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_AH166

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Bond precision:  C-C = 0.0173 A          Wavelength=0.71073

Cell:            a=10.5126(5)    b=18.8316(10)      c=12.7477(5)
                 alpha=90        beta=97.445(5)     gamma=90
Temperature:     120 K

                Calculated                Reported
Volume          2502.4(2)                 2502.4(2)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C39 H42 Cl3 N9 Nd2 O18    ?
Sum formula     C39 H42 Cl3 N9 Nd2 O18    C39 H42 Cl3 N9 Nd2 O18
Mr              1319.65                   1319.64
Dx,g cm-3       1.751                     1.751
Z               2                         2
Mu (mm-1)       2.291                     2.291
F000            1308.0                    1308.0
F000'           1308.67
h,k,lmax        12,22,15                  12,22,15
Nref            4438                      4419
Tmin,Tmax       0.872,0.892               0.772,1.000
Tmin'           0.833

Correction method= # Reported T Limits: Tmin=0.772 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.040

R(reflections)= 0.0776( 3048)     wR2(reflections)= 0.1942( 4419)

S = 1.067                 Npar= 325
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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 C Ueq(max)/Ueq(min) Range 10.0 Ratio

Author Response: it refers to the thermal ellipsoids of particular atoms in our structure.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C100 Check

Author Response: This is due to the fact that this position is shared by Cl atom and CN group.

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 N Ueq(max)/Ueq(min) Range 3.2 Ratio

Author Response: it refers to the thermal ellipsoids of particular atoms in our structure.

PLAT234_ALERT_4_C Large Hirshfeld Difference O21D --C21D 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1D --C2D 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N11D --C12D 0.18 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1D Check

Author Response: This is due to the fact that this position is shared by Cl atom and CN group.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N21D Check

Author Response: This is due to the fact that this position is shared by Cl atom and CN group.

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0173 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C5 - C6 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C12 - C16_b . 1.53 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 13 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 39.35 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 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 N100 --C100 . 18.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl11 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 C111 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 3% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C1 -C6 1.45 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C11 -C16 1.46 Ang.

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PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C1       - C100     .       1.57 Ang.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C2D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C3D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C12D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C13D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C22D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C23D Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          6 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C11      --C111           1.70 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        42 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
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 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
  16 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

PLATON version of 30/01/2018; check.def file version of 30/01/2018

Datablock shelx_Sam_AH166 - ellipsoid plot