checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0340 A   Wavelength=0.71073

Cell: a=9.226(1)   b=13.060(1)   c=17.377(2)
                alpha=90   beta=104.671(3)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2025.5(4)	2025.5(4)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	I7, C14 H26 N4 O, I3, 2(I2)	?
Sum formula	C14 H26 I14 N4 O	C14 H23 I14 N4 O
Mr	2042.99	2039.96
Dx,g cm-3	3.350	3.345
Z	2	2
Mu (mm-1)	10.714	10.714
F000	1776.0	1770.0
F000'	1763.57	
h,k,lmax	10,15,20	10,15,20
Nref	3733	2810
Tmin,Tmax	0.088,0.117	0.337,0.746
Tmin'	0.035	

Correction method= # Reported T Limits: Tmin=0.337 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.753   Theta(max)= 25.022

R(reflections)= 0.0779(2244)   wR2(reflections)= 0.2353(2810)

S = 1.090   Npar= 187

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 A

```
PLAT434_ALERT_2_A Short Inter HL..HL Contact I8       ..I9              3.23 Ang.
                                                x,y,z  =      1_555 Check
```

Author Response: these are long intramolecular distances featuring the I7-polyiodides or short I...I secondary bonds. All these distances are discussed in the manuscr

```
PLAT434_ALERT_2_A Short Inter HL..HL Contact I8       ..I9              3.23 Ang.
                                             x,1/2-y,z  =      4_565 Check
```

Author Response: these are long intramolecular distances featuring the I7-polyiodides or short I...I secondary bonds. All these distances are discussed in the manuscr

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🟠 Alert level B

```
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .     0.954 Why?
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............     0.034 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor       O1      --H1      .     Please Check
PLAT434_ALERT_2_B Short Inter HL..HL Contact I3       ..I10             3.46 Ang.
                                             -1+x,y,z  =      1_455 Check
```

Author Response: these are long intramolecular distances featuring the I7-polyiodides or short I...I secondary bonds. All these distances are discussed in the manuscr

```
PLAT434_ALERT_2_B Short Inter HL..HL Contact I3       ..I10             3.46 Ang.
                                           -1+x,3/2-y,z  =      4_475 Check
```

Author Response: these are long intramolecular distances featuring the I7-polyiodides or short I...I secondary bonds. All these distances are discussed in the manuscr

```
PLAT434_ALERT_2_B Short Inter HL..HL Contact I3       ..I10'            3.49 Ang.
                                             -1+x,y,z  =      1_455 Check
```

Author Response: these are long intramolecular distances featuring the I7-polyiodides or short I...I secondary bonds. All these distances are discussed in the manuscr

```
PLAT434_ALERT_2_B Short Inter HL..HL Contact I3       ..I10'            3.49 Ang.
                                           -1+x,3/2-y,z  =      4_475 Check
```

Author Response: these are long intramolecular distances featuring the I7-polyiodides or short I...I secondary bonds. All these distances are discussed in the manuscr

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🟡 **Alert level C**

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ    Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..      3.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference N2      --C5      .      0.16 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N2 Check
```

⚪ **Alert level G**

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C14 H23 I14 N4 O1
             Atom count from the _atom_site data:  C14 H27 I14 N4 O1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z     2
           From the CIF: _chemical_formula_sum  C14 H23 I14 N4 O
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C          28.00    28.00    0.00
           H          46.00    54.00   -8.00
           I          28.00    28.00    0.00
           N           8.00     8.00    0.00
           O           2.00     2.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        16 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     31.88 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H1          Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8A         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8C         Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      26% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )      50% Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.21 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         7 Check
           I10  -I3   -I10'   1.455   1.555   1.455        3.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        11 Check
           I10  -I9   -I10'   1.555   1.555   1.555        4.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        15 Check
           I5'  -I4   -I5     2.547   1.555   2.547        9.80 Deg.
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set    Please Do !
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        96 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
```

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   2 ALERT level A = Most likely a serious problem - resolve or explain
   7 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected
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 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check
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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.

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