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: 1_18srv178

```
Bond precision:   C-C = 0.0063 A          Wavelength=0.71073

Cell:             a=26.964(2)     b=27.059(2)         c=22.8873(17)
                  alpha=90        beta=94.601(3)      gamma=90
Temperature:      120 K
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	Calculated	Reported
Volume	16645(2)	16645(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C49 H35, Cl2 I, C H2 Cl2	Cl2 I, C H2 Cl2, C49 H35
Sum formula	C50 H37 Cl4 I	C50 H37 Cl4 I
Mr	906.50	906.49
Dx,g cm-3	1.447	1.447
Z	16	16
Mu (mm-1)	1.061	1.061
F000	7328.0	7328.0
F000'	7332.04	
h,k,lmax	36,36,30	36,36,30
Nref	42218	42199
Tmin,Tmax	0.765,0.890	0.866,1.000
Tmin'	0.727	

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Correction method= # Reported T Limits: Tmin=0.866 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 28.500

R(reflections)= 0.0531( 30112)                  wR2(reflections)=
                                                0.1495( 42199)
S = 1.033                 Npar= 1978
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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

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.32 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          3 Check
             Cl7S    Cl8S    C4SA
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 4  C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        I1C Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      62.00 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Cl7S       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl8S       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4SA       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SC       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SD       Constrained at       0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl7B       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl8B       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4SB       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SA       Constrained at       0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4SB       Constrained at       0.35 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13  )        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 12  )       3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 13  )       1.75 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H55B     ..H4SA     .       2.11 Ang.
                                          x,3/2-y,1/2+z  =      4_576 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         12 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       57.0 Degree
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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
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  17 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 18/12/2021; check.def file version of 18/12/2021

Datablock 1_18srv178 - ellipsoid plot