

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 20220110-hjp-3195

Bond precision:	C-C = 0.0035 A	Wavelength=0.71073
Cell:	a=8.8644 (3) alpha=90	b=9.5173 (3) beta=90.765 (3) c=30.8497 (9) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	2602.41 (14)	2602.41 (14)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C33 H26 N2 O S	C33 H26 N2 O S
Sum formula	C33 H26 N2 O S	C33 H26 N2 O S
Mr	498.62	498.62
Dx, g cm ⁻³	1.273	1.273
Z	4	4
Mu (mm ⁻¹)	0.154	0.154
F000	1048.0	1048.0
F000'	1048.87	
h, k, lmax	12, 13, 42	11, 12, 41
Nref	6969	6201
Tmin, Tmax	0.949, 0.959	0.437, 1.000
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.437 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.890 Theta(max)= 29.102

R(reflections)= 0.0567 (4138)	wR2(reflections)= 0.1483 (6201)
S = 1.069	Npar= 334

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O1	--C6	.	7.0 s.u.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		S1 Check



Alert level G

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	 (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	 (K)	293	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1		102.8	Degree
PLAT793_ALERT_4_G	Model has Chirality at C8	(Centro SPGR)	R	Verify
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.6	Low

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
5 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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

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.

