checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: 41026am

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=5.0633(2) b=7.8476(3) c=28.8648(9)
alpha=92.227(2) beta=93.436(2) gamma=102.045(2)
Temperature: 273 K

	Calculated	Reported
Volume	1118.12(7)	1118.12(7)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C21 H38 N O, Cl, O	?
Sum formula	C21 H38 Cl N O2	C21 H38 Cl N O
Mr	371.97	355.97
Dx,g cm-3	1.105	1.057
Z	2	2
Mu (mm-1)	0.184	0.178
F000	408.0	392.0
F000'	408.44	
h,k,lmax	6,10,38	6,10,37
Nref	5436	5404
Tmin,Tmax	0.982,0.984	0.717,0.916
Tmin'	0.982	

Correction method= NONE

Data completeness= 0.994 Theta(max)= 28.040

R(reflections)= 0.0564(3348) wR2(reflections)= 0.1997(5404)

S = 1.071 Npar= 229

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) O2

Alert level C
ABSTY03_ALERT_1_C The _exptl_absorpt_correction_type has been given as none.
However values have been given for Tmin and Tmax. Remove

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            these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.717
  From the CIF: _exptl_absorpt_correction_T_max   0.916
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.99 <> 1.01
           From the CIF: _cell_formula_units_Z                    2
           From the CIF: _chemical_formula_weight           355.97
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   21.00  252.23
           H         1.01   38.00   38.30
           N        14.01    1.00   14.01
           O        16.00    2.00   32.00
           Cl       35.45    1.00   35.45
           Calculated formula weight              371.99
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT431_ALERT_2_C Short Inter HL..A Contact  Cl1    ..  O2      ..       3.15 Ang.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT043_ALERT_1_C Check Reported Molecular Weight ................     355.97
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C21 H38 Cl1 N1 O1
            Atom count from the _atom_site data:  C21 H38 Cl1 N1 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C21 H38 Cl N O
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         42.00     42.00    0.00
           H         76.00     76.00    0.00
           Cl         2.00      2.00    0.00
           N          2.00      2.00    0.00
           O          2.00      4.00   -2.00
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.12
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)        200 Deg.
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        273 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        273 K
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   1 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   7 ALERT level C = Check and explain
   7 ALERT level G = General alerts; check

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/10/2010; check.def file version of 11/10/2010

Datablock 41026am - ellipsoid plot