checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 06Cl

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: 06Cl

Bond precision: C-C = 0.0086 A Wavelength=0.68882

Cell: a=7.46400 b=12.49300 c=21.02700
alpha=83.9600 beta=83.5800 gamma=83.2500
Temperature: 293 K

	Calculated	Reported
Volume	1926.478	1927
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H39.76 N2 O6, C36 H26.24 N2 O6, 2(C2 H5), 11.026(Cl), 2(C H	C21 H21.12 Cl2.77 N O3, C21 H19.88 Cl2.74 N O3
Sum formula	C84 H82 Cl11.03 N4 O12	C42 H39 Cl5.60 N2 O6
Mr	1730.41	866.09
Dx,g cm-3	1.492	1.493
Z	1	2
Mu (mm-1)	0.421	0.435
F000	897.4	896.0
F000’	899.30	
h,k,lmax	8,14,24	8,14,24
Nref	6139	5405
Tmin,Tmax	0.969,0.991	
Tmin’	0.805	

Correction method= Not given

Data completeness= 0.880 Theta(max)= 23.318

R(reflections)= 0.0934(5255) wR2(reflections)= 0.2203(5405)

S = 1.104 Npar= 535

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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5747
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.575 728 Report

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Alert level C

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
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 C7 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C31 has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C31 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C4A 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33 --C30A 0.18 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C6 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00858 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H3A ..H7BD 1.92 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H22B ..H31A 1.99 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 7.059 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 70 Note
PLAT922_ALERT_1_C wR2 in the CIF and FCF Differ by ..... 0.0015 Check

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Alert level G

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 H39 Cl5.6 N2 O6
Atom count from _chemical_formula_moiety:C42 H41 Cl5.51 N2 O6
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:C42 H39 Cl5.6 N2 O6
Atom count from the _atom_site data: C42 H41 Cl5.513 N2 O6
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

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          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C42 H39 Cl5.60 N2 O6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H         78.00     82.00   -4.00
          Cl        11.20     11.03    0.17
          N          4.00      4.00    0.00
          O         12.00     12.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          7 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
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.17 Why ?
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        13 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         8 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 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  )       14% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       21% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       50% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11  )      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  1         89.76 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  2         70.24 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  4          0.92 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  5          0.93 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  6          0.90 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  7          0.93 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  8          0.91 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  9          0.92 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 10          2.44 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 11          1.56 Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1AA           108.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1BA           108.8 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl1      ..C23             2.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl0A     ..C11             2.74 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl0A     ..C19             3.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3      ..C12             2.73 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3      ..C22             3.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3A     ..C15             2.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N2       ..C32A            2.93 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N2       ..C32             3.01 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C8A             2.43 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C8              2.43 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C6       ..C30             2.52 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C6       ..C30A            2.65 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C6       ..C33             3.09 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C8       ..C33             3.04 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C32A            2.47 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C32             2.54 Ang.
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PLAT432_ALERT_2_G Short Inter X...Y Contact  C32      ..C33             2.49 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C33      ..C32A            2.40 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........        42 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        3 Note
            C2 H5
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       46 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       92% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       11 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        1 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  34 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  65 ALERT level G = General information/check it is not something unexpected

  14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  39 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
  37 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 06Cl - ellipsoid plot