checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rgdm18

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: rgdm18

```
Bond precision:   C-C = 0.0124 A          Wavelength=0.71073

Cell:             a=31.73(3)     b=7.868(3)          c=19.131(15)
                  alpha=90       beta=125.25(3)      gamma=90
Temperature:      296 K
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	Calculated	Reported
Volume	3900(5)	3900(5)
Space group	C 2	C 1 2 1
Hall group	C 2y	C 2y
Moiety formula	C36 H42 Co N2 O6, 2(C2 H3 N)	?
Sum formula	C40 H48 Co N4 O6	C40 H48 Co N4 O6
Mr	739.75	739.75
Dx,g cm-3	1.260	1.260
Z	4	4
Mu (mm-1)	0.490	0.489
F000	1564.0	1564.0
F000'	1566.00	
h,k,lmax	39,9,23	39,9,23
Nref	8000[4303]	7950
Tmin,Tmax	0.921,0.943	0.530,0.940
Tmin'	0.907	

```
Correction method= # Reported T Limits: Tmin=0.530 Tmax=0.940
AbsCorr = MULTI-SCAN

Data completeness= 1.85/0.99        Theta(max)= 26.430

R(reflections)= 0.0508( 6802)                    wR2(reflections)=
                                                 0.1344( 7950)
S = 1.062                  Npar= 476
```

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

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PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C37 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C39 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N3      0.109 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N4      0.108 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01244 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         4 Note
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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.44 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  C2             I2 Note
PLAT303_ALERT_2_G Full Occupancy Atom H2O       with # Connections      2.00 Check
PLAT791_ALERT_4_G Model has Chirality at N1          (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at N2          (Sohnke SpGr)         R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .      1.83 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)      .      1.86 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         5 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF      0.15 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       1.9 Low
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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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 18/05/2022; check.def file version of 17/05/2022

Datablock rgdm18 - ellipsoid plot