checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3Cl-nondecomposition

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3Cl-nondecomposition

Bond precision: C-C = 0.0154 A Wavelength=0.68882

Cell: a=7.72200 b=12.87400 c=21.47700
alpha=84.2500 beta=84.1800 gamma=83.7300
Temperature: 293 K

	Calculated	Reported
Volume	2102.792	2103
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H41.04 Cl2.96 N2 O6, C42 H40.96 Cl3.04 N2 O6	2(C21 H20.48 Cl1.52 N O3)
Sum formula	C84 H82 Cl6 N4 O12	C42 H41 Cl3 N2 O6
Mr	1552.24	776.12
Dx,g cm-3	1.226	1.226
Z	1	2
Mu (mm-1)	0.240	0.245
F000	812.0	812.0
F000’	813.14	
h,k,lmax	8,14,24	8,14,24
Nref	6673	6278
Tmin,Tmax	0.971,0.976	
Tmin’	0.964	

Correction method= Not given

Data completeness= 0.941 Theta(max)= 23.320

R(reflections)= 0.1561(4793) wR2(reflections)= 0.4645(6278)

S = 1.840 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 A

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PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..................       0.46 Report
PLAT330_ALERT_2_A Large Average Phenyl C-C Dist C14      -C22           1.44 Ang.
PLAT330_ALERT_2_A Large Average Phenyl C-C Dist C2BA     -C19A          1.44 Ang.
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Alert level B

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RINTA01_ALERT_3_B  The value of Rint is greater than 0.18
           Rint given   0.183
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5747
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 .........      0.183 Report
PLAT082_ALERT_2_B High R1 Value ..................................       0.16 Report
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          6 Report
PLAT220_ALERT_2_B Non-Solvent  Resd 2  C   Ueq(max)/Ueq(min) Range        7.0 Ratio
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.01543 Ang.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C4AA     - C3AA     .       1.26 Ang.
PLAT369_ALERT_2_B Long   C(sp2)-C(sp2) Bond  C9       - C28      .       1.57 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.575        396 Report
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          5 Check
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Alert level C

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PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT141_ALERT_4_C s.u. on a - Axis Small or Missing ..............    0.00000 Ang.
PLAT142_ALERT_4_C s.u. on b - Axis Small or Missing ..............    0.00000 Ang.
PLAT143_ALERT_4_C s.u. on c - Axis Small or Missing ..............    0.00000 Ang.
PLAT144_ALERT_4_C s.u. on alpha    Small or Missing ..............     0.0000 Degree
PLAT145_ALERT_4_C s.u. on beta     Small or Missing ..............     0.0000 Degree
PLAT146_ALERT_4_C s.u. on gamma    Small or Missing ..............     0.0000 Degree
PLAT151_ALERT_1_C No s.u. (esd) Given on Volume ..................     Please Do !
PLAT213_ALERT_2_C Atom C3              has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C2AA            has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C6AA            has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.7 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        4.1 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 2  H   Uiso(max)/Uiso(min) Range        8.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C31      --C33             0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31      --C33A            0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1BA     --C25             0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C3AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C30 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.1 Note
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C6       - C27      .       1.55 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C7       - C24      .       1.56 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C13      - C25      .       1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     14.040 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.011 Check
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          7 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H15A            -0.31 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C42 H41 Cl3 N2 O6
           Atom count from _chemical_formula_moiety:C42 H40.96 Cl3.04 N2 O6
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         13 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         18 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.68882 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)         0. Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         6 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       26% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2  )       19% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C0BA     -C21_b          1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C14      -C22A           1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C0AA     -C8AA_a         1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C2BA     -C19            1.44 Ang.
PLAT343_ALERT_2_G Unusual       sp3Angle Range in Main Residue for       C2AA Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O3            108.5 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2AA          108.8 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        45 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2       --C32A          1.72 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       154 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       47% Note
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3 **ALERT level A** = Most likely a serious problem - resolve or explain
13 **ALERT level B** = A potentially serious problem, consider carefully
33 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
27 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
35 ALERT type 2 Indicator that the structure model may be wrong or deficient
17 ALERT type 3 Indicator that the structure quality may be low
15 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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* or *IUCrData*, 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 23/04/2018; check.def file version of 23/04/2018

Datablock 3Cl-nondecomposition - ellipsoid plot