

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: jof882c_sp

Bond precision:	C-C = 0.0041 A	Wavelength=0.71073	
Cell:	a=17.0215(8)	b=12.1750(5)	c=15.8959(7)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	3294.2(3)	3294.2(3)	
Space group	P n a 21	P na2(1)	
Hall group	P 2c -2n	?	
Moiety formula	C31 H31 N2 O2, C F3 O3 S, C H2 Cl2	?	
Sum formula	C33 H33 Cl2 F3 N2 O5 S	C33 H33 Cl2 F3 N2 O5 S	
Mr	697.58	697.57	
Dx,g cm-3	1.407	1.407	
Z	4	4	
Mu (mm-1)	0.321	0.321	
F000	1448.0	1448.0	
F000'	1450.42		
h,k,lmax	22,16,21	22,16,21	
Nref	4256[8222]	8153	
Tmin,Tmax	0.959,0.997	0.852,0.901	
Tmin'	0.938		

Correction method= MULTI-SCAN

Data completeness= 1.92/0.99 Theta(max)= 28.350

R(reflections)= 0.0548(7244) wR2(reflections)= 0.1515(8153)

S = 1.044 Npar= 442

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

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 1

● **Alert level C**

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 7
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0041 Ang

● **Alert level G**

HYDTR01_ALERT_1_G Extra text has been found in the `_refine_ls_hydrogen_treatment` field.
Explanatory text should be in the `_publ_section_refinement` field.
Hydrogen treatment given as The NH hydrogens free, ordered methyl gr
Hydrogen treatment identified as riding

RADNT01_ALERT_1_G Extra text has been found in the `_diffrn_radiation_type` field.
Radiation given as high brilliance microfocus sealed tube MoK\alpha
Radiation identified as Mo K\alpha

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 25
PLAT005_ALERT_5_G No `_iucr_refine_instructions_details` in the CIF ?
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of S1
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C98
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C98'
PLAT301_ALERT_3_G Note: Main Residue Disorder 3 Perc.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder 100 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 36
C15' -O1 -C15 1.555 1.555 1.555 24.50 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 54

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
2 **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
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
2 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*, 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.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

