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Ethyl 2-(2-chloro-1,4-dihydro-1,4-dioxonaphthalen-3-ylamino)-4-phenylthiazole-5-carboxylate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.094
wR factor = 0.251
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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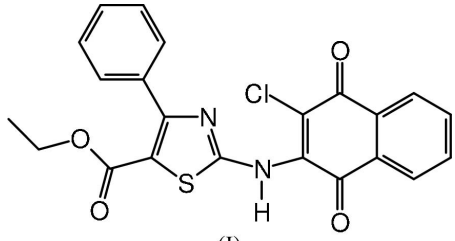
The structure of the title compound, $C_{22}H_{15}ClN_2O_4S$, comprises non-planar molecules that form a one-dimensional hydrogen-bonded chain *via* a single N—H···O interaction, which runs parallel to the *b* axis. The dihedral angle between the thiazole and quinone rings is 50.43 (7)° and the dihedral angle between the thiazole and the phenyl rings is 52.4 (1)°.

Comment

The title compound, (I), was prepared with the intention of merging two separate studies that we have recently undertaken. One study involved the synthesis and structural properties of 2-substituted 3-chloro-1,4-naphthoquinones (Lynch & McClenaghan, 2002; 2003), while the other involved 2-aminothiazoles. From the latter study came the structure of the thiazole derivative used to prepare (I), *viz*. ethyl 2-amino-4-phenylthiazole-5-carboxylate (Lynch & McClenaghan, 2000). By bringing together the two series of molecules, we are interested in examining the combined structural aspects of the resultant covalently linked products, especially considering the forced proximity of one N—H hydrogen-bond donor with five hydrogen-bond acceptors (*viz*. two O atoms, one N atom, one Cl atom and one S atom). The structure of (I) comprises non-planar molecules, the dihedral angle between the thiazole and quinone rings being 50.43 (7)° and the dihedral angle between the thiazole and phenyl rings being 52.4 (1)°. The equivalent dihedral angle in the parent thiazole molecule is 42.41 (6)°.



(I)

Molecules of (I) form a one-dimensional hydrogen-bonded chain *via* a single N—H···O interaction [graph set *C*(6); Etter, 1990], which runs parallel to the *b* axis; hydrogen-bonding geometry is given in Table 1. A close contact C25—H25···O21^{i} [C···O^{i} = 3.165 (3) Å, H···O^{i} = 2.22 Å and C—H···O^{i} = 172°; symmetry code: (i) *x*, 1 + *y*, *z*] exists adjacent to the N—H···O interaction and thus completes an $R_2^2(10)$ graph-set motif.

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

Crystal data

$C_{22}H_{15}ClN_2O_4S$
M_r = 438.87
Monoclinic, $P2_1/c$
a = 19.191 (5) Å
b = 7.719 (2) Å
c = 12.640 (3) Å
β = 94.845 (18)°
V = 1865.6 (8) Å^3
Z = 4
D_x = 1.563 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4585 reflections
θ = 2.9–27.5°
μ = 0.35 mm^{-1}
T = 120 (2) K
Plate, orange
0.18 × 0.14 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.939, T_{max} = 0.993
34099 measured reflections
3678 independent reflections
3672 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 26.0°
$h = -23 \rightarrow 23$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.251
S = 1.14
3678 reflections
276 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0933P)^2 + 12.2716P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···O24^{i}	0.86 (2)	2.27 (2)	3.066 (3)	154 (2)

Symmetry code: (i) $x, y-1, z$.

The amino H atom was located in a difference Fourier synthesis and its positional parameters were refined. Other H atoms were included in the refinement at calculated positions in the riding-model approximation, with C—H distances of 0.95 (aromatic H atoms), 0.98 (CH_3 H atoms) and 0.99 Å (CH_2 H atoms). The isotropic displacement parameters for all H atoms were set equal to 1.25U_{eq} of the carrier atom. The high R value in this structure was a direct consequence of poor data from poor-quality twinned crystals; the non-merohedral twinning was refined as two components with ratio 0.5207 (8):0.4793 (8).

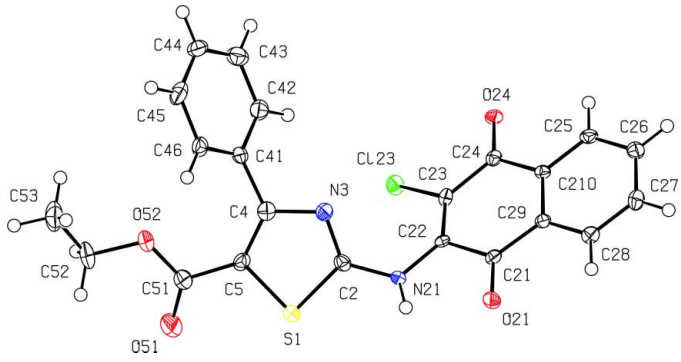


Figure 1
The molecular configuration and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radius.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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supporting information

Acta Cryst. (2005). E**61**, o790–o791 [https://doi.org/10.1107/S1600536805005647]

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$V = 1865.6\ (8)$ Å^3
$Z = 4$
$F(000) = 904$
$D_x = 1.563$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4585 reflections
$\theta = 2.9–27.5°$
$\mu = 0.35$ mm^{-1}
$T = 120$ K
Plate, orange
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Data collection

Nonius KappaCCD diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.939$, $T_{max} = 0.993$
34099 measured reflections
3678 independent reflections
3672 reflections with $I > 2\sigma(I)$
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$\theta_{max} = 26.0°$, $\theta_{min} = 3.2°$
$h = -23\rightarrow23$
$k = -9\rightarrow9$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.094$
$wR(F^2) = 0.251$
$S = 1.14$
3678 reflections
276 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0933P)^2 + 12.2716P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Special details

Geometry. Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
16.4712 (0.0108) *x* + 0.7887 (0.0076) *y* + 5.4172 (0.0114) *z* = 6.6141 (0.0074)
* -0.0087 (0.0017) C41 * 0.0073 (0.0018) C42 * -0.0018 (0.0017) C43 * -0.0024 (0.0018) C44 * 0.0009 (0.0018) C45 * 0.0046 (0.0017) C46
Rms deviation of fitted atoms = 0.0052
6.6939 (0.0215) *x* - 4.4720 (0.0052) *y* + 8.9054 (0.0083) *z* = 3.3544 (0.0063)
Angle to previous plane (with approximate e.s.d.) = 52.36 (0.10)
* -0.0093 (0.0011) S1 * 0.0086 (0.0013) C2 * -0.0030 (0.0015) N3 * -0.0064 (0.0016) C4 * 0.0100 (0.0014) C5
Rms deviation of fitted atoms = 0.0079
- 3.7776 (0.0170) *x* + 0.2173 (0.0070) *y* + 12.5531 (0.0042) *z* = 2.9615 (0.0099)
Angle to previous plane (with approximate e.s.d.) = 50.43 (0.07)
* -0.0131 (0.0016) C21 * 0.0529 (0.0017) C22 * -0.0496 (0.0017) C23 * 0.0052 (0.0017) C24 * 0.0327 (0.0017) C210 * -0.0280 (0.0016) C29
Rms deviation of fitted atoms = 0.0349

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.26243 (3)	0.31468 (8)	0.33640 (5)	0.02098 (16)
C2	0.31564 (12)	0.4837 (3)	0.38331 (19)	0.0170 (5)
N21	0.38181 (10)	0.4994 (3)	0.34992 (16)	0.0141 (5)
H21	0.4059 (12)	0.406 (3)	0.349 (2)	0.018*
N3	0.29030 (10)	0.5864 (3)	0.45263 (16)	0.0183 (5)
C4	0.22472 (12)	0.5310 (3)	0.4737 (2)	0.0180 (6)
C5	0.20140 (12)	0.3859 (3)	0.4202 (2)	0.0192 (6)
C21	0.49776 (12)	0.6183 (3)	0.37395 (19)	0.0147 (5)
O21	0.51830 (8)	0.4685 (2)	0.37840 (14)	0.0209 (4)
C22	0.42034 (12)	0.6500 (3)	0.35537 (18)	0.0133 (5)
C23	0.39744 (12)	0.8138 (3)	0.33748 (19)	0.0154 (5)
Cl23	0.31275 (3)	0.85753 (8)	0.28897 (5)	0.02148 (16)
C24	0.44328 (12)	0.9673 (3)	0.35298 (19)	0.0145 (5)
O24	0.41967 (8)	1.1139 (2)	0.34265 (13)	0.0174 (4)
C25	0.56428 (12)	1.0748 (3)	0.39453 (19)	0.0172 (6)
H25	0.5466	1.1899	0.3921	0.021*
C26	0.63557 (12)	1.0457 (3)	0.41421 (19)	0.0183 (6)
H26	0.6667	1.1407	0.4265	0.022*
C27	0.66129 (12)	0.8779 (3)	0.41589 (19)	0.0194 (6)
H27	0.7102	0.8584	0.4274	0.023*
C28	0.61666 (11)	0.7400 (4)	0.40112 (18)	0.0163 (5)
H28	0.6349	0.6255	0.4023	0.020*
C29	0.54527 (11)	0.7662 (3)	0.38451 (18)	0.0139 (5)
C210	0.51889 (11)	0.9356 (3)	0.37848 (18)	0.0125 (5)
C41	0.18920 (11)	0.6379 (3)	0.5512 (2)	0.0171 (6)
C42	0.18634 (13)	0.8157 (3)	0.5369 (2)	0.0228 (6)
H42	0.2048	0.8660	0.4767	0.027*
C43	0.15663 (13)	0.9210 (4)	0.6103 (2)	0.0269 (7)
H43	0.1541	1.0427	0.5993	0.032*
C44	0.13116 (13)	0.8496 (4)	0.6980 (2)	0.0274 (7)

H44	0.1110	0.9215	0.7483	0.033*
C45	0.13472 (13)	0.6730 (4)	0.7135 (2)	0.0277 (7)
H45	0.1170	0.6235	0.7746	0.033*
C46	0.16405 (11)	0.5670 (3)	0.6404 (2)	0.0200 (6)
H46	0.1668	0.4455	0.6520	0.024*
C51	0.13485 (13)	0.2902 (3)	0.4126 (2)	0.0238 (6)
O51	0.12084 (11)	0.1819 (3)	0.34567 (18)	0.0498 (6)
O52	0.09298 (8)	0.3353 (2)	0.48486 (15)	0.0293 (5)
C52	0.02647 (12)	0.2460 (4)	0.4842 (2)	0.0349 (7)
H51	0.0326	0.1213	0.4691	0.042*
H52	−0.0073	0.2951	0.4287	0.042*
C53	0.00022 (14)	0.2688 (4)	0.5906 (2)	0.0426 (8)
H53	0.0344	0.2214	0.6451	0.064*
H54	−0.0444	0.2077	0.5929	0.064*
H55	−0.0066	0.3924	0.6041	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0197 (3)	0.0181 (3)	0.0254 (4)	−0.0030 (3)	0.0036 (3)	−0.0041 (3)
C2	0.0186 (12)	0.0146 (13)	0.0177 (13)	−0.0010 (11)	0.0007 (11)	0.0028 (11)
N21	0.0152 (10)	0.0104 (11)	0.0171 (11)	−0.0003 (9)	0.0040 (9)	−0.0015 (10)
N3	0.0149 (10)	0.0182 (11)	0.0219 (12)	0.0018 (9)	0.0020 (9)	0.0002 (10)
C4	0.0181 (12)	0.0171 (14)	0.0184 (14)	0.0032 (11)	−0.0015 (10)	0.0053 (12)
C5	0.0172 (12)	0.0168 (14)	0.0240 (14)	0.0040 (11)	0.0043 (11)	0.0022 (12)
C21	0.0171 (12)	0.0144 (13)	0.0130 (13)	0.0025 (10)	0.0046 (10)	−0.0002 (10)
O21	0.0197 (9)	0.0098 (9)	0.0338 (11)	0.0020 (8)	0.0052 (8)	0.0032 (8)
C22	0.0163 (12)	0.0153 (14)	0.0091 (12)	−0.0009 (11)	0.0060 (10)	−0.0051 (11)
C23	0.0129 (11)	0.0178 (13)	0.0160 (13)	0.0012 (10)	0.0034 (10)	0.0018 (11)
Cl23	0.0146 (3)	0.0194 (3)	0.0298 (4)	0.0023 (3)	−0.0016 (3)	0.0021 (3)
C24	0.0171 (12)	0.0175 (14)	0.0094 (12)	−0.0007 (11)	0.0041 (10)	−0.0002 (11)
O24	0.0201 (9)	0.0091 (9)	0.0235 (10)	0.0042 (7)	0.0050 (8)	0.0014 (8)
C25	0.0231 (13)	0.0115 (13)	0.0179 (14)	0.0029 (11)	0.0069 (11)	0.0005 (11)
C26	0.0214 (13)	0.0193 (14)	0.0146 (13)	−0.0032 (11)	0.0037 (11)	−0.0031 (11)
C27	0.0159 (12)	0.0248 (15)	0.0176 (14)	−0.0011 (11)	0.0014 (10)	0.0014 (12)
C28	0.0181 (11)	0.0147 (12)	0.0163 (13)	0.0042 (12)	0.0021 (10)	0.0033 (11)
C29	0.0171 (11)	0.0123 (13)	0.0129 (12)	−0.0002 (11)	0.0053 (9)	−0.0001 (11)
C210	0.0151 (11)	0.0118 (13)	0.0105 (12)	0.0006 (10)	0.0006 (10)	−0.0008 (10)
C41	0.0091 (11)	0.0207 (15)	0.0207 (14)	0.0004 (11)	−0.0038 (10)	−0.0054 (12)
C42	0.0203 (13)	0.0240 (15)	0.0244 (15)	0.0003 (11)	0.0036 (11)	0.0008 (13)
C43	0.0232 (14)	0.0210 (16)	0.0359 (18)	0.0013 (12)	−0.0007 (13)	−0.0042 (13)
C44	0.0170 (13)	0.0301 (18)	0.0352 (18)	0.0001 (13)	0.0032 (12)	−0.0177 (14)
C45	0.0210 (14)	0.0423 (18)	0.0207 (15)	−0.0014 (13)	0.0076 (12)	−0.0045 (14)
C46	0.0123 (12)	0.0204 (15)	0.0275 (15)	0.0014 (11)	0.0023 (11)	0.0027 (13)
C51	0.0189 (13)	0.0263 (18)	0.0260 (15)	−0.0040 (11)	0.0012 (11)	−0.0039 (13)
O51	0.0413 (12)	0.0531 (15)	0.0573 (15)	−0.0240 (11)	0.0181 (11)	−0.0294 (13)
O52	0.0196 (9)	0.0287 (11)	0.0403 (12)	−0.0105 (8)	0.0070 (9)	−0.0090 (10)
C52	0.0184 (12)	0.0387 (16)	0.0480 (19)	−0.0134 (15)	0.0050 (12)	−0.0016 (17)

C53	0.0273 (14)	0.045 (2)	0.057 (2)	−0.0103 (16)	0.0147 (14)	0.0055 (18)

Geometric parameters (Å, º)

S1—C2	1.731 (2)	C27—H27	0.95
S1—C5	1.733 (2)	C28—C29	1.383 (3)
C2—N3	1.306 (3)	C28—H28	0.95
C2—N21	1.377 (3)	C29—C210	1.402 (3)
N21—C22	1.376 (3)	C41—C46	1.377 (3)
N21—H21	0.86 (2)	C41—C42	1.384 (3)
N3—C4	1.377 (3)	C42—C43	1.391 (3)
C4—C5	1.365 (3)	C42—H42	0.95
C4—C41	1.489 (3)	C43—C44	1.365 (4)
C5—C51	1.471 (3)	C43—H43	0.95
C21—O21	1.222 (3)	C44—C45	1.377 (4)
C21—C29	1.460 (3)	C44—H44	0.95
C21—C22	1.504 (3)	C45—C46	1.388 (3)
C22—C23	1.351 (3)	C45—H45	0.95
C23—C24	1.479 (3)	C46—H46	0.95
C23—Cl23	1.721 (2)	C51—O51	1.204 (3)
C24—O24	1.222 (3)	C51—O52	1.313 (3)
C24—C210	1.480 (3)	O52—C52	1.450 (3)
C25—C210	1.388 (3)	C52—C53	1.486 (4)
C25—C26	1.388 (3)	C52—H51	0.99
C25—H25	0.95	C52—H52	0.99
C26—C27	1.386 (3)	C53—H53	0.98
C26—H26	0.95	C53—H54	0.98
C27—C28	1.369 (3)	C53—H55	0.98
C2—S1—C5	87.78 (12)	C28—C29—C21	120.2 (2)
N3—C2—N21	123.9 (2)	C210—C29—C21	120.3 (2)
N3—C2—S1	116.45 (18)	C25—C210—C29	119.7 (2)
N21—C2—S1	119.59 (18)	C25—C210—C24	119.7 (2)
C2—N21—C22	124.3 (2)	C29—C210—C24	120.6 (2)
C2—N21—H21	116.4 (16)	C46—C41—C42	119.2 (2)
C22—N21—H21	115.1 (16)	C46—C41—C4	122.0 (2)
C2—N3—C4	109.9 (2)	C42—C41—C4	118.6 (2)
C5—C4—N3	115.2 (2)	C41—C42—C43	120.4 (3)
C5—C4—C41	129.2 (2)	C41—C42—H42	119.8
N3—C4—C41	115.6 (2)	C43—C42—H42	119.8
C4—C5—C51	133.7 (2)	C44—C43—C42	120.0 (3)
C4—C5—S1	110.68 (18)	C44—C43—H43	120.0
C51—C5—S1	115.40 (19)	C42—C43—H43	120.0
O21—C21—C29	122.6 (2)	C43—C44—C45	119.9 (3)
O21—C21—C22	118.1 (2)	C43—C44—H44	120.1
C29—C21—C22	119.2 (2)	C45—C44—H44	120.1
C23—C22—N21	128.0 (2)	C44—C45—C46	120.4 (3)
C23—C22—C21	118.7 (2)	C44—C45—H45	119.8

N21—C22—C21	113.0 (2)	C46—C45—H45	119.8
C22—C23—C24	123.1 (2)	C41—C46—C45	120.0 (3)
C22—C23—Cl23	121.81 (18)	C41—C46—H46	120.0
C24—C23—Cl23	115.03 (18)	C45—C46—H46	120.0
O24—C24—C23	121.1 (2)	O51—C51—O52	124.0 (2)
O24—C24—C210	121.6 (2)	O51—C51—C5	122.4 (2)
C23—C24—C210	117.2 (2)	O52—C51—C5	113.6 (2)
C210—C25—C26	119.9 (2)	C51—O52—C52	117.4 (2)
C210—C25—H25	120.1	O52—C52—C53	107.7 (2)
C26—C25—H25	120.1	O52—C52—H51	110.2
C27—C26—C25	119.9 (2)	C53—C52—H51	110.2
C27—C26—H26	120.0	O52—C52—H52	110.2
C25—C26—H26	120.0	C53—C52—H52	110.2
C28—C27—C26	120.4 (2)	H51—C52—H52	108.5
C28—C27—H27	119.8	C52—C53—H53	109.5
C26—C27—H27	119.8	C52—C53—H54	109.5
C27—C28—C29	120.5 (2)	H53—C53—H54	109.5
C27—C28—H28	119.8	C52—C53—H55	109.5
C29—C28—H28	119.8	H53—C53—H55	109.5
C28—C29—C210	119.5 (2)	H54—C53—H55	109.5

C5—S1—C2—N3	−1.5 (2)	O21—C21—C29—C28	−0.5 (4)
C5—S1—C2—N21	176.1 (2)	C22—C21—C29—C28	−179.7 (2)
N3—C2—N21—C22	−22.7 (4)	O21—C21—C29—C210	179.8 (2)
S1—C2—N21—C22	159.94 (19)	C22—C21—C29—C210	0.7 (3)
N21—C2—N3—C4	−176.5 (2)	C26—C25—C210—C29	1.4 (4)
S1—C2—N3—C4	0.9 (3)	C26—C25—C210—C24	−177.4 (2)
C2—N3—C4—C5	0.3 (3)	C28—C29—C210—C25	−3.2 (3)
C2—N3—C4—C41	−179.5 (2)	C21—C29—C210—C25	176.4 (2)
N3—C4—C5—C51	−175.2 (3)	C28—C29—C210—C24	175.5 (2)
C41—C4—C5—C51	4.5 (5)	C21—C29—C210—C24	−4.8 (3)
N3—C4—C5—S1	−1.4 (3)	O24—C24—C210—C25	2.1 (4)
C41—C4—C5—S1	178.3 (2)	C23—C24—C210—C25	−179.6 (2)
C2—S1—C5—C4	1.54 (19)	O24—C24—C210—C29	−176.7 (2)
C2—S1—C5—C51	176.6 (2)	C23—C24—C210—C29	1.7 (3)
C2—N21—C22—C23	−38.4 (4)	C5—C4—C41—C46	54.9 (4)
C2—N21—C22—C21	147.6 (2)	N3—C4—C41—C46	−125.4 (2)
O21—C21—C22—C23	−172.1 (2)	C5—C4—C41—C42	−130.2 (3)
C29—C21—C22—C23	7.1 (3)	N3—C4—C41—C42	49.6 (3)
O21—C21—C22—N21	2.5 (3)	C46—C41—C42—C43	−1.8 (4)
C29—C21—C22—N21	−178.3 (2)	C4—C41—C42—C43	−176.9 (2)
N21—C22—C23—C24	175.7 (2)	C41—C42—C43—C44	1.2 (4)
C21—C22—C23—C24	−10.7 (4)	C42—C43—C44—C45	−0.2 (4)
N21—C22—C23—Cl23	−7.3 (4)	C43—C44—C45—C46	0.0 (4)
C21—C22—C23—Cl23	166.42 (17)	C42—C41—C46—C45	1.6 (4)
C22—C23—C24—O24	−175.2 (2)	C4—C41—C46—C45	176.5 (2)
Cl23—C23—C24—O24	7.6 (3)	C44—C45—C46—C41	−0.7 (4)
C22—C23—C24—C210	6.5 (4)	C4—C5—C51—O51	166.3 (3)

Cl23—C23—C24—C210	−170.78 (17)	S1—C5—C51—O51	−7.3 (4)
C210—C25—C26—C27	1.1 (4)	C4—C5—C51—O52	−13.3 (4)
C25—C26—C27—C28	−1.8 (4)	S1—C5—C51—O52	173.10 (18)
C26—C27—C28—C29	−0.1 (4)	O51—C51—O52—C52	1.1 (4)
C27—C28—C29—C210	2.6 (4)	C5—C51—O52—C52	−179.2 (2)
C27—C28—C29—C21	−177.0 (2)	C51—O52—C52—C53	160.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21···O24^{i}	0.86 (2)	2.27 (2)	3.066 (3)	154 (2)

Symmetry code: (i) *x*, *y*−1, *z*.