checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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

Bond precision: C-C = 0.0096 A Wavelength=1.54178

Cell: a=6.1777(2) b=9.1606(3) c=9.4231(3)
alpha=108.188(1) beta=102.805(1) gamma=99.970(1)
Temperature: 298 K

	Calculated	Reported
Volume	476.83(3)	476.82(3)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C18 H26 N2 O4 S	?
Sum formula	C18 H26 N2 O4 S	C18 H26 N2 O4 S
Mr	366.47	366.47
Dx,g cm-3	1.276	1.276
Z	1	1
Mu (mm-1)	1.713	1.713
F000	196.0	196.0
F000'	196.89	
h,k,lmax	7,11,11	7,11,11
Nref	3498[1749]	3060
Tmin,Tmax	0.720,0.722	
Tmin'	0.653	

Correction method= Not given

Data completeness= 1.75/0.87 Theta(max)= 68.436

R(reflections)= 0.0487(3041) wR2(reflections)= 0.1298(3060)

S = 0.949 Npar= 234

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

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PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........       7.36 Note
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.1 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00962 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C3       - C4       .       1.35 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C1       - C6       .       1.34 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H3A      ..H4B      .       1.92 Ang.
                                             x,y,z  =      1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H3B      ..H4A      .       1.92 Ang.
                                             x,y,z  =      1_555 Check
PLAT481_ALERT_4_C Long D...A H-Bond Reported C12      ..O1       .       3.76 Ang.
PLAT482_ALERT_4_C Small D-H..A Angle Rep for C15      ..O4       .      95.10 Degree
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         25 Report
               -2 -1  1,  -4  0  1,   0  1  1,   4  3  1,   0  5  1,  -1 -2  2,
                0  1  2,   0  2  2,  -1  3  2,   0  3  2,   1  3  2,   0  1  3,
               -4  2  3,  -3  2  3,  -1  2  3,   0  1  4,  -1  2  4,   0  2  4,
               -1  1  5,  -2  4  5,  -1  4  5,  -1  2  6,  -1  0  7,   0  0  7,
               -2  1  7,
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         76 %
PLAT927_ALERT_1_C Reported and Calculated  wR2 Differ by .........     0.0014 Check
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.167 Note
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.001 Degree
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0080 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C10 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C10      - C11      .       1.52 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C10      - C12      .       1.52 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11C     ..O4       .       2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H18A     ..O3       .       2.66 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H12A     ..O1       .       2.85 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H15B     ..O4       .       2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H18A     ..O3       .       2.66 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11C     ..O4       .       2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H16      ..O2       .       2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H18A     ..O3       .       2.66 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11C     ..O4       .       2.64 Ang.
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PLAT480_ALERT_4_G Long H...A H-Bond Reported H16      ..O2       .       2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H18A     ..O3       .       2.66 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11C     ..O4       .       2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H16      ..O2       .       2.62 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11C     ..O4       .       2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H16      ..O2       .       2.62 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        41 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         2 Note
                1  2 -2,  -1 -2  2,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       3.71 Note
             Predicted wR2: Based on SigI**2  3.50 or SHELX Weight 14.23
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 Info
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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
22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
32 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 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
21 ALERT type 4 Improvement, methodology, query or suggestion
2 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 06/01/2024; check.def file version of 05/01/2024

Datablock 1 - ellipsoid plot