checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: TP_H_108_3

Bond precision: C-C = 0.0147 A Wavelength=1.54178

Cell: **a=17.1367(3)** **b=17.1367(3)** **c=28.9848(11)**
alpha=90 **beta=90** **gamma=90**
Temperature: **100 K**

	Calculated	Reported
Volume	8511.9(4)	8511.9(4)
Space group	P 43 21 2	P 43 21 2
Hall group	P 4nw 2abw	P 4nw 2abw
Moiety formula	C26 H34.22 Cl1.78 N5.78 O7.56 S1.78 [+ solvent]	1.77779(C117 H154 Cl8 N26 O34 S8)
Sum formula	C26 H34.22 Cl1.78 N5.78 O7.56 S1.78 [+ solvent]	C208 H273.78 Cl14.22 N46.22 O60.44 S14.22
Mr	668.61	5348.61
Dx,g cm-3	1.043	1.043
Z	8	1
Mu (mm-1)	2.405	2.404
F000	2798.2	2798.0
F000’	2815.96	
h,k,lmax	18,18,30	18,18,30
Nref	5213[3024]	5205
Tmin,Tmax	0.764,0.805	0.774,1.000
Tmin’	0.391	

Correction method= # Reported T Limits: Tmin=0.774 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.72/1.00 **Theta(max)= 54.264**

R(reflections)= 0.0645(3395) **wR2(reflections)= 0.2002(5205)**

S = 1.044 **Npar= 419**

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
THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5265

Author Response: Crystals did not diffract past ca. 0.95 A resolution

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Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01467 Ang.

Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ..... 7.21 Note
PLAT230_ALERT_2_C Hirshfeld Test Diff for C22 --C23 . 5.6 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cl48 --C45 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O51 --C52 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C5 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N37 --C36 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N54 --C53 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23 --C25 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35 --C36 . 0.19 Ang.
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of C33 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of C32 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl18 0.142 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C12 -C17 1.37 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.526 3 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info
PLAT987_ALERT_1_C The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12 Note
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 ..... 8 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.045 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 8.00 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for S39 --C42 . 5.6 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl18 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl48 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S9 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S39 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O40 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O41 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N34 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15 Constrained at 0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16 Constrained at 0.8889 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of C17       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C35       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C36       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C38       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C43       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C44       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C45       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C46       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C47       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AA      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AB      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6        Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8A       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8B       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8C       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33A      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33B      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35A      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35B      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H36       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H38A      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H38B      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H38C      Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H46       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H47       Constrained at     0.8889 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BC      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BD      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BE      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BA      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BB      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33C      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33D      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33E      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37A      Constrained at     0.1111 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37B      Constrained at     0.1111 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        58% Note
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          7 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        204 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
84 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 79 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 22/12/2019; check.def file version of 13/12/2019

Datablock TP_H_108_3 - ellipsoid plot