

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2090225

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: 2090225

Bond precision:	C-C = 0.0045 A	Wavelength=0.71073
Cell:	a=10.4027 (7)	b=14.8477 (7) c=13.9101 (8)
	alpha=90	beta=101.425 (6) gamma=90
Temperature:	290 K	
	Calculated	Reported
Volume	2105.9 (2)	2105.9 (2)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2 (C8 H6 O4), C6 H4 N2 Se	C6 H4 N2 Se, 2 (C8 H6 O4)
Sum formula	C22 H16 N2 O8 Se	C22 H16 N2 O8 Se
Mr	515.33	515.33
Dx, g cm ⁻³	1.625	1.625
Z	4	4
Mu (mm ⁻¹)	1.837	1.837
F000	1040.0	1040.0
F000'	1040.17	
h, k, lmax	13, 19, 18	13, 19, 18
Nref	2652	2387
Tmin, Tmax	0.615, 0.668	0.440, 1.000
Tmin'	0.603	

Correction method= # Reported T Limits: Tmin=0.440 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.900 Theta (max)= 28.449

R(reflections)= 0.0548 (1766)	wR2(reflections)= 0.0988 (2387)
S = 1.131	Npar= 152

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	15.935	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.971	Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	6	Note



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	2	Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF		Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	260	Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	4	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
1 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-
-

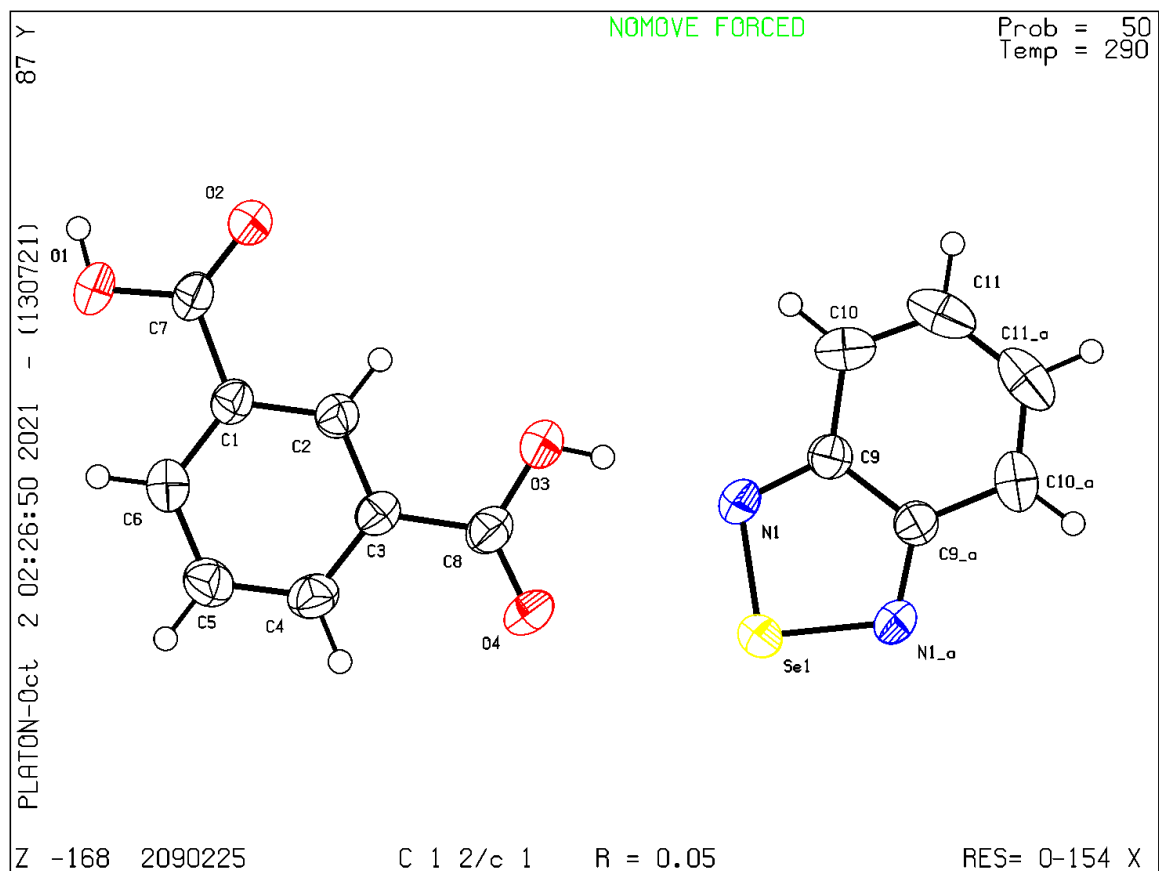
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



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R(reflections)= 0.0318( 1404)      wR2(reflections)=
S = 1.120                        0.0726( 1627)
Npar= 101
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Click on the hyperlinks for more details of the test.



Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.457 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF	Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	156 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	3 Info

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