

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) EG101156\_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: EG101156 1**

Bond precision:	C-C = 0.0016 Å	Wavelength=0.71073		
Cell:	a=8.1998 (7)	b=40.439 (3)	c=10.0135 (8)	
	alpha=90	beta=90	gamma=90	
Temperature:	100 K			

	Calculated	Reported
Volume	3320.4 (5)	3320.4 (5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C43 H30 O4 S2	?
Sum formula	C43 H30 O4 S2	C43 H30 O4 S2
Mr	674.79	674.79
Dx, g cm <sup>-3</sup>	1.350	1.350
Z	4	4
Mu (mm <sup>-1</sup> )	0.206	0.206
F000	1408.0	1408.0
F000'	1409.58	
h, k, lmax	12, 60, 14	12, 59, 14
Nref	5851	5796
Tmin, Tmax	0.934, 0.969	0.900, 0.970
Tmin'	0.934	

```
Correction method= # Reported T Limits: Tmin=0.900 Tmax=0.970
AbsCorr = MULTI-SCAN
```

Data completeness= 0.991                      Theta (max)= 32.030

R(reflections)= 0.0385( 4907)	wR2(reflections)= 0.1037( 5796)
S = 1.073	Npar= 264

---

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

PLAT767\_ALERT\_4\_C INS Embedded LIST 6 Instruction Should be LIST 4      Please Check  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..      1 Check  
                  3    0    6,

---



### Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
                  \_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
                  Atom count from \_chemical\_formula\_sum: C43 H30 O4 S2  
                  Atom count from the \_atom\_site data: C43 H32 O4 S2  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
                  symmetry error - see SYMMG tests  
                  From the CIF: \_cell\_formula\_units\_Z      4  
                  From the CIF: \_chemical\_formula\_sum C43 H30 O4 S2  
                  TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	172.00	172.00	0.00
H	120.00	128.00	-8.00
O	16.00	16.00	0.00
S	8.00	8.00	0.00

PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for C6      --C7      .      5.3 s.u.  
PLAT299\_ALERT\_4\_G Atom Site Occupancy Constrained at .....      0.5 Check  
                  H22A    H22C    H23A    H23B  
PLAT367\_ALERT\_2\_G Long? C(sp?)-C(sp?) Bond C21      - C22      .      1.53 Ang.  
PLAT367\_ALERT\_2\_G Long? C(sp?)-C(sp?) Bond C21      - C23      .      1.54 Ang.  
PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C4      - C5      .      1.42 Ang.  
PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C6      - C7      .      1.43 Ang.  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels .....      1 Note  
                  S001  
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      53 Note  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value .....      3.903 Note  
                  Predicted wR2: Based on SigI\*\*2 2.66 or SHELX Weight 9.67  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density.      20 Info

---

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
14 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
4 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.

