

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1a2a

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: 1a2a

Bond precision:	C-C = 0.0033 A	Wavelength=0.71073
Cell:	a=15.0533 (5)	b=15.1878 (5) c=10.6375 (3)
	alpha=90	beta=107.8093 (13) gamma=90
Temperature:	223 K	
	Calculated	Reported
Volume	2315.47 (13)	2315.47 (13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C25 H18 F6 O3.57 S2	?
Sum formula	C25 H18 F6 O3.57 S2	C25 H18 F6 O3.57 S2
Mr	553.60	553.60
Dx, g cm ⁻³	1.588	1.588
Z	4	4
Mu (mm ⁻¹)	0.309	0.311
F000	1130.2	1130.2
F000'	1131.96	
h, k, lmax	18, 18, 13	18, 18, 13
Nref	2367	2367
Tmin, Tmax	0.933, 0.956	0.910, 0.960
Tmin'	0.861	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.960
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 26.370

R(reflections)= 0.0529 (2162)	wR2(reflections)= 0.1420 (2367)
S = 1.245	Npar= 201

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.113 Check



Alert level G

PLAT230_ALERT_2_G	Hirshfeld Test Diff for F1A --C12 .	5.5 s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C12 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F2A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F2B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F4 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	29% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	54.57 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C11 - C12 .	1.51 Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.44 Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	15.80 Deg.
	C13 -C12 -C13 2_556 1_555 1_555 #	34 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	40.40 Deg.
	F3 -C13 -F3 2_556 1_555 1_555 #	40 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	26.00 Deg.
	C13 -C13 -F4 2_556 1_555 2_556 #	53 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	20.00 Deg.
	C13 -F3 -C13 2_556 1_555 1_555 #	61 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	8.30 Deg.
	C13 -F4 -C13 1_555 1_555 2_556 #	66 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8 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
22 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
15 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

