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: 20141114d517_0m

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Bond precision:  C-C = 0.0041 A          Wavelength=0.71073

Cell:           a=11.1889(8)    b=9.4659(7)         c=25.6944(17)
                alpha=90        beta=108.125(3)     gamma=90
Temperature:    296 K

                Calculated                Reported
Volume          2586.3(3)                 2586.3(3)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C48 H44 Cl2 Co3 N8 O16    C48 H44 Cl2 Co3 N8 O16
Sum formula     C48 H44 Cl2 Co3 N8 O16    C48 H44 Cl2 Co3 N8 O16
Mr              1236.60                   1236.60
Dx,g cm-3       1.588                     1.588
Z               2                         2
Mu (mm-1)       1.132                     1.132
F000            1262.0                    1262.0
F000'           1265.21
h,k,lmax        13,11,31                  13,11,31
Nref            4827                      4825
Tmin,Tmax       0.797,0.863
Tmin'           0.797

Correction method= Not given

Data completeness= 1.000          Theta(max)= 25.496

R(reflections)= 0.0347( 3875)     wR2(reflections)= 0.0799( 4825)

S = 1.027                 Npar= 368
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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 C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT215_ALERT_3_C Disordered O2 has ADP max/min Ratio ..... 3.1 Note
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check

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Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/c P21/n Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for Cl1 --C14 .. 8.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for Cl1' --C4 .. 15.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for N1 --C4 .. 15.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for N1' --C14 .. 8.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1' Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1' Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2' Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1' Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 9% Note
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 111.3 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O4 110.6 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 12 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
11 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 20141114d517_0m - ellipsoid plot