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Dioxopromethazinium picrate

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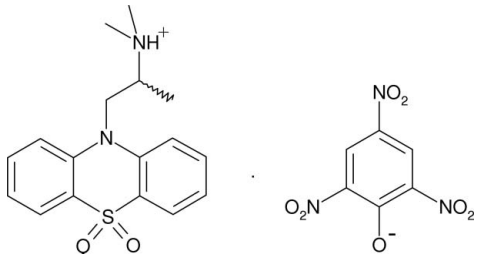
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.154; data-to-parameter ratio = 13.6.

The title compound {systematic name: [1-(9,9-dioxo-10*H*-phenothiazin-10-yl)-2-propyl]dimethylammonium 2,4,6-trinitrophenolate}, $C_{17}H_{21}N_2O_2S^+\cdot C_6H_2N_3O_7^-$, is a molecular salt arising from the reaction of racemic dioxopromethazine and picric acid, crystallizing with three ion pairs in the asymmetric unit. The conformations of the three distinct cations are very similar and each associates with a nearby picrate anion by way of hydrogen bonds. In one case, a simple N—H···O link occurs to the acceptor deprotonated phenol O atom; the other two ion pairs are linked by bifurcated N—H···(O,*O*) hydrogen bonds, where the second O atom is part of a nitro group. In the crystal structure, there is weak π–π stacking involving two of the picrate aromatic rings [ring–centroid separation = 3.676 (2) Å].

Related literature

For a related structure, see: Harrison *et al.* (2007). For background literature, see: Shi *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{21}N_2O_2S^+\cdot C_6H_2N_3O_7^-$
M_r = 545.52
Triclinic, $P\overline{1}$
a = 11.1260 (7) Å
b = 17.6054 (10) Å
c = 20.2297 (12) Å
α = 108.302 (1)°
β = 90.751 (1)°
γ = 95.536 (1)°
V = 3740.6 (4) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 295 (2) K
0.52 × 0.37 × 0.34 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.906, T_{max} = 0.937
23750 measured reflections
14116 independent reflections
7577 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.154
S = 0.93
14116 reflections
1036 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···O61	0.91	1.75	2.620 (3)	160
N22—H22*A*···O71	0.91	1.86	2.689 (3)	151
N22—H22*A*···O77	0.91	2.37	3.046 (4)	131
N42—H42*A*···O81	0.91	1.89	2.681 (4)	144
N42—H42*A*···O82	0.91	2.29	3.018 (4)	137

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2393).

References

Bruker (1999). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harrison, W. T. A., Bindya, S., Ashok, M. A., Yathirajan, H. S. & Narayana, B. (2007). *Acta Cryst.* E**63**, o3143.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shi, L.-H., Liu, X.-J., Li, H.-J. & Xu, G. B. (2006). *Anal. Chem.* **78**, 7330–7334.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

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Dioxopromethazinium picrate

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Comment

Dioxopromethazine, $C_{17}H_{20}N_2O_2S$, is an important antihistamine drug. It is frequently used as a reference standard in the electrochemiluminescence analysis of trace quantities of drugs (Shi *et al.*, 2006). As part of our ongoing studies (Harrison *et al.*, 2007) of the crystal structures of pharmaceutical molecules, we now report the title compound, (I), $C_{17}H_{21}N_2O_2S{\cdot}C_6H_2N_3O_7$, a molecular salt of dioxopromethazine and picric acid (Fig. 1).

Compound (I) formally arises *via* proton transfer from the phenol group of the picric acid to the tertiary amine N atom of the dioxopromethazine side chain. The structure features the rather uncommon situation of $Z' = 3$ for space group $P\bar{1}$, thus there are three cations and three anions in the asymmetric unit. The cation is chiral; in the arbitrarily chosen asymmetric unit, each chiral carbon centre (atoms C14, C34 and C54 in the first, second and third asymmetric cations, respectively) has S configuration, but crystal symmetry generates a racemic mixture.

The dihedral angles between the aromatic rings in the cation are 37.45 (7)°, 33.46 (10)°, and 40.57 (7)° for the C1, C21 and C41 molecules, respectively. Otherwise, the conformations of the three cations are almost identical with only a handful of distances and angles differing by more than 3σ [calculations performed with *PLATON* (Spek, 2003)].

In the crystal, the cations and anions associate into ion pairs, linked by hydrogen bonds (Table 1). One pair (the C1 cation and the C61 anion) are linked by a simple N—H···O link, with the acceptor being the deprotonated phenolic O atom. The linkages for the other two ion pairs are better described as bifurcated N—H···(O,*O*) bonds, where the second O atom is part of a nitro group *ortho* to the phenolic O atom. A similar cation-to-anion bifurcated N—H···(O,*O*) link was recently seen in imipraminium picrate (Harrison *et al.*, 2007).

In the crystal of (I), π-π stacking occurs between two of the picrate aromatic rings, with a centroid separation of 3.676 (2) Å. The crystal packing for (I) results in a dense, complex, array of molecules and it is not clear why three asymmetric cations and anions are present.

Experimental

Separate solutions of dioxopromethazine hydrochloride (1.765 g, 0.05 mol) and picric acid (1.146 g, 0.05 mol) in 100 ml of water were made up. Upon mixing the solutions at room temperature, a bright yellow precipiate instantaneously formed, which was filtered, washed with water and dried over P_2O_5. Dark orange chunks of (I) were recrystallized from a 1:1 *v*/*v* acetone and ethanol mixture (m.p.: 483 K).

Refinement

The displacement ellipsoids for several of the nitro group O atoms are elongated, suggesting disorder, but no convincing models could be developed to describe this.

The H atoms were geometrically placed (C—H = 0.93–0.98 Å, N—H = 0.91 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate, but not to tip, to best fit the electron density.

Figures

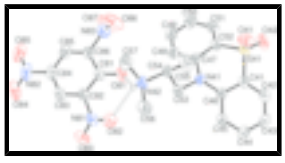


Fig. 1. View of the association of the C41 cation and the C81 anion in (I) showing 40% displacement ellipsoids (arbitrary sphere for the H atom). The hydrogen bonds are shown as double-dashed lines. All C-bound H atoms omitted for clarity.

[1-(9,9-dioxo-10*H*-phenothiazin-10-yl)-2-propyl]dimethylammonium 2,4,6-trinitrophenolate

Crystal data

$C_{17}H_{21}N_2O_2S^+\cdot C_6H_2N_3O_7^-$	Z = 6
M_r = 545.52	F_{000} = 1704
Triclinic, $P\overline{1}$	D_x = 1.453 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.1260 (7) Å	Cell parameters from 5649 reflections
b = 17.6054 (10) Å	θ = 4.4–25.6º
c = 20.2297 (12) Å	μ = 0.19 mm^{-1}
α = 108.302 (1)º	T = 295 (2) K
β = 90.751 (1)º	Chunk, dark orange
γ = 95.536 (1)º	0.52 × 0.37 × 0.34 mm
V = 3740.6 (4) Å^3	

Data collection

Bruker SMART1000 CCD diffractometer	14116 independent reflections
Radiation source: fine-focus sealed tube	7577 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 295(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 4.5º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −13→13
T_{min} = 0.906, T_{max} = 0.937	k = −21→21
23750 measured reflections	l = −21→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H-atom parameters constrained

$wR(F^2) = 0.154$	$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.93$	$(\Delta/\sigma)_{max} = 0.001$
14116 reflections	$\Delta\rho_{max} = 0.50$ e Å^{-3}
1036 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7130 (3)	0.16108 (16)	0.39410 (15)	0.0468 (7)
C2	0.7426 (3)	0.08233 (18)	0.37471 (18)	0.0590 (9)
H2	0.7437	0.0554	0.4075	0.071*
C3	0.7699 (3)	0.04485 (19)	0.30797 (19)	0.0679 (10)
H3	0.7888	−0.0080	0.2945	0.081*
C4	0.7691 (3)	0.08650 (18)	0.26010 (17)	0.0583 (8)
H4	0.7871	0.0606	0.2143	0.070*
C5	0.7425 (3)	0.16429 (17)	0.27817 (15)	0.0487 (7)
H5	0.7439	0.1908	0.2450	0.058*
C6	0.7134 (3)	0.20423 (15)	0.34645 (14)	0.0421 (7)
C7	0.7256 (3)	0.33560 (15)	0.43631 (14)	0.0411 (7)
C8	0.7628 (3)	0.41766 (17)	0.45155 (16)	0.0516 (8)
H8	0.7588	0.4416	0.4167	0.062*
C9	0.8049 (3)	0.46300 (18)	0.51715 (17)	0.0586 (9)
H9	0.8298	0.5174	0.5260	0.070*
C10	0.8117 (3)	0.43008 (19)	0.57098 (16)	0.0593 (9)
H10	0.8424	0.4616	0.6151	0.071*
C11	0.7725 (3)	0.35067 (18)	0.55815 (15)	0.0516 (8)
H11	0.7762	0.3277	0.5936	0.062*
C12	0.7272 (3)	0.30418 (16)	0.49203 (14)	0.0436 (7)
C13	0.6387 (3)	0.32103 (17)	0.31951 (15)	0.0501 (8)
H13A	0.6327	0.2829	0.2727	0.060*
H13B	0.6884	0.3692	0.3190	0.060*
C14	0.5114 (3)	0.34192 (17)	0.34426 (15)	0.0484 (7)
H14	0.5194	0.3718	0.3942	0.058*

C15	0.4254 (3)	0.2665 (2)	0.33462 (19)	0.0722 (10)
H15A	0.3459	0.2812	0.3468	0.108*
H15B	0.4527	0.2377	0.3641	0.108*
H15C	0.4234	0.2330	0.2868	0.108*
C16	0.4303 (4)	0.3566 (2)	0.23319 (16)	0.0731 (10)
H16A	0.4089	0.3964	0.2132	0.110*
H16B	0.3624	0.3168	0.2282	0.110*
H16C	0.4973	0.3312	0.2096	0.110*
C17	0.3624 (4)	0.4374 (2)	0.3453 (2)	0.0851 (12)
H17A	0.3392	0.4750	0.3232	0.128*
H17B	0.3878	0.4655	0.3930	0.128*
H17C	0.2948	0.3985	0.3436	0.128*
N1	0.6923 (2)	0.28597 (13)	0.36823 (11)	0.0447 (6)
N2	0.4645 (2)	0.39541 (14)	0.30798 (12)	0.0511 (6)
H2A	0.5257	0.4345	0.3103	0.061*
S1	0.66292 (8)	0.20591 (4)	0.47708 (4)	0.0517 (2)
O1	0.7128 (2)	0.17294 (13)	0.52667 (11)	0.0734 (7)
O2	0.5333 (2)	0.20397 (13)	0.47275 (12)	0.0676 (6)
C21	0.2859 (3)	0.57290 (17)	0.18495 (15)	0.0480 (7)
C22	0.3149 (3)	0.61617 (19)	0.25421 (16)	0.0570 (8)
H22	0.2882	0.5957	0.2892	0.068*
C23	0.3829 (3)	0.6890 (2)	0.27096 (18)	0.0671 (10)
H23	0.4040	0.7181	0.3173	0.081*
C24	0.4202 (3)	0.7190 (2)	0.21807 (18)	0.0633 (9)
H24	0.4634	0.7697	0.2296	0.076*
C25	0.3949 (3)	0.67596 (18)	0.14931 (17)	0.0566 (8)
H25	0.4225	0.6971	0.1149	0.068*
C26	0.3278 (3)	0.60029 (17)	0.13051 (15)	0.0477 (7)
C27	0.2907 (3)	0.46875 (17)	0.04208 (15)	0.0508 (8)
C28	0.3265 (4)	0.4204 (2)	−0.02207 (18)	0.0695 (10)
H28	0.3586	0.4441	−0.0540	0.083*
C29	0.3145 (4)	0.3376 (2)	−0.0383 (2)	0.0842 (12)
H29	0.3373	0.3063	−0.0816	0.101*
C30	0.2697 (4)	0.3004 (2)	0.0082 (2)	0.0777 (11)
H30	0.2635	0.2446	−0.0032	0.093*
C31	0.2345 (3)	0.34628 (19)	0.07092 (19)	0.0649 (9)
H31	0.2046	0.3218	0.1028	0.078*
C32	0.2427 (3)	0.42927 (17)	0.08769 (15)	0.0503 (8)
C33	0.2992 (3)	0.59358 (18)	0.00695 (15)	0.0568 (9)
H33A	0.2891	0.5536	−0.0389	0.068*
H33B	0.3743	0.6274	0.0089	0.068*
C34	0.1934 (3)	0.64479 (17)	0.01944 (15)	0.0482 (8)
H34	0.2042	0.6821	0.0671	0.058*
C35	0.0728 (3)	0.5959 (2)	0.01381 (18)	0.0701 (10)
H35A	0.0096	0.6306	0.0199	0.105*
H35B	0.0698	0.5702	0.0492	0.105*
H35C	0.0622	0.5558	−0.0313	0.105*
C36	0.1703 (4)	0.6479 (2)	−0.10397 (18)	0.0906 (14)
H36A	0.1795	0.6835	−0.1315	0.136*

H36B	0.0886	0.6229	−0.1096	0.136*
H36C	0.2247	0.6073	−0.1190	0.136*
C37	0.1202 (4)	0.7619 (2)	−0.0050 (2)	0.0889 (13)
H37A	0.1440	0.7935	0.0422	0.133*
H37B	0.0372	0.7400	−0.0072	0.133*
H37C	0.1292	0.7953	−0.0345	0.133*
N21	0.3040 (3)	0.55325 (14)	0.06097 (12)	0.0538 (7)
N22	0.1985 (2)	0.69456 (15)	−0.02915 (13)	0.0574 (7)
H22A	0.2760	0.7177	−0.0262	0.069*
S21	0.18308 (7)	0.48703 (5)	0.16372 (4)	0.0502 (2)
O21	0.06833 (19)	0.50805 (12)	0.14654 (10)	0.0576 (6)
O22	0.1869 (2)	0.44888 (13)	0.21664 (11)	0.0671 (6)
C41	−0.0722 (3)	−0.21677 (16)	0.75063 (14)	0.0457 (7)
C42	−0.0417 (3)	−0.29501 (18)	0.73408 (17)	0.0545 (8)
H42	−0.0375	−0.3191	0.7688	0.065*
C43	−0.0178 (3)	−0.33687 (18)	0.66718 (18)	0.0596 (9)
H43	0.0022	−0.3894	0.6560	0.072*
C44	−0.0240 (3)	−0.29984 (18)	0.61638 (17)	0.0586 (8)
H44	−0.0094	−0.3284	0.5706	0.070*
C45	−0.0515 (3)	−0.22153 (18)	0.63219 (15)	0.0535 (8)
H45	−0.0543	−0.1980	0.5970	0.064*
C46	−0.0750 (3)	−0.17716 (16)	0.70011 (14)	0.0429 (7)
C47	−0.0540 (3)	−0.04232 (16)	0.78455 (14)	0.0466 (7)
C48	−0.0111 (3)	0.03736 (17)	0.79427 (16)	0.0558 (8)
H48	−0.0165	0.0583	0.7576	0.067*
C49	0.0396 (3)	0.08571 (19)	0.85799 (18)	0.0659 (9)
H49	0.0671	0.1390	0.8636	0.079*
C50	0.0502 (3)	0.0568 (2)	0.91348 (17)	0.0656 (9)
H50	0.0868	0.0897	0.9557	0.079*
C51	0.0061 (3)	−0.02137 (19)	0.90543 (16)	0.0568 (8)
H51	0.0128	−0.0418	0.9424	0.068*
C52	−0.0483 (3)	−0.06976 (17)	0.84251 (14)	0.0478 (7)
C53	−0.1352 (3)	−0.06260 (17)	0.66486 (14)	0.0566 (9)
H53A	−0.1562	−0.1062	0.6219	0.068*
H53B	−0.0685	−0.0277	0.6563	0.068*
C54	−0.2438 (3)	−0.01496 (17)	0.68650 (15)	0.0513 (8)
H54	−0.2216	0.0270	0.7311	0.062*
C55	−0.3557 (4)	−0.0651 (2)	0.6966 (2)	0.0807 (12)
H55A	−0.4220	−0.0327	0.7062	0.121*
H55B	−0.3413	−0.0846	0.7350	0.121*
H55C	−0.3751	−0.1099	0.6550	0.121*
C57	−0.3509 (4)	0.0887 (2)	0.6574 (2)	0.0792 (11)
H57A	−0.3240	0.1237	0.7031	0.119*
H57B	−0.4303	0.0630	0.6594	0.119*
H57C	−0.3533	0.1195	0.6259	0.119*
C56	−0.3025 (4)	−0.0285 (2)	0.56120 (16)	0.0774 (11)
H56A	−0.2393	−0.0620	0.5437	0.116*
H56B	−0.3163	0.0026	0.5310	0.116*
H56C	−0.3753	−0.0617	0.5629	0.116*

N41	−0.0976 (2)	−0.09558 (13)	0.71895 (11)	0.0501 (6)
N42	−0.2660 (2)	0.02647 (14)	0.63255 (12)	0.0533 (7)
H42A	−0.1938	0.0535	0.6287	0.064*
O41	−0.2448 (2)	−0.16545 (14)	0.83084 (12)	0.0713 (7)
O42	−0.0643 (2)	−0.19653 (13)	0.88425 (11)	0.0752 (7)
S41	−0.11557 (8)	−0.16563 (5)	0.83371 (4)	0.0525 (2)
C61	0.6430 (3)	0.58926 (19)	0.34143 (18)	0.0582 (9)
C62	0.6458 (3)	0.6590 (2)	0.40116 (18)	0.0602 (9)
C63	0.6699 (3)	0.73566 (19)	0.40111 (19)	0.0632 (9)
H63	0.6708	0.7784	0.4423	0.076*
C64	0.6931 (3)	0.74922 (18)	0.33866 (19)	0.0598 (9)
C65	0.6935 (3)	0.6872 (2)	0.27744 (18)	0.0614 (9)
H65	0.7114	0.6971	0.2359	0.074*
C66	0.6669 (3)	0.60951 (18)	0.27892 (17)	0.0585 (9)
N61	0.6298 (4)	0.6472 (2)	0.4700 (2)	0.0875 (10)
N62	0.7210 (4)	0.83140 (19)	0.3371 (2)	0.0935 (12)
N63	0.6672 (4)	0.5462 (2)	0.2137 (2)	0.0939 (11)
O61	0.6298 (2)	0.51927 (14)	0.34498 (15)	0.0871 (8)
O62	0.7018 (4)	0.6852 (3)	0.51697 (17)	0.1345 (14)
O63	0.5463 (4)	0.6005 (3)	0.4747 (2)	0.1379 (14)
O64	0.7145 (4)	0.88604 (18)	0.3912 (2)	0.1491 (16)
O65	0.7505 (4)	0.84116 (18)	0.2821 (2)	0.1320 (14)
O66	0.7349 (5)	0.55476 (19)	0.16933 (16)	0.1410 (16)
O67	0.6010 (4)	0.4845 (2)	0.2039 (2)	0.181 (2)
C71	0.4771 (3)	0.83901 (18)	0.02212 (18)	0.0579 (9)
C72	0.5249 (4)	0.9013 (2)	0.08413 (19)	0.0737 (11)
C73	0.6046 (3)	0.9657 (2)	0.0854 (2)	0.0726 (11)
H73	0.6338	1.0033	0.1275	0.087*
C74	0.6407 (3)	0.97356 (18)	0.0232 (2)	0.0578 (9)
C75	0.5958 (3)	0.9205 (2)	−0.03893 (19)	0.0627 (9)
H75	0.6203	0.9277	−0.0805	0.075*
C76	0.5136 (3)	0.85573 (18)	−0.03995 (18)	0.0590 (9)
N71	0.4847 (6)	0.8968 (3)	0.1521 (2)	0.1290 (19)
N72	0.7236 (3)	1.04294 (18)	0.0237 (2)	0.0737 (9)
N73	0.4600 (3)	0.8069 (2)	−0.10755 (19)	0.0821 (10)
O71	0.4102 (2)	0.77931 (14)	0.02629 (13)	0.0755 (7)
O72	0.3758 (6)	0.8843 (3)	0.1589 (2)	0.1701 (18)
O73	0.5493 (5)	0.9015 (4)	0.1958 (3)	0.234 (3)
O74	0.7523 (2)	1.09445 (16)	0.08022 (17)	0.0905 (8)
O75	0.7605 (3)	1.04652 (17)	−0.03091 (19)	0.1129 (11)
O76	0.4750 (3)	0.83105 (18)	−0.15751 (15)	0.0948 (9)
O77	0.3995 (3)	0.74367 (19)	−0.11302 (15)	0.1299 (14)
C81	−0.0353 (3)	0.19452 (18)	0.67000 (16)	0.0523 (8)
C82	−0.0071 (3)	0.20372 (18)	0.60389 (16)	0.0526 (8)
C83	0.0301 (3)	0.2763 (2)	0.59475 (18)	0.0588 (9)
H83	0.0488	0.2789	0.5508	0.071*
C84	0.0393 (3)	0.34501 (19)	0.6512 (2)	0.0567 (8)
C85	0.0179 (3)	0.34209 (19)	0.71783 (19)	0.0593 (9)
H85	0.0276	0.3886	0.7561	0.071*

C86	−0.0176 (3)	0.26935 (18)	0.72560 (16)	0.0533 (8)
N81	−0.0155 (3)	0.13259 (19)	0.54153 (15)	0.0693 (8)
N82	0.0758 (3)	0.4215 (2)	0.6404 (2)	0.0768 (9)
N83	−0.0385 (4)	0.26582 (18)	0.79560 (16)	0.0723 (8)
O81	−0.0666 (2)	0.12896 (13)	0.68027 (11)	0.0704 (7)
O82	−0.0810 (3)	0.07272 (16)	0.54032 (13)	0.0868 (8)
O83	0.0459 (3)	0.13650 (18)	0.49275 (14)	0.1125 (11)
O84	0.0980 (3)	0.42246 (17)	0.58133 (18)	0.0973 (10)
O85	0.0811 (3)	0.48207 (18)	0.6914 (2)	0.1073 (10)
O86	−0.1345 (3)	0.2366 (2)	0.80790 (16)	0.1183 (12)
O87	0.0443 (4)	0.2892 (2)	0.83836 (16)	0.1223 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0517 (19)	0.0394 (16)	0.0530 (18)	0.0059 (14)	0.0009 (15)	0.0194 (13)
C2	0.073 (2)	0.0417 (18)	0.069 (2)	0.0098 (16)	0.0000 (19)	0.0268 (16)
C3	0.082 (3)	0.0382 (18)	0.081 (3)	0.0119 (17)	0.002 (2)	0.0136 (17)
C4	0.064 (2)	0.0463 (18)	0.0566 (19)	0.0096 (16)	−0.0024 (17)	0.0035 (15)
C5	0.058 (2)	0.0455 (17)	0.0429 (17)	0.0070 (14)	−0.0011 (15)	0.0140 (13)
C6	0.0437 (18)	0.0375 (15)	0.0465 (17)	0.0041 (13)	−0.0036 (14)	0.0158 (12)
C7	0.0444 (18)	0.0368 (15)	0.0437 (16)	0.0073 (13)	0.0014 (13)	0.0140 (12)
C8	0.062 (2)	0.0420 (17)	0.0535 (19)	0.0056 (15)	0.0008 (16)	0.0183 (14)
C9	0.062 (2)	0.0401 (17)	0.066 (2)	0.0023 (15)	0.0015 (18)	0.0078 (15)
C10	0.061 (2)	0.057 (2)	0.0501 (19)	0.0082 (16)	−0.0091 (16)	0.0025 (15)
C11	0.058 (2)	0.057 (2)	0.0404 (17)	0.0152 (16)	−0.0011 (15)	0.0140 (14)
C12	0.0472 (18)	0.0420 (16)	0.0443 (17)	0.0101 (13)	0.0018 (14)	0.0159 (13)
C13	0.068 (2)	0.0410 (16)	0.0471 (17)	0.0129 (15)	0.0020 (16)	0.0202 (13)
C14	0.053 (2)	0.0462 (17)	0.0469 (17)	0.0009 (14)	−0.0051 (15)	0.0176 (13)
C15	0.077 (3)	0.066 (2)	0.077 (2)	−0.0153 (19)	−0.007 (2)	0.0357 (19)
C16	0.088 (3)	0.076 (2)	0.057 (2)	0.013 (2)	−0.016 (2)	0.0231 (18)
C17	0.076 (3)	0.085 (3)	0.090 (3)	0.037 (2)	0.003 (2)	0.015 (2)
N1	0.0611 (17)	0.0373 (13)	0.0390 (13)	0.0116 (11)	−0.0032 (12)	0.0151 (10)
N2	0.0532 (17)	0.0444 (14)	0.0538 (15)	0.0051 (12)	−0.0005 (13)	0.0134 (11)
S1	0.0643 (6)	0.0475 (4)	0.0502 (5)	0.0050 (4)	0.0043 (4)	0.0255 (3)
O1	0.109 (2)	0.0646 (14)	0.0606 (14)	0.0111 (13)	0.0001 (13)	0.0394 (11)
O2	0.0584 (16)	0.0695 (15)	0.0771 (16)	−0.0025 (12)	0.0131 (12)	0.0286 (12)
C21	0.052 (2)	0.0485 (17)	0.0458 (18)	0.0070 (14)	−0.0038 (15)	0.0175 (14)
C22	0.066 (2)	0.062 (2)	0.0456 (18)	0.0052 (17)	−0.0038 (16)	0.0214 (15)
C23	0.073 (3)	0.069 (2)	0.053 (2)	0.0044 (19)	−0.0180 (19)	0.0118 (17)
C24	0.065 (2)	0.0517 (19)	0.069 (2)	−0.0041 (16)	−0.0165 (19)	0.0172 (17)
C25	0.055 (2)	0.0563 (19)	0.061 (2)	−0.0023 (16)	−0.0055 (17)	0.0252 (16)
C26	0.051 (2)	0.0462 (17)	0.0484 (18)	0.0060 (14)	−0.0038 (15)	0.0180 (14)
C27	0.060 (2)	0.0461 (18)	0.0473 (18)	0.0074 (15)	−0.0031 (15)	0.0153 (14)
C28	0.091 (3)	0.058 (2)	0.062 (2)	0.0146 (19)	0.012 (2)	0.0193 (17)
C29	0.109 (3)	0.060 (2)	0.077 (3)	0.023 (2)	0.016 (2)	0.007 (2)
C30	0.093 (3)	0.044 (2)	0.095 (3)	0.0099 (19)	0.002 (2)	0.019 (2)
C31	0.073 (3)	0.051 (2)	0.075 (2)	0.0069 (17)	−0.003 (2)	0.0262 (18)

C32	0.055 (2)	0.0472 (18)	0.0536 (18)	0.0047 (14)	−0.0056 (15)	0.0235 (14)
C33	0.081 (3)	0.0495 (18)	0.0422 (17)	0.0005 (17)	0.0039 (16)	0.0189 (14)
C34	0.061 (2)	0.0468 (17)	0.0394 (16)	−0.0069 (15)	−0.0056 (15)	0.0209 (13)
C35	0.072 (2)	0.076 (2)	0.071 (2)	−0.0233 (19)	−0.0120 (19)	0.0450 (19)
C36	0.114 (3)	0.108 (3)	0.055 (2)	−0.030 (3)	−0.020 (2)	0.046 (2)
C37	0.080 (3)	0.070 (3)	0.130 (4)	0.000 (2)	−0.019 (3)	0.056 (2)
N21	0.079 (2)	0.0455 (14)	0.0405 (14)	0.0057 (13)	0.0011 (13)	0.0190 (11)
N22	0.0583 (18)	0.0539 (16)	0.0657 (17)	−0.0170 (13)	−0.0145 (14)	0.0343 (13)
S21	0.0550 (5)	0.0535 (5)	0.0485 (4)	0.0019 (4)	−0.0035 (4)	0.0265 (4)
O21	0.0491 (13)	0.0687 (14)	0.0584 (13)	0.0066 (11)	−0.0031 (11)	0.0251 (11)
O22	0.0801 (17)	0.0737 (15)	0.0613 (14)	0.0015 (12)	−0.0024 (12)	0.0433 (12)
C41	0.0469 (19)	0.0424 (16)	0.0507 (17)	−0.0005 (13)	−0.0008 (14)	0.0203 (13)
C42	0.056 (2)	0.0477 (18)	0.067 (2)	−0.0013 (15)	−0.0045 (17)	0.0313 (16)
C43	0.062 (2)	0.0373 (17)	0.078 (2)	0.0072 (15)	−0.0016 (19)	0.0155 (16)
C44	0.067 (2)	0.0429 (18)	0.060 (2)	0.0075 (16)	0.0021 (17)	0.0077 (15)
C45	0.067 (2)	0.0495 (18)	0.0457 (18)	0.0058 (15)	0.0021 (16)	0.0170 (14)
C46	0.0479 (18)	0.0404 (16)	0.0420 (16)	0.0062 (13)	−0.0004 (14)	0.0146 (12)
C47	0.057 (2)	0.0408 (16)	0.0431 (17)	0.0123 (14)	0.0004 (15)	0.0131 (13)
C48	0.074 (2)	0.0455 (18)	0.0508 (19)	0.0102 (16)	−0.0023 (17)	0.0182 (14)
C49	0.080 (3)	0.0454 (19)	0.069 (2)	0.0023 (17)	−0.007 (2)	0.0148 (16)
C50	0.074 (3)	0.058 (2)	0.055 (2)	0.0054 (18)	−0.0108 (18)	0.0047 (16)
C51	0.064 (2)	0.061 (2)	0.0453 (18)	0.0088 (17)	−0.0016 (16)	0.0166 (15)
C52	0.053 (2)	0.0487 (17)	0.0422 (17)	0.0053 (14)	0.0011 (15)	0.0154 (13)
C53	0.089 (3)	0.0444 (17)	0.0399 (16)	0.0173 (17)	−0.0016 (17)	0.0151 (13)
C54	0.070 (2)	0.0423 (16)	0.0456 (17)	0.0032 (15)	−0.0062 (16)	0.0211 (13)
C55	0.089 (3)	0.070 (2)	0.096 (3)	−0.010 (2)	−0.010 (2)	0.050 (2)
C57	0.102 (3)	0.069 (2)	0.085 (3)	0.034 (2)	0.011 (2)	0.042 (2)
C56	0.110 (3)	0.071 (2)	0.051 (2)	0.005 (2)	−0.020 (2)	0.0210 (17)
N41	0.0775 (19)	0.0364 (13)	0.0380 (13)	0.0125 (12)	−0.0026 (13)	0.0123 (10)
N42	0.0702 (19)	0.0469 (14)	0.0484 (15)	0.0051 (13)	−0.0057 (13)	0.0237 (11)
O41	0.0548 (16)	0.0872 (17)	0.0643 (15)	−0.0023 (12)	0.0114 (12)	0.0158 (12)
O42	0.105 (2)	0.0736 (15)	0.0565 (14)	−0.0113 (14)	−0.0137 (13)	0.0408 (12)
S41	0.0591 (6)	0.0576 (5)	0.0441 (4)	−0.0031 (4)	0.0000 (4)	0.0235 (4)
C61	0.046 (2)	0.050 (2)	0.081 (2)	0.0016 (15)	−0.0074 (17)	0.0267 (18)
C62	0.056 (2)	0.060 (2)	0.066 (2)	0.0084 (17)	0.0027 (18)	0.0221 (17)
C63	0.065 (2)	0.050 (2)	0.069 (2)	0.0147 (16)	−0.0043 (19)	0.0082 (16)
C64	0.062 (2)	0.0385 (17)	0.077 (2)	0.0024 (15)	−0.0150 (19)	0.0172 (16)
C65	0.063 (2)	0.063 (2)	0.061 (2)	0.0020 (17)	−0.0114 (18)	0.0256 (17)
C66	0.059 (2)	0.0430 (18)	0.063 (2)	0.0036 (15)	−0.0118 (17)	0.0028 (15)
N61	0.084 (3)	0.099 (3)	0.089 (3)	0.020 (2)	0.019 (2)	0.040 (2)
N62	0.118 (3)	0.047 (2)	0.116 (3)	0.0026 (18)	−0.034 (3)	0.030 (2)
N63	0.124 (3)	0.067 (2)	0.070 (2)	−0.003 (2)	−0.003 (2)	−0.0022 (19)
O61	0.0807 (19)	0.0502 (15)	0.134 (2)	−0.0066 (12)	−0.0196 (16)	0.0396 (14)
O62	0.121 (3)	0.206 (4)	0.074 (2)	0.012 (3)	−0.007 (2)	0.042 (2)
O63	0.146 (3)	0.156 (3)	0.132 (3)	−0.014 (3)	0.026 (3)	0.081 (3)
O64	0.249 (5)	0.0439 (17)	0.140 (3)	0.007 (2)	−0.027 (3)	0.0128 (19)
O65	0.198 (4)	0.076 (2)	0.139 (3)	0.000 (2)	−0.018 (3)	0.064 (2)
O66	0.261 (5)	0.093 (2)	0.0544 (18)	−0.009 (3)	0.011 (3)	0.0113 (16)
O67	0.194 (4)	0.105 (3)	0.159 (4)	−0.065 (3)	0.038 (3)	−0.058 (2)

C71	0.051 (2)	0.0456 (18)	0.075 (2)	−0.0034 (15)	−0.0093 (18)	0.0197 (16)
C72	0.088 (3)	0.068 (2)	0.068 (2)	−0.020 (2)	−0.017 (2)	0.0343 (19)
C73	0.074 (3)	0.064 (2)	0.078 (3)	−0.0170 (19)	−0.023 (2)	0.0273 (19)
C74	0.042 (2)	0.0443 (18)	0.083 (3)	−0.0036 (14)	0.0001 (18)	0.0168 (17)
C75	0.052 (2)	0.062 (2)	0.074 (2)	0.0077 (17)	0.0225 (18)	0.0193 (18)
C76	0.049 (2)	0.0468 (18)	0.070 (2)	0.0006 (15)	0.0109 (17)	0.0036 (16)
N71	0.148 (5)	0.139 (4)	0.100 (3)	−0.083 (3)	−0.053 (3)	0.070 (3)
N72	0.0494 (19)	0.0568 (19)	0.112 (3)	0.0005 (15)	0.009 (2)	0.024 (2)
N73	0.078 (2)	0.073 (2)	0.072 (2)	−0.0094 (18)	0.0265 (19)	−0.0050 (18)
O71	0.0753 (17)	0.0637 (15)	0.0886 (17)	−0.0247 (13)	−0.0163 (14)	0.0358 (13)
O72	0.199 (5)	0.198 (4)	0.102 (3)	−0.043 (4)	0.024 (3)	0.050 (3)
O73	0.198 (5)	0.375 (8)	0.163 (4)	−0.135 (5)	−0.091 (4)	0.188 (5)
O74	0.0780 (19)	0.0571 (16)	0.123 (2)	−0.0190 (14)	−0.0126 (17)	0.0186 (16)
O75	0.115 (3)	0.084 (2)	0.128 (3)	−0.0222 (18)	0.055 (2)	0.0253 (19)
O76	0.093 (2)	0.103 (2)	0.0749 (19)	0.0047 (17)	0.0108 (17)	0.0105 (17)
O77	0.154 (3)	0.095 (2)	0.087 (2)	−0.064 (2)	0.041 (2)	−0.0260 (16)
C81	0.057 (2)	0.0524 (19)	0.0570 (19)	0.0049 (15)	0.0021 (16)	0.0304 (16)
C82	0.059 (2)	0.0562 (19)	0.0524 (19)	0.0104 (16)	0.0042 (16)	0.0298 (15)
C83	0.054 (2)	0.067 (2)	0.071 (2)	0.0110 (17)	0.0065 (17)	0.0433 (19)
C84	0.045 (2)	0.052 (2)	0.088 (3)	0.0068 (15)	0.0052 (18)	0.0419 (19)
C85	0.053 (2)	0.0499 (19)	0.077 (2)	0.0112 (15)	0.0043 (18)	0.0214 (16)
C86	0.055 (2)	0.0531 (19)	0.057 (2)	0.0068 (15)	0.0094 (16)	0.0249 (15)
N81	0.098 (3)	0.069 (2)	0.0515 (18)	0.0211 (18)	0.0121 (17)	0.0308 (16)
N82	0.056 (2)	0.065 (2)	0.129 (3)	0.0117 (16)	0.005 (2)	0.057 (2)
N83	0.089 (3)	0.069 (2)	0.060 (2)	0.0040 (18)	0.007 (2)	0.0241 (16)
O81	0.0988 (19)	0.0550 (14)	0.0641 (14)	−0.0094 (12)	−0.0022 (13)	0.0340 (11)
O82	0.126 (2)	0.0588 (16)	0.0737 (17)	0.0043 (16)	0.0128 (16)	0.0196 (13)
O83	0.182 (3)	0.104 (2)	0.0631 (17)	0.027 (2)	0.051 (2)	0.0382 (16)
O84	0.088 (2)	0.100 (2)	0.137 (3)	−0.0060 (16)	0.0032 (18)	0.089 (2)
O85	0.111 (3)	0.0535 (17)	0.165 (3)	0.0099 (16)	0.018 (2)	0.0456 (19)
O86	0.103 (3)	0.174 (3)	0.085 (2)	−0.003 (2)	0.0333 (19)	0.056 (2)
O87	0.143 (3)	0.145 (3)	0.075 (2)	−0.028 (2)	−0.022 (2)	0.043 (2)

Geometric parameters (Å, °)

C1—C2	1.391 (4)	C43—C44	1.383 (4)
C1—C6	1.402 (4)	C43—H43	0.9300
C1—S1	1.740 (3)	C44—C45	1.380 (4)
C2—C3	1.357 (4)	C44—H44	0.9300
C2—H2	0.9300	C45—C46	1.393 (4)
C3—C4	1.387 (4)	C45—H45	0.9300
C3—H3	0.9300	C46—N41	1.414 (3)
C4—C5	1.365 (4)	C47—C48	1.389 (4)
C4—H4	0.9300	C47—C52	1.404 (4)
C5—C6	1.398 (4)	C47—N41	1.411 (3)
C5—H5	0.9300	C48—C49	1.379 (4)
C6—N1	1.410 (3)	C48—H48	0.9300
C7—C8	1.398 (4)	C49—C50	1.379 (4)
C7—N1	1.402 (3)	C49—H49	0.9300

C7—C12	1.404 (4)	C50—C51	1.374 (4)
C8—C9	1.366 (4)	C50—H50	0.9300
C8—H8	0.9300	C51—C52	1.382 (4)
C9—C10	1.389 (4)	C51—H51	0.9300
C9—H9	0.9300	C52—S41	1.734 (3)
C10—C11	1.365 (4)	C53—N41	1.464 (3)
C10—H10	0.9300	C53—C54	1.528 (4)
C11—C12	1.389 (4)	C53—H53A	0.9700
C11—H11	0.9300	C53—H53B	0.9700
C12—S1	1.739 (3)	C54—C55	1.510 (5)
C13—N1	1.465 (3)	C54—N42	1.520 (3)
C13—C14	1.547 (4)	C54—H54	0.9800
C13—H13A	0.9700	C55—H55A	0.9600
C13—H13B	0.9700	C55—H55B	0.9600
C14—N2	1.489 (3)	C55—H55C	0.9600
C14—C15	1.517 (4)	C57—N42	1.487 (4)
C14—H14	0.9800	C57—H57A	0.9600
C15—H15A	0.9600	C57—H57B	0.9600
C15—H15B	0.9600	C57—H57C	0.9600
C15—H15C	0.9600	C56—N42	1.489 (4)
C16—N2	1.479 (4)	C56—H56A	0.9600
C16—H16A	0.9600	C56—H56B	0.9600
C16—H16B	0.9600	C56—H56C	0.9600
C16—H16C	0.9600	N42—H42A	0.9100
C17—N2	1.496 (4)	O41—S41	1.438 (2)
C17—H17A	0.9600	O42—S41	1.435 (2)
C17—H17B	0.9600	C61—O61	1.251 (4)
C17—H17C	0.9600	C61—C62	1.424 (4)
N2—H2A	0.9100	C61—C66	1.439 (5)
S1—O1	1.437 (2)	C62—C63	1.351 (4)
S1—O2	1.440 (2)	C62—N61	1.482 (5)
C21—C22	1.385 (4)	C63—C64	1.380 (5)
C21—C26	1.402 (4)	C63—H63	0.9300
C21—S21	1.739 (3)	C64—C65	1.371 (4)
C22—C23	1.366 (4)	C64—N62	1.461 (4)
C22—H22	0.9300	C65—C66	1.381 (4)
C23—C24	1.385 (5)	C65—H65	0.9300
C23—H23	0.9300	C66—N63	1.435 (4)
C24—C25	1.369 (4)	N61—O63	1.205 (4)
C24—H24	0.9300	N61—O62	1.212 (5)
C25—C26	1.400 (4)	N62—O64	1.218 (4)
C25—H25	0.9300	N62—O65	1.221 (5)
C26—N21	1.397 (4)	N63—O67	1.212 (5)
C27—C28	1.397 (4)	N63—O66	1.216 (5)
C27—C32	1.401 (4)	C71—O71	1.254 (4)
C27—N21	1.407 (4)	C71—C76	1.432 (5)
C28—C29	1.383 (5)	C71—C72	1.437 (5)
C28—H28	0.9300	C72—C73	1.364 (5)
C29—C30	1.377 (5)	C72—N71	1.475 (6)

C29—H29	0.9300	C73—C74	1.370 (5)
C30—C31	1.359 (5)	C73—H73	0.9300
C30—H30	0.9300	C74—C75	1.363 (5)
C31—C32	1.386 (4)	C74—N72	1.455 (4)
C31—H31	0.9300	C75—C76	1.385 (4)
C32—S21	1.736 (3)	C75—H75	0.9300
C33—N21	1.481 (3)	C76—N73	1.452 (4)
C33—C34	1.527 (4)	N71—O73	1.108 (5)
C33—H33A	0.9700	N71—O72	1.228 (6)
C33—H33B	0.9700	N72—O75	1.202 (4)
C34—C35	1.504 (4)	N72—O74	1.231 (4)
C34—N22	1.507 (3)	N73—O77	1.216 (4)
C34—H34	0.9800	N73—O76	1.221 (4)
C35—H35A	0.9600	C81—O81	1.254 (3)
C35—H35B	0.9600	C81—C82	1.432 (4)
C35—H35C	0.9600	C81—C86	1.433 (4)
C36—N22	1.490 (4)	C82—C83	1.374 (4)
C36—H36A	0.9600	C82—N81	1.466 (4)
C36—H36B	0.9600	C83—C84	1.372 (5)
C36—H36C	0.9600	C83—H83	0.9300
C37—N22	1.500 (5)	C84—C85	1.388 (4)
C37—H37A	0.9600	C84—N82	1.452 (4)
C37—H37B	0.9600	C85—C86	1.361 (4)
C37—H37C	0.9600	C85—H85	0.9300
N22—H22A	0.9100	C86—N83	1.457 (4)
S21—O21	1.431 (2)	N81—O82	1.216 (4)
S21—O22	1.4335 (19)	N81—O83	1.223 (4)
C41—C42	1.389 (4)	N82—O85	1.223 (4)
C41—C46	1.408 (4)	N82—O84	1.229 (4)
C41—S41	1.739 (3)	N83—O86	1.203 (4)
C42—C43	1.366 (4)	N83—O87	1.204 (4)
C42—H42	0.9300		
C2—C1—C6	121.5 (3)	C42—C41—C46	121.5 (3)
C2—C1—S1	120.2 (2)	C42—C41—S41	121.1 (2)
C6—C1—S1	118.1 (2)	C46—C41—S41	117.3 (2)
C3—C2—C1	120.0 (3)	C43—C42—C41	120.5 (3)
C3—C2—H2	120.0	C43—C42—H42	119.8
C1—C2—H2	120.0	C41—C42—H42	119.8
C2—C3—C4	119.0 (3)	C42—C43—C44	118.9 (3)
C2—C3—H3	120.5	C42—C43—H43	120.6
C4—C3—H3	120.5	C44—C43—H43	120.6
C5—C4—C3	122.0 (3)	C45—C44—C43	121.4 (3)
C5—C4—H4	119.0	C45—C44—H44	119.3
C3—C4—H4	119.0	C43—C44—H44	119.3
C4—C5—C6	120.2 (3)	C44—C45—C46	120.9 (3)
C4—C5—H5	119.9	C44—C45—H45	119.5
C6—C5—H5	119.9	C46—C45—H45	119.5
C5—C6—C1	117.2 (2)	C45—C46—C41	116.8 (3)
C5—C6—N1	121.9 (2)	C45—C46—N41	122.5 (2)

C1—C6—N1	120.8 (2)	C41—C46—N41	120.7 (2)
C8—C7—N1	121.9 (2)	C48—C47—C52	117.4 (3)
C8—C7—C12	116.9 (2)	C48—C47—N41	122.3 (3)
N1—C7—C12	121.2 (2)	C52—C47—N41	120.3 (2)
C9—C8—C7	120.6 (3)	C49—C48—C47	120.5 (3)
C9—C8—H8	119.7	C49—C48—H48	119.8
C7—C8—H8	119.7	C47—C48—H48	119.8
C8—C9—C10	121.8 (3)	C50—C49—C48	121.5 (3)
C8—C9—H9	119.1	C50—C49—H49	119.2
C10—C9—H9	119.1	C48—C49—H49	119.2
C11—C10—C9	119.0 (3)	C51—C50—C49	119.0 (3)
C11—C10—H10	120.5	C51—C50—H50	120.5
C9—C10—H10	120.5	C49—C50—H50	120.5
C10—C11—C12	119.9 (3)	C50—C51—C52	120.1 (3)
C10—C11—H11	120.0	C50—C51—H51	119.9
C12—C11—H11	120.0	C52—C51—H51	119.9
C11—C12—C7	121.7 (3)	C51—C52—C47	121.4 (3)
C11—C12—S1	120.4 (2)	C51—C52—S41	120.6 (2)
C7—C12—S1	117.8 (2)	C47—C52—S41	117.9 (2)
N1—C13—C14	107.6 (2)	N41—C53—C54	111.2 (2)
N1—C13—H13A	110.2	N41—C53—H53A	109.4
C14—C13—H13A	110.2	C54—C53—H53A	109.4
N1—C13—H13B	110.2	N41—C53—H53B	109.4
C14—C13—H13B	110.2	C54—C53—H53B	109.4
H13A—C13—H13B	108.5	H53A—C53—H53B	108.0
N2—C14—C15	112.0 (2)	C55—C54—N42	112.0 (3)
N2—C14—C13	110.1 (2)	C55—C54—C53	113.8 (3)
C15—C14—C13	111.4 (3)	N42—C54—C53	107.7 (2)
N2—C14—H14	107.7	C55—C54—H54	107.7
C15—C14—H14	107.7	N42—C54—H54	107.7
C13—C14—H14	107.7	C53—C54—H54	107.7
C14—C15—H15A	109.5	C54—C55—H55A	109.5
C14—C15—H15B	109.5	C54—C55—H55B	109.5
H15A—C15—H15B	109.5	H55A—C55—H55B	109.5
C14—C15—H15C	109.5	C54—C55—H55C	109.5
H15A—C15—H15C	109.5	H55A—C55—H55C	109.5
H15B—C15—H15C	109.5	H55B—C55—H55C	109.5
N2—C16—H16A	109.5	N42—C57—H57A	109.5
N2—C16—H16B	109.5	N42—C57—H57B	109.5
H16A—C16—H16B	109.5	H57A—C57—H57B	109.5
N2—C16—H16C	109.5	N42—C57—H57C	109.5
H16A—C16—H16C	109.5	H57A—C57—H57C	109.5
H16B—C16—H16C	109.5	H57B—C57—H57C	109.5
N2—C17—H17A	109.5	N42—C56—H56A	109.5
N2—C17—H17B	109.5	N42—C56—H56B	109.5
H17A—C17—H17B	109.5	H56A—C56—H56B	109.5
N2—C17—H17C	109.5	N42—C56—H56C	109.5
H17A—C17—H17C	109.5	H56A—C56—H56C	109.5
H17B—C17—H17C	109.5	H56B—C56—H56C	109.5

C7—N1—C6	120.5 (2)	C47—N41—C46	119.3 (2)
C7—N1—C13	118.9 (2)	C47—N41—C53	119.1 (2)
C6—N1—C13	120.6 (2)	C46—N41—C53	119.4 (2)
C16—N2—C14	115.3 (2)	C57—N42—C56	111.6 (3)
C16—N2—C17	110.3 (3)	C57—N42—C54	111.3 (2)
C14—N2—C17	111.5 (3)	C56—N42—C54	115.2 (2)
C16—N2—H2A	106.4	C57—N42—H42A	106.0
C14—N2—H2A	106.4	C56—N42—H42A	106.0
C17—N2—H2A	106.4	C54—N42—H42A	106.0
O1—S1—O2	116.79 (15)	O42—S41—O41	117.31 (15)
O1—S1—C12	110.09 (14)	O42—S41—C52	110.86 (14)
O2—S1—C12	109.04 (13)	O41—S41—C52	109.02 (15)
O1—S1—C1	111.00 (14)	O42—S41—C41	110.42 (15)
O2—S1—C1	108.80 (14)	O41—S41—C41	107.95 (14)
C12—S1—C1	99.75 (13)	C52—S41—C41	99.83 (14)
C22—C21—C26	121.9 (3)	O61—C61—C62	122.9 (3)
C22—C21—S21	119.9 (2)	O61—C61—C66	125.0 (3)
C26—C21—S21	117.9 (2)	C62—C61—C66	111.9 (3)
C23—C22—C21	119.8 (3)	C63—C62—C61	125.3 (3)
C23—C22—H22	120.1	C63—C62—N61	116.6 (3)
C21—C22—H22	120.1	C61—C62—N61	117.9 (3)
C22—C23—C24	119.2 (3)	C62—C63—C64	118.6 (3)
C22—C23—H23	120.4	C62—C63—H63	120.7
C24—C23—H23	120.4	C64—C63—H63	120.7
C25—C24—C23	121.7 (3)	C65—C64—C63	121.8 (3)
C25—C24—H24	119.2	C65—C64—N62	118.3 (4)
C23—C24—H24	119.2	C63—C64—N62	119.9 (3)
C24—C25—C26	120.4 (3)	C64—C65—C66	118.3 (3)
C24—C25—H25	119.8	C64—C65—H65	120.8
C26—C25—H25	119.8	C66—C65—H65	120.8
N21—C26—C25	122.1 (3)	C65—C66—N63	116.7 (3)
N21—C26—C21	121.0 (3)	C65—C66—C61	124.0 (3)
C25—C26—C21	116.9 (3)	N63—C66—C61	119.3 (3)
C28—C27—C32	116.9 (3)	O63—N61—O62	125.3 (4)
C28—C27—N21	121.9 (3)	O63—N61—C62	117.3 (4)
C32—C27—N21	121.2 (3)	O62—N61—C62	117.4 (4)
C29—C28—C27	120.3 (3)	O64—N62—O65	124.1 (4)
C29—C28—H28	119.8	O64—N62—C64	117.6 (4)
C27—C28—H28	119.8	O65—N62—C64	118.3 (4)
C30—C29—C28	121.6 (3)	O67—N63—O66	120.8 (4)
C30—C29—H29	119.2	O67—N63—C66	119.6 (4)
C28—C29—H29	119.2	O66—N63—C66	119.6 (4)
C31—C30—C29	119.0 (3)	O71—C71—C76	127.4 (3)
C31—C30—H30	120.5	O71—C71—C72	120.4 (3)
C29—C30—H30	120.5	C76—C71—C72	112.2 (3)
C30—C31—C32	120.5 (3)	C73—C72—C71	125.1 (4)
C30—C31—H31	119.8	C73—C72—N71	116.5 (3)
C32—C31—H31	119.8	C71—C72—N71	118.4 (3)
C31—C32—C27	121.6 (3)	C72—C73—C74	118.3 (3)

C31—C32—S21	120.4 (2)	C72—C73—H73	120.9
C27—C32—S21	117.8 (2)	C74—C73—H73	120.9
N21—C33—C34	109.3 (2)	C75—C74—C73	121.6 (3)
N21—C33—H33A	109.8	C75—C74—N72	119.4 (4)
C34—C33—H33A	109.8	C73—C74—N72	118.9 (3)
N21—C33—H33B	109.8	C74—C75—C76	119.8 (3)
C34—C33—H33B	109.8	C74—C75—H75	120.1
H33A—C33—H33B	108.3	C76—C75—H75	120.1
C35—C34—N22	112.1 (2)	C75—C76—C71	122.7 (3)
C35—C34—C33	113.0 (3)	C75—C76—N73	116.6 (3)
N22—C34—C33	109.3 (2)	C71—C76—N73	120.5 (3)
C35—C34—H34	107.4	O73—N71—O72	119.6 (6)
N22—C34—H34	107.4	O73—N71—C72	122.3 (6)
C33—C34—H34	107.4	O72—N71—C72	118.0 (4)
C34—C35—H35A	109.5	O75—N72—O74	123.8 (3)
C34—C35—H35B	109.5	O75—N72—C74	118.2 (3)
H35A—C35—H35B	109.5	O74—N72—C74	118.0 (4)
C34—C35—H35C	109.5	O77—N73—O76	121.5 (4)
H35A—C35—H35C	109.5	O77—N73—C76	119.5 (4)
H35B—C35—H35C	109.5	O76—N73—C76	119.0 (3)
N22—C36—H36A	109.5	O81—C81—C82	125.2 (3)
N22—C36—H36B	109.5	O81—C81—C86	122.4 (3)
H36A—C36—H36B	109.5	C82—C81—C86	112.3 (3)
N22—C36—H36C	109.5	C83—C82—C81	123.8 (3)
H36A—C36—H36C	109.5	C83—C82—N81	116.7 (3)
H36B—C36—H36C	109.5	C81—C82—N81	119.6 (3)
N22—C37—H37A	109.5	C84—C83—C82	119.3 (3)
N22—C37—H37B	109.5	C84—C83—H83	120.4
H37A—C37—H37B	109.5	C82—C83—H83	120.4
N22—C37—H37C	109.5	C83—C84—C85	121.3 (3)
H37A—C37—H37C	109.5	C83—C84—N82	118.7 (3)
H37B—C37—H37C	109.5	C85—C84—N82	120.0 (3)
C26—N21—C27	120.5 (2)	C86—C85—C84	118.2 (3)
C26—N21—C33	119.0 (2)	C86—C85—H85	120.9
C27—N21—C33	120.4 (2)	C84—C85—H85	120.9
C36—N22—C37	110.9 (3)	C85—C86—C81	125.1 (3)
C36—N22—C34	114.8 (2)	C85—C86—N83	118.4 (3)
C37—N22—C34	110.6 (3)	C81—C86—N83	116.5 (3)
C36—N22—H22A	106.7	O82—N81—O83	122.9 (3)
C37—N22—H22A	106.7	O82—N81—C82	119.6 (3)
C34—N22—H22A	106.7	O83—N81—C82	117.5 (3)
O21—S21—O22	117.23 (14)	O85—N82—O84	123.6 (3)
O21—S21—C32	108.60 (13)	O85—N82—C84	117.4 (4)
O22—S21—C32	110.69 (14)	O84—N82—C84	118.9 (4)
O21—S21—C21	108.20 (13)	O86—N83—O87	122.4 (4)
O22—S21—C21	110.51 (13)	O86—N83—C86	119.7 (3)
C32—S21—C21	100.24 (15)	O87—N83—C86	117.9 (4)
C6—C1—C2—C3	−1.6 (5)	C50—C51—C52—S41	−174.6 (3)
S1—C1—C2—C3	173.4 (3)	C48—C47—C52—C51	−4.8 (5)

C1—C2—C3—C4	0.7 (5)	N41—C47—C52—C51	172.9 (3)
C2—C3—C4—C5	0.5 (5)	C48—C47—C52—S41	173.4 (2)
C3—C4—C5—C6	−0.9 (5)	N41—C47—C52—S41	−8.9 (4)
C4—C5—C6—C1	0.0 (4)	N41—C53—C54—C55	−62.9 (3)
C4—C5—C6—N1	176.2 (3)	N41—C53—C54—N42	172.3 (2)
C2—C1—C6—C5	1.2 (4)	C48—C47—N41—C46	143.6 (3)
S1—C1—C6—C5	−173.9 (2)	C52—C47—N41—C46	−34.0 (4)
C2—C1—C6—N1	−175.0 (3)	C48—C47—N41—C53	−19.8 (4)
S1—C1—C6—N1	9.8 (4)	C52—C47—N41—C53	162.7 (3)
N1—C7—C8—C9	−174.1 (3)	C45—C46—N41—C47	−143.7 (3)
C12—C7—C8—C9	3.6 (4)	C41—C46—N41—C47	34.7 (4)
C7—C8—C9—C10	−0.5 (5)	C45—C46—N41—C53	19.6 (4)
C8—C9—C10—C11	−1.5 (5)	C41—C46—N41—C53	−162.1 (3)
C9—C10—C11—C12	0.2 (5)	C54—C53—N41—C47	−64.0 (4)
C10—C11—C12—C7	3.1 (5)	C54—C53—N41—C46	132.7 (3)
C10—C11—C12—S1	−173.4 (2)	C55—C54—N42—C57	67.2 (4)
C8—C7—C12—C11	−4.9 (4)	C53—C54—N42—C57	−166.9 (3)
N1—C7—C12—C11	172.8 (3)	C55—C54—N42—C56	−61.1 (4)
C8—C7—C12—S1	171.7 (2)	C53—C54—N42—C56	64.8 (4)
N1—C7—C12—S1	−10.6 (4)	C51—C52—S41—O42	−24.3 (3)
N1—C13—C14—N2	166.2 (2)	C47—C52—S41—O42	157.5 (2)
N1—C13—C14—C15	−69.0 (3)	C51—C52—S41—O41	106.3 (3)
C8—C7—N1—C6	148.0 (3)	C47—C52—S41—O41	−71.9 (3)
C12—C7—N1—C6	−29.6 (4)	C51—C52—S41—C41	−140.7 (3)
C8—C7—N1—C13	−30.2 (4)	C47—C52—S41—C41	41.1 (3)
C12—C7—N1—C13	152.2 (3)	C42—C41—S41—O42	26.1 (3)
C5—C6—N1—C7	−146.1 (3)	C46—C41—S41—O42	−157.0 (2)
C1—C6—N1—C7	30.0 (4)	C42—C41—S41—O41	−103.4 (3)
C5—C6—N1—C13	32.1 (4)	C46—C41—S41—O41	73.6 (3)
C1—C6—N1—C13	−151.8 (3)	C42—C41—S41—C52	142.8 (3)
C14—C13—N1—C7	−69.4 (3)	C46—C41—S41—C52	−40.2 (3)
C14—C13—N1—C6	112.4 (3)	O61—C61—C62—C63	174.1 (3)
C15—C14—N2—C16	−53.4 (4)	C66—C61—C62—C63	−1.1 (5)
C13—C14—N2—C16	71.1 (3)	O61—C61—C62—N61	−1.3 (5)
C15—C14—N2—C17	73.4 (3)	C66—C61—C62—N61	−176.5 (3)
C13—C14—N2—C17	−162.1 (3)	C61—C62—C63—C64	0.5 (5)
C11—C12—S1—O1	−26.4 (3)	N61—C62—C63—C64	176.0 (3)
C7—C12—S1—O1	156.9 (2)	C62—C63—C64—C65	−0.8 (5)
C11—C12—S1—O2	102.9 (3)	C62—C63—C64—N62	−179.2 (3)
C7—C12—S1—O2	−73.7 (3)	C63—C64—C65—C66	1.7 (5)
C11—C12—S1—C1	−143.2 (3)	N62—C64—C65—C66	−179.9 (3)
C7—C12—S1—C1	40.2 (3)	C64—C65—C66—N63	179.4 (3)
C2—C1—S1—O1	29.0 (3)	C64—C65—C66—C61	−2.5 (5)
C6—C1—S1—O1	−155.9 (2)	O61—C61—C66—C65	−173.0 (3)
C2—C1—S1—O2	−100.9 (3)	C62—C61—C66—C65	2.1 (5)
C6—C1—S1—O2	74.3 (3)	O61—C61—C66—N63	5.1 (5)
C2—C1—S1—C12	145.0 (3)	C62—C61—C66—N63	−179.9 (3)
C6—C1—S1—C12	−39.8 (3)	C63—C62—N61—O63	135.5 (4)
C26—C21—C22—C23	2.2 (5)	C61—C62—N61—O63	−48.7 (5)

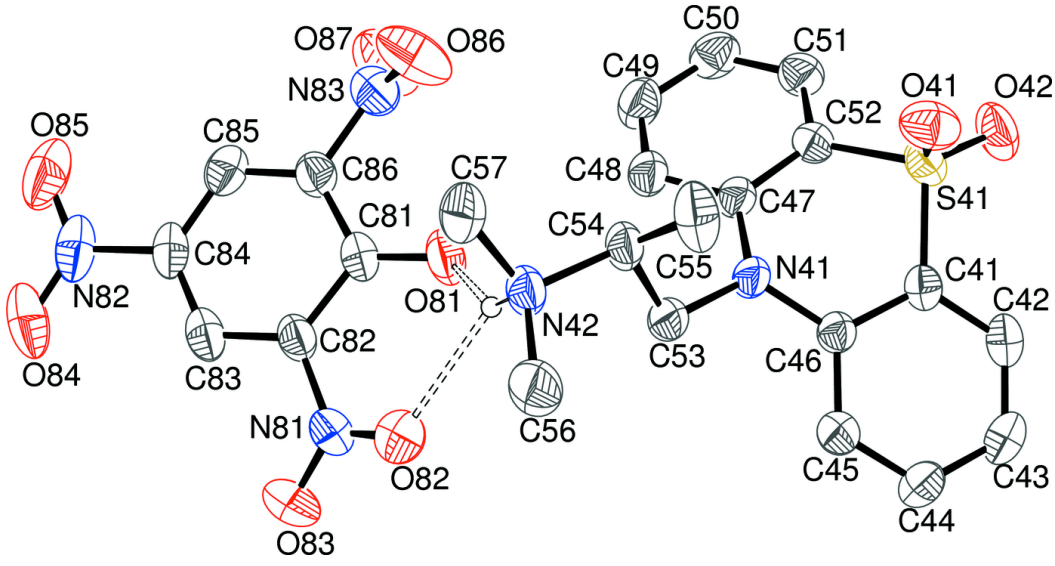
S21—C21—C22—C23	−171.4 (3)	C63—C62—N61—O62	−44.5 (5)
C21—C22—C23—C24	1.0 (5)	C61—C62—N61—O62	131.3 (4)
C22—C23—C24—C25	−2.8 (5)	C65—C64—N62—O64	176.5 (4)
C23—C24—C25—C26	1.3 (5)	C63—C64—N62—O64	−5.0 (6)
C24—C25—C26—N21	−177.5 (3)	C65—C64—N62—O65	−4.2 (5)
C24—C25—C26—C21	1.8 (4)	C63—C64—N62—O65	174.3 (4)
C22—C21—C26—N21	175.8 (3)	C65—C66—N63—O67	−149.8 (5)
S21—C21—C26—N21	−10.5 (4)	C61—C66—N63—O67	32.0 (6)
C22—C21—C26—C25	−3.6 (4)	C65—C66—N63—O66	31.1 (6)
S21—C21—C26—C25	170.1 (2)	C61—C66—N63—O66	−147.1 (4)
C32—C27—C28—C29	−0.3 (5)	O71—C71—C72—C73	175.3 (4)
N21—C27—C28—C29	178.6 (3)	C76—C71—C72—C73	−5.6 (5)
C27—C28—C29—C30	−1.3 (6)	O71—C71—C72—N71	−5.4 (6)
C28—C29—C30—C31	1.2 (6)	C76—C71—C72—N71	173.7 (4)
C29—C30—C31—C32	0.5 (6)	C71—C72—C73—C74	1.6 (6)
C30—C31—C32—C27	−2.1 (5)	N71—C72—C73—C74	−177.7 (4)
C30—C31—C32—S21	173.1 (3)	C72—C73—C74—C75	2.2 (6)
C28—C27—C32—C31	1.9 (5)	C72—C73—C74—N72	178.6 (3)
N21—C27—C32—C31	−177.0 (3)	C73—C74—C75—C76	−1.4 (5)
C28—C27—C32—S21	−173.4 (2)	N72—C74—C75—C76	−177.8 (3)
N21—C27—C32—S21	7.7 (4)	C74—C75—C76—C71	−3.3 (5)
N21—C33—C34—C35	−62.2 (3)	C74—C75—C76—N73	173.5 (3)
N21—C33—C34—N22	172.3 (2)	O71—C71—C76—C75	−174.7 (3)
C25—C26—N21—C27	149.4 (3)	C72—C71—C76—C75	6.3 (5)
C21—C26—N21—C27	−29.9 (4)	O71—C71—C76—N73	8.7 (5)
C25—C26—N21—C33	−27.4 (4)	C72—C71—C76—N73	−170.3 (3)
C21—C26—N21—C33	153.2 (3)	C73—C72—N71—O73	−51.9 (8)
C28—C27—N21—C26	−147.3 (3)	C71—C72—N71—O73	128.8 (6)
C32—C27—N21—C26	31.6 (4)	C73—C72—N71—O72	130.9 (5)
C28—C27—N21—C33	29.5 (5)	C71—C72—N71—O72	−48.4 (7)
C32—C27—N21—C33	−151.6 (3)	C75—C74—N72—O75	−8.2 (5)
C34—C33—N21—C26	−64.4 (4)	C73—C74—N72—O75	175.4 (4)
C34—C33—N21—C27	118.7 (3)	C75—C74—N72—O74	172.2 (3)
C35—C34—N22—C36	−56.0 (4)	C73—C74—N72—O74	−4.3 (5)
C33—C34—N22—C36	70.1 (3)	C75—C76—N73—O77	170.6 (4)
C35—C34—N22—C37	70.5 (3)	C71—C76—N73—O77	−12.6 (5)
C33—C34—N22—C37	−163.5 (3)	C75—C76—N73—O76	−10.7 (5)
C31—C32—S21—O21	−100.2 (3)	C71—C76—N73—O76	166.2 (3)
C27—C32—S21—O21	75.2 (3)	O81—C81—C82—C83	−178.1 (3)
C31—C32—S21—O22	29.8 (3)	C86—C81—C82—C83	−1.3 (5)
C27—C32—S21—O22	−154.8 (2)	O81—C81—C82—N81	0.7 (5)
C31—C32—S21—C21	146.4 (3)	C86—C81—C82—N81	177.5 (3)
C27—C32—S21—C21	−38.1 (3)	C81—C82—C83—C84	−1.2 (5)
C22—C21—S21—O21	99.9 (3)	N81—C82—C83—C84	179.9 (3)
C26—C21—S21—O21	−73.9 (3)	C82—C83—C84—C85	3.4 (5)
C22—C21—S21—O22	−29.7 (3)	C82—C83—C84—N82	−178.5 (3)
C26—C21—S21—O22	156.5 (2)	C83—C84—C85—C86	−2.7 (5)
C22—C21—S21—C32	−146.5 (3)	N82—C84—C85—C86	179.1 (3)
C26—C21—S21—C32	39.7 (3)	C84—C85—C86—C81	−0.1 (5)

C46—C41—C42—C43	−2.5 (5)	C84—C85—C86—N83	179.1 (3)
S41—C41—C42—C43	174.4 (2)	O81—C81—C86—C85	178.9 (3)
C41—C42—C43—C44	0.3 (5)	C82—C81—C86—C85	2.0 (5)
C42—C43—C44—C45	1.2 (5)	O81—C81—C86—N83	−0.3 (5)
C43—C44—C45—C46	−0.5 (5)	C82—C81—C86—N83	−177.2 (3)
C44—C45—C46—C41	−1.5 (4)	C83—C82—N81—O82	−157.0 (3)
C44—C45—C46—N41	176.9 (3)	C81—C82—N81—O82	24.0 (5)
C42—C41—C46—C45	3.0 (4)	C83—C82—N81—O83	23.6 (4)
S41—C41—C46—C45	−173.9 (2)	C81—C82—N81—O83	−155.4 (3)
C42—C41—C46—N41	−175.4 (3)	C83—C84—N82—O85	178.6 (3)
S41—C41—C46—N41	7.6 (4)	C85—C84—N82—O85	−3.2 (5)
C52—C47—C48—C49	2.7 (5)	C83—C84—N82—O84	−0.5 (5)
N41—C47—C48—C49	−174.9 (3)	C85—C84—N82—O84	177.7 (3)
C47—C48—C49—C50	0.6 (5)	C85—C86—N83—O86	124.7 (4)
C48—C49—C50—C51	−1.9 (6)	C81—C86—N83—O86	−56.1 (5)
C49—C50—C51—C52	−0.2 (5)	C85—C86—N83—O87	−58.8 (5)
C50—C51—C52—C47	3.6 (5)	C81—C86—N83—O87	120.5 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O61	0.91	1.75	2.620 (3)	160
N22—H22A···O71	0.91	1.86	2.689 (3)	151
N22—H22A···O77	0.91	2.37	3.046 (4)	131
N42—H42A···O81	0.91	1.89	2.681 (4)	144
N42—H42A···O82	0.91	2.29	3.018 (4)	137

Fig. 1


O87
O86
N83
O85
C85
C86
C57
C50
C51
C49
O41
O42
C52
C48
C47
S41
C81
C54
C84
C55
N41
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N82
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C53
C46
N81
C56
C45
C43
O82
C44
O83