

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 15692sadabs_P4

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: 15692sadabs P4

Bond precision:	C-C = 0.0041 A	Wavelength=0.71073		
Cell:	a=10.3270 (4)	b=10.3270 (4)	c=13.8596 (8)	
	alpha=90	beta=90	gamma=90	
Temperature:	100 K			

	Calculated	Reported
Volume	1478.08 (14)	1478.08 (14)
Space group	P 43	P 43
Hall group	P 4cw	P 4cw
Moiety formula	C14 H12 F3 N3 O3 S	C14 H12 F3 N3 O3 S
Sum formula	C14 H12 F3 N3 O3 S	C14 H12 F3 N3 O3 S
Mr	359.33	359.33
Dx, g cm-3	1.615	1.615
Z	4	4
Mu (mm-1)	0.274	0.274
F000	736.0	736.0
F000'	736.96	
h, k, lmax	14, 14, 19	14, 14, 19
Nref	4528 [2349]	4384
Tmin, Tmax	0.974, 0.988	0.968, 0.990
Tmin'	0.942	

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Correction method= # Reported T Limits: Tmin=0.968 Tmax=0.990
AbsCorr = NUMERICAL
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Data completeness= 1.87/0.97 Theta (max)= 30.536

R(reflections)= 0.0481(3920)	wR2(reflections)= 0.1188(4384)
S = 1.091	Npar= 292

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

PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.2	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00413	Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	29	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms	18	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	6	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	11	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F2' --C9 .	6.7	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F3' --C9 .	11.5	s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C9	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	50%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact S1 ..C2' .	3.15	Ang.
	y,1-x,1/4+z =	4_565	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	278	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 0 1 0,	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF 0 0 4,	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File 0 1 0,	1	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value Predicted wR2: Based on SigI**2 1.60 or SHELX Weight 10.90	7.437	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
27 **ALERT level G** = General information/check it is not something unexpected
- 1 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
11 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
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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.

