

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0032 A Wavelength=1.54184

Cell: a=4.9286(1) b=24.5232(3) c=30.1230(4)
 alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3640.82(10)	3640.80(10)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C42 H40 N2 S4	C42 H40 N2 S4
Sum formula	C42 H40 N2 S4	C42 H40 N2 S4
Mr	701.00	701.00
Dx,g cm-3	1.279	1.279
Z	4	4
Mu (mm-1)	2.640	2.640
F000	1480.0	1480.0
F000'	1488.47	
h,k,lmax	6,30,38	6,30,37
Nref	7672[4450]	7383
Tmin,Tmax	0.767,0.867	0.605,1.000
Tmin'	0.464	

Correction method= # Reported T Limits: Tmin=0.605 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.96 Theta(max)= 76.681

R(reflections)= 0.0253(6964) wR2(reflections)= 0.0679(7383)

S = 1.052 Npar= 435

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 B

PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 7.4 Ratio

🟡 Alert level C

PLAT213_ALERT_2_C Atom C36 has ADP max/min Ratio 3.8 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 8.6 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35 Check

⚪ Alert level G

PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C11 - C13 .. 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C14 - C15 .. 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C21 - C24 .. 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C25 - C26 .. 1.44 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 92 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 24 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 16 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

