checkCIF/PLATON report

Structure factors have been supplied for datablock(s) inimsqbipy

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: inimsqbipy

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Bond precision:   C-C = 0.0129 A          Wavelength=0.71073

Cell:              a=17.4861(16)      b=23.472(2)      c=26.342(4)
                   alpha=90           beta=90          gamma=90
Temperature:       298 K
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	Calculated	Reported
Volume	10812(2)	10812(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C54 H66 In N4 O2, 0.5(C6 H14)	C54 H66 In N4 O2, 0.5(C6 H14)
Sum formula	C57 H73 In N4 O2	C57 H73 In N4 O2
Mr	961.01	961.01
Dx,g cm-3	1.181	1.181
Z	8	8
Mu (mm-1)	0.479	0.479
F000	4064.0	4064.0
F000'	4059.45	
h,k,lmax	20,27,31	20,27,31
Nref	9547	9532
Tmin,Tmax	0.913,0.962	0.932,0.968
Tmin'	0.913	

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Correction method= # Reported T Limits: Tmin=0.932 Tmax=0.968
AbsCorr = ANALYTICAL

Data completeness= 0.998           Theta(max)= 25.027

R(reflections)= 0.0865( 3263)                    wR2(reflections)=
                                                 0.2356( 9532)
S = 1.005                  Npar= 597
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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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.207

Author Response: The reflectivity of crystal samples is rather low, the best single crystal suitable for SC XRD was chosen.

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.207 Report

Author Response: The reflectivity of crystal samples is rather low, the best single crystal suitable for SC XRD was chosen.

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 34% Check

Author Response: The reflectivity of crystal samples is rather low, the best single crystal suitable for SC XRD was chosen.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C1S 0.286 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01292 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 49.853 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 7.281 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.640 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 13 Report

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 14 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0050 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report

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PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0010 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C1S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6S        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1SC       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SB       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6SC       Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....            14 Note
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97000 Dev...       0.01 Ang.
             C4S      -H4SA            1_555   1_555 .......     #  147 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97000 Dev...       0.01 Ang.
             C5S      -H5SB            1_555   1_555 .......     #  151 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C6S      -H6SB            1_555   1_555 .......     #  153 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      107.70 Dev...       1.30 Degree
             C6S     -C5S     -H5SB       1_555  1_555  1_555     #  280 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         20 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....              592 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File       10 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        1 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
46 **ALERT level G** = General information/check it is not something unexpected

4 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
18 ALERT type 3 Indicator that the structure quality may be low
27 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 28/11/2022; check.def file version of 28/11/2022

Datablock inimsqbipy - ellipsoid plot