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: md496_mc187_sq

```
Bond precision:  C-C = 0.0206 A          Wavelength=0.71073

Cell:           a=28.4159(12)    b=28.4159(12)    c=19.2051(10)
                alpha=90         beta=90          gamma=90
Temperature:    293 K
```

	Calculated	Reported
Volume	15507.4(15)	15507.4(15)
Space group	I 41 c d	I 41 c d
Hall group	I 4bw -2c	I 4bw -2c
Moiety formula	C38 H47 In N2 O [+ solvent]	C38 H47 In N2 O
Sum formula	C38 H47 In N2 O [+ solvent]	C38 H47 In N2 O
Mr	662.60	662.59
Dx,g cm-3	1.135	1.135
Z	16	16
Mu (mm-1)	0.636	0.636
F000	5536.0	5536.0
F000’	5526.00	
h,k,lmax	33,33,22	33,32,22
Nref	6839[3535]	6490
Tmin,Tmax	0.808,0.903	0.574,1.000
Tmin’	0.613	

```
Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.95      Theta(max)= 24.999

R(reflections)= 0.0505( 4669)     wR2(reflections)= 0.1532( 6490)

S = 1.095                 Npar= 389
```

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02057 Ang.

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C18 -- C19 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30 -- C31 0.24 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check

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Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT014_ALERT_1_G No _shelx_fab_checksum Found in CIF ..... Please Check
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.77 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 19.85 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! 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
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

4 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
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 md496_mc187_sq - ellipsoid plot