checkCIF/PLATON report

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

Datablock: 1

Bond precision: C-C = 0.0039 A Wavelength=0.71073

Cell: a=8.813(3) b=11.082(3) c=12.620(4)
alpha=88.805(5) beta=80.440(5) gamma=75.680(5)
Temperature: 273 K

	Calculated	Reported
Volume	1177.4(6)	1177.3(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H15 N S8	C21 H15 N S8
Sum formula	C21 H15 N S8	C21 H15 N S8
Mr	537.90	537.82
Dx,g cm-3	1.517	1.517
Z	2	2
Mu (mm-1)	0.769	0.769
F000	552.0	552.0
F000'	554.10	
h,k,lmax	11,13,15	11,13,15
Nref	4801	4647
Tmin,Tmax	0.905,0.926	0.907,0.927
Tmin'	0.905	

Correction method= MULTI-SCAN

Data completeness= 0.968 Theta(max)= 26.370

R(reflections)= 0.0535(3381) wR2(reflections)= 0.1384(4647)

S = 0.998 Npar= 290

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field. Absorption correction given as multi-scan

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.968

PLAT230_ALERT_2_C Hirshfeld Test Diff for N1 -- C11 .. 6.7 su

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PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C13
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C10
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         11
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ? Do !
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........    0.00500 Deg.
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        273 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        273 K
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S7'    --  C4      ..        5.8 su
PLAT301_ALERT_3_G Note: Main Residue  Disorder ..................          7 %
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         33
              S7   -C4   -S7'     1.555   1.555   1.555             10.60 Deg.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         79
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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   3 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*, 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 01/06/2013; check.def file version of 24/05/2013

Datablock 1 - ellipsoid plot