checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 20141114d518_0m_sq

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Bond precision:  C-C = 0.0165 A          Wavelength=0.71073

Cell:          a=9.195(13)        b=12.816(18)    c=13.814(19)
               alpha=69.243(18)   beta=83.06(2)   gamma=84.178(19)
Temperature:   296 K
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	Calculated	Reported
Volume	1508(4)	1508(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H48 Cl2 Co3 N8 O18 [+ solvent]	C44 H48 Cl2 Co3 N8 O18
Sum formula	C44 H48 Cl2 Co3 N8 O18 [+ solvent]	C44 H48 Cl2 Co3 N8 O18
Mr	1224.59	1224.59
Dx,g cm-3	1.349	1.348
Z	1	1
Mu (mm-1)	0.972	0.972
F000	627.0	627.0
F000’	628.62	
h,k,lmax	10,15,16	10,15,16
Nref	5308	5237
Tmin,Tmax	0.831,0.873	
Tmin’	0.831	

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Correction method= Not given

Data completeness= 0.987          Theta(max)= 25.009

R(reflections)= 0.1080( 2175)     wR2(reflections)= 0.3006( 5237)

S = 0.867                 Npar= 343
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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

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01653 Ang.

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.30 Report
PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.013 Ang.
PLAT148_ALERT_3_C s.u. on the b - Axis is (Too) Large .... 0.018 Ang.
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large .... 0.019 Ang.
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Co1 --O8 . 5.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 -- N1 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2 -- N1 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 -- C7 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 -- C2 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 -- C3 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 -- C15 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C14 Check

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Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.18 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 112.8 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4 111.6 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 315 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 24 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 3 Note

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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
19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 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

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 09/11/2017; check.def file version of 08/11/2017

Datablock 20141114d518_0m_sq - ellipsoid plot