	0.141(4)	0.076(3)	0.135(3)	-0.023(3)	0.112(3)	0.008(3)
N(1)	0.020(1)	0.029(1)	0.028(1)	0.001(1)	0.0027(10)	0.004(1)
N(2)	0.026(1)	0.029(1)	0.028(1)	0.001(1)	0.006(1)	0.006(1)
C(1)	0.037(2)	0.032(2)	0.044(2)	0.004(2)	0.001(2)	0.009(2)
C(2)	0.028(2)	0.030(1)	0.031(2)	0.004(1)	0.006(1)	0.000(1)
C(3)	0.031(2)	0.031(2)	0.023(1)	0.001(1)	0.002(1)	0.004(1)
C(4)	0.032(2)	0.023(2)	0.031(2)	0.002(1)	0.005(1)	0.002(1)
C(5)	0.025(1)	0.023(1)	0.022(1)	-0.001(1)	-0.0028(10)	0.004(1)
C(6)	0.021(1)	0.029(2)	0.024(1)	-0.001(1)	-0.0039(10)	-0.002(1)
C(7)	0.028(2)	0.032(2)	0.036(2)	0.005(1)	-0.004(1)	0.001(2)
C(8)	0.030(2)	0.038(2)	0.044(2)	0.010(2)	-0.003(1)	-0.004(1)
C(9)	0.027(2)	0.046(2)	0.034(2)	0.002(1)	0.008(1)	-0.005(1)
C(10)	0.028(2)	0.040(2)	0.027(1)	-0.001(1)	0.004(1)	-0.001(2)
C(11)	0.023(1)	0.026(1)	0.025(1)	-0.004(1)	0.000(1)	-0.004(1)
C(12)	0.024(2)	0.027(2)	0.023(1)	-0.004(1)	0.001(1)	0.001(1)
C(13)	0.025(1)	0.020(1)	0.023(1)	-0.002(1)	-0.001(1)	-0.001(1)
C(14)	0.024(1)	0.026(2)	0.022(1)	-0.003(1)	0.001(1)	-0.002(1)
C(15)	0.022(1)	0.023(1)	0.026(1)	-0.004(1)	0.000(1)	0.001(1)
C(16)	0.026(1)	0.030(2)	0.025(1)	0.005(1)	0.002(1)	0.004(1)

C(17)	0.031(2)	0.028(2)	0.036(2)	0.000(1)	0.002(1)	0.006(1)
C(18)	0.037(2)	0.035(2)	0.047(2)	0.010(1)	0.003(1)	0.011(2)
C(19)	0.039(2)	0.040(2)	0.046(2)	0.007(2)	-0.006(2)	0.017(2)
C(20)	0.028(2)	0.040(2)	0.045(2)	0.001(1)	-0.003(1)	0.012(2)
C(21)	0.027(2)	0.029(2)	0.026(1)	0.002(1)	0.005(1)	0.007(1)
C(22)	0.026(2)	0.028(1)	0.021(1)	-0.004(1)	-0.001(1)	-0.001(1)
C(23)	0.024(1)	0.024(2)	0.024(1)	-0.005(1)	0.001(1)	-0.001(1)
C(24)	0.025(1)	0.025(2)	0.026(1)	-0.003(1)	0.001(1)	0.004(1)
C(25)	0.030(1)	0.023(1)	0.024(1)	-0.005(1)	0.004(1)	0.000(1)
C(26)	0.030(2)	0.028(2)	0.035(1)	0.002(1)	0.008(1)	0.005(1)
C(27)	0.037(2)	0.037(2)	0.028(1)	-0.003(1)	0.014(1)	0.002(1)
C(28)	0.039(2)	0.044(2)	0.029(1)	-0.003(1)	0.005(1)	0.014(2)
C(29)	0.033(2)	0.029(2)	0.031(2)	-0.003(2)	0.000(1)	0.006(1)
C(30)	0.027(1)	0.023(2)	0.028(1)	-0.008(1)	-0.001(1)	-0.002(1)
C(31)	0.029(2)	0.020(1)	0.029(1)	-0.004(1)	-0.001(1)	-0.002(1)
C(32)	0.029(2)	0.022(2)	0.025(1)	-0.004(1)	0.004(1)	-0.005(1)
C(33)	0.035(2)	0.080(4)	0.037(2)	0.002(2)	0.015(1)	-0.003(2)
C(34)	0.046(2)	0.071(3)	0.048(2)	0.011(2)	0.003(2)	0.010(2)
C(35)	0.048(2)	0.048(2)	0.044(2)	0.007(2)	0.001(2)	0.004(2)
C(36)	0.064(3)	0.044(3)	0.111(4)	0.020(2)	-0.036(3)	-0.008(3)

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_computing_cell_refinement      'PROCESS-AUTO'
_computing_data_reduction       'teXsan Ver. 1.10'
_computing_structure_solution   SIR92
_computing_structure_refinement 'teXsan Ver. 1.10'
_computing_publication_material 'teXsan Ver. 1.10'
_computing_molecular_graphics   ?
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  _geom_bond_atom_site_label_2
  _geom_bond_distance
  _geom_bond_site_symmetry_1
  _geom_bond_site_symmetry_2
  _geom_bond_publ_flag
S(1)      O(5)      1.507(4)    . . yes
S(1)      C(33)     1.771(4)    . . yes
S(1)      C(34)     1.775(5)    . . yes
S(2)      O(6)      1.459(4)    . . yes
S(2)      C(35)     1.760(5)    . . yes
S(2)      C(36)     1.750(6)    . . yes
O(1)      C(14)     1.354(4)    . . yes
O(2)      C(32)     1.357(4)    . . yes
O(3)      C(15)     1.247(4)    . . yes
O(4)      C(22)     1.250(4)    . . yes
N(1)      C(15)     1.339(4)    . . yes
N(1)      C(16)     1.468(4)    . . yes
N(2)      C(21)     1.455(4)    . . yes
N(2)      C(22)     1.333(5)    . . yes
C(1)      C(2)      1.315(5)    . . yes
C(2)      C(3)      1.509(5)    . . yes
C(2)      C(4)      1.510(5)    . . yes
C(3)      C(5)      1.523(5)    . . yes
C(4)      C(31)     1.519(5)    . . yes
C(5)      C(6)      1.422(4)    . . yes
C(5)      C(14)     1.380(5)    . . yes
C(6)      C(7)      1.416(5)    . . yes
C(6)      C(11)     1.430(5)    . . yes
C(7)      C(8)      1.362(5)    . . yes
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C(8)	C(9)	1.407(6)	. . yes
C(9)	C(10)	1.361(6)	. . yes
C(10)	C(11)	1.417(4)	. . yes
C(11)	C(12)	1.408(5)	. . yes
C(12)	C(13)	1.374(4)	. . yes
C(13)	C(14)	1.432(4)	. . yes
C(13)	C(15)	1.493(5)	. . yes
C(16)	C(17)	1.521(5)	. . yes
C(16)	C(21)	1.533(5)	. . yes
C(17)	C(18)	1.517(5)	. . yes
C(18)	C(19)	1.512(6)	. . yes
C(19)	C(20)	1.531(6)	. . yes
C(20)	C(21)	1.518(5)	. . yes
C(22)	C(23)	1.492(4)	. . yes
C(23)	C(24)	1.366(4)	. . yes
C(23)	C(32)	1.436(5)	. . yes
C(24)	C(25)	1.411(4)	. . yes
C(25)	C(26)	1.411(4)	. . yes
C(25)	C(30)	1.428(5)	. . yes
C(26)	C(27)	1.372(5)	. . yes
C(27)	C(28)	1.397(6)	. . yes
C(28)	C(29)	1.365(5)	. . yes
C(29)	C(30)	1.427(5)	. . yes
C(30)	C(31)	1.404(5)	. . yes
C(31)	C(32)	1.385(5)	. . yes

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loop_

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_2

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O(5)	S(1)	C(33)	106.0(2)	. 1_555 1_555 yes
O(5)	S(1)	C(34)	106.2(2)	. 1_555 1_555 yes
C(33)	S(1)	C(34)	97.6(2)	. 1_555 1_555 yes
O(6)	S(2)	C(35)	105.9(3)	. 1_555 1_555 yes
O(6)	S(2)	C(36)	108.3(3)	. 1_555 1_555 yes
C(35)	S(2)	C(36)	98.0(2)	. 1_555 1_555 yes
C(15)	N(1)	C(16)	122.6(3)	. 1_555 1_555 yes
C(21)	N(2)	C(22)	122.1(3)	. 1_555 1_555 yes
C(1)	C(2)	C(3)	120.5(3)	. 1_555 1_555 yes
C(1)	C(2)	C(4)	120.7(4)	. 1_555 1_555 yes
C(3)	C(2)	C(4)	118.7(3)	. 1_555 1_555 yes
C(2)	C(3)	C(5)	117.9(3)	. 1_555 1_555 yes
C(2)	C(4)	C(31)	117.2(3)	. 1_555 1_555 yes
C(3)	C(5)	C(6)	121.8(3)	. 1_555 1_555 yes
C(3)	C(5)	C(14)	119.0(3)	. 1_555 1_555 yes
C(6)	C(5)	C(14)	119.2(3)	. 1_555 1_555 yes
C(5)	C(6)	C(7)	123.1(3)	. 1_555 1_555 yes
C(5)	C(6)	C(11)	119.1(3)	. 1_555 1_555 yes
C(7)	C(6)	C(11)	117.9(3)	. 1_555 1_555 yes
C(6)	C(7)	C(8)	121.0(3)	. 1_555 1_555 yes
C(7)	C(8)	C(9)	121.1(4)	. 1_555 1_555 yes
C(8)	C(9)	C(10)	119.6(3)	. 1_555 1_555 yes
C(9)	C(10)	C(11)	121.1(3)	. 1_555 1_555 yes
C(6)	C(11)	C(10)	119.2(3)	. 1_555 1_555 yes
C(6)	C(11)	C(12)	119.6(3)	. 1_555 1_555 yes
C(10)	C(11)	C(12)	121.1(3)	. 1_555 1_555 yes

C(11)	C(12)	C(13)	121.3(3)	.	1_555	1_555	yes
C(12)	C(13)	C(14)	118.5(3)	.	1_555	1_555	yes
C(12)	C(13)	C(15)	122.6(3)	.	1_555	1_555	yes
C(14)	C(13)	C(15)	118.8(3)	.	1_555	1_555	yes
O(1)	C(14)	C(5)	118.6(3)	.	1_555	1_555	yes
O(1)	C(14)	C(13)	119.6(3)	.	1_555	1_555	yes
C(5)	C(14)	C(13)	121.8(3)	.	1_555	1_555	yes
O(3)	C(15)	N(1)	121.7(3)	.	1_555	1_555	yes
O(3)	C(15)	C(13)	120.4(3)	.	1_555	1_555	yes
N(1)	C(15)	C(13)	117.8(3)	.	1_555	1_555	yes
N(1)	C(16)	C(17)	111.8(3)	.	1_555	1_555	yes
N(1)	C(16)	C(21)	110.0(3)	.	1_555	1_555	yes
C(17)	C(16)	C(21)	110.4(3)	.	1_555	1_555	yes
C(16)	C(17)	C(18)	110.8(3)	.	1_555	1_555	yes
C(17)	C(18)	C(19)	111.2(3)	.	1_555	1_555	yes
C(18)	C(19)	C(20)	110.8(3)	.	1_555	1_555	yes
C(19)	C(20)	C(21)	112.3(3)	.	1_555	1_555	yes
N(2)	C(21)	C(16)	109.7(3)	.	1_555	1_555	yes
N(2)	C(21)	C(20)	111.4(3)	.	1_555	1_555	yes
C(16)	C(21)	C(20)	110.6(3)	.	1_555	1_555	yes
O(4)	C(22)	N(2)	121.3(3)	.	1_555	1_555	yes
O(4)	C(22)	C(23)	120.1(3)	.	1_555	1_555	yes
N(2)	C(22)	C(23)	118.5(3)	.	1_555	1_555	yes
C(22)	C(23)	C(24)	122.8(3)	.	1_555	1_555	yes
C(22)	C(23)	C(32)	118.6(3)	.	1_555	1_555	yes
C(24)	C(23)	C(32)	118.5(3)	.	1_555	1_555	yes
C(23)	C(24)	C(25)	121.6(3)	.	1_555	1_555	yes
C(24)	C(25)	C(26)	120.8(3)	.	1_555	1_555	yes
C(24)	C(25)	C(30)	118.8(3)	.	1_555	1_555	yes
C(26)	C(25)	C(30)	120.4(3)	.	1_555	1_555	yes
C(25)	C(26)	C(27)	120.4(3)	.	1_555	1_555	yes
C(26)	C(27)	C(28)	119.9(3)	.	1_555	1_555	yes
C(27)	C(28)	C(29)	121.0(3)	.	1_555	1_555	yes
C(28)	C(29)	C(30)	121.4(3)	.	1_555	1_555	yes
C(25)	C(30)	C(29)	116.7(3)	.	1_555	1_555	yes
C(25)	C(30)	C(31)	120.5(3)	.	1_555	1_555	yes
C(29)	C(30)	C(31)	122.8(3)	.	1_555	1_555	yes
C(4)	C(31)	C(30)	122.5(3)	.	1_555	1_555	yes
C(4)	C(31)	C(32)	118.9(3)	.	1_555	1_555	yes
C(30)	C(31)	C(32)	118.6(3)	.	1_555	1_555	yes
O(2)	C(32)	C(23)	119.3(3)	.	1_555	1_555	yes
O(2)	C(32)	C(31)	118.8(3)	.	1_555	1_555	yes
C(23)	C(32)	C(31)	121.8(3)	.	1_555	1_555	yes

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loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

O(1)	C(14)	C(5)	C(3)	-2.7(5)	1_555	1_555	1_555	1_555	yes
O(1)	C(14)	C(5)	C(6)	176.9(3)	1_555	1_555	1_555	1_555	yes
O(1)	C(14)	C(13)	C(12)	-174.3(3)	1_555	1_555	1_555	1_555	yes
O(1)	C(14)	C(13)	C(15)	9.2(5)	1_555	1_555	1_555	1_555	yes
O(2)	C(32)	C(23)	C(22)	6.0(5)	1_555	1_555	1_555	1_555	yes
O(2)	C(32)	C(23)	C(24)	-177.4(3)	1_555	1_555	1_555	1_555	yes

O(2)	C(32)	C(31)	C(4)	-0.9(5)	1_555	1_555	1_555	1_555	yes
O(2)	C(32)	C(31)	C(30)	178.5(3)	1_555	1_555	1_555	1_555	yes
O(3)	C(15)	N(1)	C(16)	14.4(5)	1_555	1_555	1_555	1_555	yes
O(3)	C(15)	C(13)	C(12)	167.1(3)	1_555	1_555	1_555	1_555	yes
O(3)	C(15)	C(13)	C(14)	-16.6(5)	1_555	1_555	1_555	1_555	yes
O(4)	C(22)	N(2)	C(21)	14.4(5)	1_555	1_555	1_555	1_555	yes
O(4)	C(22)	C(23)	C(24)	167.6(3)	1_555	1_555	1_555	1_555	yes
O(4)	C(22)	C(23)	C(32)	-16.0(5)	1_555	1_555	1_555	1_555	yes
N(1)	C(15)	C(13)	C(12)	-16.0(5)	1_555	1_555	1_555	1_555	yes
N(1)	C(15)	C(13)	C(14)	160.3(3)	1_555	1_555	1_555	1_555	yes
N(1)	C(16)	C(17)	C(18)	179.4(3)	1_555	1_555	1_555	1_555	yes
N(1)	C(16)	C(21)	N(2)	-57.0(3)	1_555	1_555	1_555	1_555	yes
N(1)	C(16)	C(21)	C(20)	179.7(3)	1_555	1_555	1_555	1_555	yes
N(2)	C(21)	C(16)	C(17)	179.1(3)	1_555	1_555	1_555	1_555	yes
N(2)	C(21)	C(20)	C(19)	-176.7(3)	1_555	1_555	1_555	1_555	yes
N(2)	C(22)	C(23)	C(24)	-15.7(5)	1_555	1_555	1_555	1_555	yes
N(2)	C(22)	C(23)	C(32)	160.7(3)	1_555	1_555	1_555	1_555	yes
C(1)	C(2)	C(3)	C(5)	-145.2(3)	1_555	1_555	1_555	1_555	yes
C(1)	C(2)	C(4)	C(31)	-136.8(4)	1_555	1_555	1_555	1_555	yes
C(2)	C(3)	C(5)	C(6)	64.5(4)	1_555	1_555	1_555	1_555	yes
C(2)	C(3)	C(5)	C(14)	-115.9(4)	1_555	1_555	1_555	1_555	yes
C(2)	C(4)	C(31)	C(30)	63.8(4)	1_555	1_555	1_555	1_555	yes
C(2)	C(4)	C(31)	C(32)	-116.7(4)	1_555	1_555	1_555	1_555	yes
C(3)	C(2)	C(4)	C(31)	43.1(4)	1_555	1_555	1_555	1_555	yes
C(3)	C(5)	C(6)	C(7)	-1.8(5)	1_555	1_555	1_555	1_555	yes
C(3)	C(5)	C(6)	C(11)	178.2(3)	1_555	1_555	1_555	1_555	yes
C(3)	C(5)	C(14)	C(13)	175.8(3)	1_555	1_555	1_555	1_555	yes
C(4)	C(2)	C(3)	C(5)	34.9(4)	1_555	1_555	1_555	1_555	yes
C(4)	C(31)	C(30)	C(25)	179.7(3)	1_555	1_555	1_555	1_555	yes
C(4)	C(31)	C(30)	C(29)	0.3(5)	1_555	1_555	1_555	1_555	yes
C(4)	C(31)	C(32)	C(23)	176.6(3)	1_555	1_555	1_555	1_555	yes
C(5)	C(6)	C(7)	C(8)	178.5(3)	1_555	1_555	1_555	1_555	yes
C(5)	C(6)	C(11)	C(10)	-177.4(3)	1_555	1_555	1_555	1_555	yes
C(5)	C(6)	C(11)	C(12)	4.8(4)	1_555	1_555	1_555	1_555	yes
C(5)	C(14)	C(13)	C(12)	7.2(5)	1_555	1_555	1_555	1_555	yes
C(5)	C(14)	C(13)	C(15)	-169.3(3)	1_555	1_555	1_555	1_555	yes
C(6)	C(5)	C(14)	C(13)	-4.6(5)	1_555	1_555	1_555	1_555	yes
C(6)	C(7)	C(8)	C(9)	-0.1(6)	1_555	1_555	1_555	1_555	yes
C(6)	C(11)	C(10)	C(9)	-2.3(5)	1_555	1_555	1_555	1_555	yes
C(6)	C(11)	C(12)	C(13)	-2.2(5)	1_555	1_555	1_555	1_555	yes
C(7)	C(6)	C(5)	C(14)	178.6(3)	1_555	1_555	1_555	1_555	yes
C(7)	C(6)	C(11)	C(10)	2.6(4)	1_555	1_555	1_555	1_555	yes
C(7)	C(6)	C(11)	C(12)	-175.2(3)	1_555	1_555	1_555	1_555	yes
C(7)	C(8)	C(9)	C(10)	0.5(6)	1_555	1_555	1_555	1_555	yes
C(8)	C(7)	C(6)	C(11)	-1.5(5)	1_555	1_555	1_555	1_555	yes
C(8)	C(9)	C(10)	C(11)	0.8(6)	1_555	1_555	1_555	1_555	yes
C(9)	C(10)	C(11)	C(12)	175.5(3)	1_555	1_555	1_555	1_555	yes
C(10)	C(11)	C(12)	C(13)	-180.0(3)	1_555	1_555	1_555	1_555	yes
C(11)	C(6)	C(5)	C(14)	-1.4(5)	1_555	1_555	1_555	1_555	yes
C(11)	C(12)	C(13)	C(14)	-3.6(5)	1_555	1_555	1_555	1_555	yes
C(11)	C(12)	C(13)	C(15)	172.7(3)	1_555	1_555	1_555	1_555	yes
C(13)	C(15)	N(1)	C(16)	-162.4(3)	1_555	1_555	1_555	1_555	yes
C(15)	N(1)	C(16)	C(17)	-142.1(3)	1_555	1_555	1_555	1_555	yes
C(15)	N(1)	C(16)	C(21)	94.8(4)	1_555	1_555	1_555	1_555	yes
C(16)	C(17)	C(18)	C(19)	57.9(4)	1_555	1_555	1_555	1_555	yes
C(16)	C(21)	N(2)	C(22)	92.0(4)	1_555	1_555	1_555	1_555	yes
C(16)	C(21)	C(20)	C(19)	-54.4(4)	1_555	1_555	1_555	1_555	yes
C(17)	C(16)	C(21)	C(20)	55.8(4)	1_555	1_555	1_555	1_555	yes
C(17)	C(18)	C(19)	C(20)	-55.4(4)	1_555	1_555	1_555	1_555	yes
C(18)	C(17)	C(16)	C(21)	-57.7(4)	1_555	1_555	1_555	1_555	yes
C(18)	C(19)	C(20)	C(21)	54.3(4)	1_555	1_555	1_555	1_555	yes

C(20)	C(21)	N(2)	C(22)	-145.2(3)	1_555	1_555	1_555	1_555	yes
C(21)	N(2)	C(22)	C(23)	-162.2(3)	1_555	1_555	1_555	1_555	yes
C(22)	C(23)	C(24)	C(25)	174.0(3)	1_555	1_555	1_555	1_555	yes
C(22)	C(23)	C(32)	C(31)	-171.5(3)	1_555	1_555	1_555	1_555	yes
C(23)	C(24)	C(25)	C(26)	179.2(3)	1_555	1_555	1_555	1_555	yes
C(23)	C(24)	C(25)	C(30)	-1.0(5)	1_555	1_555	1_555	1_555	yes
C(23)	C(32)	C(31)	C(30)	-3.9(5)	1_555	1_555	1_555	1_555	yes
C(24)	C(23)	C(32)	C(31)	5.0(5)	1_555	1_555	1_555	1_555	yes
C(24)	C(25)	C(26)	C(27)	177.0(3)	1_555	1_555	1_555	1_555	yes
C(24)	C(25)	C(30)	C(29)	-178.4(3)	1_555	1_555	1_555	1_555	yes
C(24)	C(25)	C(30)	C(31)	2.2(5)	1_555	1_555	1_555	1_555	yes
C(25)	C(24)	C(23)	C(32)	-2.4(5)	1_555	1_555	1_555	1_555	yes
C(25)	C(26)	C(27)	C(28)	2.4(6)	1_555	1_555	1_555	1_555	yes
C(25)	C(30)	C(29)	C(28)	0.3(5)	1_555	1_555	1_555	1_555	yes
C(25)	C(30)	C(31)	C(32)	0.3(5)	1_555	1_555	1_555	1_555	yes
C(26)	C(25)	C(30)	C(29)	1.4(5)	1_555	1_555	1_555	1_555	yes
C(26)	C(25)	C(30)	C(31)	-178.0(3)	1_555	1_555	1_555	1_555	yes
C(26)	C(27)	C(28)	C(29)	-0.6(6)	1_555	1_555	1_555	1_555	yes
C(27)	C(26)	C(25)	C(30)	-2.8(5)	1_555	1_555	1_555	1_555	yes
C(27)	C(28)	C(29)	C(30)	-0.7(6)	1_555	1_555	1_555	1_555	yes
C(28)	C(29)	C(30)	C(31)	179.7(4)	1_555	1_555	1_555	1_555	yes
C(29)	C(30)	C(31)	C(32)	-179.1(3)	1_555	1_555	1_555	1_555	yes

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  _geom_contact_atom_site_label_2
  _geom_contact_distance
  _geom_contact_site_symmetry_1
  _geom_contact_site_symmetry_2
  _geom_contact_publ_flag
S(1)      C(10)      3.556(4)    . . ?
S(1)      C(17)      3.566(4)    . 2_454 ?
O(1)      C(27)      3.461(4)    . 2_543 ?
O(1)      C(28)      3.563(4)    . 2_543 ?
O(2)      C(33)      3.270(4)    . . ?
O(2)      C(17)      3.309(5)    . 1_565 ?
O(2)      C(18)      3.487(5)    . 1_565 ?
O(3)      C(4)       3.490(4)    . 1_545 ?
O(3)      C(27)      3.541(4)    . 2_543 ?
O(4)      C(33)      3.212(5)    . . ?
O(4)      C(19)      3.337(4)    . 2_554 ?
O(5)      N(1)       3.001(4)    . 2_454 ?
O(5)      C(12)      3.308(4)    . 2_454 ?
O(6)      N(2)       2.807(4)    . 2_554 ?
O(6)      C(20)      3.269(6)    . 2_554 ?
O(6)      C(24)      3.429(6)    . 2_554 ?
O(6)      C(21)      3.440(5)    . 2_554 ?
C(8)      C(24)      3.410(5)    . 1_455 ?
C(9)      C(24)      3.445(5)    . 1_455 ?
C(10)     C(33)      3.550(6)    . . ?
C(14)     C(35)      3.569(6)    . 2_444 ?
C(27)     C(36)      3.566(7)    . 2_554 ?
C(28)     C(36)      3.362(7)    . 2_554 ?
C(29)     C(36)      3.508(6)    . 2_554 ?
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#===END
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data_6e
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# CHEMICAL DATA
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_chemical_formula_moiety	'C33 H32 N2 O6, 2(C2 H6 O S)'
_chemical_formula_weight	708.88
_chemical_melting_point	'190.0-191.5 \%
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_symmetry_space_group_name_H-M	'P 1 21 1'
_symmetry_Int_Tables_number	4
loop_	
_symmetry_equiv_pos_as_xyz	
x,y,z	
-x,1/2+y,-z	
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_cell_length_b	15.1153(6)
_cell_length_c	11.3679(6)
_cell_angle_alpha	90
_cell_angle_beta	101.640(1)
_cell_angle_gamma	90
_cell_volume	1796.6(1)
_cell_formula_units_Z	2
_cell_measurement_reflns_used	15106
_cell_measurement_theta_min	3.2
_cell_measurement_theta_max	27.5
_cell_measurement_temperature	193.2
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_exptl_crystal_colour	'yellow'
_exptl_crystal_size_max	0.410
_exptl_crystal_size_mid	0.370
_exptl_crystal_size_min	0.350
_exptl_crystal_size_rad	?
_exptl_crystal_density_diffn	1.310
_exptl_crystal_density_meas	?
_exptl_crystal_density_method	'not measured'
_exptl_absorpt_coefficient_mu	0.202
_exptl_absorpt_correction_type	multi-scan
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_diffn_measurement_device_type	'Rigaku RAXIS-RAPID Imaging Plate'
_diffn_measurement_method	\w
_diffn_detector_area_resol_mean	?
_diffn_reflns_number	18147
_diffn_reflns_av_R_equivalents	0.044
_diffn_reflns_theta_max	27.48
_diffn_measured_fraction_theta_max	0.9995
_diffn_reflns_theta_full	27.48
_diffn_measured_fraction_theta_full	0.9995
_diffn_reflns_limit_h_min	0
_diffn_reflns_limit_h_max	13
_diffn_reflns_limit_k_min	0
_diffn_reflns_limit_k_max	19
_diffn_reflns_limit_l_min	-14
_diffn_reflns_limit_l_max	14
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# REFINEMENT DATA	
_refine_special_details	


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;
Refinement using reflections with  $F^2 > 0.0 \sigma(F^2)$ . 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).
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_reflns_number_gt             3312
_reflns_threshold_expression   $F^2 > 2.0 \sigma(F^2)$ 
_refine_ls_structure_factor_coef Fsqd
_refine_ls_R_factor_gt        0.0944
_refine_ls_wR_factor_ref      0.2743
_refine_ls_hydrogen_treatment noref
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_refine_ls_number_parameters  444
_refine_ls_goodness_of_fit_ref 1.771
_refine_ls_weighting_scheme    calc
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_refine_ls_shift/su_max        1.4073
_refine_diff_density_max       1.96
_refine_diff_density_min       -2.01
_refine_ls_extinction_method    none
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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
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# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
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_atom_site_fract_z
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S(1)	S	-0.6032(2)	0.9677(9)	0.1405(2)	0.0530(5)	Uani	1.00	d	.	.	.
S(2)	S	-0.4027(3)	0.7673(9)	0.4225(4)	0.145(1)	Uani	1.00	d	.	.	.
O(1)	O	-0.1592(3)	0.5716(8)	0.3135(3)	0.0352(9)	Uani	1.00	d	.	.	.
O(2)	O	0.0209(4)	0.3174(8)	0.3883(3)	0.0346(10)	Uani	1.00	d	.	.	.
O(3)	O	-0.3660(4)	0.4961(9)	0.2126(3)	0.040(1)	Uani	1.00	d	.	.	.
O(4)	O	-0.1715(4)	0.2356(9)	0.2678(4)	0.039(1)	Uani	1.00	d	.	.	.
O(5)	O	-0.6504(3)	0.3140(9)	0.0310(3)	0.0338(9)	Uani	1.00	d	.	.	.
O(6)	O	-0.5812(3)	0.1903(9)	0.1436(4)	0.037(1)	Uani	1.00	d	.	.	.
O(7)	O	-0.6384(5)	0.8713(9)	0.1273(5)	0.058(1)	Uani	1.00	d	.	.	.
O(8)	O	-0.4713(6)	0.817(1)	0.4868(7)	0.122(3)	Uani	1.00	d	.	.	.
N(1)	N	-0.4686(4)	0.4075(9)	0.3175(4)	0.0290(10)	Uani	1.00	d	.	.	.
N(2)	N	-0.2772(4)	0.2852(8)	0.0896(4)	0.029(1)	Uani	1.00	d	.	.	.
C(1)	C	0.2959(6)	0.5874(9)	0.5354(6)	0.045(2)	Uani	1.00	d	.	.	.
C(2)	C	0.1879(5)	0.5439(9)	0.4856(5)	0.033(1)	Uani	1.00	d	.	.	.
C(3)	C	0.0610(5)	0.5824(9)	0.4941(5)	0.035(1)	Uani	1.00	d	.	.	.
C(4)	C	0.1951(4)	0.4578(9)	0.4215(4)	0.027(1)	Uani	1.00	d	.	.	.
C(5)	C	-0.0440(5)	0.5159(9)	0.5002(5)	0.031(1)	Uani	1.00	d	.	.	.
C(6)	C	-0.0338(5)	0.4537(9)	0.5954(5)	0.032(1)	Uani	1.00	d	.	.	.
C(7)	C	0.0738(5)	0.4496(9)	0.6955(5)	0.041(1)	Uani	1.00	d	.	.	.
C(8)	C	0.0835(6)	0.3857(10)	0.7804(5)	0.047(2)	Uani	1.00	d	.	.	.
C(9)	C	-0.0137(6)	0.3202(10)	0.7740(6)	0.052(2)	Uani	1.00	d	.	.	.
C(10)	C	-0.1156(5)	0.3219(9)	0.6848(6)	0.043(2)	Uani	1.00	d	.	.	.
C(11)	C	-0.1313(5)	0.3869(9)	0.5915(5)	0.033(1)	Uani	1.00	d	.	.	.
C(12)	C	-0.2378(5)	0.3885(9)	0.4979(5)	0.034(1)	Uani	1.00	d	.	.	.
C(13)	C	-0.2527(5)	0.4512(9)	0.4058(4)	0.027(1)	Uani	1.00	d	.	.	.
C(14)	C	-0.1510(5)	0.5135(9)	0.4057(5)	0.029(1)	Uani	1.00	d	.	.	.
C(15)	C	-0.3654(5)	0.4530(9)	0.3049(5)	0.030(1)	Uani	1.00	d	.	.	.
C(16)	C	-0.5762(5)	0.3949(9)	0.2194(5)	0.032(1)	Uani	1.00	d	.	.	.
C(17)	C	-0.5385(4)	0.3397(9)	0.1178(4)	0.027(1)	Uani	1.00	d	.	.	.
C(18)	C	-0.6881(5)	0.2268(9)	0.0597(5)	0.037(1)	Uani	1.00	d	.	.	.
C(19)	C	-0.8029(5)	0.2298(9)	0.1166(6)	0.043(2)	Uani	1.00	d	.	.	.
C(20)	C	-0.7140(6)	0.1737(9)	-0.0534(6)	0.050(2)	Uani	1.00	d	.	.	.
C(21)	C	-0.4779(4)	0.2506(9)	0.1583(5)	0.028(1)	Uani	1.00	d	.	.	.
C(22)	C	-0.3809(4)	0.2226(9)	0.0811(5)	0.031(1)	Uani	1.00	d	.	.	.
C(23)	C	-0.1795(4)	0.2889(9)	0.1838(4)	0.027(1)	Uani	1.00	d	.	.	.
C(24)	C	-0.0802(4)	0.3586(9)	0.1862(4)	0.025(1)	Uani	1.00	d	.	.	.
C(25)	C	-0.0782(5)	0.4122(9)	0.0864(5)	0.030(1)	Uani	1.00	d	.	.	.
C(26)	C	0.0120(5)	0.4817(9)	0.0914(4)	0.029(1)	Uani	1.00	d	.	.	.
C(27)	C	0.0149(5)	0.5343(9)	-0.0108(5)	0.036(1)	Uani	1.00	d	.	.	.
C(28)	C	0.1000(6)	0.6022(9)	-0.0052(5)	0.042(1)	Uani	1.00	d	.	.	.
C(29)	C	0.1846(5)	0.6211(9)	0.1048(6)	0.039(1)	Uani	1.00	d	.	.	.
C(30)	C	0.1838(5)	0.5711(9)	0.2046(5)	0.034(1)	Uani	1.00	d	.	.	.
C(31)	C	0.1004(4)	0.4987(9)	0.2016(4)	0.026(1)	Uani	1.00	d	.	.	.
C(32)	C	0.1005(5)	0.4445(9)	0.3022(4)	0.027(1)	Uani	1.00	d	.	.	.
C(33)	C	0.0148(4)	0.3736(9)	0.2930(4)	0.027(1)	Uani	1.00	d	.	.	.
C(34)	C	-0.6368(8)	1.0029(9)	0.2783(7)	0.058(2)	Uani	1.00	d	.	.	.
C(35)	C	-0.4367(7)	0.9731(10)	0.1747(8)	0.070(2)	Uani	1.00	d	.	.	.
C(36)	C	-0.295(1)	0.713(1)	0.490(2)	0.200(7)	Uani	1.00	d	.	.	.
C(37)	C	-0.5021(10)	0.699(1)	0.3170(8)	0.082(3)	Uani	1.00	d	.	.	.
H(1)	H	-0.2320	0.5665	0.2497	0.0423	Uiso	1.00	calc	.	.	.
H(2)	H	-0.0385	0.2652	0.3816	0.0410	Uiso	1.00	calc	.	.	.
H(3)	H	0.3758	0.5625	0.5321	0.0538	Uiso	1.00	calc	.	.	.
H(4)	H	0.2867	0.6390	0.5775	0.0538	Uiso	1.00	calc	.	.	.
H(5)	H	0.0708	0.6154	0.5639	0.0441	Uiso	1.00	calc	.	.	.
H(6)	H	0.0311	0.6159	0.4249	0.0441	Uiso	1.00	calc	.	.	.

H(7)	H	0.2796	0.4474	0.4057	0.0366	Uiso	1.00	calc	.	.	.
H(8)	H	0.1823	0.4075	0.4755	0.0366	Uiso	1.00	calc	.	.	.
H(9)	H	0.1378	0.4905	0.6982	0.0506	Uiso	1.00	calc	.	.	.
H(10)	H	0.1584	0.3805	0.8462	0.0600	Uiso	1.00	calc	.	.	.
H(11)	H	-0.0057	0.2703	0.8347	0.0637	Uiso	1.00	calc	.	.	.
H(12)	H	-0.1794	0.2737	0.6805	0.0511	Uiso	1.00	calc	.	.	.
H(13)	H	-0.3011	0.3398	0.4914	0.0399	Uiso	1.00	calc	.	.	.
H(14)	H	-0.4709	0.3762	0.3936	0.0352	Uiso	1.00	calc	.	.	.
H(15)	H	-0.6440	0.3611	0.2480	0.0393	Uiso	1.00	calc	.	.	.
H(16)	H	-0.6075	0.4475	0.1892	0.0393	Uiso	1.00	calc	.	.	.
H(17)	H	-0.4821	0.3691	0.0787	0.0332	Uiso	1.00	calc	.	.	.
H(18)	H	-0.7850	0.2644	0.1854	0.0579	Uiso	1.00	calc	.	.	.
H(19)	H	-0.8249	0.1696	0.1407	0.0579	Uiso	1.00	calc	.	.	.
H(20)	H	-0.8750	0.2507	0.0614	0.0579	Uiso	1.00	calc	.	.	.
H(21)	H	-0.6391	0.1659	-0.0879	0.0593	Uiso	1.00	calc	.	.	.
H(22)	H	-0.7807	0.1965	-0.1134	0.0593	Uiso	1.00	calc	.	.	.
H(23)	H	-0.7410	0.1107	-0.0405	0.0593	Uiso	1.00	calc	.	.	.
H(24)	H	-0.4363	0.2489	0.2413	0.0332	Uiso	1.00	calc	.	.	.
H(25)	H	-0.4225	0.2133	0.0002	0.0378	Uiso	1.00	calc	.	.	.
H(26)	H	-0.3442	0.1621	0.1089	0.0378	Uiso	1.00	calc	.	.	.
H(27)	H	-0.2785	0.3220	0.0255	0.0348	Uiso	1.00	calc	.	.	.
H(28)	H	-0.1402	0.3984	0.0141	0.0356	Uiso	1.00	calc	.	.	.
H(29)	H	-0.0418	0.5172	-0.0843	0.0442	Uiso	1.00	calc	.	.	.
H(30)	H	0.0991	0.6329	-0.0766	0.0487	Uiso	1.00	calc	.	.	.
H(31)	H	0.2381	0.6682	0.1093	0.0451	Uiso	1.00	calc	.	.	.
H(32)	H	0.2460	0.5799	0.2768	0.0412	Uiso	1.00	calc	.	.	.
H(33)	H	-0.5955	1.0552	0.3014	0.0711	Uiso	1.00	calc	.	.	.
H(34)	H	-0.7252	1.0055	0.2743	0.0711	Uiso	1.00	calc	.	.	.
H(35)	H	-0.6029	0.9574	0.3407	0.0711	Uiso	1.00	calc	.	.	.
H(36)	H	-0.4085	1.0302	0.1853	0.0856	Uiso	1.00	calc	.	.	.
H(37)	H	-0.4038	0.9396	0.2502	0.0856	Uiso	1.00	calc	.	.	.
H(38)	H	-0.4004	0.9433	0.1145	0.0856	Uiso	1.00	calc	.	.	.
H(39)	H	-0.2440	0.7287	0.5632	0.1713	Uiso	1.00	calc	.	.	.
H(40)	H	-0.2529	0.6671	0.4527	0.1713	Uiso	1.00	calc	.	.	.
H(41)	H	-0.3466	0.6547	0.5395	0.1713	Uiso	1.00	calc	.	.	.
H(42)	H	-0.4547	0.6618	0.2687	0.0917	Uiso	1.00	calc	.	.	.
H(43)	H	-0.5463	0.6521	0.3580	0.0917	Uiso	1.00	calc	.	.	.
H(44)	H	-0.5675	0.7274	0.2634	0.0917	Uiso	1.00	calc	.	.	.

loop_

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_atom_site_aniso_U_22

_atom_site_aniso_U_33

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S(1)	0.0576(10)	0.0543(9)	0.0456(9)	-0.0033(8)	0.0072(8)	0.0000(8)
S(2)	0.060(1)	0.214(4)	0.146(3)	0.037(2)	-0.015(2)	-0.128(3)
O(1)	0.033(2)	0.035(2)	0.034(2)	0.000(2)	-0.002(2)	0.005(2)
O(2)	0.038(2)	0.032(2)	0.033(2)	0.000(2)	0.005(2)	0.009(1)
O(3)	0.040(2)	0.042(2)	0.033(2)	-0.004(2)	-0.003(2)	0.007(2)
O(4)	0.042(2)	0.033(2)	0.038(2)	-0.010(2)	0.000(2)	0.011(2)
O(5)	0.027(2)	0.044(2)	0.027(2)	0.004(2)	-0.004(1)	0.000(2)
O(6)	0.029(2)	0.032(2)	0.048(2)	-0.006(1)	0.006(2)	0.009(2)
O(7)	0.061(3)	0.051(2)	0.058(3)	-0.006(2)	0.006(2)	-0.017(2)
O(8)	0.066(4)	0.189(9)	0.102(5)	0.032(5)	-0.006(4)	-0.092(6)
N(1)	0.027(2)	0.032(2)	0.026(2)	0.002(2)	0.001(1)	-0.005(2)
N(2)	0.025(2)	0.027(2)	0.035(2)	0.003(2)	0.009(1)	-0.001(2)
C(1)	0.035(3)	0.058(4)	0.039(3)	-0.010(3)	0.003(2)	-0.005(3)
C(2)	0.038(2)	0.038(2)	0.023(2)	-0.003(2)	0.004(2)	-0.004(2)

C(3)	0.035(2)	0.031(3)	0.035(3)	-0.007(2)	0.001(2)	-0.009(2)
C(4)	0.024(2)	0.028(2)	0.030(2)	0.004(2)	0.003(2)	0.001(2)
C(5)	0.029(2)	0.031(2)	0.034(2)	0.000(2)	0.006(2)	-0.010(2)
C(6)	0.026(2)	0.040(3)	0.031(2)	0.003(2)	0.005(2)	-0.007(2)
C(7)	0.031(2)	0.061(4)	0.029(2)	-0.004(3)	0.005(2)	-0.006(2)
C(8)	0.038(3)	0.073(4)	0.028(3)	0.005(3)	-0.002(2)	0.007(3)
C(9)	0.037(3)	0.075(4)	0.041(3)	0.002(3)	0.000(2)	0.018(3)
C(10)	0.033(3)	0.056(4)	0.041(3)	0.002(3)	0.004(2)	0.022(3)
C(11)	0.031(2)	0.036(3)	0.031(2)	0.003(2)	0.008(2)	-0.001(2)
C(12)	0.033(2)	0.038(3)	0.031(3)	-0.001(2)	0.007(2)	0.004(2)
C(13)	0.026(2)	0.026(2)	0.029(2)	0.004(2)	0.006(2)	-0.006(2)
C(14)	0.028(2)	0.027(2)	0.033(2)	0.001(2)	0.009(2)	-0.005(2)
C(15)	0.029(2)	0.032(3)	0.029(2)	0.005(2)	0.006(2)	-0.004(2)
C(16)	0.022(2)	0.045(3)	0.025(2)	0.007(2)	-0.003(2)	-0.004(2)
C(17)	0.024(2)	0.030(2)	0.026(2)	-0.001(2)	0.002(2)	0.001(2)
C(18)	0.028(2)	0.047(2)	0.031(2)	-0.006(2)	0.000(2)	-0.007(2)
C(19)	0.027(2)	0.048(3)	0.052(4)	-0.007(2)	0.005(2)	-0.013(3)
C(20)	0.043(3)	0.056(4)	0.045(3)	0.005(3)	0.001(3)	-0.024(3)
C(21)	0.023(2)	0.029(2)	0.031(2)	-0.001(2)	0.004(2)	0.000(2)
C(22)	0.022(2)	0.030(2)	0.041(3)	0.002(2)	0.008(2)	-0.010(2)
C(23)	0.026(2)	0.025(2)	0.031(2)	0.006(2)	0.010(2)	0.000(2)
C(24)	0.024(2)	0.024(2)	0.027(2)	0.001(2)	0.005(2)	0.000(2)
C(25)	0.024(2)	0.036(3)	0.030(2)	0.001(2)	0.004(2)	0.009(2)
C(26)	0.026(2)	0.034(2)	0.029(2)	0.002(2)	0.008(2)	0.004(2)
C(27)	0.033(3)	0.047(3)	0.029(2)	0.006(2)	0.008(2)	0.011(2)
C(28)	0.041(3)	0.051(3)	0.034(3)	-0.001(2)	0.012(2)	0.017(2)
C(29)	0.033(3)	0.044(3)	0.043(3)	-0.006(2)	0.015(2)	0.005(2)
C(30)	0.026(2)	0.040(3)	0.037(3)	-0.003(2)	0.006(2)	0.000(2)
C(31)	0.023(2)	0.029(2)	0.026(2)	0.010(2)	0.007(2)	0.000(2)
C(32)	0.028(2)	0.029(2)	0.026(2)	0.003(2)	0.008(2)	-0.001(2)
C(33)	0.025(2)	0.031(2)	0.026(2)	0.005(2)	0.006(2)	0.002(2)
C(34)	0.078(5)	0.042(3)	0.060(4)	-0.009(4)	0.031(4)	-0.009(3)
C(35)	0.057(2)	0.065(5)	0.092(6)	-0.023(4)	0.027(4)	-0.031(5)
C(36)	0.102(9)	0.16(1)	0.29(2)	0.069(9)	-0.08(1)	-0.16(1)
C(37)	0.092(6)	0.099(7)	0.056(5)	0.035(4)	0.018(4)	0.000(4)

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S(1)      O(7)      1.505(9)    . . yes
S(1)      C(34)     1.758(10)   . . yes
S(1)      C(35)     1.74(1)    . . yes
S(2)      O(8)      1.361(10)   . . yes
S(2)      C(36)     1.50(2)    . . yes
S(2)      C(37)     1.77(2)    . . yes
O(1)      C(14)     1.356(8)    . . yes
O(2)      C(33)     1.369(8)    . . yes
O(3)      C(15)     1.233(8)    . . yes

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O(4)	C(23)	1.239(8)	. . yes
O(5)	C(17)	1.441(8)	. . yes
O(5)	C(18)	1.435(10)	. . yes
O(6)	C(18)	1.441(9)	. . yes
O(6)	C(21)	1.415(8)	. . yes
N(1)	C(15)	1.332(9)	. . yes
N(1)	C(16)	1.443(8)	. . yes
N(2)	C(22)	1.446(9)	. . yes
N(2)	C(23)	1.336(9)	. . yes
C(1)	C(2)	1.35(1)	. . yes
C(2)	C(3)	1.50(1)	. . yes
C(2)	C(4)	1.501(10)	. . yes
C(3)	C(5)	1.518(10)	. . yes
C(4)	C(32)	1.531(9)	. . yes
C(5)	C(6)	1.42(1)	. . yes
C(5)	C(14)	1.402(9)	. . yes
C(6)	C(7)	1.446(10)	. . yes
C(6)	C(11)	1.44(1)	. . yes
C(7)	C(8)	1.35(1)	. . yes
C(8)	C(9)	1.42(1)	. . yes
C(9)	C(10)	1.33(1)	. . yes
C(10)	C(11)	1.43(1)	. . yes
C(11)	C(12)	1.392(10)	. . yes
C(12)	C(13)	1.398(10)	. . yes
C(13)	C(14)	1.437(9)	. . yes
C(13)	C(15)	1.486(9)	. . yes
C(16)	C(17)	1.543(9)	. . yes
C(17)	C(21)	1.524(9)	. . yes
C(18)	C(19)	1.50(1)	. . yes
C(18)	C(20)	1.49(1)	. . yes
C(21)	C(22)	1.546(9)	. . yes
C(23)	C(24)	1.491(9)	. . yes
C(24)	C(25)	1.399(9)	. . yes
C(24)	C(33)	1.434(9)	. . yes
C(25)	C(26)	1.418(10)	. . yes
C(26)	C(27)	1.413(10)	. . yes
C(26)	C(31)	1.431(9)	. . yes
C(27)	C(28)	1.36(1)	. . yes
C(28)	C(29)	1.42(1)	. . yes
C(29)	C(30)	1.36(1)	. . yes
C(30)	C(31)	1.408(10)	. . yes
C(31)	C(32)	1.406(9)	. . yes
C(32)	C(33)	1.399(9)	. . yes

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loop_

_geom_angle_atom_site_label_1

_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

_geom_angle

_geom_angle_site_symmetry_1

_geom_angle_site_symmetry_2

_geom_angle_site_symmetry_3

_geom_angle_publ_flag

O(7)	S(1)	C(34)	106.9(5)	. 1_555 1_555 yes
O(7)	S(1)	C(35)	106.9(5)	. 1_555 1_555 yes
C(34)	S(1)	C(35)	99.8(5)	. 1_555 1_555 yes
O(8)	S(2)	C(36)	117(1)	. 1_555 1_555 yes
O(8)	S(2)	C(37)	111.9(6)	. 1_555 1_555 yes
C(36)	S(2)	C(37)	108.6(9)	. 1_555 1_555 yes
C(17)	O(5)	C(18)	108.9(5)	. 1_555 1_555 yes
C(18)	O(6)	C(21)	109.0(5)	. 1_555 1_555 yes

C(15)	N(1)	C(16)	122.1(6)	.	1_555	1_555	yes
C(22)	N(2)	C(23)	123.0(6)	.	1_555	1_555	yes
C(1)	C(2)	C(3)	119.4(7)	.	1_555	1_555	yes
C(1)	C(2)	C(4)	120.3(7)	.	1_555	1_555	yes
C(3)	C(2)	C(4)	120.3(6)	.	1_555	1_555	yes
C(2)	C(3)	C(5)	115.6(6)	.	1_555	1_555	yes
C(2)	C(4)	C(32)	117.0(5)	.	1_555	1_555	yes
C(3)	C(5)	C(6)	122.0(6)	.	1_555	1_555	yes
C(3)	C(5)	C(14)	118.5(6)	.	1_555	1_555	yes
C(6)	C(5)	C(14)	119.5(6)	.	1_555	1_555	yes
C(5)	C(6)	C(7)	123.6(7)	.	1_555	1_555	yes
C(5)	C(6)	C(11)	119.7(6)	.	1_555	1_555	yes
C(7)	C(6)	C(11)	116.6(7)	.	1_555	1_555	yes
C(6)	C(7)	C(8)	121.7(7)	.	1_555	1_555	yes
C(7)	C(8)	C(9)	120.6(7)	.	1_555	1_555	yes
C(8)	C(9)	C(10)	120.0(8)	.	1_555	1_555	yes
C(9)	C(10)	C(11)	122.3(8)	.	1_555	1_555	yes
C(6)	C(11)	C(10)	118.8(7)	.	1_555	1_555	yes
C(6)	C(11)	C(12)	119.0(7)	.	1_555	1_555	yes
C(10)	C(11)	C(12)	122.2(7)	.	1_555	1_555	yes
C(11)	C(12)	C(13)	122.4(7)	.	1_555	1_555	yes
C(12)	C(13)	C(14)	118.3(6)	.	1_555	1_555	yes
C(12)	C(13)	C(15)	122.9(6)	.	1_555	1_555	yes
C(14)	C(13)	C(15)	118.8(6)	.	1_555	1_555	yes
O(1)	C(14)	C(5)	119.4(6)	.	1_555	1_555	yes
O(1)	C(14)	C(13)	119.6(6)	.	1_555	1_555	yes
C(5)	C(14)	C(13)	121.0(6)	.	1_555	1_555	yes
O(3)	C(15)	N(1)	120.1(6)	.	1_555	1_555	yes
O(3)	C(15)	C(13)	122.1(6)	.	1_555	1_555	yes
N(1)	C(15)	C(13)	117.8(6)	.	1_555	1_555	yes
N(1)	C(16)	C(17)	111.2(5)	.	1_555	1_555	yes
O(5)	C(17)	C(16)	110.7(5)	.	1_555	1_555	yes
O(5)	C(17)	C(21)	102.2(5)	.	1_555	1_555	yes
C(16)	C(17)	C(21)	114.2(6)	.	1_555	1_555	yes
O(5)	C(18)	O(6)	106.4(5)	.	1_555	1_555	yes
O(5)	C(18)	C(19)	111.2(6)	.	1_555	1_555	yes
O(5)	C(18)	C(20)	108.0(7)	.	1_555	1_555	yes
O(6)	C(18)	C(19)	109.5(6)	.	1_555	1_555	yes
O(6)	C(18)	C(20)	110.4(7)	.	1_555	1_555	yes
C(19)	C(18)	C(20)	111.3(6)	.	1_555	1_555	yes
O(6)	C(21)	C(17)	105.1(5)	.	1_555	1_555	yes
O(6)	C(21)	C(22)	110.6(5)	.	1_555	1_555	yes
C(17)	C(21)	C(22)	111.2(6)	.	1_555	1_555	yes
N(2)	C(22)	C(21)	112.0(5)	.	1_555	1_555	yes
O(4)	C(23)	N(2)	120.8(6)	.	1_555	1_555	yes
O(4)	C(23)	C(24)	120.4(6)	.	1_555	1_555	yes
N(2)	C(23)	C(24)	118.7(6)	.	1_555	1_555	yes
C(23)	C(24)	C(25)	121.5(6)	.	1_555	1_555	yes
C(23)	C(24)	C(33)	120.4(6)	.	1_555	1_555	yes
C(25)	C(24)	C(33)	118.1(6)	.	1_555	1_555	yes
C(24)	C(25)	C(26)	121.2(6)	.	1_555	1_555	yes
C(25)	C(26)	C(27)	120.7(6)	.	1_555	1_555	yes
C(25)	C(26)	C(31)	119.4(6)	.	1_555	1_555	yes
C(27)	C(26)	C(31)	119.9(6)	.	1_555	1_555	yes
C(26)	C(27)	C(28)	120.6(7)	.	1_555	1_555	yes
C(27)	C(28)	C(29)	119.6(7)	.	1_555	1_555	yes
C(28)	C(29)	C(30)	120.8(7)	.	1_555	1_555	yes
C(29)	C(30)	C(31)	121.4(7)	.	1_555	1_555	yes
C(26)	C(31)	C(30)	117.5(6)	.	1_555	1_555	yes
C(26)	C(31)	C(32)	120.0(6)	.	1_555	1_555	yes
C(30)	C(31)	C(32)	122.4(6)	.	1_555	1_555	yes

C(4)	C(32)	C(31)	122.5(6)	.	1_555	1_555	yes
C(4)	C(32)	C(33)	118.1(6)	.	1_555	1_555	yes
C(31)	C(32)	C(33)	119.4(6)	.	1_555	1_555	yes
O(2)	C(33)	C(24)	119.0(6)	.	1_555	1_555	yes
O(2)	C(33)	C(32)	119.4(6)	.	1_555	1_555	yes
C(24)	C(33)	C(32)	121.7(6)	.	1_555	1_555	yes

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loop_

_geom_torsion_atom_site_label_1

_geom_torsion_atom_site_label_2

_geom_torsion_atom_site_label_3

_geom_torsion_atom_site_label_4

_geom_torsion

_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2

_geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4

_geom_torsion_publ_flag

O(1)	C(14)	C(5)	C(3)	-1.6(9)	1_555	1_555	1_555	1_555	yes
O(1)	C(14)	C(5)	C(6)	-178.5(6)	1_555	1_555	1_555	1_555	yes
O(1)	C(14)	C(13)	C(12)	176.0(6)	1_555	1_555	1_555	1_555	yes
O(1)	C(14)	C(13)	C(15)	-0.6(9)	1_555	1_555	1_555	1_555	yes
O(2)	C(33)	C(24)	C(23)	6.5(9)	1_555	1_555	1_555	1_555	yes
O(2)	C(33)	C(24)	C(25)	-174.9(6)	1_555	1_555	1_555	1_555	yes
O(2)	C(33)	C(32)	C(4)	-2.0(9)	1_555	1_555	1_555	1_555	yes
O(2)	C(33)	C(32)	C(31)	175.6(5)	1_555	1_555	1_555	1_555	yes
O(3)	C(15)	N(1)	C(16)	9(1)	1_555	1_555	1_555	1_555	yes
O(3)	C(15)	C(13)	C(12)	-164.9(7)	1_555	1_555	1_555	1_555	yes
O(3)	C(15)	C(13)	C(14)	11.5(9)	1_555	1_555	1_555	1_555	yes
O(4)	C(23)	N(2)	C(22)	2.4(10)	1_555	1_555	1_555	1_555	yes
O(4)	C(23)	C(24)	C(25)	171.9(7)	1_555	1_555	1_555	1_555	yes
O(4)	C(23)	C(24)	C(33)	-9.5(9)	1_555	1_555	1_555	1_555	yes
O(5)	C(17)	C(16)	N(1)	169.5(6)	1_555	1_555	1_555	1_555	yes
O(5)	C(17)	C(21)	O(6)	-28.6(6)	1_555	1_555	1_555	1_555	yes
O(5)	C(17)	C(21)	C(22)	91.2(6)	1_555	1_555	1_555	1_555	yes
O(5)	C(18)	O(6)	C(21)	-4.4(7)	1_555	1_555	1_555	1_555	yes
O(6)	C(18)	O(5)	C(17)	-14.9(7)	1_555	1_555	1_555	1_555	yes
O(6)	C(21)	C(17)	C(16)	91.0(6)	1_555	1_555	1_555	1_555	yes
O(6)	C(21)	C(22)	N(2)	177.2(5)	1_555	1_555	1_555	1_555	yes
N(1)	C(15)	C(13)	C(12)	16.3(9)	1_555	1_555	1_555	1_555	yes
N(1)	C(15)	C(13)	C(14)	-167.3(6)	1_555	1_555	1_555	1_555	yes
N(1)	C(16)	C(17)	C(21)	54.9(8)	1_555	1_555	1_555	1_555	yes
N(2)	C(22)	C(21)	C(17)	60.8(7)	1_555	1_555	1_555	1_555	yes
N(2)	C(23)	C(24)	C(25)	-8.3(9)	1_555	1_555	1_555	1_555	yes
N(2)	C(23)	C(24)	C(33)	170.3(6)	1_555	1_555	1_555	1_555	yes
C(1)	C(2)	C(3)	C(5)	-148.3(7)	1_555	1_555	1_555	1_555	yes
C(1)	C(2)	C(4)	C(32)	-136.8(7)	1_555	1_555	1_555	1_555	yes
C(2)	C(3)	C(5)	C(6)	61.3(8)	1_555	1_555	1_555	1_555	yes
C(2)	C(3)	C(5)	C(14)	-115.6(7)	1_555	1_555	1_555	1_555	yes
C(2)	C(4)	C(32)	C(31)	62.6(8)	1_555	1_555	1_555	1_555	yes
C(2)	C(4)	C(32)	C(33)	-119.8(7)	1_555	1_555	1_555	1_555	yes
C(3)	C(2)	C(4)	C(32)	42.9(9)	1_555	1_555	1_555	1_555	yes
C(3)	C(5)	C(6)	C(7)	1(1)	1_555	1_555	1_555	1_555	yes
C(3)	C(5)	C(6)	C(11)	-174.6(6)	1_555	1_555	1_555	1_555	yes
C(3)	C(5)	C(14)	C(13)	179.3(6)	1_555	1_555	1_555	1_555	yes
C(4)	C(2)	C(3)	C(5)	32.0(9)	1_555	1_555	1_555	1_555	yes
C(4)	C(32)	C(31)	C(26)	178.3(6)	1_555	1_555	1_555	1_555	yes
C(4)	C(32)	C(31)	C(30)	-2.5(9)	1_555	1_555	1_555	1_555	yes
C(4)	C(32)	C(33)	C(24)	177.5(6)	1_555	1_555	1_555	1_555	yes
C(5)	C(6)	C(7)	C(8)	-175.8(7)	1_555	1_555	1_555	1_555	yes
C(5)	C(6)	C(11)	C(10)	176.6(7)	1_555	1_555	1_555	1_555	yes

C(5)	C(6)	C(11)	C(12)	-4.1(10)	1_555	1_555	1_555	1_555	yes
C(5)	C(14)	C(13)	C(12)	-4.9(9)	1_555	1_555	1_555	1_555	yes
C(5)	C(14)	C(13)	C(15)	178.5(6)	1_555	1_555	1_555	1_555	yes
C(6)	C(5)	C(14)	C(13)	2.4(10)	1_555	1_555	1_555	1_555	yes
C(6)	C(7)	C(8)	C(9)	0(1)	1_555	1_555	1_555	1_555	yes
C(6)	C(11)	C(10)	C(9)	0(1)	1_555	1_555	1_555	1_555	yes
C(6)	C(11)	C(12)	C(13)	1(1)	1_555	1_555	1_555	1_555	yes
C(7)	C(6)	C(5)	C(14)	178.7(7)	1_555	1_555	1_555	1_555	yes
C(7)	C(6)	C(11)	C(10)	0(1)	1_555	1_555	1_555	1_555	yes
C(7)	C(6)	C(11)	C(12)	179.2(7)	1_555	1_555	1_555	1_555	yes
C(7)	C(8)	C(9)	C(10)	0(1)	1_555	1_555	1_555	1_555	yes
C(8)	C(7)	C(6)	C(11)	0(1)	1_555	1_555	1_555	1_555	yes
C(8)	C(9)	C(10)	C(11)	1(1)	1_555	1_555	1_555	1_555	yes
C(9)	C(10)	C(11)	C(12)	179.8(8)	1_555	1_555	1_555	1_555	yes
C(10)	C(11)	C(12)	C(13)	-179.2(7)	1_555	1_555	1_555	1_555	yes
C(11)	C(6)	C(5)	C(14)	2.2(10)	1_555	1_555	1_555	1_555	yes
C(11)	C(12)	C(13)	C(14)	2(1)	1_555	1_555	1_555	1_555	yes
C(11)	C(12)	C(13)	C(15)	179.4(6)	1_555	1_555	1_555	1_555	yes
C(13)	C(15)	N(1)	C(16)	-171.4(6)	1_555	1_555	1_555	1_555	yes
C(15)	N(1)	C(16)	C(17)	64.5(9)	1_555	1_555	1_555	1_555	yes
C(16)	C(17)	O(5)	C(18)	-95.5(6)	1_555	1_555	1_555	1_555	yes
C(16)	C(17)	C(21)	C(22)	-149.3(5)	1_555	1_555	1_555	1_555	yes
C(17)	O(5)	C(18)	C(19)	104.2(6)	1_555	1_555	1_555	1_555	yes
C(17)	O(5)	C(18)	C(20)	-133.4(6)	1_555	1_555	1_555	1_555	yes
C(17)	C(21)	O(6)	C(18)	20.7(7)	1_555	1_555	1_555	1_555	yes
C(18)	O(5)	C(17)	C(21)	26.5(7)	1_555	1_555	1_555	1_555	yes
C(18)	O(6)	C(21)	C(22)	-99.5(6)	1_555	1_555	1_555	1_555	yes
C(19)	C(18)	O(6)	C(21)	-124.7(7)	1_555	1_555	1_555	1_555	yes
C(20)	C(18)	O(6)	C(21)	112.5(7)	1_555	1_555	1_555	1_555	yes
C(21)	C(22)	N(2)	C(23)	77.7(8)	1_555	1_555	1_555	1_555	yes
C(22)	N(2)	C(23)	C(24)	-177.4(6)	1_555	1_555	1_555	1_555	yes
C(23)	C(24)	C(25)	C(26)	176.4(6)	1_555	1_555	1_555	1_555	yes
C(23)	C(24)	C(33)	C(32)	-173.0(6)	1_555	1_555	1_555	1_555	yes
C(24)	C(25)	C(26)	C(27)	178.6(7)	1_555	1_555	1_555	1_555	yes
C(24)	C(25)	C(26)	C(31)	-1.7(10)	1_555	1_555	1_555	1_555	yes
C(24)	C(33)	C(32)	C(31)	-4.9(9)	1_555	1_555	1_555	1_555	yes
C(25)	C(24)	C(33)	C(32)	5.6(9)	1_555	1_555	1_555	1_555	yes
C(25)	C(26)	C(27)	C(28)	178.6(7)	1_555	1_555	1_555	1_555	yes
C(25)	C(26)	C(31)	C(30)	-176.7(6)	1_555	1_555	1_555	1_555	yes
C(25)	C(26)	C(31)	C(32)	2.5(9)	1_555	1_555	1_555	1_555	yes
C(26)	C(25)	C(24)	C(33)	-2.2(10)	1_555	1_555	1_555	1_555	yes
C(26)	C(27)	C(28)	C(29)	-1(1)	1_555	1_555	1_555	1_555	yes
C(26)	C(31)	C(30)	C(29)	-2.8(10)	1_555	1_555	1_555	1_555	yes
C(26)	C(31)	C(32)	C(33)	0.8(9)	1_555	1_555	1_555	1_555	yes
C(27)	C(26)	C(31)	C(30)	2.9(9)	1_555	1_555	1_555	1_555	yes
C(27)	C(26)	C(31)	C(32)	-177.9(6)	1_555	1_555	1_555	1_555	yes
C(27)	C(28)	C(29)	C(30)	1(1)	1_555	1_555	1_555	1_555	yes
C(28)	C(27)	C(26)	C(31)	-1(1)	1_555	1_555	1_555	1_555	yes
C(28)	C(29)	C(30)	C(31)	0(1)	1_555	1_555	1_555	1_555	yes
C(29)	C(30)	C(31)	C(32)	178.0(7)	1_555	1_555	1_555	1_555	yes
C(30)	C(31)	C(32)	C(33)	180.0(6)	1_555	1_555	1_555	1_555	yes

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  _geom_contact_site_symmetry_2
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S(1)      O(6)      3.372(7)    . 1_565 ?
O(1)      C(20)    3.368(9)    . 2_455 ?

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O(1)      C(36)      3.44(2)      . . ?
O(2)      C(36)      3.37(2)      . 2_546 ?
O(3)      C(20)      3.441(10)    . 2_455 ?
O(4)      C(3)       3.576(9)     . 2_546 ?
O(6)      C(34)      3.33(1)     . 1_545 ?
O(7)      N(2)       2.773(9)     . 2_455 ?
O(7)      C(22)      3.30(1)     . 2_455 ?
O(7)      C(37)      3.51(2)     . . ?
O(7)      C(25)      3.532(10)    . 2_455 ?
O(8)      N(1)       2.79(1)     . 2_456 ?
O(8)      C(12)      3.33(1)     . 2_456 ?
O(8)      C(16)      3.48(1)     . 2_456 ?
N(2)      C(28)      3.590(10)    . 2_545 ?
N(2)      C(29)      3.592(9)     . 2_545 ?
C(8)      C(27)      3.45(1)     . 1_556 ?
C(11)     C(34)      3.59(1)     . 2_446 ?
C(12)     C(34)      3.55(1)     . 2_446 ?
C(14)     C(36)      3.60(2)     . . ?
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#===END
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data_6f
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_chemical_formula_moiety   'C31 H30 N2 O4, C H2 Cl2'
_chemical_formula_weight   579.52
_chemical_melting_point    '262-264 \%C'
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_symmetry_Int_Tables_number 4
loop_
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' +x, +y, +z '
' -x, 1/2+y, -z '
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_cell_length_b             7.5530(4)
_cell_length_c             19.501(2)
_cell_angle_alpha          90
_cell_angle_beta           96.872(4)
_cell_angle_gamma          90
_cell_volume               2844.2(4)
_cell_formula_units_Z      4
_cell_measurement_reflns_used ?
_cell_measurement_theta_min ?
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_cell_measurement_temperature 296.1
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_diffrn_radiation_wavelength 0.7107
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_diffrn_detector_area_resol_mean ?
_diffrn_reflns_number        4610
_diffrn_reflns_av_R_equivalents ?
_diffrn_reflns_theta_max     26.07
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_diffrn_reflns_theta_full    26.07
_diffrn_measured_fraction_theta_full 0.7497
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_diffrn_reflns_limit_h_max    22
_diffrn_reflns_limit_k_min    0
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_diffrn_reflns_limit_l_min    -23
_diffrn_reflns_limit_l_max    23
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# REFINEMENT DATA
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  Refinement using reflections with  $F^2 > 3.0 \sigma(F^2)$ .
  The weighted R-factor (wR), goodness of fit (S) and R-factor (gt) are
  based on  $F$ , with  $F$  set to zero for negative  $F$ . The threshold expression of
   $F^2 > 2.0 \sigma(F^2)$  is used only for calculating R-factor (gt).
;
_reflns_number_gt           1929
_reflns_threshold_expression  $F^2 > 2.0 \sigma(F^2)$ 
_refine_ls_structure_factor_coef F
_refine_ls_R_factor_gt      0.0470
_refine_ls_wR_factor_ref    0.0700
_refine_ls_hydrogen_treatment ?
_refine_ls_number_reflns    1929
_refine_ls_number_parameters 781
_refine_ls_goodness_of_fit_ref 0.765
_refine_ls_weighting_scheme  calc
_refine_ls_weighting_details
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_refine_ls_shift/su_max     3.3120
_refine_diff_density_max    0.17
_refine_diff_density_min    -0.19
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_refine_ls_abs_structure_details ?
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  'H' 'H' 0.000 0.000
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International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.4)

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(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
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International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
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International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
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  _atom_site_refinement_flags
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Cl(2) Cl 1.9611(7) 0.468(1) 0.9907(5) 0.154(4) Uani 1.00 1 d . . .
Cl(3) Cl 1.8396(6) 0.5290(12) 0.8892(5) 0.156(3) Uani 1.00 1 d . . .
Cl(4) Cl 1.6661(6) 0.645(1) 0.5955(8) 0.236(6) Uani 1.00 1 d . . .
O(1) O 2.126(1) 0.299(3) 0.9071(12) 0.123(8) Uani 1.00 1 d . . .
O(5) O 2.1785(12) 0.742(2) 0.7504(12) 0.104(7) Uani 1.00 1 d . . .
O(6) O 1.4985(9) 0.799(2) 0.6701(8) 0.085(5) Uani 1.00 1 d . . .
O(7) O 2.0745(9) 0.644(2) 0.6695(8) 0.084(5) Uani 1.00 1 d . . .
O(8) O 2.0069(11) 0.401(2) 0.8353(10) 0.112(6) Uani 1.00 1 d . . .
O(9) O 1.3148(11) 0.442(2) 0.7476(9) 0.099(5) Uani 1.00 1 d . . .
O(10) O 1.4200(11) 0.557(2) 0.8290(9) 0.098(6) Uani 1.00 1 d . . .
O(12) O 1.3769(12) 0.876(3) 0.5922(11) 0.130(8) Uani 1.00 1 d . . .
N(1) N 2.165(2) 0.813(2) 0.8615(12) 0.102(8) Uani 1.00 1 d . . .
N(2) N 2.2109(12) 0.419(2) 0.8507(11) 0.083(7) Uani 1.00 1 d . . .
N(3) N 1.3368(12) 0.379(2) 0.638(1) 0.102(7) Uani 1.00 1 d . . .
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C(4) C 2.065(2) 0.803(3) 0.768(2) 0.106(9) Uani 1.00 1 d . . .
C(5) C 1.934(2) 0.615(3) 0.6298(11) 0.083(7) Uani 1.00 1 d . . .
C(6) C 1.922(2) 0.344(3) 0.706(1) 0.095(8) Uani 1.00 1 d . . .
C(17) C 1.5526(13) 0.292(3) 0.7025(10) 0.070(6) Uani 1.00 1 d . . .
C(18) C 2.142(1) 0.229(3) 0.7336(13) 0.088(8) Uani 1.00 1 d . . .
C(19) C 2.110(1) 0.293(3) 0.7861(13) 0.075(7) Uani 1.00 1 d . . .
C(20) C 1.4616(10) 0.478(2) 0.7873(11) 0.072(6) Uani 1.00 1 d . . .
C(23) C 2.1230(12) 0.077(2) 0.6162(11) 0.080(6) Uani 1.00 1 d . . .
C(24) C 1.482(1) 0.290(2) 0.6862(10) 0.071(6) Uani 1.00 1 d . . .
C(25) C 2.091(2) 0.170(3) 0.6709(12) 0.081(8) Uani 1.00 1 d . . .
C(27) C 1.518(2) 1.053(3) 0.8917(13) 0.094(7) Uani 1.00 1 d . . .
C(28) C 1.906(2) 1.004(3) 0.8378(13) 0.096(8) Uani 1.00 1 d . . .
C(29) C 1.660(2) 0.195(3) 0.6789(10) 0.098(7) Uani 1.00 1 d . . .

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C(30)	C	1.3685(12)	0.980(2)	0.7684(12)	0.080(6)	Uani	1.00	1	d	.	.	.
C(31)	C	2.035(1)	0.329(3)	0.7786(11)	0.074(7)	Uani	1.00	1	d	.	.	.
C(32)	C	1.954(2)	0.907(2)	0.793(1)	0.101(8)	Uani	1.00	1	d	.	.	.
C(33)	C	1.993(2)	0.297(2)	0.7197(13)	0.081(8)	Uani	1.00	1	d	.	.	.
C(34)	C	1.6506(13)	0.385(3)	0.7772(11)	0.082(7)	Uani	1.00	1	d	.	.	.
C(35)	C	2.140(2)	0.798(3)	0.7922(11)	0.099(8)	Uani	1.00	1	d	.	.	.
C(36)	C	1.469(2)	0.865(2)	0.7216(13)	0.086(8)	Uani	1.00	1	d	.	.	.
C(37)	C	1.531(2)	0.472(3)	0.808(1)	0.097(8)	Uani	1.00	1	d	.	.	.
C(38)	C	2.026(2)	0.215(3)	0.662(1)	0.089(8)	Uani	1.00	1	d	.	.	.
C(39)	C	1.5065(13)	0.912(3)	0.7870(12)	0.080(8)	Uani	1.00	1	d	.	.	.
C(40)	C	2.1508(13)	0.344(2)	0.8514(13)	0.076(6)	Uani	1.00	1	d	.	.	.
C(41)	C	1.4346(12)	0.390(2)	0.7243(10)	0.067(5)	Uani	1.00	1	d	.	.	.
C(42)	C	1.566(2)	0.586(3)	0.8639(13)	0.094(8)	Uani	1.00	1	d	.	.	.
C(43)	C	1.917(1)	0.818(2)	0.7332(11)	0.095(7)	Uani	1.00	1	d	.	.	.
C(44)	C	1.6092(13)	0.745(2)	0.8554(12)	0.082(7)	Uani	1.00	1	d	.	.	.
C(45)	C	1.356(2)	0.855(3)	0.6460(12)	0.103(8)	Uani	1.00	1	d	.	.	.
C(46)	C	2.238(2)	0.803(3)	0.886(2)	0.125(10)	Uani	1.00	1	d	.	.	.
C(47)	C	1.475(1)	0.998(2)	0.8366(11)	0.079(6)	Uani	1.00	1	d	.	.	.
C(48)	C	1.400(1)	0.892(2)	0.7154(11)	0.082(7)	Uani	1.00	1	d	.	.	.
C(49)	C	1.889(1)	0.459(3)	0.6529(11)	0.085(7)	Uani	1.00	1	d	.	.	.
C(50)	C	1.671(2)	0.785(4)	0.882(1)	0.107(7)	Uani	1.00	1	d	.	.	.
C(51)	C	1.369(2)	1.116(3)	0.880(1)	0.102(9)	Uani	1.00	1	d	.	.	.
C(52)	C	1.590(2)	0.191(2)	0.6637(12)	0.089(7)	Uani	1.00	1	d	.	.	.
C(53)	C	1.805(1)	0.910(2)	0.761(1)	0.109(8)	Uani	1.00	1	d	.	.	.
C(54)	C	2.259(2)	0.478(3)	0.9134(13)	0.095(8)	Uani	1.00	1	d	.	.	.
C(55)	C	1.9594(13)	0.715(2)	0.6960(10)	0.060(6)	Uani	1.00	1	d	.	.	.
C(56)	C	1.5775(10)	0.394(3)	0.7612(12)	0.072(6)	Uani	1.00	1	d	.	.	.
C(57)	C	2.0297(13)	0.887(2)	0.8097(12)	0.094(7)	Uani	1.00	1	d	.	.	.
C(58)	C	2.027(2)	0.724(2)	0.7100(12)	0.097(9)	Uani	1.00	1	d	.	.	.
C(59)	C	1.3582(13)	0.412(2)	0.702(1)	0.086(8)	Uani	1.00	1	d	.	.	.
C(60)	C	1.4856(12)	1.149(2)	0.9468(11)	0.090(6)	Uani	1.00	1	d	.	.	.
C(61)	C	1.845(1)	0.817(3)	0.719(2)	0.109(8)	Uani	1.00	1	d	.	.	.
C(62)	C	1.3988(13)	1.026(3)	0.8301(13)	0.079(7)	Uani	1.00	1	d	.	.	.
C(63)	C	2.084(2)	0.025(4)	0.559(2)	0.126(11)	Uani	1.00	1	d	.	.	.
C(64)	C	1.829(2)	0.439(3)	0.605(1)	0.096(8)	Uani	1.00	1	d	.	.	.
C(65)	C	1.987(1)	0.149(3)	0.5936(12)	0.085(6)	Uani	1.00	1	d	.	.	.
C(66)	C	1.6931(13)	0.289(3)	0.7371(12)	0.096(8)	Uani	1.00	1	d	.	.	.
C(67)	C	1.835(2)	1.008(3)	0.817(2)	0.102(11)	Uani	1.00	1	d	.	.	.
C(68)	C	2.017(2)	0.066(3)	0.549(1)	0.117(11)	Uani	1.00	1	d	.	.	.
C(69)	C	1.5890(13)	0.865(3)	0.7899(13)	0.080(6)	Uani	1.00	1	d	.	.	.
C(70)	C	1.412(1)	1.175(2)	0.9390(9)	0.087(7)	Uani	1.00	1	d	.	.	.
C(71)	C	1.2489(13)	0.557(3)	0.5560(13)	0.084(8)	Uani	1.00	1	d	.	.	.
C(72)	C	1.2430(13)	0.743(3)	0.592(1)	0.079(7)	Uani	1.00	1	d	.	.	.
C(73)	C	2.245(2)	0.653(3)	0.946(2)	0.116(11)	Uani	1.00	1	d	.	.	.
C(74)	C	1.265(2)	0.404(3)	0.6039(13)	0.086(7)	Uani	1.00	1	d	.	.	.
C(75)	C	1.5873(12)	0.579(3)	0.564(1)	0.109(7)	Uani	1.00	1	d	.	.	.
C(76)	C	2.320(2)	0.699(3)	0.983(2)	0.189(13)	Uani	1.00	1	d	.	.	.
C(77)	C	1.1804(12)	0.520(3)	0.5107(10)	0.096(6)	Uani	1.00	1	d	.	.	.
C(78)	C	2.190(2)	0.633(4)	0.995(2)	0.20(2)	Uani	1.00	1	d	.	.	.
C(79)	C	1.3073(11)	0.558(3)	0.5088(10)	0.092(7)	Uani	1.00	1	d	.	.	.
C(80)	C	1.907(2)	0.620(4)	0.947(2)	0.17(1)	Uani	1.00	1	d	.	.	.
H(1)	H	1.462(1)	0.230(2)	0.6461(10)	0.087(9)	Uiso	1.00	1	d	.	.	.
H(2)	H	1.572(2)	0.133(2)	0.6223(12)	0.109(8)	Uiso	1.00	1	d	.	.	.
H(3)	H	1.688(2)	0.129(3)	0.6514(10)	0.116(7)	Uiso	1.00	1	d	.	.	.
H(4)	H	1.7419(13)	0.281(3)	0.7484(12)	0.116(10)	Uiso	1.00	1	d	.	.	.
H(5)	H	1.6746(13)	0.443(3)	0.8161(11)	0.101(8)	Uiso	1.00	1	d	.	.	.
H(6)	H	1.567(2)	1.043(3)	0.8961(13)	0.114(8)	Uiso	1.00	1	d	.	.	.
H(7)	H	1.5132(12)	1.184(2)	0.9880(11)	0.108(7)	Uiso	1.00	1	d	.	.	.
H(8)	H	1.394(1)	1.236(2)	0.9758(9)	0.105(8)	Uiso	1.00	1	d	.	.	.
H(9)	H	1.321(2)	1.141(3)	0.871(1)	0.121(11)	Uiso	1.00	1	d	.	.	.
H(10)	H	1.3194(12)	0.987(2)	0.7645(12)	0.096(7)	Uiso	1.00	1	d	.	.	.

H(11)	H	2.190(1)	0.198(3)	0.7398(13)	0.106(9)	Uiso	1.00	1	d	.	.	.
H(12)	H	2.1715(12)	0.057(2)	0.6188(11)	0.098(7)	Uiso	1.00	1	d	.	.	.
H(13)	H	2.107(2)	-0.035(4)	0.526(2)	0.149(12)	Uiso	1.00	1	d	.	.	.
H(14)	H	1.990(2)	0.025(3)	0.508(1)	0.138(13)	Uiso	1.00	1	d	.	.	.
H(15)	H	1.939(1)	0.181(3)	0.5871(12)	0.100(7)	Uiso	1.00	1	d	.	.	.
H(16)	H	2.0502(13)	0.952(2)	0.8486(12)	0.110(8)	Uiso	1.00	1	d	.	.	.
H(17)	H	1.928(2)	1.074(3)	0.8748(13)	0.113(9)	Uiso	1.00	1	d	.	.	.
H(18)	H	1.808(2)	1.080(3)	0.844(2)	0.124(13)	Uiso	1.00	1	d	.	.	.
H(19)	H	1.756(1)	0.912(2)	0.750(1)	0.131(10)	Uiso	1.00	1	d	.	.	.
H(20)	H	1.825(1)	0.742(3)	0.683(2)	0.126(10)	Uiso	1.00	1	d	.	.	.
H(21)	H	1.2006(13)	0.730(3)	0.611(1)	0.093(7)	Uiso	1.00	1	d	.	.	.
H(22)	H	1.2394(13)	0.840(3)	0.560(1)	0.093(7)	Uiso	1.00	1	d	.	.	.
H(23)	H	1.257(2)	0.307(3)	0.5732(13)	0.102(7)	Uiso	1.00	1	d	.	.	.
H(24)	H	1.234(2)	0.398(3)	0.6379(13)	0.102(7)	Uiso	1.00	1	d	.	.	.
H(25)	H	2.261(2)	0.760(3)	0.850(2)	0.145(11)	Uiso	1.00	1	d	.	.	.
H(26)	H	2.257(2)	0.914(3)	0.902(2)	0.145(11)	Uiso	1.00	1	d	.	.	.
H(27)	H	2.245(2)	0.402(3)	0.9481(13)	0.114(8)	Uiso	1.00	1	d	.	.	.
H(28)	H	2.306(2)	0.456(3)	0.9083(13)	0.114(8)	Uiso	1.00	1	d	.	.	.
H(29)	H	1.5942(13)	0.804(3)	0.7483(13)	0.096(7)	Uiso	1.00	1	d	.	.	.
H(30)	H	1.6163(13)	0.970(3)	0.7926(13)	0.096(7)	Uiso	1.00	1	d	.	.	.
H(31)	H	1.529(2)	0.633(3)	0.8853(13)	0.113(9)	Uiso	1.00	1	d	.	.	.
H(32)	H	1.594(2)	0.512(3)	0.8956(13)	0.113(9)	Uiso	1.00	1	d	.	.	.
H(33)	H	1.901(2)	0.231(3)	0.697(1)	0.114(9)	Uiso	1.00	1	d	.	.	.
H(34)	H	1.908(2)	0.391(3)	0.747(1)	0.114(9)	Uiso	1.00	1	d	.	.	.
H(35)	H	1.971(2)	0.576(3)	0.6057(11)	0.098(8)	Uiso	1.00	1	d	.	.	.
H(36)	H	1.906(2)	0.695(3)	0.6014(11)	0.098(8)	Uiso	1.00	1	d	.	.	.
H(37)	H	1.799(2)	0.346(3)	0.615(1)	0.115(10)	Uiso	1.00	1	d	.	.	.
H(38)	H	1.816(2)	0.518(3)	0.568(1)	0.115(10)	Uiso	1.00	1	d	.	.	.
H(39)	H	1.695(2)	0.699(4)	0.911(1)	0.129(8)	Uiso	1.00	1	d	.	.	.
H(40)	H	1.690(2)	0.899(4)	0.878(1)	0.129(8)	Uiso	1.00	1	d	.	.	.
H(41)	H	1.3715(12)	0.343(2)	0.611(1)	0.121(8)	Uiso	1.00	1	d	.	.	.
H(42)	H	1.2882(12)	0.726(2)	0.6944(10)	0.101(7)	Uiso	1.00	1	d	.	.	.
H(43)	H	2.135(2)	0.844(2)	0.8947(12)	0.121(9)	Uiso	1.00	1	d	.	.	.
H(44)	H	2.2290(12)	0.436(2)	0.8080(11)	0.099(7)	Uiso	1.00	1	d	.	.	.
H(45)	H	1.888(2)	0.690(4)	0.980(2)	0.20(2)	Uiso	1.00	1	d	.	.	.
H(46)	H	1.934(2)	0.692(4)	0.920(2)	0.20(2)	Uiso	1.00	1	d	.	.	.
H(47)	H	1.5583(12)	0.544(3)	0.598(1)	0.132(8)	Uiso	1.00	1	d	.	.	.
H(48)	H	1.5959(12)	0.479(3)	0.537(1)	0.132(8)	Uiso	1.00	1	d	.	.	.
H(49)	H	2.351(2)	0.609(3)	0.972(2)	0.22(2)	Uiso	1.00	1	d	.	.	.
H(50)	H	2.336(2)	0.810(3)	0.969(2)	0.22(2)	Uiso	1.00	1	d	.	.	.
H(51)	H	2.318(2)	0.700(3)	1.032(2)	0.22(2)	Uiso	1.00	1	d	.	.	.
H(52)	H	2.159(2)	0.730(4)	0.990(2)	0.24(2)	Uiso	1.00	1	d	.	.	.
H(53)	H	2.165(2)	0.525(4)	0.990(2)	0.24(2)	Uiso	1.00	1	d	.	.	.
H(54)	H	2.216(2)	0.638(4)	1.040(2)	0.24(2)	Uiso	1.00	1	d	.	.	.
H(55)	H	1.3081(11)	0.454(3)	0.4813(10)	0.111(7)	Uiso	1.00	1	d	.	.	.
H(56)	H	1.3053(11)	0.659(3)	0.4799(10)	0.111(7)	Uiso	1.00	1	d	.	.	.
H(57)	H	1.3481(11)	0.562(3)	0.5409(10)	0.111(7)	Uiso	1.00	1	d	.	.	.
H(58)	H	1.1662(12)	0.618(3)	0.4818(10)	0.112(7)	Uiso	1.00	1	d	.	.	.
H(59)	H	1.1872(12)	0.419(3)	0.4830(10)	0.112(7)	Uiso	1.00	1	d	.	.	.
H(60)	H	1.1457(12)	0.495(3)	0.5397(10)	0.112(7)	Uiso	1.00	1	d	.	.	.

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_atom_site_aniso_label

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_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

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Cl(1)	0.118(7)	0.179(6)	0.105(5)	0.007(5)	0.010(4)	0.028(4)
Cl(2)	0.166(11)	0.173(7)	0.119(7)	0.039(6)	0.008(6)	-0.002(5)

C1(3)	0.143(8)	0.190(6)	0.133(5)	0.016(5)	0.012(4)	0.027(4)
C1(4)	0.139(9)	0.191(7)	0.36(2)	-0.026(7)	-0.053(9)	0.142(9)
O(1)	0.12(2)	0.18(2)	0.065(12)	-0.05(1)	0.001(11)	0.001(11)
O(5)	0.07(2)	0.118(11)	0.12(2)	0.016(9)	0.020(11)	0.014(9)
O(6)	0.066(10)	0.114(8)	0.075(9)	0.009(7)	0.005(7)	-0.022(7)
O(7)	0.065(11)	0.109(9)	0.079(11)	-0.002(7)	0.011(7)	-0.006(7)
O(8)	0.13(2)	0.120(10)	0.098(12)	-0.020(9)	0.050(10)	-0.008(8)
O(9)	0.086(13)	0.116(8)	0.093(11)	-0.014(7)	0.003(8)	-0.002(7)
O(10)	0.11(1)	0.085(7)	0.101(12)	0.012(7)	0.032(10)	0.004(6)
O(12)	0.11(2)	0.19(2)	0.096(12)	-0.028(12)	0.023(10)	-0.006(11)
N(1)	0.13(2)	0.104(11)	0.07(1)	0.010(10)	-0.004(12)	-0.008(9)
N(2)	0.06(2)	0.107(11)	0.08(1)	-0.001(9)	0.004(9)	0.009(9)
N(3)	0.06(2)	0.106(10)	0.14(2)	0.003(8)	-0.005(12)	-0.005(10)
N(4)	0.10(2)	0.086(9)	0.069(13)	0.002(9)	0.004(10)	-0.008(8)
C(4)	0.06(2)	0.090(11)	0.17(2)	0.024(10)	0.05(2)	0.050(13)
C(5)	0.09(2)	0.111(10)	0.049(11)	-0.007(10)	-0.006(10)	-0.014(8)
C(6)	0.10(2)	0.092(10)	0.09(2)	0.004(11)	0.012(12)	-0.018(9)
C(17)	0.05(2)	0.102(11)	0.051(11)	0.008(10)	-0.009(8)	0.010(9)
C(18)	0.07(2)	0.089(11)	0.10(2)	-0.004(9)	0.008(12)	-0.015(9)
C(19)	0.06(2)	0.096(10)	0.07(2)	0.007(10)	0.006(12)	0.014(10)
C(20)	0.028(13)	0.088(10)	0.10(1)	-0.003(8)	0.007(9)	0.009(8)
C(23)	0.08(1)	0.092(9)	0.071(12)	0.003(8)	0.032(10)	-0.001(9)
C(24)	0.10(2)	0.065(6)	0.055(11)	0.019(8)	0.027(11)	-0.001(6)
C(25)	0.07(2)	0.088(10)	0.08(1)	0.002(10)	0.012(11)	0.014(8)
C(27)	0.08(2)	0.123(13)	0.084(12)	0.030(10)	0.022(10)	-0.010(10)
C(28)	0.11(2)	0.074(11)	0.10(2)	-0.025(10)	-0.00(1)	0.003(10)
C(29)	0.13(2)	0.103(12)	0.056(12)	0.019(11)	0.000(10)	-0.009(8)
C(30)	0.053(12)	0.084(9)	0.10(1)	-0.002(6)	0.003(9)	0.029(8)
C(31)	0.08(2)	0.082(12)	0.058(13)	0.002(11)	0.011(11)	-0.018(9)
C(32)	0.11(2)	0.061(10)	0.14(2)	0.011(10)	0.05(1)	0.011(10)
C(33)	0.09(2)	0.061(9)	0.10(2)	0.005(9)	0.03(1)	0.004(8)
C(34)	0.09(2)	0.085(11)	0.076(12)	0.002(10)	0.037(11)	-0.012(8)
C(35)	0.13(3)	0.089(12)	0.067(11)	-0.024(12)	-0.029(11)	0.015(8)
C(36)	0.07(2)	0.087(8)	0.10(2)	-0.010(9)	0.01(1)	0.024(8)
C(37)	0.07(2)	0.096(10)	0.12(2)	0.007(10)	0.010(13)	0.013(10)
C(38)	0.07(2)	0.094(11)	0.11(2)	-0.002(10)	0.022(13)	0.016(9)
C(39)	0.06(2)	0.102(12)	0.08(2)	-0.008(10)	-0.000(11)	0.004(10)
C(40)	0.05(1)	0.075(8)	0.10(2)	0.012(7)	0.015(10)	0.021(8)
C(41)	0.07(2)	0.082(8)	0.046(9)	-0.008(8)	-0.003(7)	-0.016(6)
C(42)	0.08(2)	0.084(11)	0.12(2)	0.021(11)	0.012(12)	0.022(10)
C(43)	0.16(2)	0.070(7)	0.058(13)	0.011(8)	0.017(12)	-0.004(6)
C(44)	0.08(2)	0.093(9)	0.07(2)	0.025(8)	0.010(11)	0.011(8)
C(45)	0.11(2)	0.13(1)	0.068(11)	-0.010(13)	0.005(11)	-0.027(10)
C(46)	0.11(2)	0.11(2)	0.14(2)	0.005(13)	-0.04(2)	-0.004(12)
C(47)	0.13(2)	0.064(8)	0.047(11)	-0.004(9)	0.004(10)	-0.010(7)
C(48)	0.10(2)	0.065(7)	0.078(12)	-0.014(9)	0.016(11)	-0.010(7)
C(49)	0.07(2)	0.110(12)	0.078(10)	-0.018(10)	0.012(9)	-0.025(9)
C(50)	0.09(2)	0.144(13)	0.086(13)	0.019(11)	0.008(11)	0.014(9)
C(51)	0.09(3)	0.086(12)	0.12(2)	0.005(12)	-0.01(2)	-0.016(11)
C(52)	0.09(2)	0.106(10)	0.074(13)	0.040(10)	0.025(12)	-0.002(8)
C(53)	0.10(2)	0.083(10)	0.14(2)	0.003(10)	0.02(1)	-0.028(10)
C(54)	0.07(2)	0.111(11)	0.11(2)	0.008(10)	0.007(13)	-0.014(9)
C(55)	0.05(2)	0.074(10)	0.058(10)	-0.005(8)	0.007(9)	0.001(6)
C(56)	0.015(11)	0.087(12)	0.11(2)	-0.002(8)	0.011(8)	0.008(10)
C(57)	0.07(2)	0.079(9)	0.12(2)	-0.007(8)	-0.021(11)	0.013(8)
C(58)	0.17(3)	0.070(9)	0.05(1)	0.011(13)	0.02(2)	-0.005(8)
C(59)	0.07(2)	0.076(8)	0.12(2)	0.016(8)	0.038(13)	0.009(8)
C(60)	0.09(2)	0.086(9)	0.10(1)	-0.017(8)	0.010(9)	0.000(8)
C(61)	0.06(2)	0.118(12)	0.14(2)	0.007(10)	-0.040(13)	0.020(11)
C(62)	0.06(1)	0.087(11)	0.09(2)	0.008(8)	0.002(10)	-0.006(9)
C(63)	0.05(2)	0.13(2)	0.19(3)	0.03(2)	-0.01(2)	-0.04(2)

C(64)	0.10(2)	0.091(12)	0.10(2)	-0.014(11)	0.004(13)	-0.011(11)
C(65)	0.09(2)	0.097(8)	0.061(12)	-0.017(9)	-0.012(10)	0.002(8)
C(66)	0.07(2)	0.12(2)	0.10(2)	0.027(12)	0.022(11)	0.043(12)
C(67)	0.06(3)	0.097(13)	0.15(3)	-0.004(13)	0.03(2)	0.00(1)
C(68)	0.14(3)	0.14(2)	0.07(2)	0.03(2)	-0.02(2)	-0.042(13)
C(69)	0.06(1)	0.101(10)	0.08(1)	-0.008(8)	0.014(9)	0.016(8)
C(70)	0.14(2)	0.079(9)	0.042(10)	0.004(9)	0.027(9)	-0.006(6)
C(71)	0.04(2)	0.106(12)	0.10(2)	0.012(9)	-0.002(12)	-0.006(10)
C(72)	0.07(2)	0.090(11)	0.07(2)	-0.004(9)	-0.009(11)	0.003(10)
C(73)	0.14(3)	0.11(2)	0.08(2)	0.00(1)	-0.03(2)	-0.003(13)
C(74)	0.07(2)	0.099(12)	0.086(12)	-0.006(10)	-0.013(9)	0.016(8)
C(75)	0.047(13)	0.145(13)	0.14(2)	0.015(9)	0.015(10)	0.043(12)
C(76)	0.20(3)	0.11(2)	0.23(3)	0.04(2)	-0.09(3)	0.01(2)
C(77)	0.09(2)	0.113(11)	0.080(10)	-0.021(9)	-0.026(9)	-0.017(8)
C(78)	0.36(5)	0.12(2)	0.13(3)	0.04(2)	0.10(3)	0.01(2)
C(79)	0.08(1)	0.14(1)	0.062(12)	0.021(10)	0.009(8)	0.001(10)
C(80)	0.30(5)	0.10(2)	0.10(2)	-0.02(2)	0.01(2)	-0.004(12)

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C11 . C75 . 1.78(2)	yes
C12 . C80 . 1.72(3)	yes
C13 . C80 . 1.75(4)	yes
C14 . C75 . 1.66(3)	yes
O1 . C40 . 1.28(3)	yes
O5 . C35 . 1.24(3)	yes
O6 . C36 . 1.31(3)	yes
O7 . C58 . 1.42(3)	yes
O8 . C31 . 1.40(3)	yes
O9 . C59 . 1.31(3)	yes
O10 . C20 . 1.35(2)	yes
O12 . C45 . 1.18(3)	yes
N1 . C35 . 1.38(3)	yes
N1 . C46 . 1.45(4)	yes
N1 . H43 . 0.95006(6)	no
N2 . C40 . 1.30(3)	yes
N2 . C54 . 1.51(3)	yes
N2 . H44 . 0.95012(9)	no
N3 . C59 . 1.29(3)	yes
N3 . C74 . 1.49(3)	yes
N3 . H41 . 0.94990(5)	no
N4 . C45 . 1.37(3)	yes
N4 . C72 . 1.44(3)	yes
N4 . H42 . 0.95005(9)	no
C4 . C35 . 1.48(4)	yes
C4 . C57 . 1.30(3)	yes

C4	.	C58	.	1.40(4)	yes
C5	.	C49	.	1.57(3)	yes
C5	.	C55	.	1.53(3)	yes
C5	.	H35	.	0.95005(5)	no
C5	.	H36	.	0.950	no
C6	.	C33	.	1.41(3)	yes
C6	.	C49	.	1.45(3)	yes
C6	.	H33	.	0.950	no
C6	.	H34	.	0.95003(8)	no
C17	.	C24	.	1.37(3)	yes
C17	.	C52	.	1.35(3)	yes
C17	.	C56	.	1.42(3)	yes
C18	.	C19	.	1.35(3)	yes
C18	.	C25	.	1.54(4)	yes
C18	.	H11	.	0.95004(6)	no
C19	.	C31	.	1.46(3)	yes
C19	.	C40	.	1.47(3)	yes
C20	.	C37	.	1.36(3)	yes
C20	.	C41	.	1.44(3)	yes
C23	.	C25	.	1.47(3)	yes
C23	.	C63	.	1.34(4)	yes
C23	.	H12	.	0.95008(7)	no
C24	.	C41	.	1.46(3)	yes
C24	.	H1	.	0.94996(7)	no
C25	.	C38	.	1.31(4)	yes
C27	.	C47	.	1.34(3)	yes
C27	.	C60	.	1.49(3)	yes
C27	.	H6	.	0.95007(7)	no
C28	.	C32	.	1.54(4)	yes
C28	.	C67	.	1.39(4)	yes
C28	.	H17	.	0.95003(6)	no
C29	.	C52	.	1.34(3)	yes
C29	.	C66	.	1.43(3)	yes
C29	.	H3	.	0.950	no
C30	.	C48	.	1.42(3)	yes
C30	.	C62	.	1.32(3)	yes
C30	.	H10	.	0.95002(7)	no
C31	.	C33	.	1.36(4)	yes
C32	.	C43	.	1.46(4)	yes
C32	.	C57	.	1.47(3)	yes
C33	.	C38	.	1.50(3)	yes
C34	.	C56	.	1.42(3)	yes
C34	.	C66	.	1.41(3)	yes
C34	.	H5	.	0.95003(7)	no
C36	.	C39	.	1.44(3)	yes
C36	.	C48	.	1.35(3)	yes
C37	.	C42	.	1.49(3)	yes
C37	.	C56	.	1.48(3)	yes
C38	.	C65	.	1.53(4)	yes
C39	.	C47	.	1.36(3)	yes
C39	.	C69	.	1.64(3)	yes
C41	.	C59	.	1.51(3)	yes
C42	.	C44	.	1.49(3)	yes
C42	.	H31	.	0.95009(5)	no
C42	.	H32	.	0.950	no
C43	.	C55	.	1.40(3)	yes
C43	.	C61	.	1.40(4)	yes
C44	.	C50	.	1.28(3)	yes
C44	.	C69	.	1.58(3)	yes
C45	.	C48	.	1.54(3)	yes
C46	.	C73	.	1.62(4)	yes

C46	.	H25	.	0.95006(7)	no
C46	.	H26	.	0.950	no
C47	.	C62	.	1.50(4)	yes
C49	.	C64	.	1.40(4)	yes
C50	.	H39	.	0.950	no
C50	.	H40	.	0.950	no
C51	.	C62	.	1.36(3)	yes
C51	.	C70	.	1.41(3)	yes
C51	.	H9	.	0.95008(7)	no
C52	.	H2	.	0.94997(7)	no
C53	.	C61	.	1.37(4)	yes
C53	.	C67	.	1.39(4)	yes
C53	.	H19	.	0.95001(7)	no
C54	.	C73	.	1.50(3)	yes
C54	.	H27	.	0.94990(6)	no
C54	.	H28	.	0.94993(6)	no
C55	.	C58	.	1.31(4)	yes
C57	.	H16	.	0.95004(7)	no
C60	.	C70	.	1.44(3)	yes
C60	.	H7	.	0.94991(7)	no
C61	.	H20	.	0.95001(6)	no
C63	.	C68	.	1.33(4)	yes
C63	.	H13	.	0.94999(6)	no
C64	.	H37	.	0.950	no
C64	.	H38	.	0.95008(6)	no
C65	.	C68	.	1.27(4)	yes
C65	.	H15	.	0.95005(6)	no
C66	.	H4	.	0.94998(7)	no
C67	.	H18	.	0.950	no
C68	.	H14	.	0.94992(7)	no
C69	.	H29	.	0.94993(8)	no
C69	.	H30	.	0.950	no
C70	.	H8	.	0.94990(7)	no
C71	.	C72	.	1.58(3)	yes
C71	.	C74	.	1.49(3)	yes
C71	.	C77	.	1.53(3)	yes
C71	.	C79	.	1.55(3)	yes
C72	.	H21	.	0.94999(6)	no
C72	.	H22	.	0.95004(5)	no
C73	.	C76	.	1.58(4)	yes
C73	.	C78	.	1.53(5)	yes
C74	.	H23	.	0.95002(5)	no
C74	.	H24	.	0.94994(7)	no
C75	.	H47	.	0.94992(6)	no
C75	.	H48	.	0.950	no
C76	.	H49	.	0.950	no
C76	.	H50	.	0.950	no
C76	.	H51	.	0.94993(11)	no
C77	.	H58	.	0.950	no
C77	.	H59	.	0.950	no
C77	.	H60	.	0.95003(6)	no
C78	.	H52	.	0.950	no
C78	.	H53	.	0.950	no
C78	.	H54	.	0.95004(8)	no
C79	.	H55	.	0.950	no
C79	.	H56	.	0.950	no
C79	.	H57	.	0.95007(6)	no
C80	.	H45	.	0.94998(6)	no
C80	.	H46	.	0.950	no

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_geom_angle_atom_site_label_3
_geom_angle_site_symmetry_3
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_geom_angle_publ_flag
C35 . N1 . C46 . 122.3(28)    yes
C35 . N1 . H43 . 121.3(18)    no
C46 . N1 . H43 . 116.0(16)    no
C40 . N2 . C54 . 125.9(22)    yes
C40 . N2 . H44 . 119.6(14)    no
C54 . N2 . H44 . 114.5(14)    no
C59 . N3 . C74 . 125.7(25)    yes
C59 . N3 . H41 . 115.6(14)    no
C74 . N3 . H41 . 118.5(16)    no
C45 . N4 . C72 . 123.2(20)    yes
C45 . N4 . H42 . 114.6(12)    no
C72 . N4 . H42 . 121.6(14)    no
C35 . C4 . C57 . 112.7(27)    yes
C35 . C4 . C58 . 131.0(26)    yes
C57 . C4 . C58 . 116.2(26)    yes
C49 . C5 . C55 . 105.4(17)    yes
C49 . C5 . H35 . 112.8(12)    no
C55 . C5 . H35 . 112.8(15)    no
C49 . C5 . H36 . 109.7(14)    no
C55 . C5 . H36 . 106.5(12)    no
H35 . C5 . H36 . 109.457(6)    no
C33 . C6 . C49 . 128.5(24)    yes
C33 . C6 . H33 . 101.5(11)    no
C49 . C6 . H33 . 104.9(12)    no
C33 . C6 . H34 . 108.6(13)    no
C49 . C6 . H34 . 103.0(14)    no
H33 . C6 . H34 . 109.463(4)    no
C24 . C17 . C52 . 117.4(20)    yes
C24 . C17 . C56 . 115.4(21)    yes
C52 . C17 . C56 . 127.0(24)    yes
C19 . C18 . C25 . 113.3(25)    yes
C19 . C18 . H11 . 121.7(16)    no
C25 . C18 . H11 . 123.2(14)    no
C18 . C19 . C31 . 122.2(23)    yes
C18 . C19 . C40 . 119.7(24)    yes
C31 . C19 . C40 . 118.0(21)    yes
O10 . C20 . C37 . 118.9(21)    yes
O10 . C20 . C41 . 122.2(20)    yes
C37 . C20 . C41 . 118.8(19)    yes
C25 . C23 . C63 . 120.0(25)    yes
C25 . C23 . H12 . 122.4(15)    no
C63 . C23 . H12 . 117.5(17)    no
C17 . C24 . C41 . 123.7(20)    yes
C17 . C24 . H1 . 120.2(12)    no
C41 . C24 . H1 . 115.9(13)    no
C18 . C25 . C23 . 115.5(24)    yes
C18 . C25 . C38 . 123.2(21)    yes
C23 . C25 . C38 . 120.8(24)    yes
C47 . C27 . C60 . 117.2(25)    yes
C47 . C27 . H6 . 124.2(16)    no
C60 . C27 . H6 . 118.4(14)    no
C32 . C28 . C67 . 119.7(24)    yes
C32 . C28 . H17 . 116.7(16)    no
C67 . C28 . H17 . 123.0(16)    no

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C52 . C29 . C66 . 122.3(23)	yes
C52 . C29 . H3 . 119.7(11)	no
C66 . C29 . H3 . 118.0(16)	no
C48 . C30 . C62 . 127.1(24)	yes
C48 . C30 . H10 . 118.6(15)	no
C62 . C30 . H10 . 113.2(15)	no
O8 . C31 . C19 . 118.1(19)	yes
O8 . C31 . C33 . 118.3(23)	yes
C19 . C31 . C33 . 123.6(21)	yes
C28 . C32 . C43 . 113.2(26)	yes
C28 . C32 . C57 . 125.2(23)	yes
C43 . C32 . C57 . 121.4(22)	yes
C6 . C33 . C31 . 126.7(19)	yes
C6 . C33 . C38 . 117.3(24)	yes
C31 . C33 . C38 . 115.8(26)	yes
C56 . C34 . C66 . 123.0(23)	yes
C56 . C34 . H5 . 122.4(12)	no
C66 . C34 . H5 . 114.6(16)	no
O5 . C35 . N1 . 120.5(28)	yes
O5 . C35 . C4 . 115.9(22)	yes
N1 . C35 . C4 . 121.8(28)	yes
O6 . C36 . C39 . 123.2(25)	yes
O6 . C36 . C48 . 120.8(22)	yes
C39 . C36 . C48 . 116.0(21)	yes
C20 . C37 . C42 . 123.4(21)	yes
C20 . C37 . C56 . 119.6(23)	yes
C42 . C37 . C56 . 114.5(24)	yes
C25 . C38 . C33 . 120.3(27)	yes
C25 . C38 . C65 . 113.6(21)	yes
C33 . C38 . C65 . 125.3(26)	yes
C36 . C39 . C47 . 121.7(24)	yes
C36 . C39 . C69 . 111.8(22)	yes
C47 . C39 . C69 . 126.3(19)	yes
O1 . C40 . N2 . 123.3(24)	yes
O1 . C40 . C19 . 116.6(22)	yes
N2 . C40 . C19 . 120.0(23)	yes
C20 . C41 . C24 . 118.7(20)	yes
C20 . C41 . C59 . 116.1(18)	yes
C24 . C41 . C59 . 125.2(18)	yes
C37 . C42 . C44 . 126.8(21)	yes
C37 . C42 . H31 . 103.1(15)	no
C44 . C42 . H31 . 102.5(13)	no
C37 . C42 . H32 . 108.3(12)	no
C44 . C42 . H32 . 105.7(13)	no
H31 . C42 . H32 . 109.462(5)	no
C32 . C43 . C55 . 113.3(22)	yes
C32 . C43 . C61 . 123.6(23)	yes
C55 . C43 . C61 . 122.6(20)	yes
C42 . C44 . C50 . 130.8(21)	yes
C42 . C44 . C69 . 117.8(21)	yes
C50 . C44 . C69 . 109.0(20)	yes
O12 . C45 . N4 . 121.5(23)	yes
O12 . C45 . C48 . 122.5(29)	yes
N4 . C45 . C48 . 115.4(22)	yes
N1 . C46 . C73 . 106.4(25)	yes
N1 . C46 . H25 . 108.0(16)	no
C73 . C46 . H25 . 106.8(16)	no
N1 . C46 . H26 . 112.5(13)	no
C73 . C46 . H26 . 113.4(14)	no
H25 . C46 . H26 . 109.461(4)	no
C27 . C47 . C39 . 115.8(25)	yes

C27 . C47 . C62 . 122.3(22)	yes
C39 . C47 . C62 . 121.9(20)	yes
C30 . C48 . C36 . 120.7(20)	yes
C30 . C48 . C45 . 118.9(24)	yes
C36 . C48 . C45 . 119.6(20)	yes
C5 . C49 . C6 . 116.1(21)	yes
C5 . C49 . C64 . 109.7(21)	yes
C6 . C49 . C64 . 132.4(21)	yes
C44 . C50 . H39 . 117.6(14)	no
C44 . C50 . H40 . 122.0(14)	no
H39 . C50 . H40 . 120.000(4)	no
C62 . C51 . C70 . 119.1(28)	yes
C62 . C51 . H9 . 118.0(17)	no
C70 . C51 . H9 . 122.8(16)	no
C17 . C52 . C29 . 117.6(22)	yes
C17 . C52 . H2 . 124.4(15)	no
C29 . C52 . H2 . 117.2(11)	no
C61 . C53 . C67 . 122.1(28)	yes
C61 . C53 . H19 . 119.5(15)	no
C67 . C53 . H19 . 118.3(19)	no
N2 . C54 . C73 . 118.8(22)	yes
N2 . C54 . H27 . 101.5(13)	no
C73 . C54 . H27 . 98.7(17)	no
N2 . C54 . H28 . 111.8(13)	no
C73 . C54 . H28 . 114.5(18)	no
H27 . C54 . H28 . 109.455(5)	no
C5 . C55 . C43 . 124.1(22)	yes
C5 . C55 . C58 . 114.4(21)	yes
C43 . C55 . C58 . 120.5(18)	yes
C17 . C56 . C34 . 112.7(20)	yes
C17 . C56 . C37 . 122.4(21)	yes
C34 . C56 . C37 . 123.9(21)	yes
C4 . C57 . C32 . 120.0(21)	yes
C4 . C57 . H16 . 123.5(16)	no
C32 . C57 . H16 . 115.9(13)	no
O7 . C58 . C4 . 108.0(28)	yes
O7 . C58 . C55 . 124.5(20)	yes
C4 . C58 . C55 . 127.4(23)	yes
O9 . C59 . N3 . 121.7(24)	yes
O9 . C59 . C41 . 121.1(23)	yes
N3 . C59 . C41 . 116.6(20)	yes
C27 . C60 . C70 . 119.3(19)	yes
C27 . C60 . H7 . 120.1(14)	no
C70 . C60 . H7 . 120.5(11)	no
C43 . C61 . C53 . 119.8(23)	yes
C43 . C61 . H20 . 116.4(14)	no
C53 . C61 . H20 . 123.5(15)	no
C30 . C62 . C47 . 111.8(21)	yes
C30 . C62 . C51 . 126.7(25)	yes
C47 . C62 . C51 . 120.6(24)	yes
C23 . C63 . C68 . 120.1(26)	yes
C23 . C63 . H13 . 115.8(17)	no
C68 . C63 . H13 . 124.0(17)	no
C49 . C64 . H37 . 115.9(15)	no
C49 . C64 . H38 . 123.9(15)	no
H37 . C64 . H38 . 119.994(4)	no
C38 . C65 . C68 . 122.6(28)	yes
C38 . C65 . H15 . 113.6(14)	no
C68 . C65 . H15 . 123.7(20)	no
C29 . C66 . C34 . 117.2(24)	yes
C29 . C66 . H4 . 120.0(16)	no

C34 . C66 . H4 . 122.8(16)	no
C28 . C67 . C53 . 121.3(25)	yes
C28 . C67 . H18 . 117.0(16)	no
C53 . C67 . H18 . 121.7(19)	no
C63 . C68 . C65 . 122.6(30)	yes
C63 . C68 . H14 . 118.1(17)	no
C65 . C68 . H14 . 119.2(20)	no
C39 . C69 . C44 . 107.5(17)	yes
C39 . C69 . H29 . 106.3(12)	no
C44 . C69 . H29 . 111.7(12)	no
C39 . C69 . H30 . 111.3(10)	no
C44 . C69 . H30 . 110.5(12)	no
H29 . C69 . H30 . 109.461(5)	no
C51 . C70 . C60 . 121.3(20)	yes
C51 . C70 . H8 . 123.2(16)	no
C60 . C70 . H8 . 115.5(11)	no
C72 . C71 . C74 . 115.7(22)	yes
C72 . C71 . C77 . 108.1(17)	yes
C74 . C71 . C77 . 108.7(19)	yes
C72 . C71 . C79 . 110.7(19)	yes
C74 . C71 . C79 . 105.4(18)	yes
C77 . C71 . C79 . 108.0(19)	yes
N4 . C72 . C71 . 114.9(19)	yes
N4 . C72 . H21 . 104.1(14)	no
C71 . C72 . H21 . 100.9(13)	no
N4 . C72 . H22 . 112.1(12)	no
C71 . C72 . H22 . 114.2(14)	no
H21 . C72 . H22 . 109.458(5)	no
C46 . C73 . C54 . 108.5(24)	yes
C46 . C73 . C76 . 100.1(26)	yes
C54 . C73 . C76 . 101.0(24)	yes
C46 . C73 . C78 . 120.5(26)	yes
C54 . C73 . C78 . 110.6(26)	yes
C76 . C73 . C78 . 114.1(27)	yes
N3 . C74 . C71 . 119.4(21)	yes
N3 . C74 . H23 . 104.9(13)	no
C71 . C74 . H23 . 101.4(13)	no
N3 . C74 . H24 . 108.8(15)	no
C71 . C74 . H24 . 112.0(14)	no
H23 . C74 . H24 . 109.461(5)	no
C11 . C75 . C14 . 111.5(14)	yes
C11 . C75 . H47 . 108.0(8)	no
C14 . C75 . H47 . 115.3(10)	no
C11 . C75 . H48 . 109.2(9)	no
C14 . C75 . H48 . 103.3(10)	no
H47 . C75 . H48 . 109.456(3)	no
C73 . C76 . H49 . 108.3(16)	no
C73 . C76 . H50 . 111.9(15)	no
H49 . C76 . H50 . 109.468(5)	no
C73 . C76 . H51 . 108.1(20)	no
H49 . C76 . H51 . 109.472(6)	no
H50 . C76 . H51 . 109.471(6)	no
C71 . C77 . H58 . 111.9(11)	no
C71 . C77 . H59 . 107.5(11)	no
H58 . C77 . H59 . 109.476(7)	no
C71 . C77 . H60 . 108.9(13)	no
H58 . C77 . H60 . 109.466(4)	no
H59 . C77 . H60 . 109.468(5)	no
C73 . C78 . H52 . 110.8(15)	no
C73 . C78 . H53 . 113.7(15)	no
H52 . C78 . H53 . 109.478(5)	no

C73	.	C78	.	H54	.	103.8(18)	no
H52	.	C78	.	H54	.	109.473(3)	no
H53	.	C78	.	H54	.	109.470(4)	no
C71	.	C79	.	H55	.	113.2(11)	no
C71	.	C79	.	H56	.	112.1(11)	no
H55	.	C79	.	H56	.	109.477(7)	no
C71	.	C79	.	H57	.	102.8(11)	no
H55	.	C79	.	H57	.	109.472(4)	no
H56	.	C79	.	H57	.	109.464(4)	no
C12	.	C80	.	C13	.	115.1(17)	yes
C12	.	C80	.	H45	.	107.2(11)	no
C13	.	C80	.	H45	.	109.4(13)	no
C12	.	C80	.	H46	.	108.0(14)	no
C13	.	C80	.	H46	.	107.6(11)	no
H45	.	C80	.	H46	.	109.461(4)	no

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<u>geom_torsion_atom_site_label_1</u>							
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<u>geom_torsion_atom_site_label_3</u>							
<u>geom_torsion_site_symmetry_3</u>							
<u>geom_torsion_atom_site_label_4</u>							
<u>geom_torsion_site_symmetry_4</u>							
<u>geom_torsion</u>							
<u>geom_torsion_publ_flag</u>							
C46	.	N1	.	C35	.	O5	. 14.177 yes
C46	.	N1	.	C35	.	C4	. 177.912 yes
C35	.	N1	.	C46	.	C73	. -126.978 yes
C54	.	N2	.	C40	.	O1	. -4.645 yes
C54	.	N2	.	C40	.	C19	. 179.922 yes
C40	.	N2	.	C54	.	C73	. -81.710 yes
C74	.	N3	.	C59	.	O9	. 13.224 yes
C74	.	N3	.	C59	.	C41	. -175.509 yes
C59	.	N3	.	C74	.	C71	. 105.041 yes
C72	.	N4	.	C45	.	O12	. -13.404 yes
C72	.	N4	.	C45	.	C48	. 174.768 yes
C45	.	N4	.	C72	.	C71	. 92.110 yes
C57	.	C4	.	C35	.	O5	. -170.782 yes
C57	.	C4	.	C35	.	N1	. 24.780 yes
C58	.	C4	.	C35	.	O5	. 14.211 yes
C58	.	C4	.	C35	.	N1	. -150.228 yes
C35	.	C4	.	C57	.	C32	. 179.257 yes
C58	.	C4	.	C57	.	C32	. -4.939 yes
C35	.	C4	.	C58	.	O7	. -6.541 yes
C35	.	C4	.	C58	.	C55	. 170.490 yes
C57	.	C4	.	C58	.	O7	. 178.593 yes
C57	.	C4	.	C58	.	C55	. -4.376 yes
C55	.	C5	.	C49	.	C6	. -54.820 yes
C55	.	C5	.	C49	.	C64	. 138.314 yes
C49	.	C5	.	C55	.	C43	. -70.322 yes
C49	.	C5	.	C55	.	C58	. 120.761 yes
C49	.	C6	.	C33	.	C31	. 119.501 yes
C49	.	C6	.	C33	.	C38	. -56.352 yes
C33	.	C6	.	C49	.	C5	. -31.203 yes
C33	.	C6	.	C49	.	C64	. 131.962 yes
C52	.	C17	.	C24	.	C41	. 178.593 yes
C56	.	C17	.	C24	.	C41	. 2.023 yes
C24	.	C17	.	C52	.	C29	. 179.133 yes
C56	.	C17	.	C52	.	C29	. -4.747 yes

C24	.	C17	.	C56	.	C34	.	177.316	yes
C24	.	C17	.	C56	.	C37	.	8.190	yes
C52	.	C17	.	C56	.	C34	.	1.129	yes
C52	.	C17	.	C56	.	C37	.	-167.997	yes
C25	.	C18	.	C19	.	C31	.	-9.495	yes
C25	.	C18	.	C19	.	C40	.	175.575	yes
C19	.	C18	.	C25	.	C23	.	-172.218	yes
C19	.	C18	.	C25	.	C38	.	15.927	yes
C25	.	C18	.	C19	.	C31	.	-9.495	yes
C25	.	C18	.	C19	.	C40	.	175.575	yes
C18	.	C19	.	C31	.	O8	.	-177.949	yes
C18	.	C19	.	C31	.	C33	.	1.270	yes
C40	.	C19	.	C31	.	O8	.	-2.937	yes
C40	.	C19	.	C31	.	C33	.	176.282	yes
C18	.	C19	.	C40	.	O1	.	-138.222	yes
C18	.	C19	.	C40	.	N2	.	37.509	yes
C31	.	C19	.	C40	.	O1	.	46.637	yes
C31	.	C19	.	C40	.	N2	.	-137.632	yes
O10	.	C20	.	C37	.	C42	.	-15.984	yes
O10	.	C20	.	C37	.	C56	.	-177.148	yes
C41	.	C20	.	C37	.	C42	.	168.140	yes
C41	.	C20	.	C37	.	C56	.	6.976	yes
O10	.	C20	.	C41	.	C24	.	-173.082	yes
O10	.	C20	.	C41	.	C59	.	8.538	yes
C37	.	C20	.	C41	.	C24	.	2.652	yes
C37	.	C20	.	C41	.	C59	.	-175.729	yes
C63	.	C23	.	C25	.	C18	.	-178.010	yes
C63	.	C23	.	C25	.	C38	.	-5.943	yes
C25	.	C23	.	C63	.	C68	.	4.256	yes
C52	.	C17	.	C24	.	C41	.	178.593	yes
C56	.	C17	.	C24	.	C41	.	2.023	yes
C17	.	C24	.	C41	.	C20	.	-7.666	yes
C17	.	C24	.	C41	.	C59	.	170.554	yes
C19	.	C18	.	C25	.	C23	.	-172.218	yes
C19	.	C18	.	C25	.	C38	.	15.927	yes
C63	.	C23	.	C25	.	C18	.	-178.010	yes
C63	.	C23	.	C25	.	C38	.	-5.943	yes
C18	.	C25	.	C38	.	C33	.	-13.075	yes
C18	.	C25	.	C38	.	C65	.	176.637	yes
C23	.	C25	.	C38	.	C33	.	175.486	yes
C23	.	C25	.	C38	.	C65	.	5.197	yes
C60	.	C27	.	C47	.	C39	.	179.645	yes
C60	.	C27	.	C47	.	C62	.	-1.272	yes
C47	.	C27	.	C60	.	C70	.	0.859	yes
C67	.	C28	.	C32	.	C43	.	-2.901	yes
C67	.	C28	.	C32	.	C57	.	-177.527	yes
C32	.	C28	.	C67	.	C53	.	6.422	yes
C66	.	C29	.	C52	.	C17	.	5.260	yes
C52	.	C29	.	C66	.	C34	.	-2.403	yes
C62	.	C30	.	C48	.	C36	.	-7.640	yes
C62	.	C30	.	C48	.	C45	.	-177.824	yes
C48	.	C30	.	C62	.	C47	.	7.552	yes
C48	.	C30	.	C62	.	C51	.	177.182	yes
C18	.	C19	.	C31	.	O8	.	-177.949	yes
C18	.	C19	.	C31	.	C33	.	1.270	yes
C40	.	C19	.	C31	.	O8	.	-2.937	yes
C40	.	C19	.	C31	.	C33	.	176.282	yes
O8	.	C31	.	C33	.	C6	.	5.887	yes
O8	.	C31	.	C33	.	C38	.	-178.206	yes
C19	.	C31	.	C33	.	C6	.	-173.331	yes
C19	.	C31	.	C33	.	C38	.	2.576	yes

C67 . C28 . C32 . C43 . -2.901	yes
C67 . C28 . C32 . C57 . -177.527	yes
C28 . C32 . C43 . C55 . -174.321	yes
C28 . C32 . C43 . C61 . -1.677	yes
C57 . C32 . C43 . C55 . 0.537	yes
C57 . C32 . C43 . C61 . 173.181	yes
C28 . C32 . C57 . C4 . -179.126	yes
C43 . C32 . C57 . C4 . 6.661	yes
C49 . C6 . C33 . C31 . 119.501	yes
C49 . C6 . C33 . C38 . -56.352	yes
O8 . C31 . C33 . C6 . 5.887	yes
O8 . C31 . C33 . C38 . -178.206	yes
C19 . C31 . C33 . C6 . -173.331	yes
C19 . C31 . C33 . C38 . 2.576	yes
C6 . C33 . C38 . C25 . 179.893	yes
C6 . C33 . C38 . C65 . -11.025	yes
C31 . C33 . C38 . C25 . 3.585	yes
C31 . C33 . C38 . C65 . 172.667	yes
C66 . C34 . C56 . C17 . 2.021	yes
C66 . C34 . C56 . C37 . 170.960	yes
C56 . C34 . C66 . C29 . -1.438	yes
C46 . N1 . C35 . O5 . 14.177	yes
C46 . N1 . C35 . C4 . 177.912	yes
C57 . C4 . C35 . O5 . -170.782	yes
C57 . C4 . C35 . N1 . 24.780	yes
C58 . C4 . C35 . O5 . 14.211	yes
C58 . C4 . C35 . N1 . -150.228	yes
O6 . C36 . C39 . C47 . 172.676	yes
O6 . C36 . C39 . C69 . -2.221	yes
C48 . C36 . C39 . C47 . -7.867	yes
C48 . C36 . C39 . C69 . 177.236	yes
O6 . C36 . C48 . C30 . -173.786	yes
O6 . C36 . C48 . C45 . -3.667	yes
C39 . C36 . C48 . C30 . 6.743	yes
C39 . C36 . C48 . C45 . 176.862	yes
O10 . C20 . C37 . C42 . -15.984	yes
O10 . C20 . C37 . C56 . -177.148	yes
C41 . C20 . C37 . C42 . 168.140	yes
C41 . C20 . C37 . C56 . 6.976	yes
C20 . C37 . C42 . C44 . -104.124	yes
C56 . C37 . C42 . C44 . 57.901	yes
C20 . C37 . C56 . C17 . -13.140	yes
C20 . C37 . C56 . C34 . 178.958	yes
C42 . C37 . C56 . C17 . -175.898	yes
C42 . C37 . C56 . C34 . 16.200	yes
C18 . C25 . C38 . C33 . -13.075	yes
C18 . C25 . C38 . C65 . 176.637	yes
C23 . C25 . C38 . C33 . 175.486	yes
C23 . C25 . C38 . C65 . 5.197	yes
C6 . C33 . C38 . C25 . 179.893	yes
C6 . C33 . C38 . C65 . -11.025	yes
C31 . C33 . C38 . C25 . 3.585	yes
C31 . C33 . C38 . C65 . 172.667	yes
C25 . C38 . C65 . C68 . -3.672	yes
C33 . C38 . C65 . C68 . -173.387	yes
O6 . C36 . C39 . C47 . 172.676	yes
O6 . C36 . C39 . C69 . -2.221	yes
C48 . C36 . C39 . C47 . -7.867	yes
C48 . C36 . C39 . C69 . 177.236	yes
C36 . C39 . C47 . C27 . -172.056	yes
C36 . C39 . C47 . C62 . 8.857	yes

C69	.	C39	.	C47	.	C27	.	2.066	yes
C69	.	C39	.	C47	.	C62	.	-177.021	yes
C36	.	C39	.	C69	.	C44	.	-125.816	yes
C47	.	C39	.	C69	.	C44	.	59.572	yes
C54	.	N2	.	C40	.	O1	.	-4.645	yes
C54	.	N2	.	C40	.	C19	.	179.922	yes
C18	.	C19	.	C40	.	O1	.	-138.222	yes
C18	.	C19	.	C40	.	N2	.	37.509	yes
C31	.	C19	.	C40	.	O1	.	46.637	yes
C31	.	C19	.	C40	.	N2	.	-137.632	yes
O10	.	C20	.	C41	.	C24	.	-173.082	yes
O10	.	C20	.	C41	.	C59	.	8.538	yes
C37	.	C20	.	C41	.	C24	.	2.652	yes
C37	.	C20	.	C41	.	C59	.	-175.729	yes
C17	.	C24	.	C41	.	C20	.	-7.666	yes
C17	.	C24	.	C41	.	C59	.	170.554	yes
C20	.	C41	.	C59	.	O9	.	-27.614	yes
C20	.	C41	.	C59	.	N3	.	161.060	yes
C24	.	C41	.	C59	.	O9	.	154.124	yes
C24	.	C41	.	C59	.	N3	.	-17.203	yes
C20	.	C37	.	C42	.	C44	.	-104.124	yes
C56	.	C37	.	C42	.	C44	.	57.901	yes
C37	.	C42	.	C44	.	C50	.	-126.973	yes
C37	.	C42	.	C44	.	C69	.	33.127	yes
C28	.	C32	.	C43	.	C55	.	-174.321	yes
C28	.	C32	.	C43	.	C61	.	-1.677	yes
C57	.	C32	.	C43	.	C55	.	0.537	yes
C57	.	C32	.	C43	.	C61	.	173.181	yes
C32	.	C43	.	C55	.	C5	.	-177.428	yes
C32	.	C43	.	C55	.	C58	.	-9.151	yes
C61	.	C43	.	C55	.	C5	.	9.845	yes
C61	.	C43	.	C55	.	C58	.	178.122	yes
C32	.	C43	.	C61	.	C53	.	2.872	yes
C55	.	C43	.	C61	.	C53	.	174.849	yes
C37	.	C42	.	C44	.	C50	.	-126.973	yes
C37	.	C42	.	C44	.	C69	.	33.127	yes
C42	.	C44	.	C69	.	C39	.	51.590	yes
C50	.	C44	.	C69	.	C39	.	-144.230	yes
C72	.	N4	.	C45	.	O12	.	-13.404	yes
C72	.	N4	.	C45	.	C48	.	174.768	yes
O12	.	C45	.	C48	.	C30	.	137.879	yes
O12	.	C45	.	C48	.	C36	.	-32.416	yes
N4	.	C45	.	C48	.	C30	.	-50.387	yes
N4	.	C45	.	C48	.	C36	.	139.319	yes
C35	.	N1	.	C46	.	C73	.	-126.978	yes
N1	.	C46	.	C73	.	C54	.	91.708	yes
N1	.	C46	.	C73	.	C76	.	-162.970	yes
N1	.	C46	.	C73	.	C78	.	-37.103	yes
C60	.	C27	.	C47	.	C39	.	179.645	yes
C60	.	C27	.	C47	.	C62	.	-1.272	yes
C36	.	C39	.	C47	.	C27	.	-172.056	yes
C36	.	C39	.	C47	.	C62	.	8.857	yes
C69	.	C39	.	C47	.	C27	.	2.066	yes
C69	.	C39	.	C47	.	C62	.	-177.021	yes
C27	.	C47	.	C62	.	C30	.	172.812	yes
C27	.	C47	.	C62	.	C51	.	2.463	yes
C39	.	C47	.	C62	.	C30	.	-8.160	yes
C39	.	C47	.	C62	.	C51	.	-178.509	yes
C62	.	C30	.	C48	.	C36	.	-7.640	yes
C62	.	C30	.	C48	.	C45	.	-177.824	yes
O6	.	C36	.	C48	.	C30	.	-173.786	yes

O6 . C36 . C48 . C45 . -3.667	yes
C39 . C36 . C48 . C30 . 6.743	yes
C39 . C36 . C48 . C45 . 176.862	yes
O12 . C45 . C48 . C30 . 137.879	yes
O12 . C45 . C48 . C36 . -32.416	yes
N4 . C45 . C48 . C30 . -50.387	yes
N4 . C45 . C48 . C36 . 139.319	yes
C55 . C5 . C49 . C6 . -54.820	yes
C55 . C5 . C49 . C64 . 138.314	yes
C33 . C6 . C49 . C5 . -31.203	yes
C33 . C6 . C49 . C64 . 131.962	yes
C70 . C51 . C62 . C30 . -171.844	yes
C70 . C51 . C62 . C47 . -3.046	yes
C62 . C51 . C70 . C60 . 2.680	yes
C24 . C17 . C52 . C29 . 179.133	yes
C56 . C17 . C52 . C29 . -4.747	yes
C66 . C29 . C52 . C17 . 5.260	yes
C67 . C53 . C61 . C43 . 0.674	yes
C61 . C53 . C67 . C28 . -5.425	yes
C40 . N2 . C54 . C73 . -81.710	yes
N2 . C54 . C73 . C46 . -50.998	yes
N2 . C54 . C73 . C76 . -155.683	yes
N2 . C54 . C73 . C78 . 83.179	yes
C49 . C5 . C55 . C43 . -70.322	yes
C49 . C5 . C55 . C58 . 120.761	yes
C32 . C43 . C55 . C5 . -177.428	yes
C32 . C43 . C55 . C58 . -9.151	yes
C61 . C43 . C55 . C5 . 9.845	yes
C61 . C43 . C55 . C58 . 178.122	yes
C5 . C55 . C58 . O7 . -1.919	yes
C5 . C55 . C58 . C4 . -178.494	yes
C43 . C55 . C58 . O7 . -171.271	yes
C43 . C55 . C58 . C4 . 12.155	yes
C24 . C17 . C56 . C34 . 177.316	yes
C24 . C17 . C56 . C37 . 8.190	yes
C52 . C17 . C56 . C34 . 1.129	yes
C52 . C17 . C56 . C37 . -167.997	yes
C66 . C34 . C56 . C17 . 2.021	yes
C66 . C34 . C56 . C37 . 170.960	yes
C20 . C37 . C56 . C17 . -13.140	yes
C20 . C37 . C56 . C34 . 178.958	yes
C42 . C37 . C56 . C17 . -175.898	yes
C42 . C37 . C56 . C34 . 16.200	yes
C35 . C4 . C57 . C32 . 179.257	yes
C58 . C4 . C57 . C32 . -4.939	yes
C28 . C32 . C57 . C4 . -179.126	yes
C43 . C32 . C57 . C4 . 6.661	yes
C35 . C4 . C58 . O7 . -6.541	yes
C35 . C4 . C58 . C55 . 170.490	yes
C57 . C4 . C58 . O7 . 178.593	yes
C57 . C4 . C58 . C55 . -4.376	yes
C5 . C55 . C58 . O7 . -1.919	yes
C5 . C55 . C58 . C4 . -178.494	yes
C43 . C55 . C58 . O7 . -171.271	yes
C43 . C55 . C58 . C4 . 12.155	yes
C74 . N3 . C59 . O9 . 13.224	yes
C74 . N3 . C59 . C41 . -175.509	yes
C20 . C41 . C59 . O9 . -27.614	yes
C20 . C41 . C59 . N3 . 161.060	yes
C24 . C41 . C59 . O9 . 154.124	yes
C24 . C41 . C59 . N3 . -17.203	yes

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C47 . C27 . C60 . C70 . 0.859    yes
C27 . C60 . C70 . C51 . -1.554   yes
C32 . C43 . C61 . C53 . 2.872    yes
C55 . C43 . C61 . C53 . 174.849   yes
C67 . C53 . C61 . C43 . 0.674    yes
C48 . C30 . C62 . C47 . 7.552    yes
C48 . C30 . C62 . C51 . 177.182   yes
C27 . C47 . C62 . C30 . 172.812   yes
C27 . C47 . C62 . C51 . 2.463    yes
C39 . C47 . C62 . C30 . -8.160    yes
C39 . C47 . C62 . C51 . -178.509  yes
C70 . C51 . C62 . C30 . -171.844  yes
C70 . C51 . C62 . C47 . -3.046    yes
C25 . C23 . C63 . C68 . 4.256    yes
C23 . C63 . C68 . C65 . -2.683    yes
C25 . C38 . C65 . C68 . -3.672    yes
C33 . C38 . C65 . C68 . -173.387  yes
C38 . C65 . C68 . C63 . 2.324    yes
C52 . C29 . C66 . C34 . -2.403    yes
C56 . C34 . C66 . C29 . -1.438    yes
C32 . C28 . C67 . C53 . 6.422    yes
C61 . C53 . C67 . C28 . -5.425    yes
C23 . C63 . C68 . C65 . -2.683    yes
C38 . C65 . C68 . C63 . 2.324    yes
C36 . C39 . C69 . C44 . -125.816  yes
C47 . C39 . C69 . C44 . 59.572    yes
C42 . C44 . C69 . C39 . 51.590    yes
C50 . C44 . C69 . C39 . -144.230  yes
C62 . C51 . C70 . C60 . 2.680    yes
C27 . C60 . C70 . C51 . -1.554   yes
C74 . C71 . C72 . N4 . 40.225    yes
C77 . C71 . C72 . N4 . 162.308    yes
C79 . C71 . C72 . N4 . -79.632    yes
C72 . C71 . C74 . N3 . -76.592    yes
C77 . C71 . C74 . N3 . 161.635    yes
C79 . C71 . C74 . N3 . 46.112    yes
C45 . N4 . C72 . C71 . 92.110    yes
C74 . C71 . C72 . N4 . 40.225    yes
C77 . C71 . C72 . N4 . 162.308    yes
C79 . C71 . C72 . N4 . -79.632    yes
N1 . C46 . C73 . C54 . 91.708    yes
N1 . C46 . C73 . C76 . -162.970  yes
N1 . C46 . C73 . C78 . -37.103    yes
N2 . C54 . C73 . C46 . -50.998    yes
N2 . C54 . C73 . C76 . -155.683  yes
N2 . C54 . C73 . C78 . 83.179    yes
C59 . N3 . C74 . C71 . 105.041    yes
C72 . C71 . C74 . N3 . -76.592    yes
C77 . C71 . C74 . N3 . 161.635    yes
C79 . C71 . C74 . N3 . 46.112    yes
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C11 . H1 2_856 3.05(2)    no
C11 . H2 2_856 3.33(3)    no
C11 . H41 2_856 3.14(3)   no

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C11	.	H47	2_856	3.54(3)	no
C11	.	H48	2_856	3.27(3)	no
C11	.	H55	2_856	3.29(2)	no
C11	.	H57	2_856	3.44(2)	no
C12	.	H16	2_947	3.17(3)	no
C12	.	H17	2_947	3.29(3)	no
C12	.	H43	2_947	3.22(3)	no
C12	.	H46	2_947	3.26(4)	no
C12	.	H52	2_947	3.00(4)	no
C13	.	H18	1_545	3.54(3)	no
C13	.	H52	2_947	3.26(3)	no
C13	.	H54	2_947	3.49(3)	no
C14	.	H55	2_856	2.85(2)	no
O1	.	C80	2_947	3.29(4)	yes
O1	.	H16	1_545	3.15(3)	no
O1	.	H43	1_545	3.45(3)	no
O1	.	H45	2_947	2.40(4)	no
O5	.	O9	1_655	3.492(11)	yes
O5	.	N4	1_655	3.14(3)	yes
O5	.	C72	1_655	3.48(4)	yes
O5	.	H10	1_655	3.29(3)	no
O5	.	H11	1_565	3.46(3)	no
O5	.	H12	1_565	3.49(3)	no
O5	.	H21	1_655	2.81(4)	no
O5	.	H42	1_655	2.51(3)	no
O6	.	C52	1_565	3.47(3)	yes
O6	.	H1	1_565	3.35(2)	no
O6	.	H2	1_565	3.10(3)	no
O7	.	C23	1_565	3.59(2)	yes
O7	.	H21	1_655	2.90(3)	no
O7	.	H60	1_655	3.23(2)	no
O8	.	C28	1_545	3.58(3)	yes
O8	.	H16	1_545	3.49(2)	no
O8	.	H17	1_545	3.05(3)	no
O9	.	N2	1_455	3.02(3)	yes
O9	.	C54	1_455	3.55(3)	yes
O9	.	H9	1_545	3.31(3)	no
O9	.	H10	1_545	3.45(2)	no
O9	.	H11	1_455	3.05(3)	no
O9	.	H25	1_455	3.36(4)	no
O9	.	H28	1_455	3.16(3)	no
O9	.	H44	1_455	2.16(3)	no
O10	.	H25	1_455	3.51(4)	no
O10	.	H28	1_455	2.95(3)	no
O10	.	H49	1_455	3.26(4)	no
O12	.	C75	2_856	3.55(3)	yes
O12	.	H1	1_565	3.25(3)	no
O12	.	H41	1_565	3.55(3)	no
O12	.	H48	2_856	2.74(3)	no
N2	.	H9	1_645	2.99(3)	no
N4	.	H12	1_465	3.19(3)	no
C4	.	C25	1_565	3.42(3)	yes
C5	.	H13	2_956	3.24(4)	no
C5	.	H14	2_956	3.29(4)	no
C17	.	C39	1_545	3.48(3)	yes
C17	.	H30	1_545	3.17(3)	no
C18	.	C35	1_545	3.45(3)	yes
C18	.	H24	1_655	3.01(4)	no
C19	.	C57	1_545	3.50(3)	yes
C19	.	H16	1_545	3.13(3)	no
C23	.	C72	1_645	3.51(3)	yes

C23	.	H21	1_645	3.04(3)	no
C23	.	H22	1_645	3.18(3)	no
C23	.	H23	1_655	3.31(3)	no
C23	.	H24	1_655	3.23(3)	no
C23	.	H60	1_655	3.54(3)	no
C24	.	C36	1_545	3.30(2)	yes
C24	.	C39	1_545	3.47(2)	yes
C24	.	C48	1_545	3.49(3)	yes
C25	.	H24	1_655	3.39(4)	no
C27	.	C37	1_565	3.59(3)	yes
C27	.	H49	2_957	3.48(4)	no
C27	.	H51	2_957	3.54(5)	no
C28	.	H33	1_565	3.22(4)	no
C28	.	H34	1_565	3.42(3)	no
C29	.	H19	1_545	3.07(3)	no
C29	.	H29	1_545	3.54(3)	no
C29	.	H30	1_545	2.99(3)	no
C29	.	H56	2_846	3.26(3)	no
C30	.	C41	1_565	3.50(2)	yes
C30	.	C59	1_565	3.51(2)	yes
C30	.	H25	1_455	3.23(4)	no
C31	.	C32	1_545	3.58(3)	yes
C31	.	C57	1_545	3.39(3)	yes
C31	.	H16	1_545	3.15(2)	no
C31	.	H17	1_545	3.54(3)	no
C32	.	C33	1_565	3.40(3)	yes
C32	.	H33	1_565	3.18(3)	no
C33	.	C57	1_545	3.59(3)	yes
C34	.	H30	1_545	3.22(3)	no
C35	.	H11	1_565	3.36(3)	no
C36	.	H1	1_565	3.12(2)	no
C36	.	H2	1_565	3.58(3)	no
C40	.	H16	1_545	3.54(3)	no
C41	.	C62	1_545	3.55(3)	yes
C42	.	H7	2_847	3.51(3)	no
C42	.	H8	2_847	3.33(3)	no
C43	.	H33	1_565	3.20(3)	no
C44	.	H8	2_847	3.30(3)	no
C45	.	H1	1_565	3.51(4)	no
C46	.	C51	1_655	3.50(4)	yes
C46	.	H9	1_655	3.06(4)	no
C46	.	H10	1_655	3.32(4)	no
C48	.	H1	1_565	3.19(3)	no
C49	.	H13	2_956	3.49(4)	no
C50	.	H8	2_847	3.20(3)	no
C50	.	H51	2_957	3.55(4)	no
C51	.	C54	1_465	3.59(3)	yes
C51	.	H25	1_455	3.42(4)	no
C51	.	H26	1_455	2.75(5)	no
C51	.	H28	1_465	2.93(3)	no
C51	.	H50	1_455	3.01(4)	no
C52	.	C69	1_545	3.48(3)	yes
C52	.	H29	1_545	3.35(3)	no
C52	.	H30	1_545	3.01(3)	no
C53	.	C66	1_565	3.592(18)	yes
C53	.	H3	1_565	3.37(4)	no
C53	.	H4	1_565	3.058(18)	no
C53	.	H33	1_565	3.38(3)	no
C54	.	H8	1_645	3.31(4)	no
C54	.	H9	1_645	2.97(3)	no
C56	.	H30	1_545	3.33(3)	no

C59	.	H10	1_545	3.55(2)	no
C59	.	H44	1_455	3.44(3)	no
C60	.	H31	2_857	3.32(3)	no
C60	.	H49	2_957	3.38(4)	no
C61	.	H33	1_565	3.36(3)	no
C62	.	H25	1_455	3.41(4)	no
C62	.	H26	1_455	3.36(4)	no
C62	.	H50	1_455	3.51(5)	no
C63	.	H21	1_645	3.26(4)	no
C63	.	H22	1_645	3.33(4)	no
C63	.	H35	2_946	3.27(4)	no
C63	.	H36	2_946	3.40(4)	no
C63	.	H38	2_946	3.33(4)	no
C64	.	H13	2_956	2.98(4)	no
C64	.	H22	2_846	3.43(4)	no
C64	.	H58	2_846	2.97(3)	no
C65	.	H14	2_956	3.52(3)	no
C65	.	H58	2_846	3.17(3)	no
C66	.	H18	1_545	3.27(4)	no
C66	.	H19	1_545	3.098(18)	no
C66	.	H30	1_545	3.10(3)	no
C67	.	H4	1_565	2.96(3)	no
C67	.	H33	1_565	3.27(4)	no
C67	.	H34	1_565	3.57(3)	no
C67	.	H54	2_957	3.22(5)	no
C68	.	H35	2_946	3.05(3)	no
C68	.	H36	2_946	3.59(4)	no
C68	.	H58	2_846	3.56(4)	no
C68	.	H60	2_846	3.46(4)	no
C70	.	H28	1_465	2.97(3)	no
C70	.	H31	2_857	3.50(3)	no
C70	.	H32	2_857	3.47(3)	no
C70	.	H49	1_465	3.56(3)	no
C70	.	H50	1_455	3.21(4)	no
C72	.	H12	1_465	2.83(3)	no
C72	.	H13	1_465	3.26(4)	no
C74	.	H11	1_455	3.54(4)	no
C74	.	H12	1_455	3.22(3)	no
C76	.	H6	2_947	3.24(4)	no
C76	.	H7	2_947	3.22(5)	no
C76	.	H40	2_947	3.56(4)	no
C77	.	H14	2_856	3.29(5)	no
C77	.	H15	2_856	3.08(3)	no
C77	.	H36	2_846	3.57(3)	no
C77	.	H37	2_856	3.53(3)	no
C78	.	H18	2_947	3.16(5)	no
C79	.	H3	2_856	3.18(3)	no
C80	.	H52	2_947	3.49(4)	no
H2	.	H29	1_545	3.49(3)	no
H2	.	H30	1_545	3.55(3)	no
H2	.	H55	2_846	3.53(3)	no
H2	.	H56	2_846	3.29(3)	no
H3	.	H19	1_545	2.75(3)	no
H3	.	H30	1_545	3.45(3)	no
H3	.	H55	2_846	2.92(3)	no
H3	.	H56	2_846	2.59(3)	no
H4	.	H18	1_545	2.61(4)	no
H4	.	H19	1_545	2.801(19)	no
H4	.	H30	1_545	3.57(3)	no
H5	.	H51	2_947	3.48(4)	no
H6	.	H8	2_847	3.42(3)	no

H6	.	H32	1_565	3.58(3)	no
H6	.	H49	2_957	2.90(4)	no
H6	.	H51	2_957	2.76(4)	no
H7	.	H31	2_857	2.72(3)	no
H7	.	H32	1_565	3.53(3)	no
H7	.	H32	2_857	3.51(3)	no
H7	.	H49	2_957	2.72(5)	no
H7	.	H50	2_957	3.10(4)	no
H7	.	H51	2_957	3.35(5)	no
H8	.	H27	1_465	3.15(4)	no
H8	.	H28	1_465	2.63(3)	no
H8	.	H31	2_857	3.04(3)	no
H8	.	H32	2_857	3.01(3)	no
H8	.	H39	2_857	2.98(3)	no
H8	.	H49	1_465	2.93(3)	no
H8	.	H50	1_455	3.41(3)	no
H9	.	H11	1_465	3.43(4)	no
H9	.	H25	1_455	3.12(4)	no
H9	.	H26	1_455	2.25(4)	no
H9	.	H27	1_465	2.97(3)	no
H9	.	H28	1_465	2.51(3)	no
H9	.	H44	1_465	3.03(3)	no
H9	.	H50	1_455	3.14(4)	no
H10	.	H11	1_465	2.98(2)	no
H10	.	H25	1_455	2.73(4)	no
H10	.	H26	1_455	3.12(4)	no
H11	.	H24	1_655	2.72(3)	no
H12	.	H21	1_645	2.55(3)	no
H12	.	H22	1_645	2.47(3)	no
H12	.	H23	1_655	2.73(3)	no
H12	.	H24	1_655	2.85(3)	no
H12	.	H42	1_645	3.58(3)	no
H13	.	H15	2_946	3.12(4)	no
H13	.	H21	1_645	2.91(4)	no
H13	.	H22	1_645	2.75(4)	no
H13	.	H35	2_946	2.94(4)	no
H13	.	H36	2_946	3.01(4)	no
H13	.	H37	2_946	3.58(4)	no
H13	.	H38	2_946	2.52(4)	no
H13	.	H58	1_645	3.03(3)	no
H14	.	H15	2_946	3.56(3)	no
H14	.	H35	2_946	2.46(4)	no
H14	.	H36	1_545	3.60(4)	no
H14	.	H36	2_946	3.37(4)	no
H14	.	H58	2_846	3.15(4)	no
H14	.	H59	2_846	3.56(4)	no
H14	.	H60	2_846	2.70(4)	no
H15	.	H58	2_846	2.36(3)	no
H15	.	H59	2_846	3.32(3)	no
H15	.	H60	2_846	3.14(3)	no
H17	.	H34	1_565	3.44(3)	no
H17	.	H52	2_957	3.50(4)	no
H17	.	H53	2_957	3.40(5)	no
H17	.	H54	2_957	3.46(5)	no
H18	.	H52	2_957	3.42(5)	no
H18	.	H53	2_957	3.25(5)	no
H18	.	H54	2_957	2.41(5)	no
H20	.	H59	2_856	3.48(3)	no
H22	.	H23	1_565	3.54(3)	no
H22	.	H37	2_856	3.40(4)	no
H22	.	H38	2_856	2.94(4)	no

H24	.	H44	1_455	3.34(3)	no
H25	.	H42	1_655	3.15(4)	no
H27	.	H39	2_947	3.23(4)	no
H27	.	H40	2_947	3.48(4)	no
H27	.	H45	2_947	3.47(5)	no
H32	.	H50	2_947	3.20(4)	no
H32	.	H51	2_947	3.15(4)	no
H36	.	H59	2_856	2.85(3)	no
H37	.	H56	2_846	2.93(3)	no
H37	.	H58	2_846	2.70(3)	no
H38	.	H58	2_846	3.21(3)	no
H38	.	H59	2_856	3.19(3)	no
H40	.	H49	2_957	3.51(5)	no
H40	.	H51	2_957	2.89(4)	no
H40	.	H54	2_957	2.91(4)	no
H42	.	H44	1_455	3.412(12)	no
H45	.	H53	2_957	2.82(4)	no
H48	.	H56	2_846	3.13(3)	no

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