

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 ⁻³	1.350	1.350
Z	4	4
Mu (mm ⁻¹)	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.

