checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MG2

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: MG2

Bond precision: C-C = 0.0066 A Wavelength=1.54184

Cell: a=15.0285(2) b=20.1098(3) c=15.4228(2)
alpha=90 beta=92.319(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	4657.26(11)	4657.26(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C100 H82 Co2 N10 O8, 2(C H2 Cl2)	?
Sum formula	C102 H86 Cl4 Co2 N10 O8	C102 H86 Cl4 Co2 N10 O8
Mr	1839.47	1839.46
Dx,g cm-3	1.312	1.312
Z	2	2
Mu (mm-1)	4.344	4.344
F000	1908.0	1908.0
F000’	1906.36	
h,k,lmax	17,22,17	16,22,17
Nref	7191	7066
Tmin,Tmax	0.171,0.338	0.363,0.363
Tmin’	0.076	

Correction method= # Reported T Limits: Tmin=0.363 Tmax=0.363
AbsCorr = MULTI-SCAN

Data completeness= 0.983 Theta(max)= 61.400

R(reflections)= 0.0703(6234) wR2(reflections)= 0.1975(7066)

S = 1.042 Npar= 626

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

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THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
            Calculated sin(theta_max)/wavelength =    0.5694
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Alert level C

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PLAT214_ALERT_2_C Atom C51C      (Anion/Solvent) ADP max/min Ratio        4.7 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O2       --C30      .        5.3 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C28 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C29 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C40 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C41 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C44 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C39 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C42 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl1A      0.178 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl1B      0.166 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl1C      0.208 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C39      -C44            1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00661 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.569       116 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        11 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      6.50 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as     mixed Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )      2.47 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )      1.54 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )      0.99 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         1 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         3 Note
              C H2 Cl2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         4 Note
              C H2 Cl2
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .      2.24 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        64 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       77% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.1 Low
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
  1 ALERT level B = A potentially serious problem, consider carefully
 18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 26 ALERT level G = General information/check it is not something unexpected

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 20 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
 13 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 03/06/2021; check.def file version of 02/06/2021

Datablock MG2 - ellipsoid plot