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: shelx_Sam_AH148

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Bond precision:  C-C = 0.0107 A          Wavelength=0.71073

Cell:            a=9.5974(2)    b=16.4105(3)       c=15.3719(3)
                 alpha=90       beta=91.111(2)     gamma=90
Temperature:     120 K

                Calculated                Reported
Volume          2420.59(8)                2420.59(8)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C33 Ce2 Cl3 N3 O18 S6     ?
Sum formula     C33 Ce2 Cl3 N3 O18 S6     C33 Ce2 Cl3 N3 O18 S6
Mr              1305.30                   1305.31
Dx,g cm-3       1.791                     1.791
Z               2                         2
Mu (mm-1)       2.351                     2.351
F000            1252.0                    1252.0
F000'           1253.91
h,k,lmax        12,21,20                  11,21,19
Nref            5845                      4858
Tmin,Tmax       0.868,0.932               0.934,1.000
Tmin'           0.848

Correction method= # Reported T Limits: Tmin=0.934 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.831          Theta(max)= 28.009

R(reflections)= 0.0612( 4062)     wR2(reflections)= 0.1612( 4858)

S = 1.066                 Npar= 338
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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

PLAT220_ALERT_2_B Non-Solvent Resd 1 S Ueq(max)/Ueq(min) Range 10.0 Ratio

Author Response: This alert refers to the thermal ellipsoids of particular atom of S in

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C2D Check

Author Response: thi is due to atoms in the disordered coordinated DMSO solvent. Several of the atoms are still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

Alert level C

PLAT213_ALERT_2_C Atom S21D has ADP max/min Ratio ..... 3.1 oblate
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.1 Ratio

Author Response: This alert refers to the thermal ellipsoids of particular atom of S in

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1D Check

Author Response: thi is due to atoms in the disordered coordinated DMSO solvent. Several of the atoms are still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C12D Check

Author Response: thi is due to atoms in the disordered coordinated DMSO solvent. Several of the atoms are still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22D Check

Author Response: thi is due to atoms in the disordered coordinated DMSO solvent. Several of the atoms are still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01067 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 27.10 Why ?

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PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   Cl4      --C4        .       10.4 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   Cl11     --C11       .        9.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S1D      --C1D       .       12.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S1D      --C2D       .       15.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S2D      --C1D       .        7.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S2D      --C2D       .       10.4 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S11D     --C11D      .        8.6 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S11D     --C12D      .        5.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S21D     --C21D      .        5.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S21D     --C22D      .       18.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   S22D     --O21D      .       13.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C4       --C40       .       10.4 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl11       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S1D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S2D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S11D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S12D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S21D       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S22D       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S23D       Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N40        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N100       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N111       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C100       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C111       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         20% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl11     ..S11D             3.20 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C11      --C111            1.79 Ang.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        37 Note
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
40 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
20 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 30/01/2018; check.def file version of 30/01/2018

Datablock shelx_Sam_AH148 - ellipsoid plot