



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4b

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: 4b

Bond precision: C-C = 0.0025 A

Wavelength=0.71073

Cell: a=9.5327 (9) alpha=68.260 (3)

b=10.9970 (11) beta=76.402 (3)

c=14.2276 (13) gamma=79.973 (3)

Temperature: 273 K

	Calculated	Reported
Volume	1340.3 (2)	1340.3 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H28 N2 O3 S	C32 H28 N2 O3 S, 0.2 [CH3CN]
Sum formula	C32 H28 N2 O3 S	C32 H28 N2 O3 S
Mr	520.62	520.62
Dx, g cm ⁻³	1.290	1.290
Z	2	2
Mu (mm ⁻¹)	0.157	0.157
F000	548.0	548.0
F000'	548.47	
h, k, lmax	12, 14, 18	12, 14, 18
Nref	5993	5898
Tmin, Tmax	0.995, 0.997	0.601, 0.746
Tmin'	0.995	

Correction method= # Reported T Limits: Tmin=0.601 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.984

Theta (max)= 27.228

R(reflections)= 0.0417 (4890)

wR2(reflections)=
0.1192 (5898)

S = 1.027

Npar= 346

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 12 Note
1 0 0, -1 1 0, 0 1 0, 1 1 0, 0 -1 1, -1 0 1,
0 0 1, 1 0 1, 0 1 1, 1 1 1, 0 0 2, 0 1 2,

Author Response: The missing reflections below Theta(Min) are acknowledged. These reflect deviations in their intensities for symmetry equivalent measurements and omitted during initial data reduction.

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc.: C32 H28 N2 O3 S
Rep.: C32 H28 N2 O3 S, 0.2[CH3CN]

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C010 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C00Z Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 42 Report
2 0 0, 3 0 0, 2 1 0, 5 1 0, -5 2 0, 0 2 0,
2 2 0, 1 3 0, -1 -2 1, 0 -2 1, 1 -2 1, -2 -1 1,
1 -1 1, 2 0 1, -1 1 1, -1 2 1, 2 2 1, 1 3 1,
7 4 1, 0 -2 2, -1 -1 2, 0 -1 2, -2 0 2, 1 0 2,
2 0 2, -1 1 2, 2 1 2, 2 2 2, 3 2 2, 4 -2 3,
-2 -1 3, 0 0 3, 0 1 3, 2 1 3, -1 2 3, 1 3 3,
-1 -2 4, 2 -2 4, 2 1 4, 1 2 4, 2 2 4, 5 2 4,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 15 Note
2 0 0, 2 1 0, -1 -2 1, 0 -2 1, -2 -1 1, 2 0 1,
-1 2 1, 2 2 1, 0 -1 2, 2 0 2, -1 1 2, 2 1 2,
2 1 3, -1 2 3, 2 2 4,

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C32 H28 N2 O3 S1
Atom count from _chemical_formula_moiety: C32.4 H28.6 N2.2 O3 S1

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 273 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 66 Note

S001	O002	O003	N004	O005	N006	C007	C008
C009	H009	C00A	C00B	H00B	C00C	H00C	C00D
H00D	C00E	H00E	C00F	C00G	C00H	C00I	H00I
C00J	H00J	C00K	C00L	C00M	H00M	C00N	H00N
C00O	H00O	C00P	H00A	H00F	H00G	C00Q	H00Q
C00R	H00R	C00S	H00S	C00T	H00T	C00U	H00U
C00V	C00W	H00W	C00X	H00X	C00Y	H00H	H00K

	H00L	C00Z	C010	H010	C011	H011	C012	H01A										
	H01B	H01C																
PLAT793_ALERT_4_G	Model has Chirality at C00D						(Centro SpGr)		R Verify									
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 !									
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600								41 Note									
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File								27 Note									
	-5	2	0,	-2	-1	3,	-2	0	2,	-1	-1	2,	-1	0	1,	-1	1	0,
	-1	1	1,	0	-2	2,	0	-1	1,	0	0	3,	0	1	0,	0	1	1,
	0	1	2,	0	1	3,	1	-2	1,	1	-1	1,	1	0	0,	1	1	1,
	1	2	4,	1	3	0,	1	3	1,	1	3	3,	2	-2	4,	2	2	0,
	4	-2	3,	5	1	0,	5	2	4,									
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value								2.780 Note									
	Predicted wR2: Based on SigI**2 4.29 or SHELX Weight 11.60																	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.								14 Info									

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
5 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.

