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: 20150107d610_0m_sq

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=11.0545(13) b=11.2647(14) c=12.9730(16)
alpha=69.274(2) beta=72.603(2) gamma=82.921(2)
Temperature: 296 K

	Calculated	Reported
Volume	1441.5(3)	1441.5(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H42 Cl2 Co3 N6 O18 [+ solvent]	C40 H42 Cl2 Co3 N6 O18
Sum formula	C40 H42 Cl2 Co3 N6 O18 [+ solvent]	C40 H42 Cl2 Co3 N6 O18
Mr	1142.49	1142.48
Dx,g cm-3	1.316	1.316
Z	1	1
Mu (mm-1)	1.011	1.011
F000	583.0	583.0
F000’	584.61	
h,k,lmax	14,15,17	14,15,17
Nref	7236	7125
Tmin,Tmax	0.777,0.825	0.786,0.831
Tmin’	0.777	

Correction method= # Reported T Limits: Tmin=0.786 Tmax=0.831
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 28.397

R(reflections)= 0.0486(5228) wR2(reflections)= 0.1578(7125)

S = 1.020 Npar= 318

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

PLAT420_ALERT_2_B D-H Without Acceptor O9 --H9 . Please Check

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.09 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for Cl1 --C14 .. 6.7 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C14 Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 113.7 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4 114.5 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 333 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 6 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 ... 8 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
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
5 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 20150107d610_0m_sq - ellipsoid plot