

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) EG1013010132021

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: EG1013010132021

Bond precision: C-C = 0.0030 A

Wavelength=0.71073

Cell: a=8.5406(2) b=11.0477(3) c=18.4450(5)
 alpha=101.060(1) beta=101.236(1) gamma=91.429(1)
Temperature: 100 K

	Calculated	Reported
Volume	1671.78(8)	1671.78(8)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C40 H14 F10 O4 S3	?
Sum formula	C40 H14 F10 O4 S3	C40 H14 F10 O4 S3
Mr	844.69	844.72
Dx, g cm ⁻³	1.678	1.678
Z	2	2
Mu (mm ⁻¹)	0.324	0.324
F000	848.0	848.0
F000'	849.35	
h, k, lmax	10, 13, 22	10, 13, 22
Nref	6123	6098
Tmin, Tmax	0.943, 0.962	0.930, 0.960
Tmin'	0.943	

Correction method= # Reported T Limits: Tmin=0.930 Tmax=0.960
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 25.340

R(reflections)= 0.0345(5361)

wR2(reflections)=
0.0830(6098)

S = 1.148

Npar= 514

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
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.163 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 19 Report
1 1 0, 2 1 0, -1 3 0, 1 -3 1, 1 -2 1, 2 -2 1,
-1 -1 1, -1 1 1, 2 1 1, -2 2 1, 4 2 1, -2 2 2,
1 2 2, 0 0 3, 2 1 3, 1 0 4, -2 -2 6, -2 1 6,
0 -1 7,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 11 Note
2 1 0, -1 3 0, 1 -3 1, 2 -2 1, 2 1 1, -2 2 1,
-2 2 2, 1 2 2, 2 1 3, 1 0 4, -2 1 6,

● **Alert level G**

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C8 - C9 . 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C10 - C11 . 1.41 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C14 - C15 . 1.42 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C16 - C17 . 1.44 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F2 ..F5 . 2.75 Ang.
2-x,1-y,1-z = 2_766 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 73% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
0 1 0, 0 -1 1, 0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.664 Note
Predicted wR2: Based on SigI**2 1.47 or SHELX Weight 7.23
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 17 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

2 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
5 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

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.

