checkCIF/PLATON report

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

Datablock: 8b

Bond precision: C-C = 0.0150 A Wavelength=1.54184

Cell: a=7.1152(5) b=16.3138(7) c=28.6832(19)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	3329.4(4)	3329.4(4)
Space group	Pbc21	P b c 21
Hall group	P 2c -2b	P 2c -2b
Moiety formula	C14 H8 Cl2 N5 O5	C14 H9 CL2 N5 O5
Sum formula	C14 H8 Cl2 N5 O5	C14 H9 CL2 N5 O5
Mr	397.15	398.16
Dx,g cm-3	1.585	1.589
Z	8	8
Mu (mm-1)	3.875	3.876
F000	1608.0	1616.0
F000'	1618.80	
h,k,lmax	8,20,36	8,20,36
Nref	3562[6976]	3555
Tmin,Tmax	0.691,0.762	
Tmin'	0.202	

Correction method= Not given

Data completeness= 1.00/0.51 Theta(max)= 76.320

R(reflections)= 0.0634(2010) wR2(reflections)= 0.2009(3555)

S = 1.033 Npar= 489

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 B
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang .. 15

Alert level C
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax .LT. 18) 7.27
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1A -- C1A .. 6.64 su

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    C1A    --  C2A     ..       5.17 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C3A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        N5A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C1A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        N1B
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C4A    -   C5A    ...      1.36 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C2B    -   C3B    ...      1.37 Ang.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT234_ALERT_4_C Large Hirshfeld Difference N2A    --  C13A    ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1A    --  C6A     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C3A    --  C4A     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1B    --  C2B     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C4B    --  C5B     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5B    --  C6B     ..       0.15 Ang.
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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:C14 H9 Cl2 N5 O5
           Atom count from the _atom_site data:  C14 H8 Cl2 N5 O5
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    8
          From the CIF: _chemical_formula_sum  C14 H9 Cl2 N5 O5
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        112.00    112.00    0.00
          H         72.00     64.00    8.00
          Cl        16.00     16.00    0.00
          N         40.00     40.00    0.00
          O         40.00     40.00    0.00
REFLT03_ALERT_4_G  WARNING: Large fraction of Friedel related reflns may
                     be needed to determine absolute structure
          From the CIF: _diffrn_reflns_theta_max          76.32
          From the CIF: _reflns_number_total              3555
          Count of symmetry unique reflns         3562
          Completeness (_total/calc)            99.80%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured         0
          Fraction of Friedel pairs measured     0.000
          Are heavy atom types Z>Si present        yes
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large..       0.10
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................       4.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          4
PLAT128_ALERT_4_G Non-standard setting of Space-group Pca21   ....      Pbc21
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C14A
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C14B
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   0 ALERT level A = In general: serious problem
   1 ALERT level B = Potentially serious problem
  18 ALERT level C = Check and explain
  12 ALERT level G = General alerts; check

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
 10 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 13/08/2009; check.def file version of 12/08/2009

Datablock 8b - ellipsoid plot