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data_fc1

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_chemical_formula_sum
 'C21 H21 Cl2 N O3'
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0311   0.0180
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 'O'  'O'   0.0492   0.0322
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 'Cl'  'Cl'   0.3639   0.7018
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_symmetry_cell_setting            Monoclinic
_symmetry_space_group_name_H-M    P2(1)/n

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                    8.6530(10)
_cell_length_b                    23.257(2)
_cell_length_c                    10.6200(10)
_cell_angle_alpha                 90.00
_cell_angle_beta                  109.410(10)
_cell_angle_gamma                 90.00
_cell_volume                      2015.7(3)
_cell_formula_units_Z             4
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_diffrn_ambient_temperature       289(2)
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_computing_cell_refinement        'Bruker XSCANS'
_computing_data_reduction         'Bruker XSCANS'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'PLATON'
_computing_publication_material   'PLATON'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
```

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 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^ > 2sigma(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.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.1511P)^2^+0.5796P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0019(6)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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N1 N 0.5056(4) 0.93202(16) 0.0976(4) 0.0469(11) Uani 1 1 d . . .
H1A H 0.4437 0.9510 0.0300 0.056 Uiso 1 1 calc R . .
C2 C 0.6378(6) 0.9604(2) 0.1746(5) 0.0509(13) Uani 1 1 d . . .
C3 C 0.7439(6) 0.9320(2) 0.2994(5) 0.0600(15) Uani 1 1 d . . .
H3A H 0.7159 0.9471 0.3743 0.072 Uiso 1 1 calc R . .
H3B H 0.8572 0.9420 0.3133 0.072 Uiso 1 1 calc R . .
C4 C 0.7280(6) 0.8673(2) 0.2977(5) 0.0547(14) Uani 1 1 d . . .
H4A H 0.7828 0.8530 0.3872 0.066 Uiso 1 1 calc R . .
H4B H 0.7848 0.8517 0.2404 0.066 Uiso 1 1 calc R . .
C5 C 0.5502(6) 0.84466(19) 0.2491(5) 0.0474(13) Uani 1 1 d . . .
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```
C6 C 0.4509(5) 0.87359(18) 0.1113(5) 0.0432(12) Uani 1 1 d . . .
O7 O 0.6724(4) 1.00847(16) 0.1429(4) 0.0765(13) Uani 1 1 d . . .
C8 C 0.5563(7) 0.7805(2) 0.2153(6) 0.0600(15) Uani 1 1 d . . .
H8A H 0.6566 0.7627 0.2722 0.072 Uiso 1 1 calc R . .
H8B H 0.4632 0.7599 0.2247 0.072 Uiso 1 1 calc R . .
C9 C 0.5501(6) 0.7816(2) 0.0726(5) 0.0537(14) Uani 1 1 d . . .
C10 C 0.4879(5) 0.8337(2) 0.0132(5) 0.0453(13) Uani 1 1 d . . .
C11 C 0.5929(7) 0.7384(3) -0.0022(7) 0.0724(17) Uani 1 1 d . . .
H11A H 0.6343 0.7033 0.0364 0.087 Uiso 1 1 calc R . .
C12 C 0.5716(7) 0.7495(3) -0.1348(7) 0.0768(19) Uani 1 1 d . . .
H12A H 0.6017 0.7217 -0.1853 0.092 Uiso 1 1 calc R . .
C13 C 0.5068(7) 0.8007(3) -0.1938(6) 0.0707(17) Uani 1 1 d . . .
H13A H 0.4908 0.8067 -0.2839 0.085 Uiso 1 1 calc R . .
C14 C 0.4655(5) 0.8432(2) -0.1204(5) 0.0542(14) Uani 1 1 d . . .
H14A H 0.4229 0.8779 -0.1602 0.065 Uiso 1 1 calc R . .
C15 C 0.4746(6) 0.8539(2) 0.3566(5) 0.0560(14) Uani 1 1 d . . .
O16 O 0.4417(6) 0.81648(19) 0.4209(5) 0.0951(15) Uani 1 1 d . . .
O17 O 0.4492(5) 0.90883(17) 0.3757(4) 0.0696(11) Uani 1 1 d . . .
C18 C 0.3678(10) 0.9220(3) 0.4711(7) 0.103(2) Uani 1 1 d . . .
H18A H 0.3672 0.9628 0.4836 0.124 Uiso 1 1 calc R . .
H18B H 0.4251 0.9038 0.5548 0.124 Uiso 1 1 calc R . .
H18C H 0.2571 0.9081 0.4383 0.124 Uiso 1 1 calc R . .
C19 C 0.2643(5) 0.8745(2) 0.0865(5) 0.0448(13) Uani 1 1 d . . .
C20 C 0.1711(6) 0.8248(2) 0.0459(5) 0.0537(14) Uani 1 1 d . . .
H20A H 0.2217 0.7909 0.0342 0.064 Uiso 1 1 calc R . .
C21 C 0.0033(6) 0.8253(3) 0.0227(5) 0.0634(16) Uani 1 1 d . . .
H21A H -0.0572 0.7917 -0.0027 0.076 Uiso 1 1 calc R . .
C22 C -0.0733(6) 0.8752(3) 0.0372(6) 0.0636(16) Uani 1 1 d . . .
H22A H -0.1860 0.8757 0.0196 0.076 Uiso 1 1 calc R . .
C23 C 0.0154(6) 0.9241(3) 0.0772(6) 0.0652(16) Uani 1 1 d . . .
H23A H -0.0370 0.9578 0.0876 0.078 Uiso 1 1 calc R . .
C24 C 0.1850(6) 0.9243(2) 0.1031(5) 0.0534(14) Uani 1 1 d . . .
H24A H 0.2447 0.9579 0.1314 0.064 Uiso 1 1 calc R . .
C25 C 0.9906(9) 0.9135(4) 0.7337(8) 0.114(3) Uani 1 1 d D . .
H25A H 1.0573 0.8860 0.7961 0.170 Uiso 0.529(12) 1 d P A 1
H25B H 1.0022 0.9505 0.7828 0.170 Uiso 0.529(12) 1 d P A 1
Cl26 Cl 0.7950(8) 0.8922(10) 0.6830(7) 0.312(9) Uani 0.529(12) 1 d PD A 1
Cl27 Cl 1.0598(7) 0.9228(3) 0.6056(5) 0.105(2) Uani 0.529(12) 1 d PD A 1
H25C H 1.0062 0.8869 0.8065 0.170 Uiso 0.471(12) 1 d P A 2
H25D H 1.0661 0.9458 0.7726 0.170 Uiso 0.471(12) 1 d P A 2
Cl28 Cl 0.7979(11) 0.9400(4) 0.6962(9) 0.206(6) Uani 0.471(12) 1 d PD A 2
Cl29 Cl 1.0476(17) 0.8887(10) 0.6256(13) 0.304(10) Uani 0.471(12) 1 d PD A 2

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N1 0.028(2) 0.051(2) 0.056(2) 0.0109(19) 0.0062(19) -0.0062(19)
C2 0.038(3) 0.049(3) 0.062(3) 0.007(3) 0.012(3) -0.007(3)
C3 0.041(3) 0.066(4) 0.064(4) 0.009(3) 0.005(3) -0.014(3)
C4 0.038(3) 0.061(3) 0.060(3) 0.012(3) 0.010(2) 0.002(2)
C5 0.041(3) 0.045(3) 0.055(3) 0.008(2) 0.015(2) -0.005(2)
C6 0.029(3) 0.042(3) 0.058(3) 0.008(2) 0.014(2) -0.006(2)
```

```
O7 0.058(2) 0.062(3) 0.090(3) 0.020(2) -0.002(2) -0.024(2)
C8 0.055(3) 0.051(3) 0.073(4) 0.007(3) 0.020(3) 0.003(3)
C9 0.041(3) 0.050(3) 0.070(4) -0.001(3) 0.018(3) 0.001(2)
C10 0.025(2) 0.057(3) 0.055(3) 0.000(3) 0.015(2) -0.004(2)
C11 0.053(4) 0.067(4) 0.096(5) -0.009(3) 0.024(3) 0.006(3)
C12 0.052(4) 0.093(5) 0.091(5) -0.029(4) 0.032(3) -0.004(3)
C13 0.051(3) 0.093(5) 0.072(4) -0.014(4) 0.027(3) -0.005(3)
C14 0.036(3) 0.064(3) 0.066(4) 0.001(3) 0.022(3) -0.007(2)
C15 0.053(3) 0.057(4) 0.059(3) 0.007(3) 0.020(3) -0.011(3)
O16 0.130(4) 0.078(3) 0.104(3) 0.016(3) 0.074(3) -0.015(3)
O17 0.081(3) 0.070(3) 0.071(3) 0.0004(19) 0.042(2) 0.001(2)
C18 0.118(6) 0.116(6) 0.097(5) -0.014(4) 0.065(5) -0.003(5)
C19 0.033(3) 0.053(3) 0.050(3) 0.005(2) 0.016(2) -0.004(2)
C20 0.039(3) 0.055(3) 0.069(3) 0.000(3) 0.020(3) -0.009(2)
C21 0.044(3) 0.076(4) 0.074(4) -0.006(3) 0.024(3) -0.022(3)
C22 0.033(3) 0.086(4) 0.075(4) -0.001(3) 0.022(3) -0.010(3)
C23 0.043(3) 0.075(4) 0.084(4) -0.005(3) 0.030(3) 0.009(3)
C24 0.040(3) 0.051(3) 0.070(4) -0.005(3) 0.021(3) -0.004(2)
C25 0.091(5) 0.158(7) 0.088(5) -0.001(5) 0.023(4) -0.007(5)
Cl26 0.094(4) 0.73(3) 0.105(4) 0.098(9) 0.017(3) -0.117(8)
Cl27 0.105(4) 0.142(4) 0.066(3) -0.016(2) 0.025(2) -0.047(4)
Cl28 0.176(8) 0.256(10) 0.138(5) -0.048(6) -0.011(5) 0.131(8)
Cl29 0.205(12) 0.42(2) 0.216(11) -0.161(12) -0.031(8) 0.162(12)

_geom_special_details
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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N1 C6 1.462(6) . ?
N1 H1A 0.8600 . ?
C2 O7 1.234(6) . ?
C2 C3 1.492(7) . ?
C3 C4 1.511(7) . ?
C3 H3A 0.9700 . ?
C3 H3B 0.9700 . ?
C4 C5 1.544(7) . ?
C4 H4A 0.9700 . ?
C4 H4B 0.9700 . ?
C5 C15 1.508(7) . ?
C5 C8 1.540(7) . ?
C5 C6 1.580(7) . ?
C6 C10 1.507(7) . ?
C6 C19 1.547(6) . ?
C8 C9 1.499(7) . ?
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C8 H8A 0.9700 . ?
C8 H8B 0.9700 . ?
C9 C10 1.388(7) . ?
C9 C11 1.406(8) . ?
C10 C14 1.385(7) . ?
C11 C12 1.383(9) . ?
C11 H11A 0.9300 . ?
C12 C13 1.375(8) . ?
C12 H12A 0.9300 . ?
C13 C14 1.377(8) . ?
C13 H13A 0.9300 . ?
C14 H14A 0.9300 . ?
C15 O16 1.197(6) . ?
C15 O17 1.324(6) . ?
O17 C18 1.445(7) . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 C24 1.387(7) . ?
C19 C20 1.393(6) . ?
C20 C21 1.390(7) . ?
C20 H20A 0.9300 . ?
C21 C22 1.371(8) . ?
C21 H21A 0.9300 . ?
C22 C23 1.359(8) . ?
C22 H22A 0.9300 . ?
C23 C24 1.401(7) . ?
C23 H23A 0.9300 . ?
C24 H24A 0.9300 . ?
C25 Cl29 1.506(12) . ?
C25 Cl28 1.696(10) . ?
C25 Cl26 1.671(9) . ?
C25 Cl27 1.672(8) . ?
C25 H25A 0.963(8) . ?
C25 H25B 0.994(9) . ?
C25 H25C 0.965(8) . ?
C25 H25D 0.991(8) . ?
Cl28 H25B 1.718(10) . ?
Cl29 H25A 1.785(16) . ?

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C2 N1 H1A 115.2 . . ?
C6 N1 H1A 115.2 . . ?
O7 C2 N1 121.1(4) . . ?
O7 C2 C3 120.6(4) . . ?
N1 C2 C3 118.3(4) . . ?
C2 C3 C4 113.7(4) . . ?
C2 C3 H3A 108.8 . . ?
C4 C3 H3A 108.8 . . ?
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C2 C3 H3B 108.8 . . ?
C4 C3 H3B 108.8 . . ?
H3A C3 H3B 107.7 . . ?
C3 C4 C5 114.9(4) . . ?
C3 C4 H4A 108.6 . . ?
C5 C4 H4A 108.6 . . ?
C3 C4 H4B 108.6 . . ?
C5 C4 H4B 108.6 . . ?
H4A C4 H4B 107.5 . . ?
C15 C5 C8 111.8(4) . . ?
C15 C5 C4 109.5(4) . . ?
C8 C5 C4 107.5(4) . . ?
C15 C5 C6 113.7(4) . . ?
C8 C5 C6 104.3(4) . . ?
C4 C5 C6 109.8(4) . . ?
N1 C6 C10 110.7(4) . . ?
N1 C6 C19 108.9(4) . . ?
C10 C6 C19 109.9(4) . . ?
N1 C6 C5 113.2(4) . . ?
C10 C6 C5 101.7(4) . . ?
C19 C6 C5 112.3(4) . . ?
C9 C8 C5 103.0(4) . . ?
C9 C8 H8A 111.2 . . ?
C5 C8 H8A 111.2 . . ?
C9 C8 H8B 111.2 . . ?
C5 C8 H8B 111.2 . . ?
H8A C8 H8B 109.1 . . ?
C10 C9 C11 120.2(5) . . ?
C10 C9 C8 110.7(4) . . ?
C11 C9 C8 129.1(5) . . ?
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C14 C10 C6 128.4(4) . . ?
C12 C11 C9 118.1(6) . . ?
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C12 C13 H13A 119.8 . . ?
C14 C13 H13A 119.8 . . ?
C13 C14 C10 119.4(5) . . ?
C13 C14 H14A 120.3 . . ?
C10 C14 H14A 120.3 . . ?
O16 C15 O17 122.0(5) . . ?
O16 C15 C5 125.0(5) . . ?
O17 C15 C5 112.9(4) . . ?
C15 O17 C18 117.2(5) . . ?
O17 C18 H18A 109.5 . . ?
O17 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
O17 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
C24 C19 C20 118.2(4) . . ?
C24 C19 C6 121.4(4) . . ?
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C20 C19 C6 120.3(4) . . ?
C21 C20 C19 120.7(5) . . ?
C21 C20 H20A 119.6 . . ?
C19 C20 H20A 119.6 . . ?
C22 C21 C20 120.2(5) . . ?
C22 C21 H21A 119.9 . . ?
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C19 C24 C23 120.2(5) . . ?
C19 C24 H24A 119.9 . . ?
C23 C24 H24A 119.9 . . ?
Cl29 C25 Cl28 120.4(7) . . ?
Cl29 C25 Cl26 101.2(8) . . ?
Cl28 C25 Cl26 38.8(7) . . ?
Cl29 C25 Cl27 29.9(10) . . ?
Cl28 C25 Cl27 110.6(6) . . ?
Cl26 C25 Cl27 112.0(5) . . ?
Cl29 C25 H25A 89.8(9) . . ?
Cl28 C25 H25A 136.1(7) . . ?
Cl26 C25 H25A 109.6(8) . . ?
Cl27 C25 H25A 110.5(6) . . ?
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Cl26 C25 H25B 110.0(10) . . ?
Cl27 C25 H25B 108.3(6) . . ?
H25A C25 H25B 106.3(7) . . ?
Cl29 C25 H25C 111.7(12) . . ?
Cl28 C25 H25C 106.6(6) . . ?
Cl26 C25 H25C 85.7(6) . . ?
Cl27 C25 H25C 137.9(7) . . ?
H25A C25 H25C 29.5(3) . . ?
H25B C25 H25C 99.9(7) . . ?
Cl29 C25 H25D 105.7(11) . . ?
Cl28 C25 H25D 106.5(8) . . ?
Cl26 C25 H25D 144.7(11) . . ?
Cl27 C25 H25D 82.9(5) . . ?
H25A C25 H25D 93.1(6) . . ?
H25B C25 H25D 35.7(3) . . ?
H25C C25 H25D 104.7(7) . . ?
C25 Cl28 H25B 33.8(4) . . ?
C25 Cl29 H25A 32.7(5) . . ?

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 _geom_torsion_site_symmetry_3
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C6 N1 C2 O7 174.6(5) . . . . ?
C6 N1 C2 C3 -4.7(7) . . . . ?
O7 C2 C3 C4 -156.8(5) . . . . ?
N1 C2 C3 C4 22.4(7) . . . . ?
C2 C3 C4 C5 -47.0(6) . . . . ?
C3 C4 C5 C15 -74.4(6) . . . . ?
C3 C4 C5 C8 164.0(4) . . . . ?
C3 C4 C5 C6 51.1(6) . . . . ?
C2 N1 C6 C10 -103.3(5) . . . . ?
C2 N1 C6 C19 135.7(5) . . . . ?
C2 N1 C6 C5 10.1(7) . . . . ?
C15 C5 C6 N1 91.5(5) . . . . ?
C8 C5 C6 N1 -146.5(4) . . . . ?
C4 C5 C6 N1 -31.5(5) . . . . ?
C15 C5 C6 C10 -149.7(4) . . . . ?
C8 C5 C6 C10 -27.8(4) . . . . ?
C4 C5 C6 C10 87.2(4) . . . . ?
C15 C5 C6 C19 -32.3(5) . . . . ?
C8 C5 C6 C19 89.6(4) . . . . ?
C4 C5 C6 C19 -155.4(4) . . . . ?
C15 C5 C8 C9 152.2(4) . . . . ?
C4 C5 C8 C9 -87.6(5) . . . . ?
C6 C5 C8 C9 29.0(5) . . . . ?
C5 C8 C9 C10 -19.9(5) . . . . ?
C5 C8 C9 C11 162.0(5) . . . . ?
C11 C9 C10 C14 0.9(7) . . . . ?
C8 C9 C10 C14 -177.5(4) . . . . ?
C11 C9 C10 C6 -179.9(4) . . . . ?
C8 C9 C10 C6 1.8(5) . . . . ?
N1 C6 C10 C9 137.1(4) . . . . ?
C19 C6 C10 C9 -102.6(4) . . . . ?
C5 C6 C10 C9 16.6(5) . . . . ?
N1 C6 C10 C14 -43.8(6) . . . . ?
C19 C6 C10 C14 76.6(5) . . . . ?
C5 C6 C10 C14 -164.3(4) . . . . ?
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C8 C9 C11 C12 178.2(5) . . . . ?
C9 C11 C12 C13 -1.6(8) . . . . ?
C11 C12 C13 C14 1.9(8) . . . . ?
C12 C13 C14 C10 -0.8(7) . . . . ?
C9 C10 C14 C13 -0.6(7) . . . . ?
C6 C10 C14 C13 -179.7(4) . . . . ?
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C4 C5 C15 O16 -110.1(6) . . . . ?
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C8 C5 C15 O17 -172.1(4) . . . . ?
C4 C5 C15 O17 68.9(5) . . . . ?
C6 C5 C15 O17 -54.3(5) . . . . ?
O16 C15 O17 C18 -4.7(8) . . . . ?
C5 C15 O17 C18 176.3(5) . . . . ?
N1 C6 C19 C24 -23.0(6) . . . . ?
C10 C6 C19 C24 -144.4(4) . . . . ?
C5 C6 C19 C24 103.2(5) . . . . ?
N1 C6 C19 C20 156.7(4) . . . . ?
C10 C6 C19 C20 35.2(6) . . . . ?
C5 C6 C19 C20 -77.2(5) . . . . ?
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C24 C19 C20 C21 0.0(7) . . . . ?
C6 C19 C20 C21 -179.7(4) . . . . ?
C19 C20 C21 C22 1.2(8) . . . . ?
C20 C21 C22 C23 -1.5(8) . . . . ?
C21 C22 C23 C24 0.5(9) . . . . ?
C20 C19 C24 C23 -1.0(7) . . . . ?
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